

ÉCOLE DE PHYSIQUE DES HOUCHES – UJF & INPG – GRENOBLE

a NATO Advanced Study Institute

LES HOUCHES

SESSION LXXII

27 July – 27 August 1999

Coherent atomic matter waves

Ondes de matière cohérentes

Edited by

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Les Ulis, Paris, Cambridge



Springer

*Berlin, Heidelberg, New York,
Barcelona, Hong Kong, London
Milan, Paris, Singapore, Tokyo*

Published in cooperation with the NATO Scientific Affair Division

Preface

Progress in atomic physics has been so vigorous during the past decade that one is hard pressed to follow all the new developments. In the early 1990s the first atom interferometers opened a new field in which we have been able to use the wave nature of atoms to probe fundamental quantum mechanics questions as well as to make precision measurements. Coming fast on the heels of this development was the demonstration of Bose–Einstein condensation in dilute atomic vapors which intensified research interest in studying the wave nature of matter, especially in a domain in which “macroscopic” quantum effects (vortices, stimulated scattering of atomic beams) are visible.

At the same time there has been much progress in our understanding of the behavior of waves (notably electromagnetic) in complex media, both periodic and disordered. An obvious topic of speculation and probably of future research is whether any new insight or applications will develop if one examines the behavior of de Broglie waves in analogous situations.

Finally, our ability to manipulate atoms has allowed us not only to create macroscopically occupied quantum states but also to exercise fine control over the quantum states of a small number of atoms. This has advanced to the study of quantum entanglement and its relation to the theory of measurement and the theory of information. The 1990s have also seen an explosion of interest in an exciting potential application of this fine control: quantum computation and quantum cryptography.

Despite this bewildering variety of phenomena, we scientists must continually make attempts to synthesize and explain our progress both to our students, the researchers of tomorrow, and to the general public. Thus, the purpose of this school was to bring together some of the participants in the trends mentioned above and ask them to give synthetic and pedagogical lectures on these topics in the hope of setting the stage for the research of the next decade, in which a large number of the students at the school will surely participate. At this task the invited lecturers succeeded admirably, generally attending each others’ lectures and commenting on them in their own. The students did their part as well by asking a lot of questions during the lectures, continuing the discussions in the lounge afterwards, and organizing sessions, devoted talks and posters. In addition, thanks to Bill Phillips, our school has contributed to informing the general public about some of our recent progress.

The first part of this volume is devoted to several aspects of Bose-Einstein condensation. Yvan Castin begins with a “simple” theoretical introduction, along with a discussion of experimental tests of the theory. Wolfgang Ketterle follows up with an extensive discussion of recent experiments and experimental techniques in this field. Finally Henk Stoof’s contribution complements the approach of Yvan Castin with a field theoretic approach to a number of current problems. Steven Chu discusses atom interferometry, which has enabled a number of striking precision measurements in recent years. These techniques are also interesting because they are being reapplied to Bose-Einstein condensates instead of just to individual atoms. Unfortunately, Eric Cornell, who also gave a series of lectures on Bose-Einstein condensation, was unable to contribute a written manuscript.

The second part of the book contains some discussions of wave behavior in complex media. Bart van Tiggelen discusses wave propagation in disordered media with some special remarks directed toward the atomic matter wave community, and Dominique Delande discusses the problem of the quantum behavior of classically chaotic systems. Sajeev John contributed a set of lectures on photonic band gaps.

The third part of the book is devoted to the quantum manipulation of systems with few atoms, but which may be coupled to a large reservoir. Wojciech Zurek and Juan-Pablo Paz teamed up to discuss the problems of quantum coherence and decoherence and its relation to quantum information theory. These lectures had an interesting resonance with those of Dominique Delande on quantum chaos. Michel Brune then discusses recent experiments on decoherence and entanglement. Finally, Artur Ekert contributed some lectures on quantum information processing, and in particular on quantum computing.

We were fortunate to benefit from two visitors who gave seminars, Guillaume Labeyrie, who has contributed a short article to this volume, and to Bill Phillips. Bill Phillips also entertained us and the citizens of the town of Les Houches with a public lecture on the nature of absolute zero temperature. A standing-room-only crowd of more than 300 people came to see Bill dip balloons and flowers in liquid nitrogen and talk about laser cooling. Many thanks to Robert Romestain, who ferried the liquid nitrogen all the way from Grenoble.

The Les Houches Physics School benefits from support from the French MENRT, CNRS and CEA. We thank the Les Houches Scientific Advisory Board for its support and advice. This session would not have been possible without the generous financial support of the NATO Advanced Study Institute program. We also thank the “Formation permanente” program of the French CNRS for a substantial contribution. The American NSF also contributed funds to defray the expenses of some

students. We wish to warmly thank the staff of the school, Isabel Lelièvre, Brigitte Rousset and Ghislaine d'Henry, for their friendly and efficient assistance in the preparation and running of the session. We don't know how we would have organized the school without them. Finally, thanks to the restaurant staff for the excellent meals which we could usually enjoy out in the open in full view of the mountains.

Robin Kaiser
Chris Westbrook
François David

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COURSE 1

**BOSE–EINSTEIN CONDENSATES IN ATOMIC GASES:
SIMPLE THEORETICAL RESULTS**

Y. CASTIN

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BOSE–EINSTEIN CONDENSATES IN ATOMIC GASES: SIMPLE THEORETICAL RESULTS

Y. Castin

1 Introduction

1.1 1925: Einstein's prediction for the ideal Bose gas

Einstein considered N non-interacting bosonic and non-relativistic particles in a cubic box of volume L^3 with periodic boundary conditions. In the *thermodynamic limit*, defined as

$$N, L \rightarrow \infty \quad \text{with} \quad \frac{N}{L^3} = \rho = \text{constant}, \quad (1.1)$$

a phase transition occurs at a temperature T_c defined by:

$$\rho \lambda_{\text{dB}}^3(T_c) = \zeta(3/2) = 2.612... \quad (1.2)$$

where we have defined the thermal de Broglie wavelength of the gas as function of the temperature T :

$$\lambda_{\text{dB}}(T) = \left(\frac{2\pi\hbar^2}{mk_B T} \right)^{1/2} \quad (1.3)$$

and where $\zeta(\alpha) = \sum_{k=1}^{\infty} 1/k^\alpha$ is the Riemann Zeta function.

The order parameter of this phase transition is the fraction N_0/N of particles in the ground state of the box, that is in the plane wave with momentum $\vec{p} = \vec{0}$. For temperatures lower than T_c this fraction N_0/N remains finite at the thermodynamic limit, whereas it tends to zero when $T > T_c$:

$$T > T_c \quad \frac{N_0}{N} \rightarrow 0 \quad (1.4)$$

$$T < T_c \quad \frac{N_0}{N} \rightarrow 1 - \left(\frac{T}{T_c} \right)^{3/2}. \quad (1.5)$$

For $T < T_c$ the system has formed a Bose–Einstein condensate in $\vec{p} = \vec{0}$. The number N_0 of particles in the condensate is on the order of N , that is macroscopic. As we will see, the *macroscopic population of a single quantum state* is the key feature of a Bose–Einstein condensate, and gives rise to interesting properties, *e.g.* coherence (as for the laser).

1.2 Experimental proof?

The major problem encountered experimentally to verify Einstein's predictions is that at densities and temperatures required by equation (1.2) at thermodynamic equilibrium almost all materials are in the solid state.

An exception is He^4 which is a fluid at $T = 0$. However He^4 is a strongly interacting system. In He^4 in sharp contrast with the prediction for the ideal gas equation (1.5), $N_0/N < 10\%$ even at zero temperature [1]¹.

The solution which victoriously led to Bose–Einstein condensation in atomic gases is to bring the system to extremely low densities (much lower than in a normal gas) and to cool it rapidly enough so that it has no time to recombine and solidify. The price to pay for an ultralow density is the necessity to cool at extremely low temperatures. Typically one has in the experiments with condensates:

$$\rho < 10^{15} \text{ atoms/cm}^3 \quad (1.6)$$

$$T < 1 \text{ } \mu\text{K}. \quad (1.7)$$

The critical temperatures range from 20 nK to the μK range.

Bose–Einstein condensation was achieved for the first time in atomic gases in 1995. The group of Eric Cornell and Carl Wieman at JILA was first, with ^{87}Rb atoms [2]. They were closely followed by the group of Wolfgang Ketterle at MIT with ^{23}Na atoms [3] and the group of Randy Hulet at Rice University with ^7Li atoms [4]. Nowadays there are many condensates mainly with rubidium or sodium atoms. No other alkali than the ones of year 1995 has been condensed. Atomic hydrogen has been condensed in 1998 at MIT in the group of Dan Kleppner [5]; the experiments on hydrogen were actually the first ones to start and played a fundamental pioneering role in developing many of the experimental techniques having led the alkalis atoms to success, such as magnetic trapping and evaporative cooling of atoms.

In our lectures we do not consider the experimental techniques used to obtain and to study Bose–Einstein condensates as they are treated in the lectures of Wolfgang Ketterle and of Eric Cornell at this school.

1.3 Why interesting?

1.3.1 Simple systems for the theory

An important theoretical frame for Bose–Einstein condensation in interacting systems was developed in the 50's by Beliaev, Bogoliubov, Gross,

¹Amusingly the ideal gas prediction equation (1.2) does not give a too wrong result for the transition temperature in helium. Note that the condensate fraction N_0/N should not be confused with the superfluid fraction: at $T = 0$ the superfluid fraction is equal to unity.

Pitaevskii in the context of superfluid helium. This theory however is supposed to work better if applied to Bose condensed gases where the interactions are much weaker.

The interactions in ultracold atomic gases can be described by a single parameter a , the so-called *scattering length*, as interactions take place between atoms with very low relative kinetic energy. The gaseous condensates are *dilute* systems as the mean interparticle separation is much larger than the scattering length a :

$$\rho|a|^3 \ll 1. \quad (1.8)$$

This provides a small parameter to the theory and, as we shall see, simple mean field approaches can be used with success to describe most of the properties of the atomic condensates.

1.3.2 New features

Atomic gases offer some new interesting features with respect to superfluid helium 4:

- *Spatial inhomogeneity*: This feature can be used as a tool to detect the presence of a Bose–Einstein condensate inside the trap: in an inhomogeneous gas Bose-Einstein condensation occurs not only in momentum space but also in position space!
- *Finite size effects*: The number of atoms in condensates of alkali gases is usually $N_0 < 10^7$. The hydrogen condensate obtained at MIT by Kleppner is larger $N_0 \simeq 10^9$. Interesting finite size effects, that is effects which disappear at the thermodynamic limit, such as Bose–Einstein condensates with effective attractive interactions ($a < 0$), can be studied in relatively small condensates;

It is also interesting to consider small condensates where some interesting quantum aspects concerning coherence properties of the condensates, such as collapses and revivals of the relative phase between two condensates [6], could perhaps be measured [7];

- *Tunability*: Condensates in atomic gases can be manipulated and studied using the powerful techniques of atomic physics (see the lectures of Ketterle and Cornell). Almost all the parameters can be controlled at will, including the interaction strength a between the particles. The atoms can be imaged not only in position space, but also in momentum space, allowing one to see the momentum distribution of atoms in the condensate! One can also tailor the shape and intensity of the trapping potential containing the condensate.

2 The ideal Bose gas in a trap

Let us consider a gas of non-interacting bosonic particles trapped in a potential $U(\vec{r})$ at thermal equilibrium. As the particles do not interact thermal equilibrium has to be provided by coupling to an external reservoir. In the grand-canonical ensemble the state of the gas is described by the equilibrium N -body density matrix

$$\hat{\rho} = \frac{1}{\Xi} \exp \left[-\beta \left(\hat{H} - \mu \hat{N} \right) \right] \quad (2.1)$$

where Ξ is a normalization factor, $\hat{H}$ is the Hamiltonian containing the kinetic energy and trapping potential energy of all the particles, $\hat{N}$ is the operator giving the total number of particles, $\beta = 1/k_B T$ where T is the temperature, and μ is the chemical potential. One more conveniently introduces the fugacity:

$$z = \exp[\beta\mu]. \quad (2.2)$$

2.1 Bose–Einstein condensation in a harmonic trap

Let us consider the case of a harmonic trapping potential $U(\vec{r})$:

$$U(\vec{r}) = \frac{1}{2}m(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2). \quad (2.3)$$

We wish to determine the properties of the trapped gas at thermal equilibrium; the calculations can be done in the basis of harmonic levels or in position space.

2.1.1 In the basis of harmonic levels

Let us consider the single particle eigenstates of the harmonic potential with eigenvalues $\epsilon_{\vec{l}}$ labeled by the vector:

$$\vec{l} = (l_x, l_y, l_z) \quad l_\alpha = 0, 1, 2, 3 \dots (\alpha = x, y, z). \quad (2.4)$$

One has:

$$\epsilon_{\vec{l}} = l_x \hbar \omega_x + l_y \hbar \omega_y + l_z \hbar \omega_z \quad (2.5)$$

where the zero-point energy $(\hbar/2)(\omega_x + \omega_y + \omega_z)$ has been absorbed for convenience in the definition of the chemical potential. Let us consider the case of an isotropic potential for which all the ω_α 's are equal to ω , so that $\epsilon_{\vec{l}} = l \hbar \omega$ with $l \equiv l_x + l_y + l_z$.

The mean occupation number of each single particle eigenstate in the trap is given by the Bose distribution:

$$n_{\vec{l}} = \frac{1}{\exp[\beta(\epsilon_{\vec{l}} - \mu)] - 1} = \left[\frac{1}{z} \exp(\beta l \hbar \omega) - 1 \right]^{-1}. \quad (2.6)$$

Since $n_{\vec{l}}$ has to remain positive (for $l = 0, 1, 2, \dots$), the range of variation of the fugacity z is given by

$$0 < z < 1. \quad (2.7)$$

The average total number of particles N is obtained by summing over all the occupation numbers: $N = \sum_{\vec{l}} n_{\vec{l}}$, a relation that can be used in principle to eliminate z in terms of N . It is useful to keep in mind that for a fixed temperature T , N is an increasing function of z .

In the limit $z \rightarrow 0$ one recovers Boltzmann statistics: $n_{\vec{l}} \propto \exp(-\beta \epsilon_{\vec{l}})$. We are interested here in the opposite, quantum degenerate limit where the occupation number of the ground state $l = 0$ of the trap, given by

$$N_0 = n_{\vec{0}} = \frac{z}{1 - z}, \quad (2.8)$$

diverges when $z \rightarrow 1$, which indicates the presence of a Bose–Einstein condensate in the ground state of the trap.

We wish to watch the formation of the condensate when z is getting closer to one, that is when one gradually increases the total number of particles N . The essence of Bose–Einstein condensation is actually the phenomenon of *saturation* of the population of the excited levels in the trap, a direct consequence of the Bose distribution function. Consider indeed the sum of the occupation numbers of the single particle excited states in the trap:

$$N' = \sum_{\vec{l} \neq \vec{0}} n_{\vec{l}}. \quad (2.9)$$

The key point is that for a given temperature T , N' is bounded from above:

$$N' = \sum_{\vec{l} \neq \vec{0}} \left[\frac{1}{z} \exp(\beta l \hbar \omega) - 1 \right]^{-1} < \sum_{\vec{l} \neq \vec{0}} [\exp(\beta l \hbar \omega) - 1]^{-1} \equiv N'_{\max}. \quad (2.10)$$

Note that we can safely set $z = 1$ since the above sum excludes the term $l = 0$.

If the temperature T is fixed and we start adding particles to the system, particles will be forced to pile up in the ground state of the trap when $N > N'_{\max}$, where they will form a condensate. Let us now estimate the “critical” value of particle number $N'_{\max}$.

We will restrict to the interesting regime $k_B T \gg \hbar\omega$: in this regime Bose statistics allows one to accumulate most of the particles in a single quantum state of the trap while having the system in contact with a thermostat at a temperature much higher than the quantum of oscillation $\hbar\omega$, a very counter-intuitive result for someone used to Boltzmann statistics! On the contrary the regime $k_B T \ll \hbar\omega$ would lead to a large occupation number of the ground state of the trap even for Boltzmann statistics.

A first way to calculate $N'_{\max}$ is to realize that the generic term of the sum varies slowly with l as $k_B T \gg \hbar\omega$ so that one can replace the discrete sum $\sum_{\vec{l} \neq \vec{0}}$ by an integral $\int_{l_\alpha \geq 0} d^3 \vec{l}$. As we are in the case of a three-dimensional harmonic trap there is no divergence of the integral around $\vec{l} = \vec{0}$.

We will rather use a second method, which allows one to calculate also the first correction to the leading term in $k_B T / \hbar\omega$. We use the series expansion

$$\frac{1}{e^x - 1} = \frac{e^{-x}}{1 - e^{-x}} = \sum_{k=1}^{\infty} e^{-kx} \quad (2.11)$$

which leads to the following expression for $N'_{\max}$, if one exchanges the summations over $\vec{l}$ and k :

$$N'_{\max} = \sum_{k=1}^{\infty} \sum_{\vec{l} \neq \vec{0}} \exp \left[-k\beta\hbar\omega \sum_{\alpha} l_{\alpha} \right] = \sum_{k=1}^{\infty} \left[\left(\frac{1}{1 - \exp[-\beta\hbar\omega k]} \right)^3 - 1 \right]. \quad (2.12)$$

We now expand the expression inside the brackets for small x :

$$\left[\left(\frac{1}{1 - \exp[-x]} \right)^3 - 1 \right] = \frac{1}{x^3} + \frac{3}{2x^2} + \dots \quad (2.13)$$

and we sum term by term to obtain

$$N'_{\max} = \left(\frac{k_B T}{\hbar\omega} \right)^3 \zeta(3) + \frac{3}{2} \left(\frac{k_B T}{\hbar\omega} \right)^2 \zeta(2) + \dots \quad (2.14)$$

Note that the exchange of summation over k and summation over the order of expansion in equation (2.13) is no longer allowed for the next term $1/x$, which would lead to a logarithmic divergence (that one can cut “by hand” at $k \simeq k_B T / \hbar\omega$).

One then finds to leading order for the fraction of population in the single particle ground state:

$$\frac{N_0}{N} \simeq \frac{N - N'_{\max}}{N} \simeq 1 - \zeta(3) \left(\frac{k_B T}{\hbar\omega} \right)^3 \frac{1}{N} = 1 - \left(\frac{T}{T_c^0} \right)^3 \quad (2.15)$$

where the critical temperature T_c^0 is defined by:

$$\zeta(3) \left(\frac{k_B T_c^0}{\hbar \omega} \right)^3 = N \quad (2.16)$$

and $\zeta(3) = 1.202\dots$. Note that the universal law (2.15) differs from the one obtained in the homogeneous case (1.5) usually considered in the literature.

The present calculation is easily extended to the case of an anisotropic harmonic trap. To leading order one finds

$$N'_{\max} \simeq \left(\frac{k_B T}{\hbar \bar{\omega}} \right)^3 \zeta(3) \quad (2.17)$$

where $\bar{\omega} = (\omega_x \omega_y \omega_z)^{1/3}$ is the geometric mean of the trap frequencies. One can also calculate $N'_{\max}$ in two-dimensional and one-dimensional models. One also finds in these cases a finite value for $N'_{\max}$: the saturation of population in the single particle excited states applies as well and one can form a condensate, a situation very different from the thermodynamical limit in the homogeneous 1D and 2D cases.

2.1.2 Comparison with the exact calculation

One can see in Figure 1 that the first two terms in the expansion equation (2.14), combined with the approximation $N_0/N \simeq 1 - N'_{\max}/N$, give a very good approximation to the exact condensate fraction for $N = 1000$ particles only.

2.1.3 In position space

A very important object in the description of the state of the gas is the so-called one-body density matrix. We can define it as follows.

Consider a one-body observable

$$\mathcal{X} = \sum_{i=1}^{\hat{N}} X(i) \quad (2.18)$$

where $X(i)$ is the observable for particle number i and where $\hat{N}$ is the operator giving the total number of particles. The one-body density matrix $\hat{\rho}_1$ is defined by the requirement that for any χ :

$$\langle \mathcal{X} \rangle \equiv \text{Tr} [\hat{\rho}_1 X(1)]. \quad (2.19)$$

For the particular case of X equal to the identity it follows $\mathcal{X} = \hat{N}$ and $\langle \mathcal{X} \rangle = \text{Tr}[\hat{\rho}_1] = \langle \hat{N} \rangle$ so that our one-body density matrix is normalized to the mean number of particles in the system.

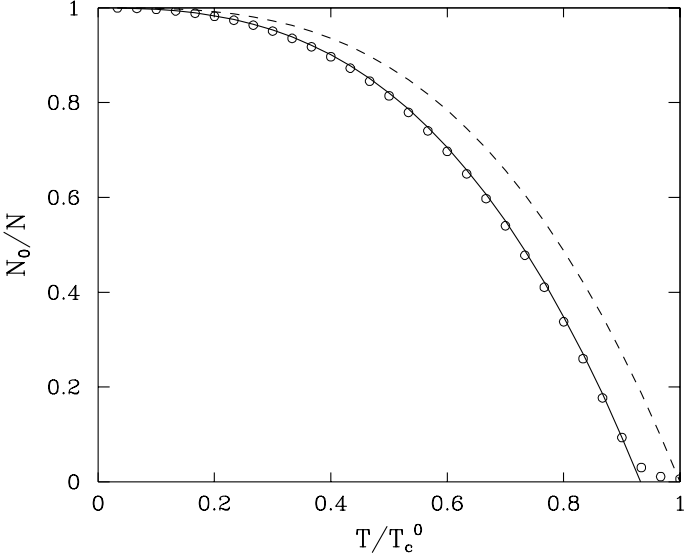


Fig. 1. Condensate fraction *versus* temperature for an ideal Bose gas in a spherically symmetric trap with $N = 1000$ particles. The circles correspond to the exact quantum calculation. The solid line corresponds to the prediction $N_0/N \simeq 1 - N'_{\max}/N$ with $N'_{\max}$ given by the two terms in the expansion equation (2.14). The dashed line corresponds to the prediction $N_0/N \simeq 1 - N'_{\max}/N$ with $N'_{\max}$ given by the leading term in equation (2.14). This figure was taken from [8].

An equivalent definition of $\hat{\rho}_1$ in the second quantized formalism is simply

$$\langle \vec{r}' | \hat{\rho}_1 | \vec{r} \rangle = \langle \hat{\psi}^\dagger(\vec{r}) \hat{\psi}(\vec{r}') \rangle \quad (2.20)$$

where $\hat{\psi}(\vec{r})$ is the atomic field operator, annihilating an atom in $\vec{r}$.

At thermal equilibrium in the grand-canonical ensemble, the one-body density matrix of the ideal Bose gas is given by

$$\hat{\rho}_1 = \frac{1}{z^{-1} \exp(\beta \hat{h}_1) - 1} \quad (2.21)$$

where the single-particle Hamiltonian in the case of a spherically symmetric harmonic trap is

$$\hat{h}_1 = \frac{\vec{p}^2}{2m} + \frac{1}{2} m \omega^2 \vec{r}^2 - \frac{3}{2} \hbar \omega. \quad (2.22)$$

Here again we have subtracted the zero-point energy for convenience. The Bose formula equation (2.6) corresponds to the diagonal element of $\hat{\rho}_1$ in the eigenbasis of the harmonic oscillator (the off-diagonal elements of course vanish). In position space the diagonal term

$$\langle \vec{r} | \hat{\rho}_1 | \vec{r} \rangle = \rho(\vec{r}) \quad (2.23)$$

gives the mean spatial density of the gas.

In order to calculate the density we use the series expansion equation (2.11) to rewrite $\hat{\rho}_1$ as follows:

$$\hat{\rho}_1 = \sum_{k=1}^{\infty} z^k e^{-\beta k \hat{h}_1}. \quad (2.24)$$

This writing takes advantage of the fact that the matrix elements

$$\langle \vec{r} | e^{-\beta k \hat{h}_1} | \vec{r}' \rangle \quad (2.25)$$

are known for an harmonic oscillator potential [9]. One then obtains explicitly:

$$\begin{aligned} \rho(\vec{r}) &= \left(\frac{m\omega}{\pi\hbar} \right)^{3/2} \sum_{k=1}^{\infty} z^k (1 - \exp(-2\beta k \hbar \omega))^{-3/2} \\ &\times \exp \left[-\frac{m\omega r^2}{\hbar} \tanh \left(\frac{\beta k \hbar \omega}{2} \right) \right]. \end{aligned} \quad (2.26)$$

One can identify the contribution of the condensate to this sum when $z \rightarrow 1^-$. When the summation index k is large, what determines the convergence of the series is indeed the factor z^k . Replacing the other factors in the summand by their asymptotic value for $k \rightarrow +\infty$ we identify the diverging part when $z = 1$:

$$\left(\frac{m\omega}{\pi\hbar} \right)^{3/2} \sum_{k=1}^{\infty} z^k \exp \left[-\frac{m\omega r^2}{\hbar} \right] = \frac{z}{1-z} |\phi_{0,0,0}(\vec{r})|^2 = N_0 |\phi_{0,0,0}(\vec{r})|^2 \quad (2.27)$$

where $\phi_{0,0,0}(\vec{r})$ is the ground state wave function of the harmonic oscillator.

Numerically we have calculated the total density $\rho(\vec{r})$ for a fixed temperature $k_B T = 20\hbar\omega$ and for increasing number of particles (see Fig. 2). Here the maximal number of particles one can put in the excited states of the trap is $N'_{\max} \simeq \zeta(3)(k_B T/\hbar\omega)^3 \simeq 10^4$. When $N \ll N'_{\max}$ the effect of an increase of N is mainly to multiply the density by some global factor (the curves in logarithmic scale in Figure 2 are parallel one to the other). When N is becoming larger than $N'_{\max}$ a peak in density grows around $r = 0$, indicating the formation of the condensate, whereas the far wings of the density distribution saturate, which reflects the saturation of the population of the excited levels of the trap.

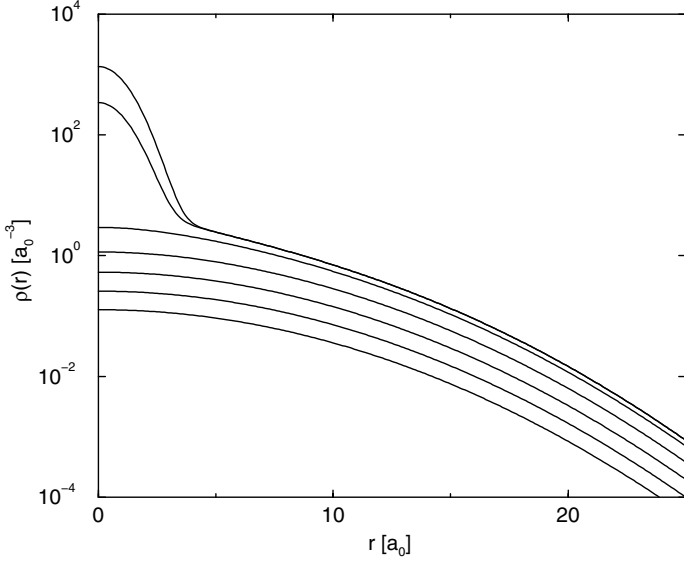


Fig. 2. Spatial density for an ideal Bose gas at thermal equilibrium in a harmonic trap of frequency ω . The temperature is fixed to $k_B T = 20\hbar\omega$ and the number of particles ranges from $N = 500$ to $N = 32000$ between the lowest curve and the upper curve, with a geometrical reason equal to 2. The unit of length for the figure is $a_0 = (\hbar/2m\omega)^{1/2}$, that is the spatial radius of the ground state of the trap.

2.1.4 Relation to Einstein's condition $\rho\lambda_{\text{dB}}^3 = \zeta(3/2)$

In the limit $k_B T \gg \hbar\omega$ we can actually calculate the value $\rho'_{\text{max}}(\vec{r})$ to which the density $\rho'(\vec{r})$ of particles in the excited states of the trap saturates when $z \rightarrow 1$. We simply use the expansion equation (2.26), subtracting from the total density $\rho(\vec{r})$ the contribution of the condensate $N_0|\phi_{0,0,0}(\vec{r})|^2$. The resulting series is converging even for $z = 1$ so that we can take safely the semiclassical limit $k_B T \gg \hbar\omega$ term by term in the sum:

$$\begin{aligned} \rho'(\vec{r}) &\simeq \frac{1}{\lambda_{\text{dB}}^3} \sum_{k=1}^{\infty} \frac{z^k}{k^{3/2}} \exp\left(-\frac{1}{2}k\beta m\omega^2 r^2\right) \\ &= \frac{1}{\lambda_{\text{dB}}^3} g_{3/2} \left[z \exp\left(-\beta \frac{1}{2} m\omega^2 r^2\right) \right] \end{aligned} \quad (2.28)$$

where

$$g_{\alpha}(x) = \sum_{k=1}^{\infty} \frac{x^k}{k^{\alpha}}. \quad (2.29)$$

We term this approximation semiclassical as (i) one can imagine that the classical limit $\hbar \rightarrow 0$ is taken in each term k of the sum, giving the usual Gaussian distribution for the density of a classical harmonic oscillator at temperature $k_B T/k$, but (ii) the distribution still reflects the quantum Bose statistics.

If now we set $z = 1$ in (2.28) to express the fact that a condensate is formed we obtain

$$\rho'_{\max}(\vec{r} = \vec{0}) \simeq \frac{1}{\lambda_{\text{dB}}^3} g_{3/2}(1) = \frac{\zeta(3/2)}{\lambda_{\text{dB}}^3}. \quad (2.30)$$

We therefore recover Einstein's condition provided one replaces the density ρ of the homogeneous case by the density at the center of the trap.

2.2 Bose–Einstein condensation in a more general trap

We now extend the idea of the previous semiclassical limit to more general non-harmonic potentials. This allows to find the condition for Bose–Einstein condensation in presence of a non-harmonic potential. This will prove useful in presence of interactions between the particles where the non-harmonicity is provided by the mean field potential.

2.2.1 The Wigner distribution

The idea is to find a representation of the one-body density matrix having a simple (non pathological) behavior when $\hbar \rightarrow 0$. Let us take as an example a single harmonic oscillator. The density matrix is then of the form:

$$\hat{\sigma} = \frac{1}{Z} e^{-\beta \hat{H}_{\text{ho}}} \quad (2.31)$$

where $\hat{H}_{\text{ho}}$ is the harmonic oscillator Hamiltonian. As shown in [9] all the matrix elements of $\hat{\sigma}$ can be calculated exactly:

$$\langle \vec{r} | \hat{\sigma} | \vec{r}' \rangle = \frac{1}{(2\pi)^{3/2} (\Delta r)^3} \exp \left[-\frac{[(\vec{r} + \vec{r}')/2]^2}{2(\Delta r)^2} \right] \exp \left[-\frac{(\vec{r} - \vec{r}')^2}{2\xi^2} \right]. \quad (2.32)$$

The relevant length scales are the spatial width of the cloud Δr :

$$(\Delta r)^2 = \frac{\hbar}{2m\omega} \coth \left(\frac{\hbar\omega}{2k_B T} \right) \quad (2.33)$$

and the coherence length ξ :

$$\xi^2 = \frac{2\hbar}{m\omega} \tanh \left(\frac{\hbar\omega}{2k_B T} \right). \quad (2.34)$$

If we now take the classical limit $\hbar \rightarrow 0$ (in more physical terms the limit $\hbar\omega \ll k_B T$) then:

$$(\Delta r)^2 \rightarrow \frac{k_B T}{m\omega^2} \quad (2.35)$$

$$\xi^2 \sim \frac{\hbar^2}{mk_B T} = \frac{\lambda_{\text{dB}}^2}{2\pi}. \quad (2.36)$$

In the limit $\hbar \rightarrow 0$ the $\hbar$ dependence of ξ causes $\langle \vec{r} | \hat{\sigma} | \vec{r}' \rangle \rightarrow 0$ for fixed values of $\vec{r}, \vec{r}'$ unless $\vec{r} = \vec{r}'$: the limit is singular.

To avoid this problem one can use the Wigner representation of the density matrix, introduced also in the lectures of Zurek and Paz:

$$W[\hat{\sigma}](\vec{r}, \vec{p}) = \int \frac{d^3 \vec{u}}{h^3} \left\langle \vec{r} - \frac{\vec{u}}{2} \left| \hat{\sigma} \right| \vec{r} + \frac{\vec{u}}{2} \right\rangle e^{i\vec{p} \cdot \vec{u}/\hbar}. \quad (2.37)$$

The Wigner distribution is the quantum analog of the classical phase space distribution. In particular one can check that the Wigner distribution is normalized to unity and that

$$\int d^3 \vec{r} W(\vec{r}, \vec{p}) = \langle \vec{p} | \hat{\sigma} | \vec{p} \rangle \quad (2.38)$$

$$\int d^3 \vec{p} W(\vec{r}, \vec{p}) = \langle \vec{r} | \hat{\sigma} | \vec{r} \rangle. \quad (2.39)$$

An important caveat is that W is not necessarily positive.

For the harmonic oscillator at thermal equilibrium the integral over $\vec{u}$ in equation (2.37) is Gaussian and can be performed exactly:

$$W(\vec{r}, \vec{p}) = \frac{1}{(2\pi\Delta r\Delta p)^3} \exp\left(-\frac{r^2}{2(\Delta r)^2}\right) \exp\left(-\frac{p^2}{2(\Delta p)^2}\right) \quad (2.40)$$

where $\Delta p \equiv \hbar/\xi$. If we take now the limit $\hbar \rightarrow 0$:

$$(\Delta r)^2 \rightarrow \frac{k_B T}{m\omega^2} \quad (2.41)$$

$$(\Delta p)^2 \rightarrow mk_B T \quad (2.42)$$

so that $W(\vec{r}, \vec{p})$ tends to the classical phase space density.

2.2.2 Critical temperature in the semiclassical limit

Let us turn back to our problem of trapped atoms in a non-harmonic trap where the single particle Hamiltonian is given by

$$\hat{h}_1 = \frac{\vec{p}^2}{2m} + U(\vec{r})$$

and the one-body density matrix is given by equation (2.24). For $\hbar \rightarrow 0$ we have:

$$W[e^{-\beta k \hat{h}_1}](\vec{r}, \vec{p}) \simeq \frac{1}{h^3} \exp \left[-k\beta \left(\frac{p^2}{2m} + U(\vec{r}) \right) \right]. \quad (2.43)$$

As we did before we put apart the contribution of the condensate. One then gets for the one-body density matrix of the non-condensed fraction of the gas in the semi classical limit:

$$W[\rho'_1]_{\text{sc}} = \frac{1}{h^3} \sum_{k=1}^{+\infty} z^k \exp \left[-k\beta \left(\frac{p^2}{2m} + U(\vec{r}) \right) \right] \quad (2.44)$$

$$= \frac{1}{h^3} \left\{ \frac{1}{z} \exp \left[\beta \left(\frac{p^2}{2m} + U(\vec{r}) \right) \right] - 1 \right\}^{-1}. \quad (2.45)$$

We are now interested in the spatial density of the non-condensed particles in the semiclassical limit. By integrating equation (2.44) over p we obtain:

$$\rho'_{\text{sc}}(\vec{r}) = \frac{1}{\lambda_{\text{dB}}^3} g_{3/2}(ze^{-\beta U(\vec{r})}) \quad (2.46)$$

where g_α is defined in equation (2.29). The condition for Bose–Einstein condensation is $z \rightarrow e^{\beta U_{\min}}$ where $U_{\min} = \min_{\vec{r}} U(\vec{r})$ is the minimal value of the trapping potential, achieved in the point $\vec{r}_{\min}$. For $z = e^{\beta U_{\min}}$ the semiclassical approximation for the non-condensed density gives in this point:

$$\rho'_{\text{sc}}(\vec{r}_{\min}) = \frac{1}{\lambda_{\text{dB}}^3} g_{3/2}(1) \quad (2.47)$$

or

$$\rho \lambda_{\text{dB}}^3 = 2.612... \quad (2.48)$$

Again Einstein's formula is recovered with ρ being the maximal density of the non-condensed cloud, that is the non-condensed density at the center of the trap.

The semiclassical calculation that we have just presented was initially put forward in [10]. We do not discuss in details the validity of this semiclassical approximation. Intuitively a necessary condition is $k_B T \gg \Delta E$ where ΔE is the maximal level spacing of the single particle Hamiltonian among the states thermally populated. Some situations, where the trapping potential is not just a single well, may actually require more care. The case of Bose–Einstein condensation in a periodic potential is an interesting example that we leave as an exercise to the reader.

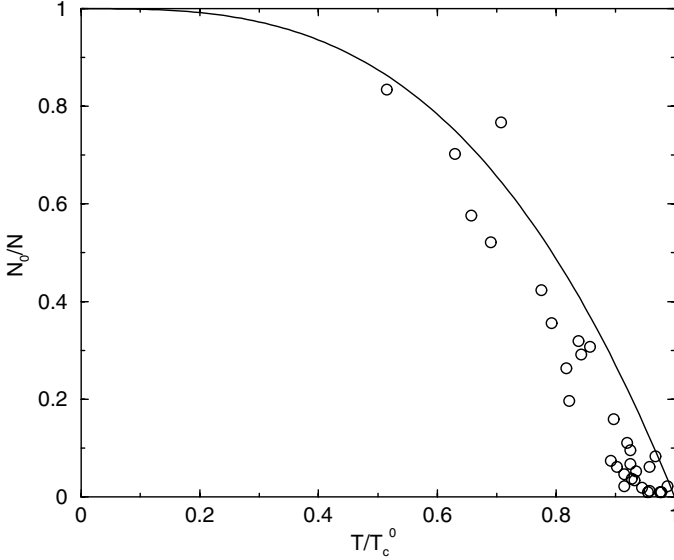


Fig. 3. Condensate fraction N_0/N as function of T/T_c^0 where T_c^0 is the leading order ideal Bose gas prediction equation (2.16). Circles are the experimental results of [11] while the dashed line is equation (2.15).

2.3 Is the ideal Bose gas model sufficient: Experimental verdict

2.3.1 Condensed fraction as a function of temperature

The groups at MIT and JILA have measured the condensate fraction N_0/N as function of temperature for a typical number of particles $N = 10^5$ or larger. We reproduce here the results of JILA [11] (see Fig. 3). This figure shows that the leading order prediction of the ideal Bose gas equation (2.15) is quite good, even if there is a clear indication from the experimental data that the actual transition temperature is lower than T_c^0 . This deviation may be due to finite size effects and interaction effects but the large experimental error has not allowed yet a fully quantitative comparison to theory.

2.3.2 Energy of the gas as a function of temperature and the number of particles

In the experiments one produces first a Bose condensed gas at thermal equilibrium. Then one switches off suddenly the trapping potential. The cloud then expands ballistically, and after a time long enough that the expansion velocity has reached a steady state value one measures the kinetic energy of the expanding cloud.

Suppose that the trap is switched off at $t = 0$. For $t = 0^-$ the total energy of the gas can be written as

$$E_{\text{tot}}(0^-) = E_{\text{kin}} + E_{\text{trap}} + E_{\text{int}}, \quad (2.49)$$

that is as the sum of kinetic energy, trapping potential energy and interaction energy. At time $t = 0^+$ there is no trapping potential anymore so that the total energy of the gas reduces to

$$E_{\text{tot}}(0^+) = E_{\text{kin}} + E_{\text{int}}. \quad (2.50)$$

In the limit $t \rightarrow +\infty$ the gas expands, the density and therefore the interaction energy drop, and all the energy $E_{\text{tot}}(0^+)$ is converted into kinetic energy, which is measured.

In Figure 4 we show the results of JILA for $E_{\text{tot}}(0^+)$ for temperatures around T_c^0 [11] together with the ideal Bose gas prediction. The main feature of the ideal Bose gas prediction is a change in the slope of the energy as function of temperature when T crosses T_c . One observes indeed a change of slope in the experimental results (see the magnified inset)!

For $T > T_c$ the ideal Bose gas model is in good agreement with the experiment. For $T < T_c$ we observe however that the experiment significantly deviates from the ideal Bose gas.

What happens at even lower values of T/T_c^0 ? We show in Figure 5 the expansion energy of the condensate per particle in the regime of an almost pure condensate [12]. This energy then depends almost only on the number of condensate particles N_0 , in a non-linear fashion. This is in complete violation with the ideal Bose gas model, which predicts an energy per particle in the condensate independent of N_0 . More precisely the ideal Bose gas prediction would be $\hbar(\omega_x + \omega_y + \omega_z)/4$ where the ω_α 's are the trap frequencies. In units of k_B this would be in the 10 nK range, an order of magnitude smaller than the measured values.

2.3.3 Density profile of the condensate

The group of Lene Hau at Rowland Institute has measured the density profile of the condensate in a cigar-shaped trap, along the weakly confining axis z of the trap. As imaging with a light beam is used the actual density obtained in the experiment is the density integrated along the direction y of propagation of the laser beam, plotted in Figure 6 for $x = 0$ as function of z [13]. The measured profile is very different from and much broader than the Gaussian density profile of the ground state wavefunction of the harmonic oscillator.

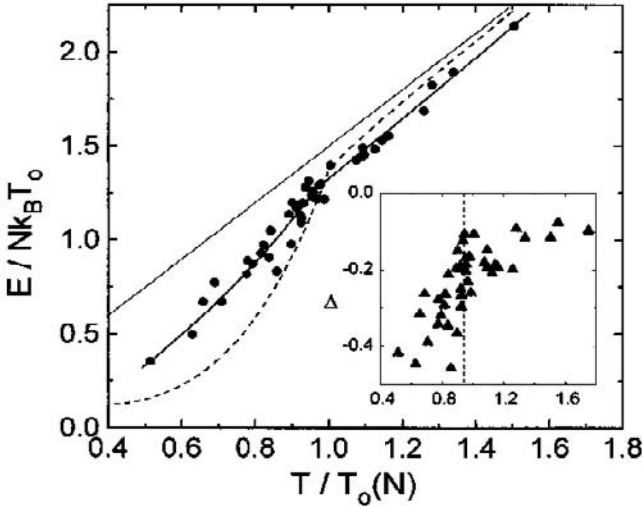


Fig. 4. Expansion energy of the gas $E_{\text{tot}}(0^+)$ per particle and in units of $k_B T_c^0$ as function of the temperature in units of T_c^0 . The disks correspond to the experimental results of [11]. The straight solid line is the prediction of Boltzmann statistics. The dashed curve exhibiting a change of slope is the ideal Bose gas prediction. The curved solid line is a piecewise polynomial fit to the data. The inset is a magnification showing the change of slope of the energy as function of T close to $T = T_c^0$. The figure is taken from [11].

2.3.4 Response frequencies of the condensate

By modulating the harmonic frequencies of the trapping potential one can excite breathing modes of the condensate. For example the group at MIT modulated the trap frequency along the slow axis z of a cigar-shaped trap and observed at $T \ll T_c$ subsequent breathing of the condensate at a frequency $1.569(4)\omega_z$. This frequency is not an integer multiple of ω_z and can therefore not be obtained in the ideal Bose gas model.

In conclusion the ideal Bose gas model may be acceptable as long as no significant condensate has been formed. If a condensate is formed interaction effects become important, and dominant at $T \ll T_c$. This serves as a motivation to the next sections of this lecture, which will deal with the interacting Bose gas problem.

3 A model for the atomic interactions

The previous Section 2 has shown that the ideal Bose gas model is insufficient to explain the experimental results when a condensate is formed.

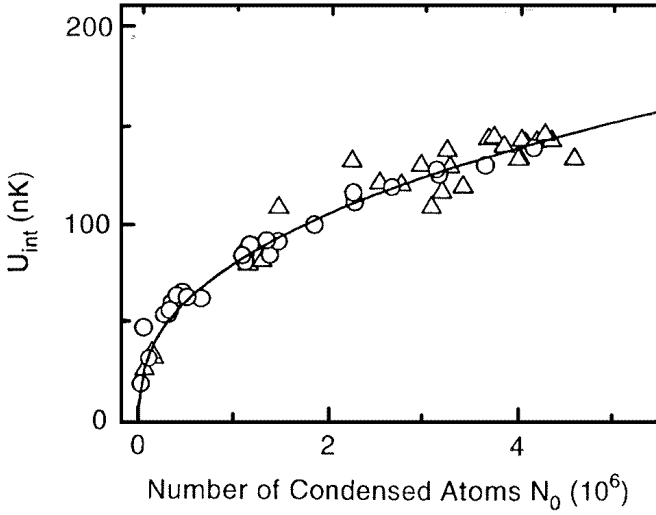


Fig. 5. Expansion energy of the condensate per particle in the condensate, divided by k_B , as a function of the number of particles in the condensate. The experiment is performed at temperatures $T \ll T_c$. The triangles correspond to cases where the non-condensed cloud was not visible experimentally. The disks correspond to case where the non-condensed cloud could be seen. The figure is taken from [12]. The solid line is a fit of the interacting Bose gas prediction of Section 5.

In this section we choose the model potential to be used in this lecture to take into account the atomic interactions. The reader interested in a more careful discussion of real interaction potentials is referred to [14].

3.1 Reminder of scattering theory

We consider two particles of mass m interacting in free space *via* the potential $V(\vec{r}_1 - \vec{r}_2)$ depending on the positions $\vec{r}_1, \vec{r}_2$ only through the relative vector $\vec{r}_1 - \vec{r}_2$. The center of mass of the two particles is then decoupled from their relative motion, and the evolution of the relative motion is governed by the Hamiltonian:

$$H_{\text{rel}} = \frac{\vec{p}^2}{2\mu} + V(\vec{r}) \quad (3.1)$$

where $\vec{r} = \vec{r}_1 - \vec{r}_2$ is the vector of coordinates of the relative motion, $\vec{p} = (\vec{p}_1 - \vec{p}_2)/2$ is the relative momentum and $\mu = m/2$ is the reduced mass. We assume in what follows that the potential $V(\vec{r})$ is vanishing in the limit $r \rightarrow \infty$.

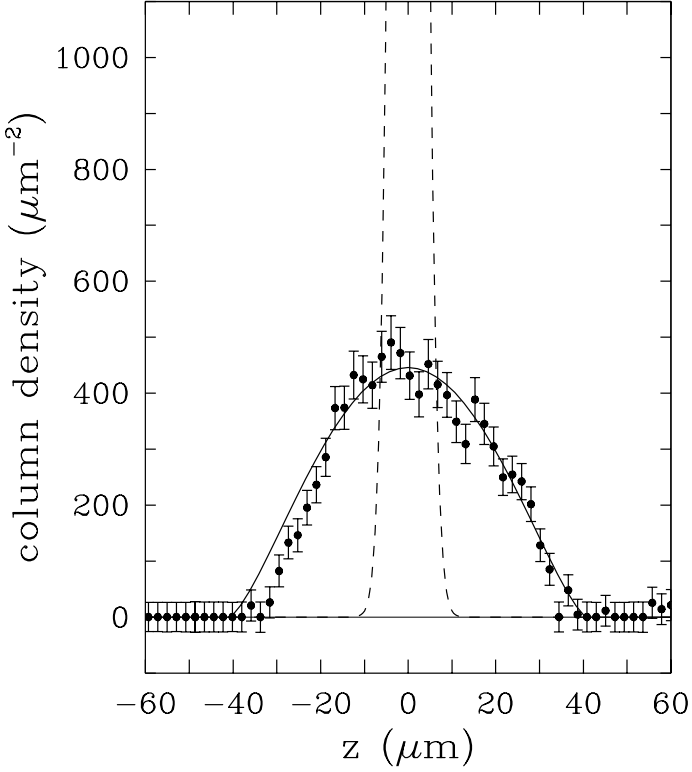


Fig. 6. Column density profile (see text) of a condensate along the weak axis z of a cigar-shaped trap. The experimental results of [13] (dots) are very different from the ideal Bose gas prediction (dashed line). The solid line corresponds to the theoretical prediction of Section 5.

3.1.1 General results of scattering theory

The scattering states $\psi(\vec{r})$ of the relative motion of the two particles are the eigenstates of H_{rel} with positive energy E . Writing $E = \hbar^2 k^2 / 2\mu$ and multiplying the eigenvalue equation by $2\mu / \hbar^2$ we obtain

$$(\Delta + k^2)\psi(\vec{r}) = \frac{2\mu}{\hbar^2}V(\vec{r})\psi(\vec{r}). \quad (3.2)$$

One has also to specify boundary conditions on ψ to get the full description of a scattering state. This is achieved by means of an integral formulation of the eigenvalue equation.

- *Integral equation*

To obtain the integral formulation of the scattering problem we write the right hand side of the eigenvalue equation (3.2) as a continuous sum of Dirac distributions:

$$(\Delta + k^2)\psi(\vec{r}) = \int d^3\vec{r}' \frac{2\mu}{\hbar^2} V(\vec{r}') \psi(\vec{r}') \delta(\vec{r} - \vec{r}'). \quad (3.3)$$

We then find a solution of this equation with a single Dirac distribution on the right hand side:

$$(\Delta_{\vec{r}} + k^2)\psi_G(\vec{r}) = \delta(\vec{r} - \vec{r}') \quad (3.4)$$

having the form of an outgoing spherical wave for $r \rightarrow \infty$:

$$\psi_G(\vec{r}) = -\frac{1}{4\pi} \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|}. \quad (3.5)$$

This is actually a Green's function of the operator $\Delta + k^2$. The scattering state of the full problem can then be written as

$$\psi(\vec{r}) = \psi_0(\vec{r}) - \frac{2\mu}{4\pi\hbar^2} \int d^3\vec{r}' \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} V(\vec{r}') \psi(\vec{r}'). \quad (3.6)$$

The first term ψ_0 is the incoming free wave of the collision, solving $(\Delta + k^2)\psi_0 = 0$; we simply assume here that the incoming wave is a plane wave of wavevector $\vec{k}$:

$$\psi_0(\vec{r}) = \exp[i\vec{k} \cdot \vec{r}]. \quad (3.7)$$

The remaining part of ψ is then simply the scattered wave.

- *Born expansion*

When the interaction potential is weak one sometimes expands the scattering state ψ in powers of V . In the integral formulation equation (3.6) of the eigenvalue equation this corresponds to successive iterations of the integral, the approximation for ψ at order $n+1$ in V being obtained by replacing ψ by its approximation at order n in the right-hand side of the integral equation. *E.g.* to zeroth order in V , $\psi = \psi_0$, and to first order in V we get the so-called Born approximation:

$$\psi_{\text{Born}}(\vec{r}) = \psi_0(\vec{r}) - \frac{2\mu}{4\pi\hbar^2} \int d^3\vec{r}' \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} V(\vec{r}') \psi_0(\vec{r}'). \quad (3.8)$$

3.1.2 Low energy limit for scattering by a finite range potential

Some results can be obtained in a simple way when the potential V has a finite range b , that is when it vanishes when $r > b$.

- *Asymptotic behavior for large r*

As the integration over the variable $\vec{r}'$ is limited to a range of radius b one can expand the distance from $\vec{r}$ to $\vec{r}'$ in powers of r when $r \gg b$:

$$|\vec{r} - \vec{r}'| = r - \vec{r}' \cdot \vec{n} + O\left(\frac{1}{r}\right) \quad (3.9)$$

where $\vec{n} = \vec{r}/r$ is the direction of scattering. The neglected term, scaling as b^2/r , has a negligible contribution to the phase $\exp[ik|\vec{r} - \vec{r}'|]$ when $r \gg kb^2$. One then enters the asymptotic regime for ψ :

$$\psi(\vec{r}) = \psi_0(\vec{r}) + \frac{e^{ikr}}{r} f_{\vec{k}}(\vec{n}) + O\left(\frac{1}{r^2}\right) \quad (3.10)$$

where the factor $f_{\vec{k}}$, the so-called scattering amplitude, does not depend on the distance r :

$$f_{\vec{k}}(\vec{n}) = -\frac{2\mu}{4\pi\hbar^2} \int d^3\vec{r}' e^{-ik\vec{n} \cdot \vec{r}'} V(\vec{r}') \psi(\vec{r}'). \quad (3.11)$$

If the mean distance between the particles in the gas, on the order of $\rho^{-1/3}$, where ρ is the density, lies in the asymptotic regime for ψ (that is $\rho^{-1/3} \gg b, kb^2$) the effect of binary interactions on the macroscopic properties of the gas will be sensitive to the scattering amplitude $f_{\vec{k}}$, and no longer to the details of the scattering potential. This is the key property that we shall use later in this low density regime to replace the exact interaction potential by a model potential having approximately the same scattering amplitude.

- *Limit of low energy collisions*

Another simplification comes from the fact that collisions take place at low energy in the Bose condensed gases: as $\hbar^2 k^2 / 2\mu$ is on the order of $k_B T$ in the thermal gas, k becomes small at low temperature.

If $kb \ll 1$ the phase factor $\exp[-ik\vec{n} \cdot \vec{r}']$ becomes close to one in the integral equation (3.11) giving the scattering amplitude. The scattering amplitude $f_{\vec{k}}$ then no longer depends on the scattering direction $\vec{n}$, the asymptotic part of the scattered wave becomes spherically symmetric (even if the scattering potential is not!): one then says that scattering takes place in the s -wave only.

Going to the mathematical limit $k \rightarrow 0$ we get for the scattering amplitude:

$$f_{\vec{k}}(\vec{n}) \rightarrow -a. \quad (3.12)$$

The quantity a is the so-called scattering amplitude; it will be the only parameter of our theory describing the interactions between the particles, and our model potential will be adjusted to have the same scattering length as the exact potential. When k is going to zero, the scattering state converges to the zero energy scattering state, behaving for large r as

$$\psi_{E=0}(\vec{r}) = 1 - \frac{a}{r} + O\left(\frac{1}{r^2}\right). \quad (3.13)$$

A numerical calculation of this zero energy scattering state is an efficient way of calculating a for a given potential V . Note that there is of course no connection between a and b , except for particular potentials like the hard sphere potential.

3.1.3 Power law potentials

In real life the interaction potential between atoms is not of finite range, as it contains the Van der Waals tail scaling as $1/r^6$ for large r ². It is fortunately possible to show for the class of power-law potentials, scaling as $1/r^n$, that several of our conclusions, obtained in the finite range case, hold provided that $n > 3$. *E.g.* in the limit of small k 's only the s -wave scattering survives, and $f_{\vec{k}}$ has a well defined limit for $k \rightarrow 0$, allowing one to define the scattering length.

3.2 The model potential used in this lecture

3.2.1 Why not keep the exact interaction potential?

For alkali atoms the exact interaction potential has a repulsive hard core, is very deep (as deep as 10^3 Kelvins times k_B for ^{133}Cs), has a minimum at a distance r_{12} on the order of 6 Å (for cesium), and contains many bound states corresponding to molecular states of two alkali atoms (see Fig. 7).

There are several disadvantages to use the exact interaction potential in a theoretical treatment of Bose–Einstein condensation:

1. V is difficult to calculate precisely, and a small error on V may result in a large error on the scattering length a . In practice a is measured experimentally, and this is the most relevant information on V in the low density, low temperature limit;

²Or even as $1/r^7$ if r is larger than the optical wavelength.

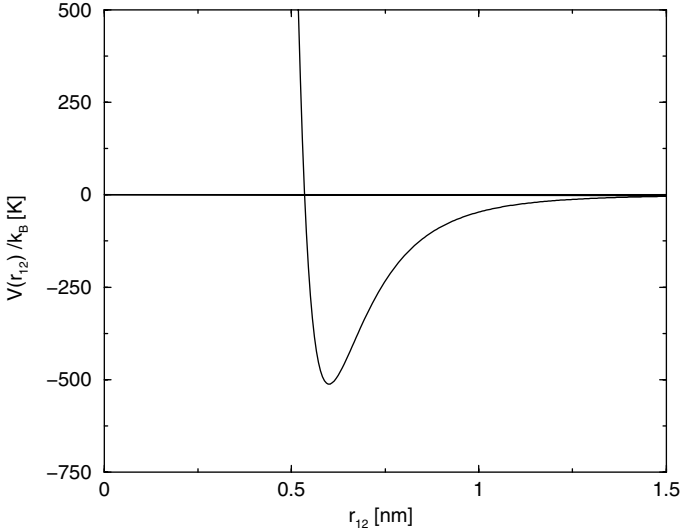


Fig. 7. Typical shape of the interaction potential between two atoms, as function of the interatomic distance r_{12} . The numbers are indicative and correspond to cesium.

2. The presence of bound states of V with a binding energy much smaller than the temperature of the gas (there are 9 orders of magnitude between the potential depth 10^3 K and the gas temperature $\simeq 1$ μ K) clearly indicates that the Bose condensed gases are in a metastable state; at the experimental temperatures and densities the complete thermal equilibrium of the system would be a solid. Direct thermal equilibrium theory, such as the thermal N -body density matrix $\exp[-\beta H]$, cannot therefore be used with V . This is why even in the exact Quantum Monte Carlo calculations performed for alkali gases [15] V is replaced by a hard sphere potential. Such a complication was absent for liquid helium, where the well-known exact V can be used [16];
3. V can not be treated in the Born approximation, because it is very strongly repulsive at short distances and has many bound states: even if the scattering length was zero, one would have to resum the whole Born series to obtain the correct result (We recall that for a potential as gentle as a square well of radius b , the Born approximation applies when the zero-point energy for confinement within a domain of radius b , $\hbar^2/2\mu b^2$, is much larger than the potential depth, which implies that no bound state is present in the well.) As a consequence naive mean

field approximations, which neglect the correlations between particles due to interactions, implicitly relying on the Born approximation, cannot be used with the exact V .

The key idea is therefore to replace the exact interaction potential by a model potential (i) having the same scattering properties at low energy, that is the same scattering length, and (ii) which should be treatable in the Born approximation, so that naive mean field approaches apply.

The model potential satisfying these requirements with the minimal number of parameters (one!) is the zero-range pseudo-potential initially introduced by Enrico Fermi [17, 18] and having the following action on any two-body wavefunction:

$$\langle \vec{r}_1, \vec{r}_2 | V | \psi_{1,2} \rangle \equiv g \delta(\vec{r}_1 - \vec{r}_2) \left[\frac{\partial}{\partial r_{12}} (r_{12} \psi_{1,2}(\vec{r}_1, \vec{r}_2)) \right]_{r_{12}=0}. \quad (3.14)$$

The factor g is the so-called coupling constant

$$g = \frac{4\pi\hbar^2}{m} a \quad (3.15)$$

where a is the scattering length of the exact potential. The pseudo-potential involves a Dirac distribution and a regularizing operator.

- *Effect of regularization*

When the wavefunction $\psi_{1,2}$ is regular close to $\vec{r}_1 = \vec{r}_2$, one can check that the regularizing operator has no effect, so that the pseudo-potential can be viewed as a mere contact potential $g\delta(\vec{r}_1 - \vec{r}_2)$.

When the wavefunction $\psi_{1,2}$ has a $1/r_{12}$ divergence:

$$\psi_{1,2}(\vec{r}_1, \vec{r}_2) = \frac{A(\vec{r}_1 + \vec{r}_2)}{r_{12}} + \text{regular} \quad (3.16)$$

where A is the function of the center of mass coordinates only the regularizing operator removes the diverging part:

$$\frac{\partial}{\partial r_{12}} \left(r_{12} \frac{A(\vec{r}_1 + \vec{r}_2)}{r_{12}} \right) = 0. \quad (3.17)$$

In this way we have extended the Hilbert space of the state vectors of the particles with wave functions diverging as $1/r_{12}$; note that these wavefunctions remain square integrable, as the element of volume scales as r_{12}^2 in 3D. As we shall see this $1/r_{12}$ divergence is a consequence of the zero-range of the pseudo-potential.

3.2.2 Scattering states of the pseudo-potential

Turning back to the relative motion of two particles we now derive the scattering states of the pseudo-potential from the integral equation (3.6). As the pseudo-potential involves a Dirac $\delta(\vec{r}')$ the integral over $\vec{r}'$ can be performed explicitly:

$$\psi(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} - a \frac{e^{ikr}}{r} \left[\frac{\partial}{\partial \vec{r}'} (r' \psi(\vec{r}')) \right]_{r'=0}. \quad (3.18)$$

As the factor

$$C = \left[\frac{\partial}{\partial \vec{r}'} (r' \psi(\vec{r}')) \right]_{r'=0} \quad (3.19)$$

does not depend on $\vec{r}$ we find that ψ has the standard asymptotic behavior of a scattering state in r but *everywhere* in space, not only for large r . This is due to the zero-range of the pseudo-potential. To calculate C , we multiply equation (3.18) by r , we take the derivative with respect to r and set r to zero. On the left hand side we recover the constant C by definition. We finally obtain:

$$C = 1 - aCik \quad (3.20)$$

so that $C = 1/(1 + ika)$ and the scattering states of the pseudo-potential are exactly given by

$$\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} - \frac{a}{1 + ika} \frac{e^{ikr}}{r}. \quad (3.21)$$

The corresponding scattering amplitude,

$$f_k = -\frac{a}{1 + ika} \quad (3.22)$$

does not depend on the direction of scattering, so that the pseudo-potential scatters only in the s -wave, whatever the modulus k is. The scattering length of the pseudo-potential, $-f_{k=0} = a$, coincides with the one of the exact potential.

Finally we note that the total cross-section for scattering of identical bosons by the pseudo-potential is given by a Lorentzian in k ,

$$\sigma = 8\pi |f_{\vec{k}}(\vec{n})|^2 = \frac{8\pi a^2}{1 + k^2 a^2}, \quad (3.23)$$

and that the pseudo-potential obeys the optical theorem.

3.2.3 Bound states of the pseudo-potential

As a mathematical curiosity we now point out that not only the scattering states but also the bound states of the pseudo-potential can be calculated. A first way of obtaining the bound states is a direct solution of Schrödinger’s equation. A more amusing way is to use the following closure relation:

$$\int \frac{d^3\vec{k}}{(2\pi)^3} |\psi_{\vec{k}}\rangle \langle \psi_{\vec{k}}| = 1 - P_{\text{bound}} \quad (3.24)$$

where $|\psi_{\vec{k}}\rangle$ is the scattering state given in equation (3.21) and P_{bound} is the projector on the bound states of the pseudo-potential.

In calculating the matrix elements of this closure relation between perfectly localized state vectors $|\vec{r}\rangle$ and $|\vec{r}'\rangle$ and using spherical coordinates for the integration over $\vec{k}$ one ultimately faces the following type of integrals:

$$I = \int_{-\infty}^{+\infty} dk \frac{e^{ik(r+r')}}{1 + ika} . \quad (3.25)$$

We calculate I using the residues formula, by extending the integration variable k to the complex plane and closing the contour of integration by a circle of infinite radius, which has to be in the upper half of the complex plane as $r + r' > 0$. As the integrand in I has a pole in $k = i/a$, we find that I vanishes for $a < 0$, as the pole is then in the lower half of the complex plane. For $a > 0$ the pole gives a non-zero contribution to the integral:

$$I = \frac{2\pi}{a} e^{-(r+r')/a} . \quad (3.26)$$

Finally we find that $P_{\text{bound}} = 0$ for $a < 0$, corresponding to the absence of bound states, and $P_{\text{bound}} = |\psi_{\text{bound}}\rangle \langle \psi_{\text{bound}}|$ for $a > 0$, corresponding to the existence of a single bound state:

$$\psi_{\text{bound}}(\vec{r}) = \frac{1}{\sqrt{2\pi a}} \frac{e^{-r/a}}{r} . \quad (3.27)$$

From Schrödinger’s equation, we find for the energy of the bound state:

$$E_{\text{bound}} = -\frac{\hbar^2}{ma^2} . \quad (3.28)$$

The existence of a bound state for $a > 0$ and its absence for $a < 0$ is a paradoxical situation. As we shall see in the mean field approximation, the case $a > 0$ corresponds to effective repulsive interactions between the atoms, whereas the case $a < 0$ corresponds to effective attractive interactions. In the purely 1D case, the situation is more intuitive, the potential $g_{1D}\delta(x)$

having a bound state only in the effective attractive case $g_{1D} < 0$. This paradox in 3D comes from the non-intuitive effect of the regularizing operator (an operation not required in 1D), which makes the pseudo-potential different from a delta potential; actually one can shown in 3D that a delta potential viewed as a limit of square well potentials with decreasing width b and constant area does not scattered in the limit $b \rightarrow 0$.

3.3 *Perturbative vs. non-perturbative regimes for the pseudo-potential*

3.3.1 Regime of the Born approximation

As we will use mean field approximations requiring that the scattering potential is treatable in the Born approximation, we identify the regime of validity of the Born approximation for the pseudo-potential.

As we have seen in the previous subsection the integral equation for the scattering states of the pseudo-potential can be reduced to the equation for C :

$$C = 1 - ikaC, \quad (3.29)$$

the scattering state being given by

$$\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k} \cdot \vec{r}} - aC \frac{e^{i\vec{k}r}}{r}. \quad (3.30)$$

The Born expansion will then reduces to iterations of equation (3.29). To zeroth order in the interaction potential, we obtain $C_0 = 0$ so that $\psi_{\vec{k}}$ reduces to the incoming wave. To first order, we get the Born approximation

$$C_1 = 1 - ikaC_0 = 1. \quad (3.31)$$

To second order and third order we obtain

$$C_2 = 1 - ikaC_1 = 1 - ika \quad (3.32)$$

$$C_3 = 1 - ikaC_2 = 1 - ika + (ika)^2 \quad (3.33)$$

so that the Born expansion is a geometrical series expansion of the exact result $C = 1/(1 + ika)$ in powers of ika .

The validity condition of the Born approximation is that the first order result is a small correction to the zeroth order result. For the scattering amplitude this requires

$$k|a| \ll 1. \quad (3.34)$$

For the scattering state this requires

$$r \gg a. \quad (3.35)$$

If one takes for r the typical distance $\rho^{-1/3}$ between the particles in the gas, where ρ is the density, this leads to

$$\rho^{1/3}|a| \ll 1. \quad (3.36)$$

- *Are the conditions for the Born approximation satisfied in the experiments?*

To estimate the order of magnitude of k we average k^2 over a Maxwell-Boltzmann distribution of atoms with a temperature $T = 1 \mu\text{K}$, typically larger than the critical temperature for alkali gases; the average gives a root mean square for k equal to

$$\Delta k = \left(\frac{3mk_B T}{2\hbar^2} \right)^{1/2}. \quad (3.37)$$

For ^{23}Na atoms used at MIT, with a scattering length of $50 a_{\text{Bohr}}$, where the Bohr radius is $a_{\text{Bohr}} = 0.53 \text{ \AA}$, we obtain $\Delta k a = 2 \times 10^{-2}$. For rubidium ^{87}Rb atoms used at JILA, with a scattering length of $110 a_{\text{Bohr}}$, we obtain $\Delta k a = 0.1$.

In the case of an almost pure condensate in a trap, the typical k is given by the inverse of the size R of the condensate, as the condensate wavefunction is not very far from a minimum uncertainty state. Generally this results in a much smaller Δk than equation (3.37), as R is much larger than the thermal de Broglie wavelength. One could however imagine a condensate in a very strongly confining trap, such that R would become close to a ; in this case, not yet realized, the mean field theory has to be revisited.

We turn to the second condition equation (3.36). The typical densities of condensates are on the order of 2×10^{14} atoms per cm^3 . For the scattering length of sodium this leads to $\rho^{1/3}a \simeq 0.015 \ll 1$. For the scattering length of rubidium this leads to $\rho^{1/3}a \simeq 0.034 \ll 1$. Both conditions for the Born approximation applied to the pseudo-potential are therefore satisfied.

3.3.2 Relevance of the pseudo-potential beyond the Born approximation

Let us try to determine necessary validity conditions for the substitution of the exact interaction potential by the pseudo-potential.

First one should be in a regime dominated by s -wave scattering, as the pseudo-potential neglects scattering in the other wave. This condition is easily satisfied in the μK temperature range for Rb, Na.

Second the scattering amplitude of the exact potential in s -wave should be well approximated by the pseudo-potential. For isotropic potentials vanishing for large r as $1/r^n$, with $n > 5$, the s -wave scattering amplitude has

the following low k expansion:

$$f_k^{s=0} = -\frac{1}{a^{-1} + ik - \frac{1}{2}k^2 r_e + \dots} \quad (3.38)$$

where r_e is the so-called effective range of the potential. To this order in k the result of the pseudo-potential corresponds to the approximation $r_e = 0$. When r_e is on the order of a (which is the case for a hard sphere potential, but not necessarily true for a more general potential) the term in r_e can be neglected if $k^2 r_e \ll 1/a$, that is $(ka)^2 \ll 1$; there is therefore no meaning to use the pseudo-potential beyond the Born regime.

Consider now the case $r_e \ll |a|$. The term $r_e k^2$ remains small as compared to $1/a$ for $k|a| < 1$. For $k|a| \gg 1$ the term ik dominates over $1/a$; $k^2 r_e$ remains small as compared to ik as long as $kr_e \ll 1$. The use of the pseudo-potential may then extend beyond the Born approximation.

An example of a situation with $r_e \ll |a|$ is the so-called zero energy resonance, where a is diverging. When a bound state of the interaction potential is arbitrarily close to the dissociation limit, the scattering length diverges $a \rightarrow +\infty$, the bound state has a large tail in r scaling as $e^{-r/a}/r$ and the bound state energy scales as $-\hbar^2/ma^2$ [19, 20]. These scaling laws hold for the pseudo-potential, as we have seen.

4 Interacting Bose gas in the Hartree–Fock approximation

Now that we have identified a simple model interaction potential treatable in the Born approximation we use it in the simplest possible mean field approximation, the so-called Hartree–Fock approximation. This approximation was applied to trapped gases for the first time in 1981 (see [21])!

4.1 BBGKY hierarchy

The Hartree–Fock mean field approximation can be implemented in a variety of ways. We have chosen here the approach in terms of the BBGKY hierarchy, truncated to first order.

4.1.1 Few body-density matrices

We have already introduced in Section 2 the concept of the one-body density matrix. We revisit here this notion and extend it to two-body density matrices.

- *For a fixed total number of particles*

Let us first consider a system with a fixed total number of particles N and let $\sigma_{1,2,\dots,N}$ be the N -body density matrix. Starting from $\sigma_{1,2,\dots,N}$ we introduce

simpler objects as the one-body and two-body density matrices $\hat{\rho}_1$ and $\hat{\rho}_{12}$, by taking the trace over the states of all the particles but one or two:

$$\hat{\rho}_1^{(N)} = N \operatorname{Tr}_{2,3,\dots,N}(\sigma_{1,2,\dots,N}) \quad (4.1)$$

$$\hat{\rho}_{12}^{(N)} = N(N-1) \operatorname{Tr}_{3,4,\dots,N}(\sigma_{1,2,\dots,N}). \quad (4.2)$$

In practice the knowledge of $\hat{\rho}_1$ and $\hat{\rho}_{12}$ is sufficient to describe most of the experimental results. As you know, $\langle \vec{r} | \hat{\rho}_1 | \vec{r} \rangle$ is the density of particles and $\langle \vec{r}_1, \vec{r}_2 | \hat{\rho}_{12} | \vec{r}_1, \vec{r}_2 \rangle$ is the pair distribution function.

- *For a fluctuating total number of particles*

If N fluctuates according to the probability distribution P_N , we define few-body density matrices by the following averages over N :

$$\hat{\rho}_1 = \sum_N P_N \hat{\rho}_1^{(N)} \quad (4.3)$$

$$\hat{\rho}_{12} = \sum_N P_N \hat{\rho}_{12}^{(N)}. \quad (4.4)$$

Alternatively one can define directly the one-body and two-body density matrices in second quantization:

$$\langle \vec{r}_1 | \hat{\rho}_1 | \vec{r}_2 \rangle = \langle \hat{\psi}^\dagger(\vec{r}_2) \hat{\psi}(\vec{r}_1) \rangle \quad (4.5)$$

$$\langle \vec{r}_1, \vec{r}_2 | \hat{\rho}_{12} | \vec{r}_3, \vec{r}_4 \rangle = \langle \hat{\psi}^\dagger(\vec{r}_3) \hat{\psi}^\dagger(\vec{r}_4) \hat{\psi}(\vec{r}_2) \hat{\psi}(\vec{r}_1) \rangle. \quad (4.6)$$

Note that the few-body density matrices are normalized as

$$\operatorname{Tr}[\hat{\rho}_1] = \langle N \rangle \quad (4.7)$$

$$\operatorname{Tr}[\hat{\rho}_{12}] = \langle N(N-1) \rangle \quad (4.8)$$

so that one can obtain the variance of the fluctuations in the number of atoms from the one-body and two-body density matrices.

4.1.2 Equations of the hierarchy

The idea of our derivation of the mean field approximation is to get an approximate closed equation for $\hat{\rho}_1$ by closing the hierarchy with some “cooking recipe” giving $\hat{\rho}_{12}$ in terms of $\hat{\rho}_1$.

To derive the first equation of the hierarchy we start from the exact master equation:

$$i\hbar \frac{d}{dt} \sigma_{1,2,\dots,N} = [H, \sigma_{1,2,\dots,N}] \quad (4.9)$$

where the Hamiltonian is the sum of one-body and two-body terms:

$$H = \sum_{i=1}^N h_i + \frac{1}{2} \sum_{i \neq j; i, j=1}^N V_{ij}. \quad (4.10)$$

The single particle Hamiltonian h_i contains the kinetic and trapping potential energy of the atom i and V_{ij} in the interaction potential between the atoms i and j . Now we take the trace of the master equation over the particles 2,3 ... N and multiply it by N , obtaining

$$i\hbar \frac{d}{dt} \hat{\rho}_1 = [h_1, \hat{\rho}_1] + N \text{Tr}_{2, \dots, N} \left\{ \sum_{j=2}^N [V_{1j}, \sigma_{1,2, \dots, N}] \right\}. \quad (4.11)$$

We have kept here only the terms involving the atom 1, as the other terms are commutators of vanishing trace. The sum over j amounts to $N - 1$ times the same contribution, *e.g.* the $j = 2$ contribution, as the atoms are indiscernible. We finally obtain the first equation of the hierarchy:

$$i\hbar \frac{d}{dt} \hat{\rho}_1 = [h_1, \hat{\rho}_1] + \text{Tr}_2 \{ [V_{12}, \hat{\rho}_{12}] \}. \quad (4.12)$$

The equation (4.12) is not closed for $\hat{\rho}_1$, as it involves $\hat{\rho}_{12}$. The next equation of the hierarchy, the equation for $\hat{\rho}_{12}$, involves $\hat{\rho}_{123}$, etc. up to the N -body density matrix, where the hierarchy terminates. The mean field approximation consists in replacing $\hat{\rho}_{12}$ by an ad hoc function of $\hat{\rho}_1$.

4.2 Hartree–Fock approximation for $T > T_c$

4.2.1 Mean field potential for the non-condensed particles

We use the following simple approximation to break the hierarchy:

$$\hat{\rho}_{12} \simeq \hat{\rho}_{12}^{\text{HF}} = \left(\frac{1 + P_{12}}{\sqrt{2}} \right) \hat{\rho}_1 \otimes \hat{\rho}_1 \left(\frac{1 + P_{12}}{\sqrt{2}} \right) = (1 + P_{12}) \hat{\rho}_1 \otimes \hat{\rho}_1 \quad (4.13)$$

where P_{12} is the permutation operator exchanging the states of the particles 1 and 2. The last identity in (4.13) is obtained by using the commutation of P_{12} and $\hat{\rho}_1 \otimes \hat{\rho}_1$, and the fact that $P_{12}^2 = 1$.

The factorized prescription $\hat{\rho}_{12} = \hat{\rho}_1 \otimes \hat{\rho}_1$ is the Hartree approximation. It assumes weak correlations between the particles. Indeed at short distances r_{12} , the real $\hat{\rho}_{12}$ is expected to be a statistical mixture of scattering states of the interaction potential. Neglecting the correlations in $\hat{\rho}_{12}$ between particles 1 and 2 amounts to considering only separable, plane wave scattering states, which corresponds to the zeroth order in the Born expansion of the scattering theory. Actually $\hat{\rho}_{12}$ appears in equation (4.12)

inside a commutator with V_{12} , so that taking the zeroth order approximation for the scattering states in $\hat{\rho}_{12}$ corresponds to the first order of the Born approximation in the equation for $\hat{\rho}_1$.

As we are dealing with bosons we have supplemented the Hartree approximation by a bosonic symmetrization procedure, involving the permutation operator P_{12} . Note that the symmetrization as it was written works only for particles 1 and 2 in orthogonal states:

$$\frac{1 + P_{12}}{\sqrt{2}}|\alpha\rangle|\beta\rangle = \frac{|\alpha\rangle|\beta\rangle + |\beta\rangle|\alpha\rangle}{\sqrt{2}} \quad (4.14)$$

as the factor $\sqrt{2}$ is the correct normalization factor only in this case. This is almost true for a non-degenerate Bose gas. This restriction forces us to treat separately the case in which a condensate is present ($T < T_c$).

We now insert the Hartree–Fock ansatz for $\hat{\rho}_{12}$ in the hierarchy³

$$i\hbar \frac{d}{dt} \hat{\rho}_1 = [h_1, \hat{\rho}_1] + \text{Tr}_2 \{ [V_{12}, \hat{\rho}_{12}^{\text{HF}}] \}. \quad (4.15)$$

In the commutator with V_{12} we will encounter

$$\delta(\vec{r}_1 - \vec{r}_2)(1 + P_{12}) = (1 + P_{12})\delta(\vec{r}_1 - \vec{r}_2) = 2\delta(\vec{r}_1 - \vec{r}_2). \quad (4.16)$$

The fact that P_{12} commutes with V_{12} is due to the parity of the delta distribution, and P_{12} acting on a state with two particles at the same position can be replaced by the identity. As a consequence, with our zero-range interaction potential, the Fock term simply doubles the Hartree term. We finally obtain

$$i\hbar \frac{d}{dt} \hat{\rho}_1 = \left[\frac{\vec{p}^2}{2m} + U(\vec{r}) + \mathcal{V}(\vec{r}), \hat{\rho}_1 \right] \quad (4.17)$$

where $\mathcal{V}(\vec{r})$ is the mean field potential

$$\mathcal{V}(\vec{r}) = 2g\langle \vec{r} | \hat{\rho}_1 | \vec{r} \rangle = 2g\rho(\vec{r}). \quad (4.18)$$

The Hartree–Fock Hamiltonian is then

$$h^{\text{HF}}(1) = \frac{\vec{p}^2}{2m} + U(\vec{r}) + 2g\rho(\vec{r}). \quad (4.19)$$

The problem is then formally reduced to the one of an ideal Bose gas moving in a self-consistent potential. For $g > 0$ the mean field corresponds to repulsive interactions, as $2g\rho(\vec{r})$ expels the atoms from the region of high density, while for $g < 0$ the mean field corresponds to attractive interactions.

³Note that for the present calculation the regularization of the pseudo-potential is not necessary. Indeed by considering plane waves as scattering states in $\hat{\rho}_{12}$ we suppress any problem of divergences in the commutator with V_{12} , and we can then take V_{12} as a simple delta distribution.

4.2.2 Effect of interactions on T_c

Let us now consider the Hartree–Fock one-body density matrix at thermal equilibrium; we use the same formula as the ideal Bose gas equation (2.21), replacing h_1 by the Hartree–Fock Hamiltonian:

$$\hat{\rho}_1 = \{\exp [\beta (h^{\text{HF}}(1) - \mu)] - 1\}^{-1}. \quad (4.20)$$

For $k_B T \gg \Delta E$ where ΔE is the level spacing of h^{HF} we can perform the semiclassical approximation. We obtain for the spatial density as in equation (2.46):

$$\rho_{\text{sc}}(\vec{r}) = \frac{1}{\lambda_{\text{dB}}^3} g_{3/2}(z \exp[-\beta(U(\vec{r}) + 2g\rho_{\text{sc}}(\vec{r}))]). \quad (4.21)$$

At $T = T_c$ the argument of $g_{3/2}$ goes to 1 in the point $\vec{r}_{\text{min}}$ where the potential is minimal, so that Einstein’s condition still holds in the Hartree–Fock approximation:

$$\rho_{\text{sc}}(\vec{r}_{\text{min}})\lambda_{\text{dB}}^3 = \zeta(3/2). \quad (4.22)$$

For the harmonic trap $U(\vec{r}) = m\omega^2 r^2/2$ the minimum occurs at the center of the trap, $\vec{r}_{\text{min}} = \vec{0}$ so that the chemical potential at the phase transition is given by

$$\mu = 2g\rho_{\text{sc}}(\vec{0}). \quad (4.23)$$

It is shifted by the mean field effect with respect to the ideal Bose gas. Using as a small parameter $\rho_{\text{sc}}(\vec{0})g/k_B T_c^0$, one can derive at constant N [22] the first order change in the critical temperature with respect to T_c^0 , the transition temperature of the ideal Bose gas:

$$\frac{\delta T_c}{T_c^0} = -2.5\rho_{\text{sc}}^{1/3}(\vec{0})a = -1.33 \frac{a}{(\hbar/m\omega)^{1/2}} N^{1/6}. \quad (4.24)$$

For $N = 10^7$ atoms of ^{23}Na in a trap of harmonic frequency $\omega = 2\pi \times 100$ Hz, with a scattering length $a = 50 a_{\text{Bohr}}$ we find $T_c^0 \simeq 1 \mu\text{K}$, and $\delta T_c/T_c^0 \simeq -2.5 \times 10^{-2}$, an effect for the moment smaller than the experimental accuracy. The fact that δT_c is negative for effective repulsive interactions ($a > 0$) is intuitive: for fixed values of N and T the interacting gas has a lower density at the center of the trap than the ideal Bose gas, so that one needs to further cool the gas to get Bose–Einstein condensation.

- *A calculation of δT_c beyond mean field*

The purest situation to study the effect of the interactions on the critical temperature T_c is the case of atoms trapped in a flat bottom potential; in

this case the density is uniform, the previously mentioned intuitive mean field effect is suppressed, and our Hartree–Fock theory predicts the same critical temperature as the ideal Bose gas. This prediction is actually not correct, and rigorous results for the first order correction of T_c in $a\rho^{1/3}$ have been obtained recently, by a combination of perturbative theory and Quantum Monte Carlo calculations [23]:

$$\frac{\delta T_c^{\text{box}}}{T_c^0} = (2.2 \pm 0.25)a\rho^{1/3} + o(a\rho^{1/3}). \quad (4.25)$$

Recent calculations in the many body Green’s function formalism confirm this result [24]. This effect, if heuristically extended to the trap, is of opposite sign and of the same order of magnitude as the mean-field prediction.

4.3 Hartree–Fock approximation in presence of a condensate

4.3.1 Improved Hartree–Fock Ansatz

As already emphasized in the previous subsection the symmetrization procedure of the Hartree–Fock prescription equation (4.13) has to be modified in presence of a condensate. To this end we split the one-body density matrix as

$$\hat{\rho}_1 = \langle N_0 \rangle |\phi\rangle\langle\phi| + \hat{\rho}'_1 \quad (4.26)$$

where ϕ is the condensate wavefunction, $\langle N_0 \rangle$ is the mean number of particles in the condensate and $\hat{\rho}'_1$ is the one-body density matrix of the non-condensed fraction. The Hartree approximation for the two-body density matrix now reads:

$$\hat{\rho}_1 \otimes \hat{\rho}_1 = \langle N_0 \rangle^2 |\phi, \phi\rangle\langle\phi, \phi| + \text{remaining Hartree part}. \quad (4.27)$$

The first term in the right hand side is already symmetrized; the second term can be symmetrized as in equation (4.13) as it does not involve coexistence of two atoms in the (only) macroscopically populated state ϕ . We therefore put forward the following Hartree–Fock ansatz:

$$\hat{\rho}_{12}^{\text{HF}} = \langle N_0 \rangle^2 |\phi, \phi\rangle\langle\phi, \phi| + \left(\frac{1 + P_{12}}{\sqrt{2}} \right) \text{remaining Hartree part} \left(\frac{1 + P_{12}}{\sqrt{2}} \right). \quad (4.28)$$

Eliminating the remaining Hartree part with the help of equation (4.27), we finally obtain

$$\hat{\rho}_{12}^{\text{HF}} = \left(\frac{1 + P_{12}}{\sqrt{2}} \right) \hat{\rho}_1 \otimes \hat{\rho}_1 \left(\frac{1 + P_{12}}{\sqrt{2}} \right) - \langle N_0 \rangle^2 |\phi, \phi\rangle\langle\phi, \phi|. \quad (4.29)$$

In this way we have avoided the double counting of the condensate contribution that would have resulted from the prescription equation (4.13).

4.3.2 Mean field seen by the condensate

We replace $\hat{\rho}_{12}$ in the first equation of the hierarchy by the improved Hartree–Fock ansatz. The first bit of the ansatz gives the same result as in the case $T > T_c$, the second bit involves the term:

$$\text{Tr}_2 ([\delta(\vec{r}_1 - \vec{r}_2), |\phi, \phi\rangle\langle\phi, \phi|]) = [|\phi(\vec{r}_1)|^2, |\phi\rangle\langle\phi|]. \quad (4.30)$$

Splitting $\hat{\rho}_1$ as condensate and non-condensed contribution we arrive at

$$i\hbar \frac{d}{dt} \hat{\rho}_1 = \left[\frac{\vec{p}^2}{2m} + U(\vec{r}) + 2g\rho(\vec{r}) - \langle N_0 \rangle g |\phi(\vec{r})|^2, \langle N_0 \rangle |\phi\rangle\langle\phi| \right] \quad (4.31)$$

$$+ \left[\frac{\vec{p}^2}{2m} + U(\vec{r}) + 2g\rho(\vec{r}), \hat{\rho}'_1 \right]. \quad (4.32)$$

The non-condensed particles still move in the mean field potential $2g\rho(\vec{r})$. On the contrary the atoms in the condensate see a different mean field potential:

$$2g\rho(\vec{r}) - g\langle N_0 \rangle |\phi(\vec{r})|^2 = 2g\rho'(\vec{r}) + g\langle N_0 \rangle |\phi(\vec{r})|^2 \quad (4.33)$$

where ρ' is the non-condensed density and $\langle N_0 \rangle |\phi|^2$ is the condensate density⁴. This result can be interpreted as follows: an atom in the condensate interacts with non-condensed particles with the effective coupling constant $2g$, and it interacts with another particle of the condensate with the effective coupling constant g .

For repulsive effective interactions ($g > 0$) this is at the basis of Nozières' argument against fragmentation of the condensate in several orthogonal states: in a box of size L in the thermodynamical limit, transferring a finite fraction of condensate particles from the plane wave $\vec{p} = \vec{0}$ to an excited plane wave $p = O(\hbar/L)$ costs a negligible amount of kinetic energy per particle but a finite amount of interaction energy. The transferred fraction would indeed be repelled with a stronger amplitude ($2g$ rather than g) by the atoms remaining in the condensate.

4.3.3 At thermal equilibrium

At thermal equilibrium the one-body density matrix of non-condensed atoms is given by the usual Bose distribution for the ideal Bose gas, with

⁴A careful reader may argue that we forget here the condition of orthogonality of the eigenstates of $\hat{\rho}'_1$ to ϕ . Inclusion of this condition is beyond accuracy of the Hartree–Fock approximation. It will be carefully included in the more precise number conserving Bogoliubov approach of Section 7.

the trapping potential being supplemented by the mean-field potential:

$$\hat{\rho}'_1 = \frac{1}{\exp \left\{ \beta \left[\frac{\vec{p}^2}{2m} + U(\vec{r}) + 2g\rho(\vec{r}) - \mu \right] \right\} - 1}. \quad (4.34)$$

The condensate wave function has to be a steady state of the total, mean field plus trapping potential seen by an atom in the condensate:

$$\lambda \phi(\vec{r}) = -\frac{\hbar^2}{2m} \Delta \phi + [U(\vec{r}) + g\langle N_0 \rangle |\phi(\vec{r})|^2 + 2g\rho'(\vec{r})] \phi(\vec{r}). \quad (4.35)$$

The Hartree–Fock single particle energy λ should not be confused with the energy per particle in the condensate, as it will become clear in the next section. The occupation number of the condensate is related to λ by the Bose formula:

$$\langle N_0 \rangle = \frac{1}{e^{\beta(\lambda - \mu)} - 1}. \quad (4.36)$$

We now have to solve in a self consistent way the three equations (4.34–4.36). In practice, when $\langle N_0 \rangle$ is already large, one can assume $\lambda = \mu$, which eliminates one unknown λ and one equation (4.36).

4.4 Comparison of Hartree–Fock to exact results

4.4.1 Quantum Monte Carlo calculations

The Quantum Monte Carlo method developed by Ceperley *et al* allows to sample in an exact way the N -body distribution function of a gas of N interacting bosons at thermal equilibrium. *I.e.* the algorithm generates random positions $\vec{r}_1, \dots, \vec{r}_N$ for the N particles with a probability distribution given by the exact N -body distribution function of the atoms.

In Figure 8 the Hartree–Fock prediction for the radial density of particles in a spherical harmonic trap, $r^2\rho(r)$, is compared to the Quantum Monte Carlo result for several temperatures below T_c . The Hartree–Fock prediction is in good agreement with the exact result, except close to T_c where it tends to underestimate the number of particles in the condensate [25].

4.4.2 Experimental results for the energy of the gas

At JILA the sum of kinetic and interaction energy of the atoms was measured as function of temperature, as we have already explained in Section 2.3. Whereas the ideal Bose gas model was clearly getting wrong for $T < T_c$, the Hartree–Fock prediction [26] is consistent with the experimental results over the whole considered temperature range (see Fig. 9).

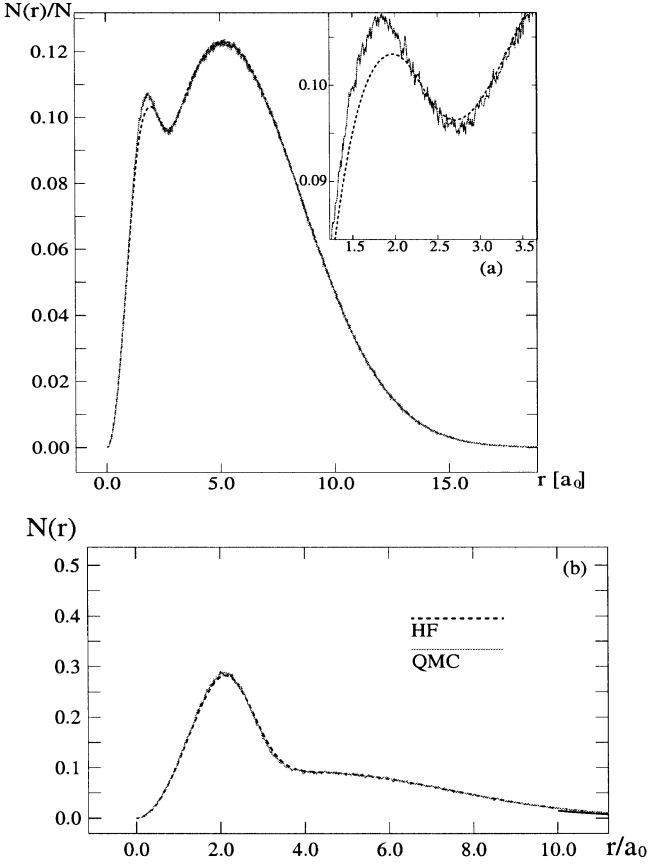


Fig. 8. Radial density of particles, $r^2 \rho(r)$, for an interacting Bose gas at thermal equilibrium in an isotropic harmonic trap. Noisy lines: results of a Quantum Monte Carlo simulation. Smooth solid lines: Hartree-Fock prediction. The curves corresponds to the temperatures $T/T_c^0 = 0.88$ (a), $T/T_c^0 = 0.7$ (b). The number of particles is $N = 10^4$ and the parameters are the ones of ^{87}Rb . These figures are taken from [25].

At very low temperatures ($T < T_c/2$), measurements at MIT have shown that the same energy becomes mainly a function of the number of particles N_0 in the condensate. By setting $\rho' = 0$ in the Hartree-Fock approximation, and using approximations presented in the coming section Section 5.3, an analytical expression can be obtained for the energy, in excellent agreement with the experimental results (see Fig. 5): the energy per particle has a power law dependence with N_0 , with an exponent $2/5$, to be contrasted

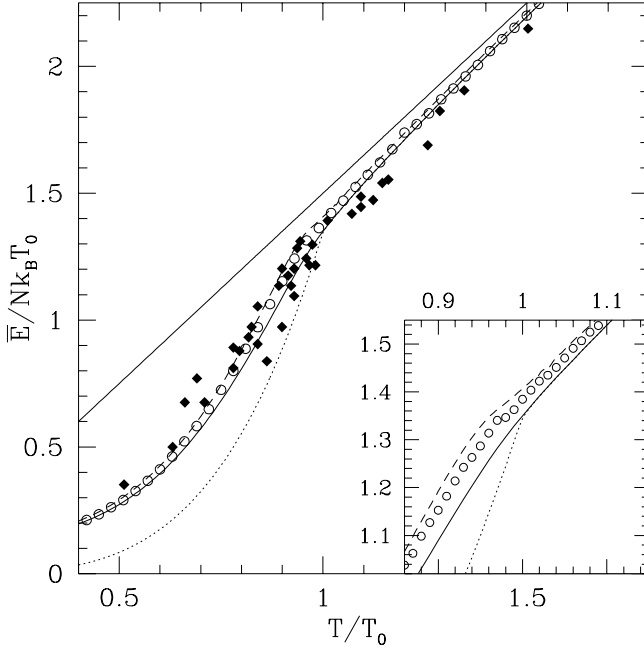


Fig. 9. Expansion energy of the gas per particle and in units of $k_B T_c^0$ as function of the temperature in units of T_c^0 . The filled rhombi correspond to the experimental results of [11]. The straight solid line is the prediction of Boltzmann statistics. The dotted curve is the ideal Bose gas prediction. The circles are the numerical solution to the Hartree–Fock approach. The curved solid line and the dashed line are approximate solutions to the Hartree–Fock equations. The inset is a magnification showing the change of slope of the energy as function of T close to $T = T_c^0$. The figure is taken from [26].

with the constant ideal Bose gas result, and has typical values an order of magnitude larger than the zero-point energy of the harmonic oscillator.

5 Properties of the condensate wavefunction

In this section we consider the regime of an almost pure condensate, where the non-condensed cloud has a negligible effect on the condensate. At thermal equilibrium with temperature T this regime corresponds to the limit $T \ll T_c$. As we shall see most of the experimental results obtained with almost pure condensates can be well reproduced by a single equation for the

condensate wavefunction, the so-called Gross–Pitaevskii equation, derived independently by Gross [27] and Pitaevskii [28].

5.1 The Gross–Pitaevskii equation

5.1.1 From Hartree–Fock

Let us assume that the density of non-condensed particles is much smaller than the density of condensate particles over the spatial width of the condensate:

$$\rho'(\vec{r}) \ll N_0 |\phi(\vec{r})|^2 \quad (5.1)$$

where N_0 is the mean number of particles in the condensate, ϕ is the condensate wavefunction normalized to unity:

$$\int d^3\vec{r} \phi(\vec{r}, t) \phi^*(\vec{r}, t) = 1. \quad (5.2)$$

In the Hartree–Fock expression of the mean field potential seen by the condensate, derived in the previous Section 4, we can drop the contribution of the non-condensed particles, to get for the evolution of the condensate contribution to the 1-body density matrix:

$$i\hbar \frac{d}{dt} (N_0 |\phi\rangle \langle \phi|) = \left[\frac{\vec{p}^2}{2m} + U(\vec{r}, t) + g N_0 |\phi(\vec{r}, t)|^2, N_0 |\phi\rangle \langle \phi| \right]. \quad (5.3)$$

This equation leads to $N_0 = \text{constant}$ and to the evolution equation for the condensate wavefunction:

$$i\hbar \partial_t \phi(\vec{r}, t) = \left[-\frac{\hbar^2}{2m} \Delta + U(\vec{r}, t) + N_0 g |\phi(\vec{r}, t)|^2 - \xi(t) \right] \phi(\vec{r}, t). \quad (5.4)$$

This non-linear Schrödinger equation is the so-called time dependent Gross–Pitaevskii equation. This equation is determined from our Hartree–Fock approach up to an arbitrary real function of time, $\xi(t)$, as equation (5.3) involves a commutator to which $\xi(t)$ does not contribute. In general the precise value of $\xi(t)$ is considered as a matter of convenience, as it can be absorbed in a redefinition of the global phase of ϕ . The knowledge of the value of $\xi(t)$ can become important when one is interested in the evolution of the relative phase of *two* Bose–Einstein condensates. The value of $\xi(t)$ has been derived in [29] assuming a well defined number of particles in the condensate. If the condensate is assumed to be in a Glauber coherent state that is a quasi-classical state of the atomic field with a well defined relative phase (see Sect. 8) one obtains $\xi(t) = 0$ as we will see in Section 5.1.3.

When the gas is at thermal equilibrium, the only time dependence left for ϕ is a global phase dependence. The most convenient choice is to assume $\partial_t \phi = 0$ so that $\xi(t)$ is a constant. As shown in Section 4.3.3 this constant is very close to the chemical potential of the gas as N_0 is large so that we get the so-called time independent Gross–Pitaevskii equation:

$$\mu \phi(\vec{r}) = \left[-\frac{\hbar^2}{2m} \Delta + U(\vec{r}) + N_0 g |\phi(\vec{r})|^2 \right] \phi(\vec{r}). \quad (5.5)$$

Both the time independent and the time dependent Gross–Pitaevskii equations can be solved numerically. But, as explained in the next part of this section, the fact that the trap is harmonic allows one to find very good approximate analytical solutions.

5.1.2 Variational formulation

Variational calculus turns out to be a very fruitful approximate technique in the solution of the Gross–Pitaevskii equation. We therefore derive here a variational formulation of the Gross–Pitaevskii equation.

- *Time independent case*

The time independent Gross–Pitaevskii equation can be obtained from extremalization over ϕ of the so-called Gross–Pitaevskii energy functional:

$$E[\phi, \phi^*] = N_0 \int d^3 \vec{r} \left[\frac{\hbar^2}{2m} |\text{grad } \phi|^2 + U(\vec{r}) |\phi(\vec{r})|^2 + \frac{1}{2} N_0 g |\phi(\vec{r})|^4 \right] \quad (5.6)$$

with the constraint that ϕ is normalized to unity.

Proof: We take into account the normalization constraint with the method of Lagrange multiplier, so that we simply have to express the fact that ϕ extremalizes without constraint the functional:

$$X[\phi, \phi^*] = E[\phi, \phi^*] - \lambda N_0 \int d^3 \vec{r} \phi(\vec{r}) \phi^*(\vec{r}). \quad (5.7)$$

The parameter λ is the Lagrange multiplier. We calculate the first order variation of X due to an infinitesimal arbitrary variation of the condensate wavefunction:

$$\phi(\vec{r}) \rightarrow \phi(\vec{r}) + \delta \phi(\vec{r}). \quad (5.8)$$

We obtain:

$$\begin{aligned} \delta X &= N_0 \int d^3 \vec{r} \left[\frac{\hbar^2}{2m} \text{grad } \delta \phi^* \cdot \text{grad } \phi + U(\vec{r}) \delta \phi^* \phi \right. \\ &\quad \left. + N_0 g \delta \phi^* \phi^* \phi^2 - \lambda \delta \phi^* \phi \right] + \text{c.c.} \end{aligned} \quad (5.9)$$

We modify the variation of the kinetic energy term by integrating by part, assuming that ϕ vanishes at infinity:

$$\int d^3\vec{r} (\vec{\text{grad}} \delta\phi^* \cdot \vec{\text{grad}} \phi + \text{c.c.}) = - \int d^3\vec{r} (\delta\phi^* \Delta\phi + \text{c.c.}). \quad (5.10)$$

The variation δX has to vanish for any $\delta\phi$. We can take as independent variables the real part and the imaginary part of $\delta\phi$, or equivalently $\delta\phi$ and $\delta\phi^*$ as it amounts to considering independent linear superpositions of the real and imaginary part. We therefore obtain:

$$N_0 \left[-\frac{\hbar^2}{2m} \Delta + U(\vec{r}) + N_0 g |\phi(\vec{r})|^2 - \lambda \right] \phi(\vec{r}) = 0. \quad (5.11)$$

We recover the time independent Gross–Pitaevskii equation, with $\lambda = \mu$, which gives a physical interpretation to the Lagrange multiplier λ .

- *Time dependent case*

The time dependent Gross–Pitaevskii equation with the choice $\xi(t) \equiv 0$ is obtained over a time interval $[t_1, t_2]$ from extremalization of the action:

$$A = \int_{t_1}^{t_2} dt \left[\frac{i\hbar}{2} \left(\langle \phi | \frac{d}{dt} | \phi \rangle - \text{c.c.} \right) N_0 - E[\phi(t), \phi^*(t)] \right] \quad (5.12)$$

with fixed values of $|\phi(t = t_1)\rangle$ and $|\phi(t = t_2)\rangle$.

- *Physical interpretation of the Gross–Pitaevskii energy functional*

We now show that $E[\phi, \phi^*]$ is simply the mean energy of the gas in the Hartree–Fock approximation in the limit of a pure condensate. As the N -body Hamiltonian is a sum of one-body and two-body (binary interaction) terms,

$$H = \sum_{i=1}^N h_i + \frac{1}{2} \sum_{i \neq j} V_{ij} \quad (5.13)$$

the mean energy of the gas involves the one-body and two-body density matrices:

$$\langle H \rangle = \text{Tr}[h_1 \hat{\rho}_1] + \frac{1}{2} \text{Tr}[V_{12} \hat{\rho}_{12}]. \quad (5.14)$$

In the limit of a pure condensate we keep only the condensate contribution to $\hat{\rho}_1$:

$$\hat{\rho}_1 \simeq N_0 |\phi\rangle \langle \phi| \quad (5.15)$$

and we approximate $\hat{\rho}_{12}$ by the Hartree ansatz

$$\hat{\rho}_{12} \simeq \hat{\rho}_1 \otimes \hat{\rho}_1. \quad (5.16)$$

We then obtain $E[\phi, \phi^*] = \langle H \rangle$. It was actually clear from the start that $E[\phi, \phi^*]$ was the sum of kinetic energy, trapping potential energy and mean field interaction energy of the condensate.

A different and interesting point of view at zero temperature is to use directly a Hartree–Fock ansatz for the ground state wavefunction $|\Psi\rangle$ of the gas, assuming that all the particles are in the condensate:

$$|\Psi\rangle = |N\rangle: \phi\rangle = |\phi\rangle \otimes \dots \otimes |\phi\rangle. \quad (5.17)$$

The mean energy of $|\Psi\rangle$ for the interaction potential $g\delta(\vec{r}_1 - \vec{r}_2)$ is then

$$\begin{aligned} E[\phi, \phi^*] = N \int d^3\vec{r} \left[\frac{\hbar^2}{2m} |\vec{\text{grad}} \phi|^2 + U(\vec{r}) |\phi(\vec{r})|^2 \right. \\ \left. + \frac{1}{2} (N-1) g |\phi(\vec{r})|^4 \right], \end{aligned} \quad (5.18)$$

which differs from equation (5.6) in the limit $N_0 = N$ only by the occurrence of a factor $(N-1)$ rather than N in front of the coupling constant g , ensuring that the interaction term disappears for $N = 1$!

- *What is the chemical potential?*

At zero temperature, assuming a pure condensate $N_0 \simeq N$, the usual thermodynamical definition of the chemical potential μ reduces to:

$$\mu = \frac{d\langle H \rangle}{dN} \simeq \frac{d}{dN_0} E[\phi, \phi^*, N_0] \quad (5.19)$$

where we have made appear the explicit dependence of E on N_0 . When one takes the total derivative of E with respect to N_0 , one gets in principle a contribution from the implicit dependence of E on N_0 through the N_0 dependence of ϕ, ϕ^* ; actually this contribution vanishes as the variation of E due to a change in ϕ, ϕ^* vanishes to first order in this change. We therefore get

$$\begin{aligned} \frac{d}{dN_0} E[\phi, \phi^*, N_0] = \frac{\partial}{\partial N_0} E[\phi, \phi^*, N_0] = \int d^3\vec{r} \left[\frac{\hbar^2}{2m} |\vec{\text{grad}} \phi|^2 \right. \\ \left. + U(\vec{r}) |\phi(\vec{r})|^2 + N_0 g |\phi(\vec{r})|^4 \right]. \end{aligned} \quad (5.20)$$

This quantity coincides with the chemical potential indeed, as can be checked by multiplying the time independent Gross–Pitaevskii equation by ϕ^* and integrating over the whole space. As g does not have the factor $1/2$ in equation (5.20), whereas it is multiplied by $1/2$ in the expression for $E[\phi, \phi^*]$, we see that in the interacting case $g \neq 0$:

$$\mu \neq \frac{E}{N_0} \quad (5.21)$$

that is the chemical potential μ differs from the mean energy per particle.

5.1.3 The fastest trick to recover the Gross–Pitaevskii equation

Starting from the second quantized form of the Hamiltonian,

$$H = \int d1 \, \hat{\psi}^\dagger(1) h_1 \hat{\psi}(1) + \frac{1}{2} \int d1 \int d2 \, \hat{\psi}^\dagger(1) \hat{\psi}^\dagger(2) V_{12} \hat{\psi}(2) \hat{\psi}(1) \quad (5.22)$$

where 1 and 2 stand for three-dimensional coordinates in real space, one first derives the Heisenberg equation of motion for the field operator:

$$i\hbar \frac{d}{dt} \hat{\psi}(1) = [\hat{\psi}(1), H] = \partial_{\hat{\psi}^\dagger(1)} H \quad (5.23)$$

$$= h_1 \hat{\psi}(1) + \int d2 \, \hat{\psi}^\dagger(2) V_{12} \hat{\psi}(2) \hat{\psi}(1) \quad (5.24)$$

and then replaces the quantum field operator by a classical field:

$$\hat{\psi} \rightarrow \psi = \sqrt{N_0} \phi. \quad (5.25)$$

As V_{12} is the pseudo-potential, the equation that we get for ϕ is the time dependent Gross–Pitaevskii equation with $\xi(t) \equiv 0$.

This sheds a new light on the Gross–Pitaevskii equation: the Gross–Pitaevskii equation is the equation of motion of the atomic field in the classical approximation, neglecting quantum fluctuations of the field. A Bose–Einstein condensate is a classical state of the atomic field, in a way similar to the laser being a classical state of the electromagnetic field.

5.2 Gaussian Ansatz

In this subsection we look for a variational solution to the Gross–Pitaevskii equation in a harmonic trap, using a Gaussian ansatz for ϕ [30]. The choice of a Gaussian is natural in the non-interacting limit $g \rightarrow 0$, where it becomes exact. It turns out to give also interesting results in presence of strong interactions.

5.2.1 Time-independent case

Consider for simplicity an isotropic harmonic trap, where the atoms have the oscillation frequency ω . We assume the following Gaussian for the condensate wavefunction:

$$\phi(\vec{r}) = \frac{1}{\pi^{3/4} \sigma^{3/2}} e^{-r^2/2\sigma^2} \quad (5.26)$$

the spatial width σ being the only variational parameter. The mean energy per particle can be calculated exactly for this ansatz:

$$\varepsilon \equiv \frac{E[\phi, \phi^*]}{N_0} = \frac{3\hbar^2}{4m\sigma^2} + \frac{3}{4}m\omega^2\sigma^2 + \frac{\hbar^2}{m} \frac{N_0 a}{\sigma^3} \frac{1}{\sqrt{2\pi}}. \quad (5.27)$$

The form of the result is intuitive: the kinetic energy term scales as Δp_x^2 , where $\Delta p_x = \hbar/(2\Delta x) = \hbar/(\sqrt{2}\sigma)$; the trapping potential energy scales as σ^2 and the interaction energy per particle is proportional to the coupling constant $g = 4\pi\hbar^2 a/m$ and to the typical density of atoms in the gas, N_0/σ^3 . Taking the harmonic oscillator length $(\hbar/m\omega)^{1/2}$ as a unit of length and the harmonic quantum of vibration $\hbar\omega$ as a unit of energy we get the simple form:

$$\varepsilon = \frac{3}{4} \left[\frac{1}{\sigma^2} + \sigma^2 \right] + \frac{\chi}{2\sigma^3} \quad (5.28)$$

where the only physical parameter left is

$$\chi = \sqrt{\frac{2}{\pi}} \frac{N_0 a}{\sqrt{\hbar/m\omega}}. \quad (5.29)$$

This parameter χ measures the effect of the interactions on the condensate density: the case $\chi \ll 1$ corresponds to the weakly interacting regime, close to the ideal Bose gas limit $\chi = 0$; the case $\chi \gg 1$ corresponds to the strongly interacting regime.

- *Case $a > 0$*

In the case of effective repulsive interactions between the particles, the dependence of ε with σ is plotted in Figure 10. In the limit $\sigma \rightarrow 0$, the energy ε is dominated by the positively diverging repulsive interaction ($\sim 1/\sigma^3$). For large σ the trapping potential term $\sim \sigma^2$ dominates. The function ε has a single minimum, in $\sigma = \sigma_0$, solving

$$\frac{d\varepsilon}{d\sigma}(\sigma_0) = 0 \rightarrow \sigma_0^5 = \sigma_0 + \chi. \quad (5.30)$$

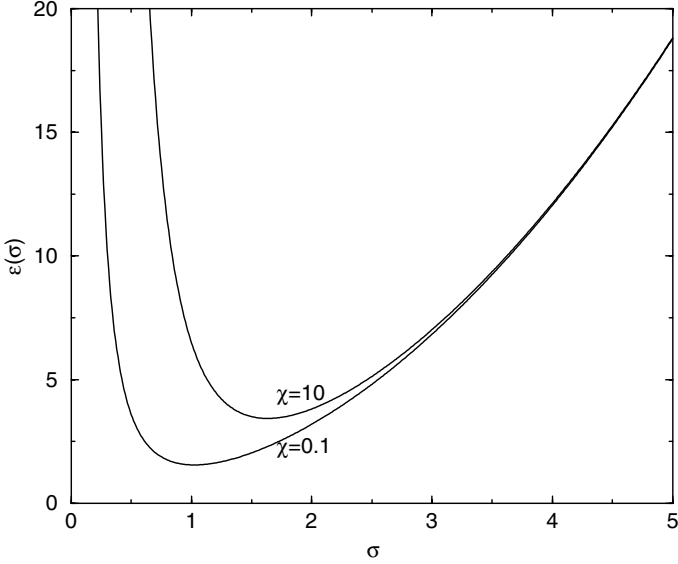


Fig. 10. Energy per particle in the condensate in units of $\hbar\omega$ as function of the variational width σ in units of $(\hbar/m\omega)^{1/2}$. Case of effective repulsive interactions $a > 0$.

For $\chi \ll 1$ one recovers the ground state of the harmonic trap, with $\sigma_0 = 1$. For $\chi \gg 1$ the condensate cloud becomes much broader than the ground state of the harmonic trap,

$$\sigma_0 \simeq \chi^{1/5} \propto N_0^{1/5}. \quad (5.31)$$

In this regime one can check that the kinetic energy term becomes negligible as compared to the trapping energy:

$$\frac{E_{\text{kin}}}{E_{\text{trap}}} = \frac{1}{\sigma^4} \simeq \frac{1}{\chi^{4/5}} \quad (5.32)$$

so that the steady state of the condensate is an equilibrium between the trapping potential and the repulsive interactions between particles. This regime will be studied in detail in the next subsection.

- *Case $a < 0$*

For effective attractive interactions between the particles the shape of ε as function of σ depends on the balance between kinetic and interaction energy (see Fig. 11). The interaction energy is negatively diverging as $\sigma \rightarrow 0$ always

faster than the positively diverging kinetic energy so that $\sigma = 0$ is always a minimum of ε , with $\varepsilon = -\infty$: the condensate is in a spatially collapsed state! Of course the Gross–Pitaevskii equation no longer applies for a too small σ , as the validity of the Born approximation requires $k|a| \simeq |a|/\sigma \ll 1$. For $|\chi|$ larger than some critical value $|\chi_c|$, this collapsed minimum is the only one of $\varepsilon(\sigma)$ so that we do not find any stable solution for the condensate wavefunction. When $|\chi|$ is smaller than $|\chi_c|$ the kinetic energy term, which is opposed to spatial compression of the gas, is able to beat the attractive energy over some range of σ , so that a local minimum of $\varepsilon(\sigma)$ appears, in $\sigma = \sigma_0$, separated from the collapsed minimum by a barrier.

To calculate $|\chi_c|$ we express the fact that the stationary point of ε in $\sigma = \sigma_0$ has now a vanishing curvature (inflexion point of ε):

$$\left(\frac{d\varepsilon}{d\sigma} \right)_{\sigma=\sigma_0}^{\chi=\chi_c} = 0 \quad (5.33)$$

$$\left(\frac{d^2\varepsilon}{d\sigma^2} \right)_{\sigma=\sigma_0}^{\chi=\chi_c} = 0. \quad (5.34)$$

By eliminating σ_0 between these two equations we obtain

$$\chi_c = -\frac{4}{5^{5/4}} = -0.5350... \quad (5.35)$$

This result can be rephrased in terms of a maximal number of atoms N_0^c that can be put in the condensate without inducing a collapse, according to a Gaussian ansatz:

$$\frac{N_0^c |a|}{\sqrt{\hbar/m\omega}} = \left(\frac{\pi}{2} \right)^{1/2} |\chi_c| \simeq -0.67. \quad (5.36)$$

A more precise result has been obtained by a numerical solution of Gross–Pitaevskii equation, not restricting to the subspace of Gaussian wavefunctions [31]: no solution of the time independent Gross–Pitaevskii equation is obtained for $N_0 > N_0^c$, where

$$\frac{N_0^c |a|}{\sqrt{\hbar/m\omega}} \simeq -0.57. \quad (5.37)$$

By a generalization of the Gaussian ansatz to the case of a non-isotropic harmonic trap one can also get a prediction of N_0^c for the parameters of the lithium experiment of Hulet’s group [32]. In the experiment the traps frequencies are $\omega_z = 2\pi \times 117$ Hz and $\omega_{x,y} = 2\pi \times 163$ Hz, and the scattering length is $a = -27$ Bohr radii. The Gaussian prediction is then $N_0^c \simeq 1500$, consistent with the experimental results.

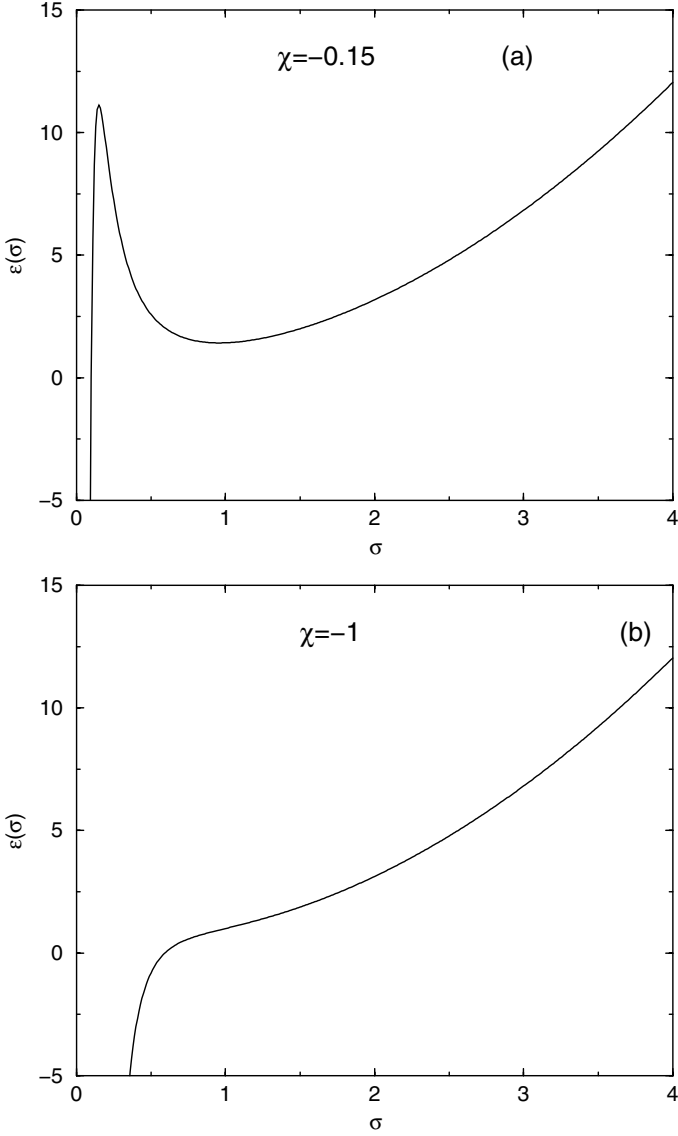


Fig. 11. For an effective attractive interaction $a < 0$ between the particles energy per particle in the condensate in units of $\hbar\omega$ as function of the variational width σ in units of $(\hbar/m\omega)^{1/2}$. The curve has two possible shapes, (a) with two minima when $|\chi|$ is smaller than a critical value $|\chi_c|$, and (b) with a single minimum for $|\chi| > |\chi_c|$.

- *Physical origin of the stabilization for $a < 0$*

In a harmonic trap, the energy of the ground state level is separated from the energy of excited states by $\hbar\omega$. At low values of χ the mean interaction energy per particle, $\sim \rho|g|$, where ρ is the density, is much smaller than $\hbar\omega$ so that it cannot efficiently induce a transition from the ground harmonic level to excited harmonic levels. Initiation of collapse on the contrary requires that the wavefunction ϕ expands on many excited levels in the trap, so that the density $|\phi|^2$ can exhibit a high density peak narrower than $\sqrt{\hbar/m\omega}$. We therefore intuitively reformulate the non-collapse condition as

$$\rho|g| < \hbar\omega. \quad (5.38)$$

Estimating ρ as $N_0/(\hbar/m\omega)^{3/2}$ we recover a N_0^c scaling as $\sqrt{\hbar/m\omega}/|a|$. This reasoning also applies to the gas confined in a cubic box with periodic boundary conditions, as we shall see in Section 6 of the lecture.

5.2.2 Time-dependent case

As done in [33, 34] the Gaussian ansatz can be generalized to the time dependent case. We assume here for simplicity that the condensate, initially in steady state, is excited only by a temporal variation of the trap frequencies $\omega_\alpha(t)$; then no oscillation of the center of mass motion of the condensate takes place, ϕ remaining of vanishing mean position and momentum. The Gaussian ansatz then contains only exponential of terms quadratic with position, its does not involve exponential of terms linear with position:

$$\phi(\vec{r}, t) = \frac{e^{i\delta(t)}}{\pi^{3/4} [\prod_\alpha \sigma_\alpha(t)]^{1/2}} \exp \left[- \sum_\alpha \frac{r_\alpha^2}{2\sigma_\alpha^2(t)} + i \sum_\alpha r_\alpha^2 \gamma_\alpha(t) \right]. \quad (5.39)$$

We do not assume that the trap is isotropic, so we have as variational parameters 3 spatial widths σ_α ($\alpha = x, y, z$), 3 factors γ_α governing the spatially quadratic phase and a global phase δ .

One gets time evolution equations for the variational parameters by inserting the ansatz for ϕ in the action A of equation (5.12) and by writing the Lagrange equations expressing the stationarity condition. It turns out that γ_α can be expressed in terms of the widths and their time derivatives:

$$\gamma_\alpha = - \frac{m\dot{\sigma}_\alpha}{2\hbar\sigma_\alpha} \quad (5.40)$$

so that one is left with equations for the σ_α 's. Taking ω^{-1} as a unit of time, $\sqrt{\hbar/m\omega}$ as a unit of length, where ω is an arbitrary reference frequency, we get:

$$\ddot{\sigma}_\alpha + \nu_\alpha^2 \sigma_\alpha = \frac{1}{\sigma_\alpha^3} + \frac{\chi}{\sigma_\alpha \sigma_x \sigma_y \sigma_z} \quad (5.41)$$

where the trap frequencies are $\omega_\alpha = \nu_a \omega$ and χ is defined in equation (5.29). In the absence of interaction ($\chi = 0$) these evolution equations become exact, and give a remarkable (and known!) result for the time dependent harmonic oscillator. In the interacting case ($\chi \neq 0$) these equations can be cast in Hamiltonian form as the “force” seen by the variable σ_α derives from a potential. The corresponding dynamics is non linear and non trivial; chaotic behavior has been obtained in [35] in the limiting regime of $\chi \gg 1$ where the $1/\sigma_\alpha^3$ can be neglected.

One can use equation (5.41) to study the response of the condensate to a weak excitation, the trap frequency ω_α in the experiments being typically slightly perturbed from its steady state value $\omega_\alpha(0)$ for a finite excitation time. Linearizing the evolution equations in terms of the deviations of the σ ’s from their steady state value:

$$\sigma_\alpha(t) = \sigma_\alpha^{\text{st}} + \delta\sigma_\alpha(t) \quad (5.42)$$

one gets a three by three system of second order differential equations for the $\delta\sigma$ ’s. Looking for eigenmodes of this system, one finds three eigenfrequencies [34]. Their values have been compared to experimental results at JILA [36], see Figure 12: the agreement is very good, not only in the weakly interacting regime $\chi \ll 1$ but also in the regime $\chi \gg 1$, where the Gaussian ansatz for the condensate wavefunction has no reason to be a good one! The explanation of this mystery is given in Section 5.4.1.

5.3 Strongly interacting regime: Thomas–Fermi approximation

In this subsection we focus on the strongly interacting regime: the scattering length is positive, with the dimensionless parameter χ of equation (5.29) much larger than one. This regime is the so-called Thomas–Fermi regime. As we now see analytical results can be obtained in this limit.

5.3.1 Time-independent case

If we put a large enough number of particles into the condensate the atoms will experience repulsive interactions that will increase the spatial radius of the condensate to a value R much larger than the one of the ground state of the harmonic trap:

$$R \gg \left(\frac{\hbar}{m\omega} \right)^{1/2}. \quad (5.43)$$

For increasing value of N_0 , R increases so that the momentum width of the condensate, scaling as $\hbar/R$ as ϕ_0 is a non-oscillating function of the position, is getting smaller and smaller. More precisely we find that

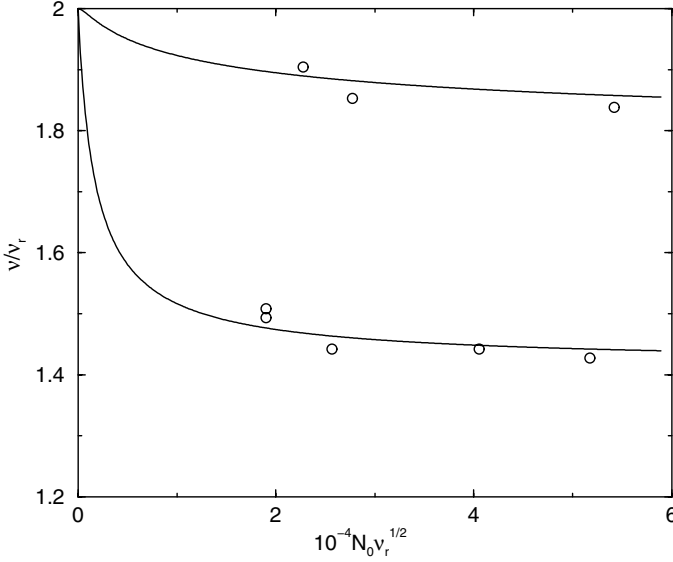


Fig. 12. Frequencies of two eigenmodes of a condensate in a cylindrically symmetric harmonic trap, in units of the radial trap frequency ν_r , as a function of a parameter proportional to χ measuring the strength of the interactions. Plotting symbols: measurements at JILA [36]. Solid lines: predictions of the Gaussian Ansatz [34].

the typical kinetic energy of the condensate becomes much smaller than the typical harmonic potential energy of the condensate:

$$\frac{E_{\text{kin}}}{E_{\text{harm}}} \simeq \frac{\frac{\hbar^2}{mR^2}}{m\omega^2 R^2} \simeq \left(\frac{\hbar}{m\omega R^2} \right)^2 \ll 1. \quad (5.44)$$

The mechanical equilibrium of the condensate in the trap then comes mainly from the balance between the expelling effect of the repulsive interactions and the confining effect of the trap.

In this large R regime we neglect the kinetic energy term in the Gross–Pitaevskii energy functional, which leads to a functional of the condensate density only (similarly to the Thomas–Fermi approximation for electrons). This approximation amounts to neglecting the $\Delta\phi$ term in the Gross–Pitaevskii equation:

$$\mu\phi(\vec{r}) \simeq U(\vec{r})\phi(\vec{r}) + N_0 g |\phi(\vec{r})|^2 \phi(\vec{r}). \quad (5.45)$$

Taking ϕ to be real we find that

$$\phi(\vec{r}) = \left(\frac{\mu - U(\vec{r})}{N_0 g} \right)^{1/2} \quad (5.46)$$

in the points of space where $\mu > U(\vec{r})$, otherwise we have $\phi(\vec{r}) = 0$.

This very important, Thomas–Fermi result equation (5.46) can also be obtained in a local density approximation point of view. A spatially uniform condensate with a chemical potential μ and in presence of a uniform external potential U has a density $N_0|\phi|^2 = (\mu - U)/g$. Applying this formula with a $\vec{r}$ dependent potential U gives again equation (5.46). A local density approximation can be used only if the density of the condensate varies slowly at the scale of the so-called “healing length” ξ , introduced in Section 5.3.4; one can check that the condition $\xi \ll R$ is indeed satisfied in the Thomas–Fermi regime.

We specialize equation (5.46) to the case of a harmonic but not necessarily isotropic trap:

$$U(\vec{r}) = \frac{1}{2} m \sum_{\alpha} \omega_{\alpha}^2 r_{\alpha}^2 \quad (5.47)$$

where $\alpha = x, y, z$ label the eigenaxis of the trap. The boundary of the condensate $\mu = U(\vec{r})$ is then an ellipsoid with a radius R_{α} along axis α given by:

$$\mu = \frac{1}{2} m \omega_{\alpha}^2 R_{\alpha}^2. \quad (5.48)$$

The condensate wavefunction can be rewritten in terms of these radii:

$$\phi(\vec{r}) = \left(\frac{\mu}{N_0 g} \right)^{1/2} \left(1 - \sum_{\alpha} \frac{r_{\alpha}^2}{R_{\alpha}^2} \right)^{1/2}. \quad (5.49)$$

Using the normalization condition of ϕ to unity we can also express the “normalization” factor $\sqrt{\mu/N_0 g}$ in terms of the radii. The integral of $|\phi|^2$ can be calculated in spherical coordinates after having made the change of variable $u_{\alpha} = r_{\alpha}/R_{\alpha}$. This leads to

$$\left(\frac{\mu}{N_0 g} \right)^{1/2} = \left(\frac{15}{8\pi \prod_{\alpha} R_{\alpha}} \right)^{1/2}. \quad (5.50)$$

Eliminating R_{α} in terms of μ thanks to equation (5.48) we can calculate the chemical potential:

$$\mu = \frac{1}{2} \hbar \bar{\omega} \left[15 \frac{N_0 a}{(\hbar/m\bar{\omega})^{1/2}} \right]^{2/5} \quad (5.51)$$

where $\bar{\omega}$ is the geometrical mean of the trap frequencies:

$$\bar{\omega} = (\omega_x \omega_y \omega_z)^{1/3}. \quad (5.52)$$

We can now see that in the limit $\chi \gg 1$ the chemical potential μ satisfies

$$\mu \gg \hbar \bar{\omega}, \quad (5.53)$$

which is a convenient way of defining the Thomas–Fermi regime.

We can now compare these Thomas–Fermi predictions to the MIT experimental results on the energy of the condensate [12]. In the experiment the trapping potential is switched off abruptly, so that the energy of the gas abruptly reduces to $E_{\text{red}} = E_{\text{kin}} + E_{\text{int}} \simeq E_{\text{int}}$; afterwards the cloud ballistically expands, E_{int} is converted in kinetic expansion energy that can be measured. In the Thomas–Fermi approximation the integral of $N_0^2 g |\phi|^4 / 2$ can be done, which leads to

$$E_{\text{int}} \simeq \frac{2}{7} N_0 \mu \propto N_0^{7/5}. \quad (5.54)$$

The resulting dependence in N_0 is in good agreement with the MIT results, see Figure 5.

From the expression of the chemical potential we can also calculate the total energy of the condensate in the trap, as $\mu = \partial_{N_0} E$: integrating over N_0 gives

$$E \simeq \frac{5}{7} \mu N_0. \quad (5.55)$$

One can then check explicitly that $\mu \neq E/N_0$!

5.3.2 How to extend the Thomas–Fermi approximation to the time-dependent case?

We would like to analyze time dependent situations encountered in the experiments, *e.g.*

- ballistic expansion of the gas: this is a crucial example, as it is a standard experimental imaging technique of the condensate;
- collective excitations: response of the condensate to a modulation of the trap frequencies;

in the strongly interacting regime. An immediate generalization of the Thomas–Fermi approximation consisting in neglecting the kinetic energy of the condensate is now too naive! In the case of ballistic expansion for example the interaction energy is gradually transformed into kinetic energy when the cloud expands so kinetic energy becomes important!

The trick is actually to split the kinetic energy in two contributions, one of them remaining small and negligible in the time dependent case. This is performed using the so-called hydrodynamic representation of the condensate classical field, split in a modulus and a phase:

$$N_0^{1/2} \phi(\vec{r}) = \rho^{1/2}(\vec{r}) e^{iS(\vec{r})/\hbar} \quad (5.56)$$

where S has the dimension of an action and ρ is simply the condensate density. The mean kinetic energy of the condensate then writes

$$\begin{aligned} E_{\text{kin}}[\phi, \phi^*] &= \int d^3\vec{r} \frac{\hbar^2}{2m} \left| \text{grad } \phi \right|^2 \\ &= \int d^3\vec{r} \left[\frac{\hbar^2}{2m} \left(\text{grad} \sqrt{\rho} \right)^2 + \rho \frac{\left(\text{grad } S \right)^2}{2m} \right]. \end{aligned} \quad (5.57)$$

As we shall see during ballistic expansion of the condensate the density ρ remains a smooth, slowly varying function of the position so that it has a very small contribution to the kinetic energy; most of the kinetic energy induced from interaction energy is stored in the spatial variation of the phase of the condensate wavefunction.

5.3.3 Hydrodynamic equations

In this subsection we rewrite the time dependent Gross–Pitaevskii equation in terms of the density ρ and the phase S . This can be done of course by a direct insertion of equation (5.56) in the Gross–Pitaevskii equation.

A more elegant way is to use the covariant nature of the Lagrangian formulation of the Gross–Pitaevskii equation, equation (5.12). We rewrite the density of Lagrangian in terms of ρ and S :

$$\mathcal{L} = - \left[\rho \partial_t S + \frac{\hbar^2}{2m} \left(\text{grad} \sqrt{\rho} \right)^2 + \rho \frac{\left(\text{grad } S \right)^2}{2m} + U(\vec{r}, t) \rho + \frac{g}{2} \rho^2 \right]. \quad (5.58)$$

An evolution equation for an arbitrary coordinate $Q(\vec{r}, t)$ of the field is obtained from the Lagrange equation:

$$\partial_t \left(\frac{\partial \mathcal{L}}{\partial(\partial_t Q)} \right) + \sum_{\alpha} \partial_{r_{\alpha}} \left(\frac{\partial \mathcal{L}}{\partial(\partial_{r_{\alpha}} Q)} \right) = \frac{\partial \mathcal{L}}{\partial Q}. \quad (5.59)$$

We first specialize the Lagrange equations to the choice $Q = \sqrt{\rho}$; dividing the resulting equation by $2\sqrt{\rho}$ we obtain

$$\partial_t S + \frac{1}{2m} \left(\text{grad } S \right)^2 + U + \rho g = \frac{\hbar^2}{2m} \frac{\Delta \sqrt{\rho}}{\sqrt{\rho}}. \quad (5.60)$$

Then we set $Q = S$ in the Lagrange equations which leads to

$$\partial_t \rho + \operatorname{div} \left[\frac{\rho}{m} \vec{\operatorname{grad}} S \right] = 0. \quad (5.61)$$

This last equation looks like a continuity equation. This is confirmed by the following physical interpretation of $\vec{\operatorname{grad}} S$. It is known in basic quantum mechanics that the probability current density associated to a single particle wavefunction ϕ is

$$\vec{j}_{\text{proba}} = \frac{\hbar}{2im} \left[\phi^* \vec{\operatorname{grad}} \phi - \text{c.c.} \right]. \quad (5.62)$$

Multiplying this expression by N_0 , as there are N_0 particles in the condensate, and introducing the (ρ, S) representation of ϕ we get the following expression for the current density of condensate particles:

$$\vec{j} = \rho \frac{\vec{\operatorname{grad}} S}{m} \equiv \rho \vec{v} \quad (5.63)$$

where $\vec{v}$ is the so-called local velocity field in the gas.

Equation (5.61) is therefore the usual continuity equation:

$$\partial_t \rho + \operatorname{div} [\rho \vec{v}] = 0. \quad (5.64)$$

The other equation (5.60) can be turned into an evolution equation for the velocity field by taking its spatial gradient:

$$m \partial_t \vec{v} + \vec{\operatorname{grad}} \left[\frac{1}{2} m v^2 + U(\vec{r}) + g \rho(\vec{r}) - \frac{\hbar^2}{2m} \frac{\Delta \sqrt{\rho}}{\sqrt{\rho}} \right] = 0. \quad (5.65)$$

This looks like the Navier–Stokes equation used in classical hydrodynamics, in the limiting case of a fluid with no viscosity. The term $\vec{\operatorname{grad}}(\frac{1}{2} m v^2)$ looks unusual but using the fact that $\vec{v}$ is the gradient of a function S/m one can put it in the usual form of a convective term:

$$\vec{\operatorname{grad}} \left(\frac{1}{2} m v^2 \right) = m (\vec{v} \cdot \vec{\operatorname{grad}}) \vec{v}. \quad (5.66)$$

A difference with classical hydrodynamics is the so-called quantum pressure term, involving

$$-\frac{\hbar^2}{2m} \frac{\Delta \sqrt{\rho}}{\sqrt{\rho}}, \quad (5.67)$$

the only term in the equations (5.64, 5.65) where $\hbar$ appears.

5.3.4 Classical hydrodynamic approximation

The classical hydrodynamic approximation consists precisely in neglecting the quantum pressure term equation (5.67) in the equation (5.65) for the velocity field of the condensate.

We can estimate simply the validity condition of this approximation. Denoting d a typical length scale for the variation of the condensate density $\rho(\vec{r})$ we obtain the estimate

$$\frac{\Delta\sqrt{\rho}}{\sqrt{\rho}} \sim \frac{1}{d^2}. \quad (5.68)$$

Comparing the quantum pressure term equation (5.67) to the classical mean field term ρg yields the condition

$$\frac{\hbar^2}{md^2} \ll g\rho(\vec{r}) \sim \rho_{\max}g \quad (5.69)$$

where $\rho_{\max}$ is the maximal density (usually at the center of the trap). This validity condition can be reformulated in terms of the healing length,

$$d \gg \xi \equiv \left(\frac{\hbar^2}{2m\rho_{\max}g} \right)^{1/2}. \quad (5.70)$$

Note that ξ is sometimes also called coherence length, which can be confusing.

Why this name of healing length for ξ ? Imagine that you cut with an infinite wall a condensate in an otherwise uniform potential. Right at the wall the condensate density vanishes; far away from the wall the density of the condensate is uniform. The condensate density adapts from zero to its constant bulk value over a length typically on the order of ξ . This can be checked by an explicit solution of the Gross–Pitaevskii equation:

$$N_0^{1/2}\phi(x, y, z) = \rho_{\max}^{1/2} \tanh\left(\frac{z}{\sqrt{2}\xi}\right) \quad (5.71)$$

where $z = 0$ is the plane of the infinite wall. This explicit solution shows that at a distance $z \gg \xi$ from the infinite wall there is no more any effect of the boundary condition $\phi(x, y, z = 0) = 0$. This is to be contrasted with the case of the ideal Bose gas: the ground state between infinite walls separated by the length L then scales as $\sin(\pi z/L)$ and depends dramatically on L .

For a moderate excitation of the condensate by a modulation of the trap frequencies, or in the course of ballistic expansion of the condensate, we shall see that the only typical length scale for the variation of the condensate density is the radius R of the condensate itself. One can then check that in

the Thomas–Fermi regime the classical hydrodynamic approximation indeed applies:

$$\frac{R}{\xi} \simeq \left(\frac{2\mu}{m\omega^2} \right)^{1/2} \times \left(\frac{2m\mu}{\hbar^2} \right)^{1/2} = \frac{2\mu}{\hbar\omega} \gg 1. \quad (5.72)$$

In the Thomas–Fermi regime we therefore neglect the quantum pressure term to obtain

$$m \left[\partial_t + \left(\vec{v} \cdot \vec{\text{grad}} \right) \right] \vec{v}(\vec{r}, t) = -\vec{\text{grad}} (U(\vec{r}, t) + g\rho(\vec{r}, t)) \equiv \vec{F}(\vec{r}, t). \quad (5.73)$$

This equation is then a purely classical equation, Newton’s equation in presence of the force field $\vec{F}$ written in Euler’s point of view. The operator between square brackets is simply the so-called convective derivative.

It is instructive to rewrite equation (5.73) in Lagrange’s point of view. One then follows a small piece of the fluid in course of its motion. Denoting $\vec{r}(t)$ the trajectory of the small piece of fluid we directly write Newton’s equation:

$$m \frac{d^2}{dt^2} \vec{r}(t) = \vec{F}(\vec{r}(t), t) = - \left[\vec{\text{grad}} (U + g\rho) \right] (\vec{r}(t), t). \quad (5.74)$$

This equation automatically implies the continuity equation (5.64) and the Euler equation (5.73). The unusual feature is that the force field depends itself on the density of the gas, so that we are facing here a self-consistent classical problem, corresponding formally to the mean field approximation for a collisionless classical gas! A surprising conclusion, knowing that we are actually studying the motion of a Bose–Einstein condensate!

5.4 Recovering time-dependent experimental results

5.4.1 The scaling solution

It turns out that the self-consistent classical problem equation (5.74) can be solved exactly for the particular conditions of a gas initially at rest and in a harmonic trap.

At time $t = 0$ we assume a steady state Bose–Einstein condensate in the trap, of course in the Thomas–Fermi regime so that the classical hydrodynamic approximation is reasonable. The steady state of equation (5.74) corresponds to a force field $\vec{F}$ vanishing everywhere, so that

$$U(\vec{r}) + g\rho(\vec{r}) = \text{constant}. \quad (5.75)$$

One recovers the stationary Thomas–Fermi density profile, the constant being determined from the normalization condition of ρ and therefore coinciding with the Thomas–Fermi approximation for μ .

At time $t > 0$ the trapping potential remains harmonic with the same eigenaxis [37] but the eigenfrequencies of the trap can have any time dependence:

$$U(\vec{r}, t) = \frac{1}{2} \sum_{\alpha=x,y,z} m\omega_{\alpha}^2(t)r_{\alpha}^2. \quad (5.76)$$

Then any small piece of the fluid with initial positions $r_{\alpha}(0)$ along axis α will move according to the trajectory

$$r_{\alpha}(t) = \lambda_{\alpha}(t)r_{\alpha}(0) \quad (5.77)$$

where the scaling factors $\lambda_{\alpha}(t)$ depend only on time, not on the initial position of the small piece of fluid. In other words the density of the gas will experience a mere (possibly anisotropic) dilatation

$$\rho(\vec{r}, t) = \frac{1}{\lambda_x(t)\lambda_y(t)\lambda_z(t)} \rho\left(\left\{\frac{r_{\alpha}}{\lambda_{\alpha}(t)}\right\}, t=0\right). \quad (5.78)$$

We can see simply why the ansatz equation (5.77) solves indeed equation (5.74) for a harmonic trap. As the initial density in the trap has a quadratic dependence on position, so will have the density at time t . The gradient $-\text{grad}(\rho g)$ appearing in the expression of the force field will then be a linear function of the coordinates; so is the harmonic force $-\text{grad}U(\vec{r}, t)$. Newton's equation is therefore linear in the coordinates; dividing it by $r_{\alpha}(0)$ one then gets equations for $\lambda_{\alpha}(t)$ irrespective of the initial coordinates $r_{\alpha}(0)$!

More details are given in [38, 39], we give here the equations for the scaling parameters:

$$\frac{d^2}{dt^2}\lambda_{\alpha}(t) = \frac{\omega_{\alpha}^2(0)}{\lambda_{\alpha}\lambda_x\lambda_y\lambda_z} - \omega_{\alpha}^2(t)\lambda_{\alpha}(t), \quad \alpha = x, y, z \quad (5.79)$$

with the initial conditions

$$\lambda_{\alpha}(0) = 0 \quad (5.80)$$

$$\frac{d}{dt}\lambda_{\alpha}(0) = 0 \quad (5.81)$$

since the condensate is initially at rest.

Finally we make the connection between these scaling solutions and the equations for the spatial widths σ_{α} obtained in equation (5.41) from a time dependent variational Gaussian ansatz for the condensate wavefunction. We are here in the Thomas-Fermi regime $\chi \gg 1$ so that the $1/\sigma_{\alpha}^3$ terms can be neglected in equation (5.41). The steady state solutions for the σ_{α} 's are then $\sigma_{\alpha}(0) \simeq \chi^{1/5}\bar{\nu}^{3/5}/\nu_{\alpha}(0)$ where $\bar{\nu}$ is the geometrical mean of the

initial frequencies $\nu_\alpha(0)$, and the quantities $\sigma_\alpha(t)/\sigma_\alpha(0)$ then obey the same equations as the λ_α 's! The Gaussian ansatz, which has the wrong shape in the Thomas–Fermi regime, is however able to capture the right scaling nature of the solution! This explains why the collective mode frequencies obtained from equation (5.41) are a good approximation, not only when $\chi \ll 1$, where the Gaussian ansatz was expected to hold, but also in the strongly interacting regime $\chi \gg 1$.

5.4.2 Ballistic expansion of the condensate

At time $t = 0^+$ the trapping potential is turned off suddenly. The scaling parameters then satisfy the simpler equations

$$\frac{d^2}{dt^2} \lambda_\alpha(t) = \frac{\omega_\alpha^2(0)}{\lambda_\alpha \lambda_x \lambda_y \lambda_z}. \quad (5.82)$$

These equations are still difficult to solve analytically. In the experimentally relevant regime of cigar-shaped traps, with $\omega_z(0) \ll \omega_x(0) = \omega_y(0)$, one can find an approximate solution [38].

Experimentally the scaling predictions have been tested carefully. First one can see if the ballistically expanded condensate density has indeed the shape of an inverted parabola [38]. Second one can measure the radii of the condensate as function of time to see if they fit the scaling predictions [40]. Both tests confirm the scaling predictions in the Thomas–Fermi regime.

5.4.3 Breathing frequencies of the condensate

A typical excitation sequence of breathing modes of the condensate proceeds as follows. One starts with a steady state condensate in the trapping potential. Then one modulates one of the trap frequencies for some finite time t_{exc} , at a frequency close to an expected resonance of the condensate. Then one lets the excited condensate evolve in the unperturbed trap for some adjustable time t_{osc} . Finally one can perform imaging of the cloud, *e.g.* by performing a ballistic expansion of the condensate and measuring the aspect ratio of the expanded cloud. By repeating the whole sequence for different values of t_{osc} one can reconstruct the aspect ratio as function of t_{osc} .

Such a procedure has been used at JILA and at MIT. In Figure 13 are shown results obtained at MIT in a cigar-shaped trap, for a modulation of the trap frequency along the slow (that is weakly confining) axis z . The solid line corresponds to the prediction of scaling theory, the input parameters being (i) the oscillation frequencies ω_α of the atoms in the trap, (ii) the precise way the excitation is performed, and (iii) the duration of ballistic expansion; the agreement between theory and experiment is good, considering the fact that there is no fitting parameter [38].

If one is interested only in the frequencies of the breathing eigenmodes of the condensate it is sufficient to linearize the equations of the scaling parameters around their steady state value:

$$\frac{d^2}{dt^2} \delta\lambda_\alpha = -2\omega_\alpha^2(0)\delta\lambda_\alpha - \omega_\alpha^2(0) \sum_\beta \delta\lambda_\beta \quad (5.83)$$

and find the eigenvalues of the corresponding three by three linear system (see also Sect. 6.3.3). For a trap with cylindrical symmetry one gets the eigenfrequencies $\Omega = \sqrt{2}\omega_\perp(0)$ and

$$\Omega^2 = \frac{1}{2} \left[3\omega_z^2(0) + 4\omega_\perp^2(0) \pm (9\omega_z^4(0) + 16\omega_\perp^4(0) - 16\omega_z^2(0)\omega_\perp^2(0))^{1/2} \right]. \quad (5.84)$$

The mode observed at MIT corresponds to the $-$ sign in the above expression; as the trap was cigar-shaped in the experiment, $\omega_\perp(0) \gg \omega_z(0)$ so that one has the approximate formula

$$\Omega \simeq \left(\frac{5}{2} \right)^{1/2} \omega_z(0). \quad (5.85)$$

6 What we learn from a linearization of the Gross–Pitaevskii equation

There are several important motivations to perform a linearization of the Gross–Pitaevskii equation around a steady state solution ϕ_0 :

- as the Gross–Pitaevskii equation is a non-linear equation it is crucial to check the so-called “dynamical” stability of the steady state solution. More precisely one has to check with a linear stability analysis that any small deviation $\delta\phi$ of the condensate wavefunction from ϕ_0 does not diverge exponentially with time. Otherwise ϕ_0 may not be physically considered as a steady state as even very small perturbations will eventually induce an evolution of the condensate wavefunction far from ϕ_0 ;
- as a byproduct of linear stability analysis we obtain a linear response theory for the condensate very useful to interpret experiments which apply a weak perturbation to the condensate;
- another important byproduct is the Bogoliubov approach which gives a description of the state of the non-condensed particles that is still approximate but more accurate at low temperature (typically $k_B T < \mu$) than the Hartree–Fock approach. This allows to check the so-called “thermodynamical stability” of the condensate and will be the subject of Section 7.

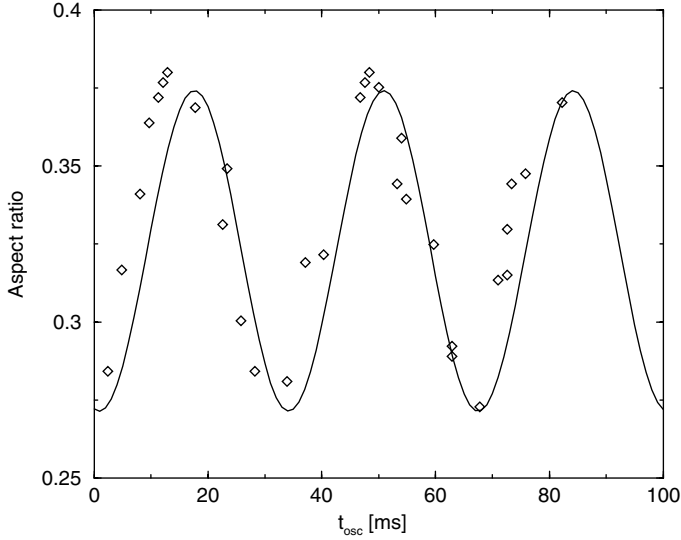


Fig. 13. Aspect ratio of the excited and ballistically expanded condensate as a function of free oscillation time t_{osc} . The expansion time is 40 ms, the unperturbed trap frequencies are $\omega_{\perp}(0) = 2\pi \times 250$ Hz, $\omega_z(0) = 2\pi \times 19$ Hz. Solid line: theory. Diamonds: experimental data obtained at MIT.

6.1 Linear response theory for the condensate wavefunction

6.1.1 Linearize the Gross–Pitaevskii solution around a steady–state solution

Let $\phi_0(\vec{r})$ be a steady state solution of the Gross–Pitaevskii solution in the time independent trapping potential $U_0(\vec{r})$:

$$0 = \left[-\frac{\hbar^2}{2m} \Delta + U_0 + gN_0|\phi_0|^2 - \mu \right] \phi_0. \quad (6.1)$$

The trapping potential is then slightly modified by a time dependent perturbation $\delta U(\vec{r}, t)$, resulting in a total trapping potential

$$U(\vec{r}, t) = U_0(\vec{r}) + \delta U(\vec{r}, t). \quad (6.2)$$

The condensate wavefunction, initially equal to ϕ_0 , evolve according to

$$i\hbar \partial_t \phi = \left[-\frac{\hbar^2}{2m} \Delta + U + gN_0|\phi|^2 - \mu \right] \phi. \quad (6.3)$$

As δU is so small we assume that ϕ experiences only a small deviation from ϕ_0 :

$$\phi(\vec{r}, t) = \phi_0(\vec{r}) + \delta\phi(\vec{r}, t) \quad (6.4)$$

so that we can linearize equation (6.3) in terms of $\delta\phi$. Neglecting the second order product of $\delta\phi$ and δU we obtain:

$$i\hbar\partial_t\delta\phi = \left[-\frac{\hbar^2}{2m}\Delta + U_0 - \mu \right] \delta\phi + 2gN_0\phi_0^*\phi_0\delta\phi + gN_0\phi_0^2\delta\phi^* + \delta U\phi_0. \quad (6.5)$$

Note the presence of the factor 2 in front of the term proportional to $g\delta\phi$; it turns out (and this should become clear in the Bogoliubov approach) that this factor 2 has the same origin as the one in the Hartree-Fock potential (4.18) for the non-condensed particles. As ϕ remains normalized to unity, as ϕ_0 was, we note that to first order in $\delta\phi$,

$$\int d^3\vec{r} [\delta\phi(\vec{r}, t)\phi_0^*(\vec{r}) + \phi_0(\vec{r})\delta\phi^*(\vec{r}, t)] = 0. \quad (6.6)$$

A peculiar feature of equation (6.5) is that, though it is obtained from a linearization procedure, it is not a linear equation for $\delta\phi$ in the strict mathematical sense: if $\delta\phi$ is a particular solution of the homogeneous part of this equation (set $\delta U = 0$), the function $\alpha\delta\phi$ (where α is a constant complex number) is generally not a solution of the homogeneous part anymore because of the coupling of $\delta\phi$ to $\delta\phi^*$. There are several possibilities to restore this linearity. A first one is to consider as unknown functions the real part and the imaginary part of $\delta\phi$. A second, more elegant method, more common in the literature, is to introduce formally as unknown the two-component column vector:

$$\begin{pmatrix} \delta\phi(\vec{r}, t) \\ \delta\phi^*(\vec{r}, t) \end{pmatrix} \quad (6.7)$$

the functions $\delta\phi$ and $\delta\phi^*$ being now considered as independent. We then rewrite equation (6.5) as the linear system:

$$i\hbar\partial_t \begin{pmatrix} \delta\phi(\vec{r}, t) \\ \delta\phi^*(\vec{r}, t) \end{pmatrix} = \mathcal{L}_{\text{GP}} \begin{pmatrix} \delta\phi(\vec{r}, t) \\ \delta\phi^*(\vec{r}, t) \end{pmatrix} + \begin{pmatrix} S(\vec{r}, t) \\ -S^*(\vec{r}, t) \end{pmatrix} \quad (6.8)$$

with a source term $S(\vec{r}, t) = \delta U(\vec{r}, t)\phi_0(\vec{r})$ and a linear operator

$$\mathcal{L}_{\text{GP}} = \begin{pmatrix} H_{\text{GP}} + gN_0|\phi_0|^2 & gN_0\phi_0^2 \\ -gN_0\phi_0^{*2} & -[H_{\text{GP}} + gN_0|\phi_0|^2]^* \end{pmatrix} \quad (6.9)$$

where we have introduced the Gross–Pitaevskii Hamiltonian:

$$H_{\text{GP}} \equiv -\frac{\hbar^2}{2m}\Delta + U_0 + gN_0|\phi_0|^2 - \mu. \quad (6.10)$$

Note the presence of complex conjugation in the second line of $\mathcal{L}_{\text{GP}}$; it also applies to the potential U_0 , without effect here as U_0 , hermitian function of $\vec{r}$, is real; it should not be forgotten in situations where the potential contains a complex term such as $-\Omega L_z$ where L_z is the angular momentum operator (inertial term in a frame rotating at angular velocity Ω).

As the operator $\mathcal{L}_{\text{GP}}$ is time independent the general method to determine the time evolution of $\delta\phi$ is to diagonalize $\mathcal{L}_{\text{GP}}$ and expand $\delta\phi$ on the corresponding eigenmodes. At this stage one faces a slight difficulty: it turns out that $\mathcal{L}_{\text{GP}}$ is not diagonalizable, that is the set of all eigenvectors of $\mathcal{L}_{\text{GP}}$ does not form a basis (in general one vector is missing to span the whole functional space). Mathematically this can be solved by putting $\mathcal{L}_{\text{GP}}$ into the so-called Jordan normal form. Here we use the more physical following procedure.

6.1.2 Extracting the “relevant part” from $\delta\phi$

We split $\delta\phi$ on a component along ϕ_0 and a part orthogonal to ϕ_0 :

$$\delta\phi(\vec{r}, t) = \eta(t)\phi_0(\vec{r}) + \delta\phi_{\perp}(\vec{r}, t). \quad (6.11)$$

From equation (6.6) valid to first order in $\delta\phi$ we realize that $\eta = \langle\phi_0|\delta\phi\rangle$ is such that $\eta(t) + \eta^*(t) = 0$, so that $\eta(t)$ is purely imaginary and can be reinterpreted as a change of phase of ϕ_0 :

$$\phi(\vec{r}, t) \simeq e^{\eta(t)}\phi_0(\vec{r}) + \delta\phi_{\perp}(\vec{r}, t). \quad (6.12)$$

One then sees that this change of phase has no consequence on the one-body density matrix of the condensate, up to first order in $\delta\phi$:

$$|\phi\rangle\langle\phi| \simeq |\phi_0\rangle\langle\phi_0| + |\phi_0\rangle\langle\delta\phi_{\perp}| + |\delta\phi_{\perp}\rangle\langle\phi_0|. \quad (6.13)$$

After a little algebra we turn equation (6.8) into a closed equation for $\delta\phi_{\perp}$:

$$i\hbar\partial_t \begin{pmatrix} \delta\phi_{\perp}(\vec{r}, t) \\ \delta\phi_{\perp}^*(\vec{r}, t) \end{pmatrix} = \mathcal{L} \begin{pmatrix} \delta\phi_{\perp}(\vec{r}, t) \\ \delta\phi_{\perp}^*(\vec{r}, t) \end{pmatrix} + \begin{pmatrix} S_{\perp}(\vec{r}, t) \\ -S_{\perp}^*(\vec{r}, t) \end{pmatrix}. \quad (6.14)$$

Introducing the projection operators orthogonally to ϕ_0 and ϕ_0^* :

$$Q = 1 - |\phi_0\rangle\langle\phi_0| \quad (6.15)$$

$$Q^* = 1 - |\phi_0^*\rangle\langle\phi_0^*| \quad (6.16)$$

we have $S_\perp = QS$ and

$$\mathcal{L} = \begin{pmatrix} H_{\text{GP}} + gN_0Q|\phi_0|^2Q & gN_0Q\phi_0^2Q^* \\ -gN_0Q^*\phi_0^{*2}Q & -[H_{\text{GP}} + gN_0Q|\phi_0|^2Q]^* \end{pmatrix} \quad (6.17)$$

where the Gross-Pitaevskii Hamiltonian H_{GP} is defined in equation (6.10). In general the operator $\mathcal{L}$ is diagonalizable.

6.1.3 Spectral properties of $\mathcal{L}$ and dynamical stability

Consider an eigenvector of $\mathcal{L}$ with eigenvalue ϵ_k :

$$\mathcal{L} \begin{pmatrix} u_k \\ v_k \end{pmatrix} = \epsilon_k \begin{pmatrix} u_k \\ v_k \end{pmatrix}. \quad (6.18)$$

The free evolution of this mode, that is for $\delta U = 0$, is given by the phase factor $\exp(-i\epsilon_k t/\hbar)$. This factor remains bounded in time provided that the imaginary part of ϵ_k is negative, which leads to the dynamical stability condition

$$\text{Im}(\epsilon_k) \leq 0 \quad \text{for all } k. \quad (6.19)$$

One has the following three interesting spectral properties.

1. ϵ_k^* is also an eigenvalue of $\mathcal{L}$;
2. $\begin{pmatrix} v_k^* \\ u_k^* \end{pmatrix}$ is also an eigenvector of $\mathcal{L}$, with eigenvalue $-\epsilon_k^*$;
3. $\begin{pmatrix} u_k \\ -v_k \end{pmatrix}$ is an eigenvector of $\mathcal{L}^\dagger$ with eigenvalue ϵ_k .

The last two of these three properties can be checked by direct substitution. They can be viewed more elegantly as a consequence of the symmetry properties:

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \mathcal{L} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}^{-1} = -\mathcal{L}^* \quad (6.20)$$

$$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \mathcal{L} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}^{-1} = \mathcal{L}^\dagger. \quad (6.21)$$

As we shall see this last property involving $\mathcal{L}^\dagger$ is useful to write $\mathcal{L}$ in diagonal form.

The first of these properties is easy to prove when ϕ_0 is real. In this case the operator $\mathcal{L}$ is a real operator (as Q , U_0 , ϕ_0^2 , Δ are real) so that complex eigenvalues come by pairs of complex conjugates. When ϕ_0 is complex

one can use the following mathematical fact: if ϵ_k is an eigenvalue of an arbitrary operator $\mathcal{L}$, ϵ_k^* is an eigenvalue of the operator $\mathcal{L}^\dagger$. Here $\mathcal{L}^\dagger$ differs from $\mathcal{L}$ by a unitary transform (6.21) so that it has the same spectrum as $\mathcal{L}$. This property of the spectrum is actually known in classical mechanics for a linearized Hamiltonian system, and the Gross–Pitaevskii equation can be viewed as a classical Hamiltonian equation for a continuous set of conjugate coordinates $q = \text{Re}(\phi)$, $p = \text{Im}(\phi)$.

As a consequence of this first spectral property of $\mathcal{L}$ the dynamical stability condition equation (6.19) can be reformulated as

$$\text{Im}(\epsilon_k) = 0 \quad \text{for all } k \quad (6.22)$$

that is all the eigenvalues of $\mathcal{L}$ have to be real to have a dynamically stable condensate wavefunction. We assume that this property is satisfied in the remaining part of this Section 6.1.

6.1.4 Diagonalization of $\mathcal{L}$

As $\mathcal{L}$ is not a Hermitian operator the eigenbasis of $\mathcal{L}$ is not orthogonal (see the minus sign in the second line of $\mathcal{L}$, due to Bose statistics; one does not have this sign in the BCS theory for interacting fermions).

To write $\mathcal{L}$ in diagonal form the knowledge of the eigenvectors is then *a priori* not sufficient. One generally proceeds as follows:

Reminder: *Let M be a diagonalizable but not necessarily Hermitian operator. Then the diagonal form of M can be written as*

$$M = \sum_k m_k |\psi_k^R\rangle \langle \psi_k^L| \quad (6.23)$$

where $|\psi_k^R\rangle$ is a right eigenvector of M with eigenvalue m_k :

$$M|\psi_k^R\rangle = m_k |\psi_k^R\rangle \quad (6.24)$$

and $\langle \psi_k^L|$ is a left eigenvector of M with eigenvalue m_k :

$$\langle \psi_k^L|M = m_k \langle \psi_k^L| \quad (6.25)$$

or equivalently

$$M^\dagger |\psi_k^L\rangle = m_k^* |\psi_k^L\rangle. \quad (6.26)$$

The normalization of the left and right eigenvectors is such that

$$\langle \psi_k^L|\psi_{k'}^R\rangle = \delta_{k,k'}. \quad (6.27)$$

$|\psi_k^L\rangle$ is then called the adjoint vector of $|\psi_k^R\rangle$.

We apply this reminder to $\mathcal{L}$. We have already defined the right eigenvector:

$$|\psi_k^R\rangle = \begin{pmatrix} |u_k\rangle \\ |v_k\rangle \end{pmatrix}, \quad \text{eigenvalue of } \mathcal{L} : \epsilon_k. \quad (6.28)$$

From the third of the above spectral properties of $\mathcal{L}$ we can easily obtain the corresponding left eigenvector up to a normalization factor:

$$|\psi_k^L\rangle = \mathcal{N}_k \begin{pmatrix} |u_k\rangle \\ -|v_k\rangle \end{pmatrix}, \quad \text{eigenvalue of } \mathcal{L}^\dagger : \epsilon_k^* = \epsilon_k. \quad (6.29)$$

The normalization condition equation (6.27) imposes

$$\langle \psi_k^L | \psi_k^R \rangle = 1 = \mathcal{N}_k^* [\langle u_k | u_k \rangle - \langle v_k | v_k \rangle]. \quad (6.30)$$

It is then natural to normalize the right eigenvectors in such a way that the quantity between square brackets is ± 1 , leading to $\mathcal{N}_k = \pm 1$.

We therefore group the eigenvectors of $\mathcal{L}$ in three families:

- the + family, such that $\langle u_k | u_k \rangle - \langle v_k | v_k \rangle = +1$;
- the – family, such that $\langle u_k | u_k \rangle - \langle v_k | v_k \rangle = -1$;
- the 0 family, such that $\langle u_k | u_k \rangle - \langle v_k | v_k \rangle = 0$.

From the spectral property number 2 we see that there is a duality between the + family and the – family. Conventionally we will refer to eigenvectors of the + family as (u_k, v_k) (eigenvalue ϵ_k) and the eigenvectors of the – family will be expressed as (v_k^*, u_k^*) (eigenvalue $-\epsilon_k$).

Generally there are only the following two members in the 0 family:

$$\begin{pmatrix} \phi_0 \\ 0 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 0 \\ \phi_0^* \end{pmatrix}. \quad (6.31)$$

One can check that these two vectors are eigenvectors of $\mathcal{L}$ with the eigenvalue zero. [In the case of $\mathcal{L}_{\text{GP}}$ one finds in general only one zero-energy eigenmode, the missing one leads to the non-diagonalizability]. In general these two vectors span the whole 0 family. As they are also eigenmodes of the operator $\mathcal{L}^\dagger$ with the eigenvalue zero they are actually their own conjugate vectors! From equation (6.27) we then get the important property:

$$\langle \phi_0 | u_k \rangle = \langle \phi_0^* | v_k \rangle = 0 \quad \text{for all } k \text{ in } + \text{ family}. \quad (6.32)$$

It is important to note that the + in the denomination “+ family” refers *a priori* to the sign of $\langle u_k | u_k \rangle - \langle v_k | v_k \rangle$ and **not** to the sign of ϵ_k !

6.1.5 General solution of the linearized problem

We expand the unknown column vector of equation (6.14) onto eigenmodes of $\mathcal{L}$. We assume that the only modes of the 0 family are the ones of equation (6.31); these modes do not contribute to the expansion as $\langle \phi_0 | \delta \phi_\perp \rangle = \langle \phi_0^* | \delta \phi_\perp^* \rangle = 0$. We then get the expansion

$$\begin{pmatrix} \delta \phi_\perp(\vec{r}, t) \\ \delta \phi_\perp^*(\vec{r}, t) \end{pmatrix} = \sum_{k \in +\text{family}} b_k(t) \begin{pmatrix} u_k(\vec{r}) \\ v_k(\vec{r}) \end{pmatrix} + b_k^*(t) \begin{pmatrix} v_k^*(\vec{r}) \\ u_k^*(\vec{r}) \end{pmatrix} \quad (6.33)$$

with the coefficients

$$\begin{aligned} b_k(t) &= (\langle u_k |, -\langle v_k |) \begin{pmatrix} |\delta \phi_\perp(t)\rangle \\ |\delta \phi_\perp^*(t)\rangle \end{pmatrix} \\ &= \int d^3\vec{r} [u_k^*(\vec{r}) \delta \phi_\perp(\vec{r}, t) - v_k^*(\vec{r}) \delta \phi_\perp^*(\vec{r}, t)]. \end{aligned} \quad (6.34)$$

As the second component of the expanded column vector is the complex conjugate of the first component the amplitudes on the $-$ family modes are the complex conjugates of the amplitudes b_k on the $+$ family modes, that is b_k^* .

Similarly one expands the source term of equation (6.14) on the eigenmodes of $\mathcal{L}$. The components on the $+$ family modes are given by

$$s_k(t) = \int d^3\vec{r} [u_k^*(\vec{r}) S_\perp(\vec{r}, t) + v_k^*(\vec{r}) S_\perp^*(\vec{r}, t)]. \quad (6.35)$$

Note the absence of $-$ sign here, due to the fact that the second component of the source column vector is the opposite of the complex conjugate of the first component. Finally the projection of equation (6.14) on the eigenmodes of the $+$ family gives the set of equations:

$$i\hbar \frac{d}{dt} b_k(t) = \epsilon_k b_k(t) + s_k(t) \quad (6.36)$$

which can be integrated including the initial condition $\delta \phi_\perp(t_0) = 0$:

$$b_k(t) = \int_0^{t-t_0} \frac{d\tau}{i\hbar} s_k(t-\tau) e^{-i\epsilon_k \tau / \hbar}. \quad (6.37)$$

6.1.6 Link between eigenmodes of $\mathcal{L}_{\text{GP}}$ and eigenmodes of $\mathcal{L}$

The linear operators $\mathcal{L}$ and $\mathcal{L}_{\text{GP}}$ describe the same physical problem, so that one expects in particular that their spectra, which correspond to the linear response frequencies of the condensate, are the same.

This expectation is confirmed by the simple result, that one can check by direct substitution: if $(|u_k^{GP}\rangle, |v_k^{GP}\rangle)$ is an eigenvector of $\mathcal{L}_{\text{GP}}$ with the eigenvalue ϵ_k then $(Q|u_k^{GP}\rangle, Q^*|v_k^{GP}\rangle)$ is an eigenvector of $\mathcal{L}$ with the *same* eigenvalue ϵ_k .

6.2 Examples of dynamical instabilities

We consider simple stationary solutions of the Gross–Pitaevskii equations that are dynamically unstable, that is with non-real eigenfrequencies $\epsilon_k/\hbar$. The situations considered correspond to a gas trapped in a cubic box with periodic boundary conditions; analytical calculations can then be performed. The conclusions remain qualitatively correct for harmonic traps.

6.2.1 Condensate in a box

The atoms are trapped in a cubic box of size L , and we assume periodic boundary conditions. An obvious solution of the time independent Gross–Pitaevskii equation is then the plane wave with vanishing momentum,

$$\phi_0(\vec{r}) = \frac{1}{L^{3/2}}. \quad (6.38)$$

It has a chemical potential

$$\mu = gN_0|\phi_0|^2 = \rho_0 g \quad (6.39)$$

where $\rho_0 = N_0/L^3$ is the density of condensate atoms.

To obtain the linear response frequencies of the condensates we calculate the spectrum of $\mathcal{L}_{\text{GP}}$, this operator takes here the very simple form:

$$\mathcal{L}_{\text{GP}} = \begin{pmatrix} -\frac{\hbar^2}{2m}\Delta + \rho_0 g & \rho_0 g \\ -\rho_0 g & -\left[-\frac{\hbar^2}{2m}\Delta + \rho_0 g\right] \end{pmatrix}. \quad (6.40)$$

Using the translational invariance of this operator we seek its eigenvectors in the form of plane waves:

$$\begin{pmatrix} u_{\vec{k}}^{GP}(\vec{r}) \\ v_{\vec{k}}^{GP}(\vec{r}) \end{pmatrix} = \frac{e^{i\vec{k}\cdot\vec{r}}}{L^{3/2}} \begin{pmatrix} U_{\vec{k}} \\ V_{\vec{k}} \end{pmatrix}. \quad (6.41)$$

Within the subspace of plane waves with wave vector $\vec{k}$, $\mathcal{L}_{\text{GP}}$ is represented by the 2×2 non-Hermitian matrix:

$$\mathcal{L}_{\text{GP}}[\vec{k}] = \begin{pmatrix} \frac{\hbar^2 k^2}{2m} + \rho_0 g & \rho_0 g \\ -\rho_0 g & -\left[\frac{\hbar^2 k^2}{2m} + \rho_0 g\right] \end{pmatrix}. \quad (6.42)$$

For $\vec{k} \neq \vec{0}$ this matrix can be diagonalized, giving one eigenvector of + family, with the eigenvalue

$$\epsilon_{\vec{k}} = \left[\frac{\hbar^2 k^2}{2m} \left(\frac{\hbar^2 k^2}{2m} + 2\rho_0 g \right) \right]^{1/2} \quad (6.43)$$

and one eigenvector of – family with the eigenvalue $-\epsilon_{\vec{k}}$. The eigenvector of the + family can be chosen as

$$\begin{aligned} U_{\vec{k}} + V_{\vec{k}} &= \left(\frac{\frac{\hbar^2 k^2}{2m}}{\frac{\hbar^2 k^2}{2m} + 2\rho_0 g} \right)^{1/4} \\ U_{\vec{k}} - V_{\vec{k}} &= \left(\frac{\frac{\hbar^2 k^2}{2m}}{\frac{\hbar^2 k^2}{2m} + 2\rho_0 g} \right)^{-1/4} \end{aligned} \quad (6.44)$$

with the correct normalization $U_{\vec{k}}^2 - V_{\vec{k}}^2 = 1$.

The spectrum equation (6.43) is the so-called Bogoliubov spectrum, as it was first derived by Bogoliubov. Physically it is a very important result. In the limiting case of the ideal Bose gas ($g = 0$) the spectrum is the usual parabola; for $g \neq 0$ the spectrum is very different, and this deserves a more detailed discussion

- *Bogoliubov spectrum for $g > 0$*

In the case of effective repulsive interactions the Bogoliubov spectrum strongly differs from the one of a free particle in the low momenta domain $\hbar^2 k^2 / 2m \ll 2\rho_0 g$ as it scales linearly with k :

$$\epsilon_{\vec{k}} \simeq \hbar k \sqrt{\frac{\rho_0 g}{m}}. \quad (6.45)$$

This linear dispersion relation leads to a propagation of low energy excitations in the condensate in the form of sound waves with a sound velocity c_s given by

$$c_s = \frac{d\omega_{\vec{k}}}{dk} = \frac{1}{\hbar} \frac{d\epsilon_{\vec{k}}}{dk} = \sqrt{\frac{\rho_0 g}{m}} \quad (6.46)$$

or equivalently by the relativistic type formula

$$mc_s^2 = \rho_0 g. \quad (6.47)$$

Superfluidity is an important consequence of this linear behavior of the spectrum at low k , as shown by an argument due to Landau and that we explain briefly. Consider a particle (of mass M) sent in the atomic gas with an initial velocity $\vec{u}$. The motion of this particle can be damped by interaction with the condensate only if the particle can create some excitation of the condensate. Imagine that such an excitation is produced, with momentum $\vec{k}$; the particle experiences a momentum recoil of $-\hbar\vec{k}$ and conservation of energy imposes

$$\epsilon_{\vec{k}} = \frac{1}{2}M\vec{u}^2 - \frac{1}{2M} \left[M\vec{u} - \hbar\vec{k} \right]^2 = \hbar\vec{k} \cdot \vec{u} - \frac{\hbar^2 k^2}{2M}. \quad (6.48)$$

The velocity u has then to satisfy the inequality:

$$u \geq \left| \frac{\vec{k} \cdot \vec{u}}{k} \right| \geq \frac{\epsilon_{\vec{k}}}{k} \geq c_s. \quad (6.49)$$

So a particle with an incoming velocity smaller than the sound velocity can move through the condensate without damping, only scattering on thermal excitations of the gas can damp its motion. This prediction has received an experimental confirmation at MIT [41].

At high momenta ($\hbar^2 k^2/2m \gg \rho_0 g$) corresponding to a velocity $\hbar k/m$ much larger than the sound velocity the Bogoliubov spectrum reduces to a shifted parabola

$$\epsilon_{\vec{k}} \simeq \frac{\hbar^2 k^2}{2m} + \rho_0 g = \frac{\hbar^2 k^2}{2m} + 2\rho_0 g - \mu. \quad (6.50)$$

This approximate form can be obtained by a series expansion of the general formula equation (6.43). It can also be derived more instructively from the observation that the off-diagonal coupling $\rho_0 g$ between the $U_{\vec{k}}$ component and the $V_{\vec{k}}$ component in the 2×2 matrix equation (6.42) becomes very non-resonant at high k (because the diagonal terms for $U_{\vec{k}}$ and $V_{\vec{k}}$ have opposite signs); neglecting this coupling one recovers equation (6.50) with $U_{\vec{k}} \simeq 1$, $V_{\vec{k}} \simeq 0$.

This last high energy property applies also in a non-uniform trapping potential: neglecting the off-diagonal coupling between u_k and v_k one approximates the high energy part of the Bogoliubov spectrum by the eigenvalues of

$$-\frac{\hbar^2}{2m}\Delta + U_0 + 2gN_0|\phi_0|^2 - \mu \quad (6.51)$$

which (up to the shift $-\mu$) is the Hartree–Fock Hamiltonian for non-condensed particles equation (4.19) in a regime of an almost pure condensate where

the density of non-condensed particles is negligible as compared to the condensate density $N_0|\phi_0|^2$.

From this we expect that the Hartree Fock approach is invalid for the low energy fraction of the non-condensed gas (energy typically less than μ); this may become a problem at temperatures $k_B T < \mu$, where one has to use the more precise Bogoliubov approach of Section 7.

- *Case of a negative g*

In the case of effective attractive interactions between particles the dynamical stability condition $\text{Im}(\epsilon_{\vec{k}}) = 0$ is satisfied if and only if

$$\frac{\hbar^2 k^2}{2m} + 2g\rho_0 \geq 0 \quad \text{for all } k > 0. \quad (6.52)$$

If one considers the thermodynamical limit of an infinite number of condensate atoms with a fixed mean density $\rho_0 = N_0/L^3$ the stability condition cannot be satisfied as k can be arbitrarily close to 0 in an infinite box. One may then be tempted to conclude that condensates with effective attractive interactions cannot be obtained experimentally, attractive interactions leading to a spatial collapse of the gas.

Experiments with atomic gases can deal however with small number of atoms and the simplifying assumption of a thermodynamical limit is not necessarily a good approximation. In the cubix box of size L with periodic boundary conditions the components of the wavevector $\vec{k}$ of an atom are integer multiples of $2\pi/L$. The smallest but non zero modulus of wavevector that can be achieved is therefore $2\pi/L$ (by taking *e.g.* $k_x = 2\pi/L, k_y = k_z = 0$). Dynamical stability condition equation (6.52) can then be rewritten as

$$\frac{\hbar^2}{2m} \left(\frac{2\pi}{L} \right)^2 \geq 2|g| \frac{N_0}{L^3} \quad (6.53)$$

or equivalently in terms of the scattering length as

$$\frac{N_0|a|}{L} \leq \frac{\pi}{4}. \quad (6.54)$$

Condensates for $a < 0$ can contain a limited number of atoms proportional to the size of the condensate.

Condition equation (6.53) has a clear physical interpretation: the energy gap in the spectrum of a particle in the box between the ground state and the first excited states should be larger than the mean field energy per particle: stabilization against collapse is thus provided by the discrete spectrum of the atoms in the trapping potential. This condition can thus be qualitatively extended to the case of an isotropic harmonic trap, $\hbar\omega > |g|N_0/a_{\text{ho}}^3$ where ω is the oscillation frequency of the atoms in the trap and $a_{\text{ho}} = (\hbar/m\omega)^{1/2}$ is the typical spatial extension of the ground state of the trap. One then recovers up to a numerical factor the results of Section 5.2.1.

6.2.2 Demixing instability

We consider here atoms with two internal states a, b ; this model is relevant for experiments performed at JILA on binary mixtures of ^{87}Rb condensates, and also (if one includes a third atomic internal level) experiments at MIT in Ketterle's group on spinor ^{23}Na condensates.

To describe the elastic interactions between the atoms with two internal states one needs three coupling constants, all positive in the case of ^{87}Rb : g_{aa} and g_{bb} for interactions between atoms in the same internal state, g_{ab} for interactions between atoms in different internal states:

$$\begin{aligned} g_{aa} : \quad a + a &\rightarrow a + a \\ g_{bb} : \quad b + b &\rightarrow b + b \\ g_{ab} : \quad a + b &\rightarrow a + b. \end{aligned} \tag{6.55}$$

In the JILA experiment internal states a and b correspond to different hyperfine levels of the atoms so that inelastic collisions such as $a + a \rightarrow a + b$ are either strongly endothermic (and do not take place) or strongly exothermic (and result in losses of atoms from the trap); we neglect these inelastic processes.

Omitting for simplicity the regularizing operator in the pseudo-potential we write the interaction Hamiltonian between the atoms in second quantized form as

$$\begin{aligned} H_{\text{int}} = \int d^3\vec{r} \left[\frac{g_{aa}}{2} \hat{\psi}_a^\dagger(\vec{r}) \hat{\psi}_a^\dagger(\vec{r}) \hat{\psi}_a(\vec{r}) \hat{\psi}_a(\vec{r}) + \frac{g_{bb}}{2} \hat{\psi}_b^\dagger(\vec{r}) \hat{\psi}_b^\dagger(\vec{r}) \hat{\psi}_b(\vec{r}) \hat{\psi}_b(\vec{r}) \right. \\ \left. + g_{ab} \hat{\psi}_b^\dagger(\vec{r}) \hat{\psi}_a^\dagger(\vec{r}) \hat{\psi}_a(\vec{r}) \hat{\psi}_b(\vec{r}) \right] \end{aligned} \tag{6.56}$$

where $\hat{\psi}_a$ and $\hat{\psi}_b$ are the atomic field operators for atoms in state a and b respectively. Note the absence of factor $1/2$ in the $a - b$ interaction term, which is best understood in first quantization point of view: all the pairs of atoms of the form $a : i, b : j$, where i running from 1 to N_a labels the atoms in a and j running from 1 to N_b labels the atoms in b , are different so that there is no double counting of these interaction terms and no factor $1/2$ is required.

Using the trick of Section 5.1.3 we can rapidly derive the Gross–Pitaevskii equations for the condensate wavefunctions ϕ_a in state a and ϕ_b in state b , both wavefunctions being normalized to unity. One simply has to write the Heisenberg equations of motion for the field operators and perform the substitution

$$\hat{\psi}_a \rightarrow N_a^{1/2} \phi_a \tag{6.57}$$

$$\hat{\psi}_b \rightarrow N_b^{1/2} \phi_b \tag{6.58}$$

where $N_{a,b}$ are the number of particles in condensates a, b . As in Section 6.2.1 we restrict to the case of atoms trapped in a cubix box of size L with periodic boundary conditions. We obtain the coupled time dependent Gross–Pitaevskii equations

$$\begin{aligned} i\hbar\partial_t\phi_a &= \left[-\frac{\hbar^2}{2m}\Delta + N_a g_{aa}|\phi_a|^2 + N_b g_{ab}|\phi_b|^2 \right] \phi_a \\ i\hbar\partial_t\phi_b &= \left[-\frac{\hbar^2}{2m}\Delta + N_b g_{bb}|\phi_b|^2 + N_a g_{ab}|\phi_a|^2 \right] \phi_b. \end{aligned} \quad (6.59)$$

Consider now a steady state solution of these coupled Gross–Pitaevskii equations. As we have not introduced any coherent coupling between the internal states a and b (no $\hat{\psi}_b^\dagger\hat{\psi}_a$ term in the Hamiltonian) ϕ_a and ϕ_b can have in steady state time dependent phase factors evolving with *different* frequencies:

$$\phi_a(\vec{r}, t) = \phi_{a,0}(\vec{r})e^{-i\mu_a t/\hbar} \quad (6.60)$$

$$\phi_b(\vec{r}, t) = \phi_{b,0}(\vec{r})e^{-i\mu_b t/\hbar}. \quad (6.61)$$

From a more thermodynamical perspective we can also observe that the number of particles N_a and N_b are separately conserved by the three elastic interactions of equation (6.55) so that *two* distinct chemical potentials μ_a and μ_b are required to describe the equilibrium state.

The time independent Gross–Pitaevskii equations for $\phi_{a,0}$ and $\phi_{b,0}$ in the box have the natural solutions

$$\phi_{a,0}(\vec{r}) = \phi_{b,0}(\vec{r}) = \frac{1}{L^{3/2}} \quad (6.62)$$

leading to the following expressions for the chemical potentials:

$$\mu_a = \rho_{a,0}g_{aa} + \rho_{b,0}g_{bb} \quad (6.63)$$

$$\mu_b = \rho_{b,0}g_{bb} + \rho_{a,0}g_{ab} \quad (6.64)$$

where $\rho_{a,b}$ are the condensate densities in a, b . Although we assume here that all the coupling constants are positive it is physically intuitive that these spatially uniform solutions should become unstable when the interactions between a and b are very repulsive; one then feels that the two condensates a and b have a tendency to spatially separate.

To test this expectation we linearize the time dependent coupled Gross–Pitaevskii equations around the steady state, setting

$$\phi_a(\vec{r}, t) = e^{-i\mu_a t/\hbar} [\phi_{a,0}(\vec{r}) + \delta\phi_a(\vec{r}, t)] \quad (6.65)$$

$$\phi_b(\vec{r}, t) = e^{-i\mu_b t/\hbar} [\phi_{b,0}(\vec{r}) + \delta\phi_b(\vec{r}, t)]. \quad (6.66)$$

We obtain

$$i\hbar\partial_t\delta\phi_a = -\frac{\hbar^2}{2m}\Delta\delta\phi_a + \rho_{a,0}g_{aa}[\delta\phi_a + \delta\phi_a^*] + \rho_{b,0}g_{ab}[\delta\phi_b + \delta\phi_b^*] \quad (6.67)$$

and a similar equation for $\delta\phi_b$ exchanging the role of a and b indices. We look for eigenmodes of these linear equations, with eigenfrequency $\epsilon/\hbar$ and a well defined wavevector $\vec{k}$. This amounts to performing the substitutions

$$\begin{aligned} \delta\phi_a(\vec{r}, t) &\rightarrow u_a e^{i(\vec{k}\cdot\vec{r} - \epsilon t/\hbar)} \\ \delta\phi_a^*(\vec{r}, t) &\rightarrow v_a e^{i(\vec{k}\cdot\vec{r} - \epsilon t/\hbar)} \end{aligned}$$

and equivalent changes for the b components. This leads to the eigensystem

$$\begin{aligned} \left[\epsilon - \frac{\hbar^2 k^2}{2m} \right] u_a &= \left[-\epsilon - \frac{\hbar^2 k^2}{2m} \right] v_a \\ &= \rho_{a,0}g_{aa} [u_a + v_a] + \rho_{b,0}g_{ab} [u_b + v_b] \end{aligned} \quad (6.68)$$

and similar equations obtained by exchanging the indices a and b . Taking as new variables the sums and the differences between u and v and using the first identity in equation (6.68) we eliminate the differences as functions of the sums:

$$u_a - v_a = \frac{2m\epsilon}{\hbar^2 k^2} [u_a + v_a]. \quad (6.69)$$

We get from the second equality in equation (6.68) (and $a \leftrightarrow b$) a two by two system for the sums $u_a + v_a$, $u_b + v_b$:

$$\left\{ \frac{\hbar^2 k^2}{2m} \left[1 - \left(\frac{2m\epsilon}{\hbar^2 k^2} \right)^2 \right] \text{Id} + M \right\} \begin{pmatrix} u_a + v_a \\ u_b + v_b \end{pmatrix} = 0 \quad (6.70)$$

where we have introduced the two by two matrix

$$M = \begin{pmatrix} \rho_{a,0}g_{aa} & \rho_{b,0}g_{ab} \\ \rho_{a,0}g_{ab} & \rho_{b,0}g_{bb} \end{pmatrix}. \quad (6.71)$$

This leads to the following condition for the spectrum:

$$\epsilon^2 = \left[\frac{\hbar^2 k^2}{2m} \left(\frac{\hbar^2 k^2}{2m} + 2\eta_{1,2} \right) \right] \quad (6.72)$$

where $\eta_{1,2}$ are the eigenvalues of M .

In the thermodynamical limit the mixture of condensates with uniform densities is dynamically stable provided that both eigenvalues $\eta_{1,2}$ are positive. This is equivalent to the requirement that the symmetric matrix M

is positive. As $g_{aa} > 0$ here this is ensured provided that the determinant of M is positive:

$$\det M = \rho_{a,0}\rho_{b,0} [g_{aa}g_{bb} - g_{ab}^2] \geq 0. \quad (6.73)$$

The mixture of spatially uniform condensates is therefore stable if

$$g_{ab} \leq (g_{aa}g_{bb})^{1/2}. \quad (6.74)$$

In this case one can check that the spectrum of the $+$ family is given by the positive solutions ϵ to equation (6.72). The spectrum of the binary mixtures of condensates is then made of two branches, which are both linear at low momenta with sound velocities $(\eta_{1,2}/m)^{1/2}$.

What happens when this stability condition is not satisfied? The condensates a and b have a tendency to separate spatially. This happens in the JILA experiment [42]. Actually our model in a box is too crude to be applied to the experimental case of particles in a harmonic trap, the stability condition equation (6.74) being marginally satisfied for ^{87}Rb ; a numerical solution of the time dependent Gross–Pitaevskii equations is required in this case [43].

The occurrence of demixing when equation (6.74) is violated can be connected with the following simple energy argument. Consider a demixed configuration with all the N_a atoms in the left part of the box in a volume νL^3 and all the N_b atoms in the right part of the box in the complementary volume $(1-\nu)L^3$. The condensate densities vanish on a scale on the order of the healing length ξ of the gas, this leads to “surface” kinetic and interaction energies negligible in the thermodynamical limit as compared to the volume interaction energy

$$\frac{N_a^2 g_{aa}}{2\nu L^3} + \frac{N_b^2 g_{bb}}{2(1-\nu)L^3}. \quad (6.75)$$

We minimize this energy over ν to obtain

$$E_{\text{demix}} = \frac{1}{2L^3} \left[N_a^2 g_{aa} + N_b^2 g_{bb} + 2N_a N_b (g_{aa}g_{bb})^{1/2} \right]. \quad (6.76)$$

We find that the demixed configuration has an energy lower than the one of the spatially uniform configuration

$$E_{\text{unif}} = \frac{1}{2L^3} [N_a^2 g_{aa} + N_b^2 g_{bb} + 2N_a N_b g_{ab}] \quad (6.77)$$

precisely when the stability condition equation (6.74) of the uniform configuration is violated.

6.3 Linear response in the classical hydrodynamic approximation

We consider in this subsection the case of a condensate in a harmonic trap. The eigenmodes of the linearized Gross–Pitaevskii equation can then in general be determined only numerically. In the Thomas–Fermi regime however approximate results can be obtained for the low energy eigenmodes of the system from the classical hydrodynamic approach, as we shall see now.

6.3.1 Linearized classical hydrodynamic equations

The classical hydrodynamic equations for the position dependent condensate density $\rho(\vec{r})$ and velocity field $\vec{v}(\vec{r})$ have been derived in Section 5.3.4:

$$\partial_t \rho + \text{div} [\rho \vec{v}] = 0 \quad (6.78)$$

$$m \left(\partial_t + \vec{v} \cdot \vec{\text{grad}} \right) \vec{v} = -\vec{\text{grad}}[U + \rho g]. \quad (6.79)$$

We linearize these equations around their steady state solution with density ρ_0 and vanishing velocity field $\vec{v}_0 = \vec{0}$ in the unperturbed trapping potential U_0 . Writing the trap potential as a perturbation of U_0 :

$$U(\vec{r}, t) = U_0(\vec{r}) + \delta U(\vec{r}, t) \quad (6.80)$$

and splitting ρ and $\vec{v}$ as

$$\rho(\vec{r}, t) = \rho_0(\vec{r}) + \delta \rho(\vec{r}, t) \quad (6.81)$$

$$\vec{v}(\vec{r}, t) = \vec{0} + \delta \vec{v}(\vec{r}, t) \quad (6.82)$$

we obtain the linearized equations:

$$\begin{aligned} \partial_t \delta \rho + \text{div} [\rho_0 \delta \vec{v}] &= 0 \\ m \partial_t \delta \vec{v} + \vec{\text{grad}} [\delta \rho g] &= -\vec{\text{grad}} \delta U. \end{aligned} \quad (6.83)$$

Taking the time derivative of the first equation we obtain a term $\partial_t \delta \vec{v}$ that we can eliminate with the second equation. This results in a closed equation for the perturbation of density:

$$\partial_t^2 \delta \rho - \text{div} \left[\frac{\rho_0 g}{m} \vec{\text{grad}} \delta \rho \right] = \text{div} \left[\frac{\rho_0}{m} \vec{\text{grad}} \delta U \right]. \quad (6.84)$$

The homogeneous part of this equation can be rewritten in a more suggestive way by introducing the position dependent velocity c_s given by

$$m c_s^2(\vec{r}) = \rho_0(\vec{r}) g. \quad (6.85)$$

The homogeneous part of equation (6.84) then reads

$$\partial_t^2 \delta \rho - \text{div} \left[c_s^2(\vec{r}) \vec{\text{grad}} \delta \rho \right] \quad (6.86)$$

which corresponds to the propagation of sound waves with a position dependent sound velocity $c_s(\vec{r})$. Note that the expression (6.85) could be expected from the result equation (6.47) obtained in the spatially homogeneous case.

The propagation of sound waves in a cigar shaped trapped condensate has been observed in Ketterle’s group at MIT; the condensate was excited mechanically by the dipole force induced by a far detuned laser beam focused at the center of the trap. It is instructive to note that to predict theoretically the velocity of sound obtained in the experiment one has to carefully solve equation (6.84), rather than to take naively the sound velocity on the axis of the trap; the naive expectation would be wrong by a factor of $\sqrt{2}$ [44, 45].

6.3.2 Validity condition of the linearized classical hydrodynamic equations

The classical hydrodynamic equations have been obtained from the time dependent Gross–Pitaevskii equation in hydrodynamic point of view by neglecting the quantum pressure term (see Sect. 5.3.4). If we keep this term and linearize the resulting equation we get extra terms with respect to equation (6.83). One of the extra terms is

$$\frac{\hbar^2}{m\rho_0}\Delta\delta\rho \quad (6.87)$$

which should be small as compared to the “classical” pressure term $g\delta\rho$:

$$\frac{\hbar^2}{m\rho_0}|\Delta\delta\rho| \ll g|\delta\rho|. \quad (6.88)$$

If we denote by k a typical wavevector for the spatial variation of $\delta\rho$, $\Delta\delta\rho \sim -k^2\delta\rho$ and the condition for neglecting the quantum pressure term reads

$$\frac{\hbar^2 k^2}{m} \ll g\rho_0. \quad (6.89)$$

This condition can be rewritten in a variety of ways. It claims that the wavevector k should satisfy

$$k\xi \ll 1 \quad (6.90)$$

where $\xi = \hbar/(2m\rho_0 g)^{1/2}$ is the healing length of the condensate. Equation (6.84) cannot be used to describe perturbations of the condensate at a length scale on the order of ξ or smaller.

The validity condition can also be written as

$$\hbar k \ll mc_s \quad \text{or} \quad \hbar k c_s \ll mc_s^2 = \rho_0 g \sim \mu. \quad (6.91)$$

In terms of the Bogoliubov spectrum for the homogeneous condensate this means that the wavevector k has to be in the *linear* part of the excitation

spectrum. The energy of the corresponding eigenmode $\sim \hbar k c_s$ has to be much smaller than μ . Therefore only the eigenmodes of equation (6.84) with eigenenergy much less than μ are relevant:

$$\epsilon \ll \mu \quad (6.92)$$

the higher energy modes are not an acceptable approximation of the exact eigenmodes of the condensate. Note that as shown in [46,47], equation (6.92) is a necessary but not sufficient condition in a trap.

6.3.3 Approximate spectrum in a harmonic trap

We look for eigenmodes of the homogeneous part of equation (6.84) with eigenenergy ϵ . They solve the eigenvalue equation

$$-\epsilon^2 \delta\rho = \text{div} \left[c_s^2(\vec{r}) \vec{\text{grad}} \delta\rho \right]. \quad (6.93)$$

In the present Thomas–Fermi regime c_s^2 is a quadratic function of the coordinates as it is proportional to the condensate density ρ_0 . We can therefore solve the eigenvalue equation using an ansatz for $\delta\rho$ polynomial in the spatial coordinates x, y, z . If $\delta\rho$ is a polynomial of total degree n , $\vec{\text{grad}} \delta\rho$ is a polynomial of total degree $n - 1$; after multiplication by c_s^2 and action of the div operator we get a polynomial of total degree $(n - 1) + 2 - 1 = n$. The subspace of polynomials of degree $\leq n$ is therefore stable.

For low values of the total degree n an analytical calculation is possible. For example in a general harmonic trap with atomic oscillation frequencies $\omega_x, \omega_y, \omega_z$ one can check that the polynomials $\delta\rho = x, y, z$ (respectively) are eigenvectors with eigenvalues $\epsilon = \hbar\omega_x, \hbar\omega_y, \hbar\omega_z$ (respectively). These three modes correspond to the oscillation of the center of mass of the gas, which is exactly decoupled from all the relative coordinates of the particles in a harmonic trap; for this specific example the frequencies (but not the modes!) predicted by classical hydrodynamics are exact. These “sloshing” modes are used experimentally to determine accurately the trap frequencies $\omega_{x,y,z}$.

Another important example is the case of a total degree $n = 2$. One can check that the subclass of polynomials involving the monomials x^2, y^2, z^2 and 1 is stable, which corresponds to the ansatz

$$\delta\rho(\vec{r}) = B + \sum_{\alpha=x,y,z} A_\alpha r_\alpha^2. \quad (6.94)$$

By inserting this ansatz into equation (6.93) we arrive at the eigenvalue system

$$(\epsilon/\hbar)^2 A_\alpha = 2\omega_\alpha^2 A_\alpha + \omega_\alpha^2 \sum_\beta A_\beta. \quad (6.95)$$

This eigenvalue system can be obtained more directly as in equation (5.83) by a linearization of the equations equation (5.79) for the scaling parameters λ_α around their steady state value $\lambda_\alpha = 1$. Physically the modes identified by the ansatz (6.94) are therefore breathing modes of the condensate. The frequency of one of these modes (the one of Sect. 5.4.3) has been measured with high precision at MIT in a cigar-shaped trap, it differs from the Thomas–Fermi prediction $\simeq (5/2)^{1/2}\omega_z$ (see Eq. (5.85)) by less than one percent [48].

In the case of an isotropic harmonic trap all the eigenenergies ϵ can be calculated analytically (keeping in mind that modes with $\epsilon > \mu$ are not properly described by classical hydrodynamics!). As shown in [49] one uses the rotational symmetry of the problem, as in the case of Schrödinger’s equation for the hydrogen atom, with the ansatz

$$\delta\rho(\vec{r}) = Y_l^m(\theta, \phi)r^l P_{l,n}(r) \quad (6.96)$$

where θ, ϕ are the polar and azimuthal angles of spherical coordinates, Y_l^m is the spherical harmonic of angular momentum l . The last factor $P_{l,n}(r)$ is a polynomial of degree n in r . As $P_{l,n}$ is a polynomial the recurrence relation obtained from equation (6.93) for the coefficients of the monomials r^j should terminate at $j = n$. This leads to the eigenfrequencies $\Omega = \epsilon/\hbar$ such that

$$\Omega^2 = (2n^2 + 2nl + 3n + l)\omega^2 \quad \text{for any } n, l \geq 0 \quad (6.97)$$

where ω is the oscillation frequency of the atoms in the trap. For $l = 1, n = 0$ we recover the sloshing modes with frequency $\Omega = \omega$.

7 Bogoliubov approach and thermodynamical stability

Imagine that we have already checked the dynamical stability of a steady state solution ϕ_0 of the Gross–Pitaevskii equation for the condensate wavefunction. We cannot relax yet and be sure that the condensate will remain in state ϕ_0 in the long run.

What is missing is a check that interaction of the condensate with the non-condensed cloud does not induce an evolution of the condensate far from the predicted ϕ_0 . We have to check what is called thermodynamical stability of the condensate as it involves the “thermal”, non-condensed component of the gas.

This check will be performed in the low temperature domain ($T \ll T_c$) using the Bogoliubov approach. We will then present examples of thermodynamical instabilities.

We give here a summarized account of the $U(1)$ -symmetry preserving Bogoliubov approach developed in [50, 51]. In contrast to the almost general attitude in the literature this approach does not assume a symmetry

breaking state with $\langle\hat{\psi}\rangle \neq 0$ but considers instead a state with a fixed total number of particles. A different $U(1)$ -symmetry preserving Bogoliubov approach was developed long ago in [52].

This allows to eliminate a technical problem of the symmetry breaking approach: if $\langle\hat{\psi}\rangle(t=0) \neq 0$ the state of the system necessarily involves a coherent superposition of states with different total number of particles; such a state *cannot be stationary* (as states with different number of particles have also different energies) and it experiences a phase collapse $\langle\hat{\psi}\rangle(t) \rightarrow 0$ making the description of the evolution of the system more involved.

7.1 Small parameter of the theory

We restrict in this section to a steady state regime where most of the atoms of the gas are in the condensate. We split the atomic field operator as

$$\hat{\psi}(\vec{r}) = \phi_0(\vec{r})\hat{a}_{\phi_0} + \delta\hat{\psi}(\vec{r}) \quad (7.1)$$

where ϕ_0 is the condensate wavefunction and $\hat{a}_{\phi_0}$ annihilates a particle in the mode ϕ_0 . The idea is to treat $\delta\hat{\psi}$ as a perturbation with respect to $\phi_0\hat{a}_{\phi_0}$: Let us compare indeed the typical matrix elements of these two operators:

$$\delta\hat{\psi} \sim \langle\delta\hat{\psi}^\dagger\delta\hat{\psi}\rangle^{1/2} \sim (\rho')^{1/2} \quad (7.2)$$

where ρ' is the density of non-condensed particles whereas

$$\phi_0\hat{a}_{\phi_0} \sim N_0^{1/2}\phi_0 \sim \rho_0^{1/2} \quad (7.3)$$

where ρ_0 is the condensate density. We will therefore assume

$$\rho' \ll \rho_0 \quad (7.4)$$

and even more

$$N' = \int d^3\vec{r} \rho'(\vec{r}) \ll N_0 \simeq N \quad (7.5)$$

where N is the total number of particles in the gas. Using these two assumptions a systematic expansion of the field equations in powers of the small parameter

$$\varepsilon = (N'/N_0)^{1/2} \ll 1 \quad (7.6)$$

can be performed. We give here a somewhat simplified presentation.

The following identities are important properties of $\delta\hat{\psi}$. First, $\delta\hat{\psi}$ is the part of the atomic field operator transverse to the condensate wavefunction:

$$\int d^3\vec{r} \phi_0^*(\vec{r})\delta\hat{\psi}(\vec{r}) = 0. \quad (7.7)$$

As a consequence the bosonic commutation relation obeyed by $\delta\hat{\psi}$ involves matrix elements of the projector Q orthogonal to ϕ_0 rather than the identity operator:

$$[\delta\hat{\psi}(\vec{r}_1), \delta\hat{\psi}^\dagger(\vec{r}_2)] = \langle \vec{r}_1 | Q | \vec{r}_2 \rangle = \delta(\vec{r}_1 - \vec{r}_2) - \phi_0(\vec{r}_1) \phi_0^*(\vec{r}_2). \quad (7.8)$$

Second, there should be no coherence in the one-body density matrix between the condensate and the non-condensed modes, or equivalently ϕ_0 should be an eigenstate of the one-body density matrix (with eigenvalue N_0):

$$\langle \hat{a}_{\phi_0}^\dagger \delta\hat{\psi} \rangle = 0. \quad (7.9)$$

This last identity is used to calculate the condensate wavefunction order by order in the small parameter [50, 51].

7.2 Zeroth order in ε : Gross–Pitaevskii equation

To zeroth order in ε all the particles are supposed to be in the condensate. In steady state one then recovers the time independent Gross–Pitaevskii equation with the further approximation $N_0 \simeq N$:

$$\mu\phi_0 = \left[-\frac{\hbar^2}{2m}\Delta + U + gN|\phi_0|^2 \right] \phi_0. \quad (7.10)$$

7.3 Next order in ε : Linear dynamics of non-condensed particles

Calculation to first order in ε corresponds to a linearization of the Heisenberg field equations around $\phi_0\hat{a}_{\phi_0}$ keeping terms up to first order in $\delta\hat{\psi}$. Equivalently it corresponds to a quadratization of the Hamiltonian around $\phi_0\hat{a}_{\phi_0}$ keeping terms up to second order in $\delta\hat{\psi}$.

We use this quadratization approach here. At this order of the calculation the regularizing operator of the pseudo-potential can be neglected, divergences due the use of the non-regularized $g\delta$ potential coming at the next order ε^2 . We therefore take the Hamiltonian

$$\hat{H} = \int d^3\vec{r} \left[\hat{\psi}^\dagger h_1 \hat{\psi} + \frac{g}{2} \hat{\psi}^\dagger \hat{\psi}^\dagger \hat{\psi} \hat{\psi} \right]. \quad (7.11)$$

The one-body Hamiltonian h_1 contains the kinetic energy and the trapping potential energy:

$$h_1 = -\frac{\hbar^2}{2m}\Delta + U. \quad (7.12)$$

It does not contain any $-\mu$ term as we use here in the canonical rather than grand canonical point of view, the total number of particles being fixed to N .

We substitute expansion (7.1) for equation (7.11) and we keep terms up to quadratic in $\delta\hat{\psi}$.

- The contribution of h_1 is quadratic in $\hat{\psi}$ so that all the terms should be kept. One of the contributions is

$$\left(\int d^3\vec{r} \phi_0^* h_1 \phi_0 \right) \hat{a}_{\phi_0}^\dagger \hat{a}_{\phi_0}. \quad (7.13)$$

One can use the following trick to express this quantity in terms of $\delta\hat{\psi}$: from equation (7.7) one sees that the total number of particles operator can be written as

$$\hat{N} \equiv \int d^3\vec{r} \hat{\psi}^\dagger \hat{\psi} = \hat{n}_{\phi_0} + \delta\hat{N} \quad (7.14)$$

that is the sum of the number operator of condensate particles:

$$\hat{n}_{\phi_0} = \hat{a}_{\phi_0}^\dagger \hat{a}_{\phi_0} \quad (7.15)$$

and the number operator of non-condensed particles:

$$\delta\hat{N} = \int d^3\vec{r} \delta\hat{\psi}^\dagger \delta\hat{\psi}. \quad (7.16)$$

We therefore obtain

$$\hat{n}_{\phi_0} = \hat{N} - \delta\hat{N}. \quad (7.17)$$

- The expansion of the interaction term gives the following up to quadratic contributions:

$$\begin{aligned} \frac{g}{2} \hat{\psi}^\dagger \hat{\psi}^\dagger \hat{\psi} \hat{\psi} &\rightarrow \frac{g}{2} |\phi_0|^4 \hat{a}_{\phi_0}^\dagger \hat{a}_{\phi_0}^\dagger \hat{a}_{\phi_0} \hat{a}_{\phi_0} \\ &+ g [\phi_0^* \phi_0^* \phi_0 \hat{a}_{\phi_0}^\dagger \hat{a}_{\phi_0}^\dagger \hat{a}_{\phi_0} \delta\hat{\psi} + \text{h.c.}] \\ &+ \frac{g}{2} [\phi_0^* \phi_0^* \hat{a}_{\phi_0}^\dagger \hat{a}_{\phi_0}^\dagger \delta\hat{\psi} \delta\hat{\psi} + \text{h.c.}] \\ &+ 2g \phi_0^* \phi_0 \hat{a}_{\phi_0}^\dagger \delta\hat{\psi}^\dagger \delta\hat{\psi} \hat{a}_{\phi_0}. \end{aligned} \quad (7.18)$$

The first line of this expression is transformed using equation (7.17):

$$\hat{a}_{\phi_0}^\dagger \hat{a}_{\phi_0}^\dagger \hat{a}_{\phi_0} \hat{a}_{\phi_0} = \hat{n}_{\phi_0} (\hat{n}_{\phi_0} - 1) = \hat{N} (\hat{N} - 1) - 2\hat{N} \delta\hat{N} + \dots \quad (7.19)$$

with $N \simeq N - 1$. When we group the above term in $\delta\hat{N}$ with the one coming from h_1 and we replace $\hat{N}$ by N we obtain

$$-\delta\hat{N} \left[\int d^3\vec{r} \phi_0^* h_1 \phi_0 + Ng |\phi_0|^4 \right] = -\mu \delta\hat{N} \quad (7.20)$$

as ϕ_0 solves the Gross–Pitaevskii equation (7.10). This is amusing: we obtain formally a grand canonical Hamiltonian for the non-condensed particles, the reservoir being formed by the condensate particles! In the second line of equation (7.18) we replace $\hat{a}_{\phi_0}^\dagger \hat{a}_{\phi_0}$ by N as the corrective term $\delta \hat{N}$ would lead to a cubic contribution in $\delta \hat{\psi}$.

Another important transformation is performed by collecting the terms linear in $\delta \hat{\psi}$ from equation (7.18) and from the contribution of h_1 , leading to

$$\int d^3\vec{r} \phi_0^* \hat{a}_{\phi_0}^\dagger [h_1 + g|\phi_0|^2 N] \delta \hat{\psi} + \text{h.c.} \quad (7.21)$$

As ϕ_0 solves the Gross–Pitaevskii equation, the operator between brackets, when acting on the left on ϕ_0^* , gives a contribution $\mu \phi_0^*$ orthogonal to $\delta \hat{\psi}$ (see Eq. (7.7)). The sum of all the terms linear in $\delta \hat{\psi}$ therefore vanishes! We shall see later that this could be expected from equation (7.9).

7.4 Bogoliubov Hamiltonian

We now collect all the terms of $\hat{H}$ up to quadratic in $\delta \hat{\psi}$ and express them in terms of the field operator

$$\hat{\Lambda}(\vec{r}) = \frac{1}{N^{1/2}} \hat{a}_{\phi_0}^\dagger \delta \hat{\psi}(\vec{r}). \quad (7.22)$$

This operator commutes with the operator $\hat{N}$ giving the total number of particles: it transfers one non-condensed particle into the condensate. As the operator $\delta \hat{\psi}$, it is transverse to ϕ_0 (see Eq. (7.7)). By definition of the condensate wavefunction $\hat{\Lambda}$ has a zero mean (see Eq. (7.9)).

In general it is difficult to exactly eliminate $\delta \hat{\psi}$ in terms of $\hat{\Lambda}$. Fortunately at the present order of the calculation we can use the assumption of a very small non-condensed fraction so that one has for example

$$\delta \hat{\psi}^\dagger \delta \hat{\psi} \simeq \delta \hat{\psi}^\dagger \hat{a}_{\phi_0} \hat{N}^{-1} \hat{a}_{\phi_0}^\dagger \delta \hat{\psi} = \hat{\Lambda}^\dagger \hat{\Lambda}. \quad (7.23)$$

To the same order of approximation $\hat{\Lambda}$ obeys the same commutation relation equation (7.8) as $\delta \hat{\psi}$.

The final result can be written in term of the operator $\mathcal{L}$ introduced in Section 6, with the approximation $N_0 \simeq N$:

$$\hat{H}_{\text{quad}} = f(\hat{N}) + \frac{1}{2} \int d^3\vec{r} (\hat{\Lambda}^\dagger, -\hat{\Lambda}) \mathcal{L} \begin{pmatrix} \hat{\Lambda} \\ \hat{\Lambda}^\dagger \end{pmatrix} \quad (7.24)$$

where the function f is specified in [51].

From this quadratic Hamiltonian the Heisenberg equations of motion for the field $\hat{\Lambda}$ have the suggestive form

$$i\hbar \frac{d}{dt} \begin{pmatrix} \hat{\Lambda} \\ \hat{\Lambda}^\dagger \end{pmatrix} = \mathcal{L} \begin{pmatrix} \hat{\Lambda} \\ \hat{\Lambda}^\dagger \end{pmatrix}. \quad (7.25)$$

We note that an hypothetic term of $\hat{H}_{\text{quad}}$ linear in $\hat{\Lambda}$ would give rise to a source term in equation (7.25) preventing one from satisfying equation (7.9) at all times!

The result equation (7.25) is really a crucial one. It shows that the linearized evolution of the non-condensed part $\delta\hat{\psi}$ of the atomic field is formally equivalent to the linearized response of the condensate to a classical perturbation (*e.g.* of the trapping potential) derived from the Gross–Pitaevskii equation; both treatments indeed exhibit the same operator $\mathcal{L}$ (see Eq. (6.14)).

All the machinery of Section 6 can therefore be used. We expand the field operator $\hat{\Lambda}$ on the eigenmodes of $\mathcal{L}$. We assume here dynamical stability and that the only eigenmodes in the 0 family are the zero-energy modes $(\phi_0, 0)$ and $(0, \phi_0^*)$ to which the field $\hat{\Lambda}$ is orthogonal according to equation (7.7). We therefore get an expansion similar to equation (6.33):

$$\begin{pmatrix} \hat{\Lambda}(\vec{r}) \\ \hat{\Lambda}^\dagger(\vec{r}) \end{pmatrix} = \sum_{k \in +\text{family}} \hat{b}_k \begin{pmatrix} u_k(\vec{r}) \\ v_k(\vec{r}) \end{pmatrix} + \hat{b}_k^\dagger \begin{pmatrix} v_k^*(\vec{r}) \\ u_k^*(\vec{r}) \end{pmatrix} \quad (7.26)$$

with the important difference that the coefficients in the expansion are now operators:

$$\hat{b}_k = \int d^3\vec{r} \left[u_k^*(\vec{r}) \hat{\Lambda}(\vec{r}) - v_k^*(\vec{r}) \hat{\Lambda}^\dagger(\vec{r}) \right]. \quad (7.27)$$

From the normalization condition between the eigenvectors of $\mathcal{L}$ and their adjoint vectors (see Sect. 6) one shows that the $\hat{b}_k$ obey bosonic commutation relations:

$$[\hat{b}_k, \hat{b}_{k'}^\dagger] = \delta_{k,k'} \quad \text{and} \quad [\hat{b}_k, \hat{b}_{k'}] = 0. \quad (7.28)$$

$\hat{b}_k$ corresponds formally to an annihilation operator; as $|v_k\rangle \neq 0$ in general $\hat{b}_k$ does not simply annihilate a particle as it is a coherent superposition of $\hat{\Lambda}$ (which transfers one non-condensed particle to the condensate) and of $\hat{\Lambda}^\dagger$ (which transfers one condensate particle to the non-condensed fraction). One then says that $\hat{b}_k$ annihilates a *quasi-particle* in mode k .

Finally we rewrite the Hamiltonian equation (7.24) in terms of the $\hat{b}_k$'s:

$$\hat{H}_{\text{quad}} = E_0(\hat{N}) + \sum_{k \in +\text{family}} \epsilon_k \hat{b}_k^\dagger \hat{b}_k. \quad (7.29)$$

We recall that ϵ_k is the eigenenergy of the mode (u_k, v_k) of the $+$ family. Our quadratic Hamiltonian describes a gas of non-interacting quasi-particles: this is the so-called Bogoliubov Hamiltonian.

The ground state of $\hat{H}_{\text{quad}}$ is obtained when no quasi-particle is present, it corresponds to all the modes k being in vacuum state:

$$\hat{H}_{\text{quad}}|0\rangle = E_0(N)|0\rangle \quad (7.30)$$

where

$$\hat{b}_k|0\rangle = 0 \quad \forall k. \quad (7.31)$$

E_0 is therefore the Bogoliubov approximation for the ground state energy of the gas. To get a finite expression for E_0 one has to include the regularizing operator in the pseudo-potential.

The excited states of the system are obtained in the Bogoliubov approximation by successive actions of the $\hat{b}_k^\dagger$'s. For this reason $\hat{b}_k^\dagger$ is said to create an *elementary* excitation k in the system, to distinguish with *collective* excitations involving all the particles of the condensate (induced *e.g.* by a perturbation δU of the trapping potential). We emphasize again that the elementary excitations of the gas have the same frequency $\epsilon_k/\hbar$ as the collective excitations in the linear response domain (δU small enough). This intriguing property is valid only at the presently considered regime of an almost pure condensate ($T \ll T_c$).

7.5 Order ε^2 : Corrections to the Gross–Pitaevskii equation

Expanding the Heisenberg field equations for $\hat{\psi}$ keeping terms up to $N^{1/2}\varepsilon^2$ one can calculate the first correction to the prediction equation (7.10) for the condensate wavefunction. This correction includes (i) the fact that the number of condensate particles N_0 rather than the total number of particles N should appear in the Gross–Pitaevskii equation, and (ii) the mechanical back-action of the non-condensed particles on the condensate in the form of mean field potentials.

The calculations are a bit involved [51] and require the use of the regularizing operator in the pseudo-potential (a fact realized in [53] but not yet in [51]). We give here only the result. The condensate wavefunction is given by an expansion

$$\phi_0 = \phi_0^{(0)} + \phi_0^{(2)} + o(\varepsilon^2) \quad (7.32)$$

where $\phi_0^{(0)}$, zeroth order approximation in ε , is the solution of equation (7.10). The correction $\phi_0^{(2)}$ is of order ε^2 ; its component on $\phi_0^{(0)}$ is purely imaginary (as both ϕ_0 and $\phi_0^{(0)}$ are normalized to unity) and can

be considered as a (not physically relevant) change of global phase of $\phi_0^{(0)}$; the part of $\phi_0^{(2)}$ orthogonal to $\phi_0^{(0)}$ is given by:

$$-\mathcal{L} \begin{pmatrix} Q\phi_0^{(2)} \\ Q^*\phi_0^{(2)*} \end{pmatrix} = \begin{pmatrix} QS \\ -Q^*S^* \end{pmatrix} \quad (7.33)$$

where Q projects orthogonally to ϕ_0 and where the source term S is equal to

$$\begin{aligned} S(\vec{r}) = & -(1 + \langle \delta \hat{N} \rangle) g |\phi_0^{(0)}(\vec{r})|^2 \phi_0^{(0)}(\vec{r}) + 2g \langle \hat{\Lambda}^\dagger(\vec{r}) \hat{\Lambda}(\vec{r}) \rangle \phi_0^{(0)}(\vec{r}) \\ & + g \left[\partial_s \left(s \langle \hat{\Lambda}(\vec{r} - \vec{s}/2) \hat{\Lambda}(\vec{r} + \vec{s}/2) \rangle \right) \right]_{s \rightarrow 0} \phi_0^{(0)*}(\vec{r}) \\ & - g \int d^3 \vec{s} |\phi_0^{(0)}(\vec{s})|^2 \left\langle \left[\hat{\Lambda}^\dagger(\vec{s}) \phi_0^{(0)}(\vec{s}) + \hat{\Lambda}(\vec{s}) \phi_0^{(0)*}(\vec{s}) \right] \hat{\Lambda}(\vec{r}) \right\rangle. \end{aligned} \quad (7.34)$$

The first line of this expression contains the effect of the depletion of the condensate, the number of non-condensed particles $\langle \delta \hat{N} \rangle$ being calculated in the Bogoliubov approximation, see discussion in Section 7.7. The other terms are mean field terms, among which one recognizes the Hartree-Fock contribution $2g \langle \hat{\Lambda}^\dagger(\vec{r}) \hat{\Lambda}(\vec{r}) \rangle$ already obtained in Section 4.

7.6 Thermal equilibrium of the gas of quasi-particles

In the Bogoliubov approximation the quasi-particles behave as an ideal Bose gas; such a gas can reach thermal equilibrium only by contact with a thermostat. There is no such thermostat in the experiments on trapped Bose gas, relaxation to thermal equilibrium has to be provided instead by interactions between the atoms.

Fortunately the full Hamiltonian equation (7.11) contains terms cubic and quartic in $\delta\hat{\psi}$: when expressed in terms of the $\hat{b}$'s and $\hat{b}^\dagger$'s they correspond to interactions between the quasi-particles which will provide thermalization. Two situations can then be considered, depending on the sign of ϵ_k .

- “Good” case: $\epsilon_k > 0$ for all k in $+$ family. We assume for simplicity thermal equilibrium in the canonical point of view (which should be equivalent to the micro-canonical point of view in the limit of large number of particles) with a N -body density matrix

$$\hat{\rho}_{1,\dots,N} = \frac{1}{Z} e^{-\beta \hat{H}} \simeq \frac{1}{Z_{\text{quad}}} e^{-\beta \hat{H}_{\text{quad}}}. \quad (7.35)$$

We suppose therefore that the interactions between quasi-particles, essential to ensure thermalization, have a weak effect on the thermal equilibrium

state. From equation (7.35) we finally obtain the mean number of quasi-particles in mode k :

$$\langle \hat{b}_k^\dagger \hat{b}_k \rangle = \frac{1}{e^{\beta \epsilon_k} - 1}. \quad (7.36)$$

This good case corresponds to a thermodynamically stable condensate in state ϕ_0 .

- “Bad” case: there is a mode k_0 in the $+$ family such that $\epsilon_{k_0} < 0$. In this case the quadratic Hamiltonian $\hat{H}_{\text{quad}}$ contains a harmonic oscillator of frequency $\omega_{k_0} = |\epsilon_{k_0}|/\hbar$ having formally a negative mass M :

$$-|\epsilon_{k_0}| \hat{b}_{k_0}^\dagger \hat{b}_{k_0} = \frac{1}{2M} [\hat{P}_{k_0}^2 + \omega_{k_0}^2 \hat{Q}_{k_0}^2] \quad (7.37)$$

where $\hat{P}_{k_0}$ and $\hat{Q}_{k_0}$ correspond formally to a momentum and position operator. By collisions with the quasi-particles of positive energy the mode k_0 can loose energy which increases its own excitation; if the number of quanta in the mode can become comparable to N the process of thermalization of the gas may lead the condensate to a state different from the predicted ϕ_0 .

This phenomenon of thermodynamical instability should not be confused with dynamical instability of the condensate, where ϵ_{k_0} is complex; *e.g.* the case of a purely imaginary ϵ_{k_0} corresponds formally to an oscillator in an expelling potential, $[\hat{P}_{k_0}^2 - |\omega_{k_0}|^2 \hat{Q}_{k_0}^2]/(2M)$.

7.7 Condensate depletion and the small parameter $(\rho a^3)^{1/2}$

We assume the situation of thermodynamical stability. We calculate the mean number $\langle \delta \hat{N} \rangle$ of particles out of the condensate, that is in all the modes orthogonal to the condensate wavefunction ϕ_0 :

$$\langle \delta \hat{N} \rangle \equiv \int d^3 \vec{r} \langle \delta \hat{\psi}^\dagger(\vec{r}) \delta \hat{\psi}(\vec{r}) \rangle. \quad (7.38)$$

In this way we can calculate explicitly the small parameter of the present theory given in equation (7.6).

To lowest order in the Bogoliubov approximation we can replace $\delta \hat{\psi}$ by $\hat{\Lambda}$ in the above expression:

$$\langle \delta \hat{N} \rangle \simeq \int d^3 \vec{r} \langle \hat{\Lambda}^\dagger(\vec{r}) \hat{\Lambda}(\vec{r}) \rangle. \quad (7.39)$$

We replace $\hat{\Lambda}$ by its modal expansion; using the approximation in equation (7.35) the only terms with non-zero mean are $\langle \hat{b}_k^\dagger \hat{b}_k \rangle$ given by equation (7.36) and

$$\langle \hat{b}_k \hat{b}_k^\dagger \rangle = \langle \hat{b}_k^\dagger \hat{b}_k \rangle + 1. \quad (7.40)$$

We therefore obtain:

$$\begin{aligned} \langle \delta \hat{N} \rangle &\simeq \sum_{k \in +\text{family}} \langle \hat{b}_k^\dagger \hat{b}_k \rangle [\langle u_k | u_k \rangle + \langle v_k | v_k \rangle] \\ &+ \sum_{k \in +\text{family}} \langle v_k | v_k \rangle. \end{aligned} \quad (7.41)$$

The contribution of the occupation numbers $\langle \hat{b}_k^\dagger \hat{b}_k \rangle$ corresponds to the so-called thermal depletion of the condensate, as it is non-zero only at finite temperature. The contribution of the +1 coming from the identity (7.40) is the so-called quantum depletion of the condensate: it expresses the fact that, even at zero temperature, there is a finite number of particles out of the condensate due to atomic interactions, contrarily to the ideal Bose gas case where all the v_k 's vanish.

It is instructive to calculate the depletion of the condensate in the homogeneous case in the thermodynamical limit, replacing the sum over the wavevector $\vec{k}$ characterizing each mode of the + family by an integral. From equation (6.44) we calculate

$$\langle u_k | u_k \rangle + \langle v_k | v_k \rangle = 1 + 2\langle v_k | v_k \rangle = \frac{\frac{\hbar^2 k^2}{2m} + \rho g}{\left[\frac{\hbar^2 k^2}{2m} \left(\frac{\hbar^2 k^2}{2m} + 2\rho g \right) \right]^{1/2}}. \quad (7.42)$$

At zero temperature we obtained for the non-condensed fraction of particles the following integral:

$$\frac{\langle \delta \hat{N} \rangle}{N}(T=0) = \frac{16}{\pi^{1/2}} (\rho a^3)^{1/2} \int_0^{+\infty} dq \, q^2 \left[\frac{q^2 + 1/2}{q(1+q^2)^{1/2}} - 1 \right] \quad (7.43)$$

where we have integrated over the solid angle in spherical coordinates and we have made the change of variable

$$\frac{\hbar^2 k^2}{2m} = 2\rho g q^2. \quad (7.44)$$

This integral can be calculated exactly:

$$\frac{\langle \delta \hat{N} \rangle}{N}(T=0) = \frac{8}{3\pi^{1/2}} (\rho a^3)^{1/2}. \quad (7.45)$$

In this way we obtain a very important small parameter of the theory, $(\rho a^3)^{1/2}$, which characterizes the domain of a weakly interacting Bose gas. This small parameter is similar to the condition obtained in equation (3.36) of Section 3 already with a totally different point of view, a condition of Born approximation on the pseudo-potential! In the typical experimental

conditions of MIT for sodium atoms we have $\rho \sim 10^{14} \text{ cm}^{-3}$ and $a \sim 25 \text{ \AA}$, which leads to a small parameter $(\rho a^3)^{1/2} \sim 10^{-3}$. The result (7.45) also gives us the opportunity to recall that the number of non-condensed particles should not be confused with the number of quasi-particles for an interacting Bose gas: one notes here that the second quantity vanishes at $T = 0$ whereas the first one does not.

At finite temperature there is, in addition to the quantum depletion, a thermal depletion of the condensate:

$$\begin{aligned} \frac{\langle \delta \hat{N} \rangle}{N}(T) - \frac{\langle \delta \hat{N} \rangle}{N}(0) &= \frac{32}{\pi^{1/2}} \int_0^{+\infty} dq \frac{q(q^2 + 1/2)}{(q^2 + 1)^{1/2}} \\ &\times \left[\exp \left(2\beta \rho g q (q^2 + 1)^{1/2} \right) - 1 \right]^{-1}. \end{aligned} \quad (7.46)$$

The integral over q depends only on the parameter $\rho g / (k_B T)$. At low temperature $k_B T \ll \rho g$ this parameter is large so that the modes with a $q \sim 1$ have a very low occupation number: one can neglect q as compared to one and one-half (which amounts to restricting to the linear part of the Bogoliubov spectrum) and one obtains a small correction to the zero temperature case:

$$\frac{\langle \delta \hat{N} \rangle}{N}(T) = \frac{\langle \delta \hat{N} \rangle}{N}(0) \left[1 + \left(\frac{\pi k_B T}{2 \rho g} \right)^2 + \dots \right]. \quad (7.47)$$

At high temperature $k_B T \gg \rho g$ the major fraction of the populated Bogoliubov modes have a q much larger than unity, so that we can now neglect one and one-half as compared to q^2 (which amounts to restricting to the quadratic part of the Bogoliubov spectrum). To this approximation we recover the ideal Bose gas result

$$\frac{\langle \delta \hat{N} \rangle}{N}(T) \simeq \frac{\zeta(3/2)}{\rho \lambda_{\text{dB}}^3} \quad (7.48)$$

where λ_{dB} is the thermal de Broglie wavelength and ζ stands for the Riemann Zeta function (see Sect. 2). For a given temperature indeed the density of non-condensed particles in presence of a condensate saturates to its maximal value $\zeta(3/2) \lambda_{\text{dB}}^{-3}$ for the ideal Bose gas in a box (see Eq. (1.5) and Eq. (1.2)).

In the high temperature regime $k_B T \gg \rho g$ our Bogoliubov approach can therefore be valid only if $\rho \lambda_{\text{dB}}^3 \gg \zeta(3/2)$. Both inequalities on ρ can be satisfied simultaneously only if $2\zeta(3/2)a/\lambda_{\text{dB}} \ll 1$. Amusingly this condition is similar to the condition $a\Delta k \ll 1$ obtained in Section 3 (see Eq. (3.37)) for the validity condition of the Born approximation for the pseudo-potential.

7.8 Fluctuations in the number of condensate particles

The Bogoliubov theory that we have presented also allows a calculation of the fluctuations of N_0 in the canonical ensemble. This has the advantage of removing the effect of fluctuations in the total number of particles present in the grand-canonical ensemble, a “trivial” contribution to the fluctuations of N_0 .

As the total number of particles is fixed to N the variance of N_0 is exactly equal to the variance of $\delta\hat{N}$, number of non-condensed particles. The mean value of $\delta\hat{N}$ has been given in the previous section, we now have to calculate the mean value of its square:

$$\langle(\delta\hat{N})^2\rangle = \int d\vec{r}_1 \int d\vec{r}_2 \langle \delta\hat{\psi}^\dagger(\vec{r}_1) \delta\hat{\psi}(\vec{r}_1) \delta\hat{\psi}^\dagger(\vec{r}_2) \delta\hat{\psi}(\vec{r}_2) \rangle \quad (7.49)$$

$$= \langle\delta\hat{N}\rangle + \int d\vec{r}_1 \int d\vec{r}_2 \langle \delta\hat{\psi}^\dagger(\vec{r}_1) \delta\hat{\psi}^\dagger(\vec{r}_2) \delta\hat{\psi}(\vec{r}_1) \delta\hat{\psi}(\vec{r}_2) \rangle \quad (7.50)$$

where we have used the commutation relation equation (7.8) and the fact equation (7.7) that ϕ is orthogonal to $\delta\hat{\psi}$. To lowest order in the Bogoliubov approximation we can replace $\delta\hat{\psi}$ by $\hat{\Lambda}$ in the above expression and take the approximation equation (7.35) for the equilibrium density operator. As $\hat{H}_{\text{quad}}$ is quadratic in the field $\hat{\Lambda}$, Wick’s theorem can be used. We finally find for the variance of the number of non-condensed particles:

$$\begin{aligned} \text{Var}(\delta\hat{N}) \simeq & \langle\delta\hat{N}\rangle + \int d\vec{r}_1 \int d\vec{r}_2 \left[\left| \langle \hat{\Lambda}^\dagger(\vec{r}_1) \hat{\Lambda}(\vec{r}_2) \rangle \right|^2 \right. \\ & \left. + \left| \langle \hat{\Lambda}(\vec{r}_1) \hat{\Lambda}(\vec{r}_2) \rangle \right|^2 \right]. \end{aligned} \quad (7.51)$$

The variance in equation (7.51) is simple to calculate in the homogeneous case of a gas in a cubic box of size L with periodic boundary conditions. The eigenmodes (u, v) are simply plane waves equation (6.41) with real coefficients U_k, V_k given in equation (6.44) and depending only on the modulus k of the wavevector $\vec{k}$. We find for the two correlation functions appearing in equation (7.51) the simple expression:

$$\langle \hat{\Lambda}^\dagger(\vec{r}_1) \hat{\Lambda}(\vec{r}_2) \rangle = \frac{1}{L^3} \sum_{\vec{k} \neq \vec{0}} [(U_k^2 + V_k^2) n_k + V_k^2] e^{i\vec{k} \cdot (\vec{r}_1 - \vec{r}_2)} \quad (7.52)$$

$$\langle \hat{\Lambda}(\vec{r}_1) \hat{\Lambda}(\vec{r}_2) \rangle = \frac{1}{L^3} \sum_{\vec{k} \neq \vec{0}} U_k V_k (1 + 2n_k) e^{i\vec{k} \cdot (\vec{r}_1 - \vec{r}_2)} \quad (7.53)$$

where we have introduced the mean occupation numbers $n_k = \langle \hat{b}_k^\dagger \hat{b}_k \rangle$.

After spatial integration of the square modulus of these quantities we obtain

$$\text{Var}(\delta\hat{N}) = \langle\delta\hat{N}\rangle + \sum_{\vec{k}\neq\vec{0}} [(U_k^2 + V_k^2) n_k + V_k^2]^2 + U_k^2 V_k^2 (1 + 2n_k)^2 \quad (7.54)$$

where the mean number of non-condensed particles $\langle\delta\hat{N}\rangle$ is already given in equation (7.41):

$$\langle\delta\hat{N}\rangle = \sum_{\vec{k}\neq\vec{0}} (U_k^2 + V_k^2) n_k + V_k^2. \quad (7.55)$$

We first apply formula (7.54) to the limiting case of zero temperature. All the occupation numbers n_k vanish. For the ideal Bose gas ($g = 0$) all the V_k 's are zero and the variance of $\delta\hat{N}$ vanishes as expected, since all the particles are in the ground state of the box. For the interacting Bose gas we find

$$\text{Var}(\delta\hat{N})(T = 0) = \frac{1}{8} \sum_{\vec{k}\neq\vec{0}} \frac{1}{q^2 (1 + q^2)} \quad (7.56)$$

where q is given as function of k by equation (7.44). In the thermodynamical limit we replace the discrete sum by an integral and this leads to a variance scaling as the number of particles for a fixed density:

$$\frac{\text{Var}(\delta\hat{N})(T = 0)}{N} = 2\pi^{1/2} (\rho a^3)^{1/2}. \quad (7.57)$$

In the regime of validity of the Bogoliubov approach one has $\rho a^3 \ll 1$ so that the fluctuations of N_0 are sub-poissonian.

The situation can be totally different at finite temperature. Consider first the case of the ideal Bose gas [54]:

$$\begin{aligned} \text{Var}(\delta\hat{N}) &= \sum_{\vec{k}\neq\vec{0}} n_k (1 + n_k) \\ &= \sum_{\vec{k}\neq\vec{0}} \frac{1}{4 \sinh^2(\beta \epsilon_k / 2)} \end{aligned} \quad (7.58)$$

with $\epsilon_k = \hbar^2 k^2 / (2m)$. In the thermodynamical limit one may be tempted to replace in the usual manner the sum over $\vec{k}$ by an integral. This leads however to an integral divergent in $k = 0$: the integrand scales as $1/k^4$, which is not compensated by the Jacobian k^2 of three-dimensional integration in spherical coordinates. In this case the contribution of the sum in

the thermodynamical limit is dominated by the terms close to $k = 0$ where $\beta\epsilon_k \ll 1$ and the function $\sinh$ can be linearized. We then obtain

$$\text{Var}(\delta\hat{N})_{g=0} \simeq \left(\frac{k_B T}{\Delta}\right)^2 \sum_{\vec{n} \neq \vec{0}} \frac{1}{n^4}. \quad (7.59)$$

In this expression we have introduced the kinetic energy difference between the ground state and the first excited state for a single particle in the box:

$$\Delta = \frac{\hbar^2}{2mL^2} \quad (7.60)$$

and the sum ranges over all the vectors $\vec{n}$ with integer components and a non-vanishing norm n . By a numerical calculation we obtain

$$\sum_{\vec{n} \neq \vec{0}} \frac{1}{n^4} = 16.53 \dots \quad (7.61)$$

A remarkable feature is that the variance of N_0 scales as L^4 that is as the volume of the box to the power 4/3, or equivalently as the number of particles to the power 4/3 in the thermodynamical limit. This is much larger than N in the thermodynamical limit.

Do the fluctuations of N_0 remain large in presence of interactions? As the spectrum ϵ_k is linear at small k the divergence of n_k^2 is only as $1/k^2$, which has a finite integral in three dimensions. However the mode functions U_k, V_k are also diverging in $k = 0$, each as $1/k^{1/2}$, so that one recovers the $1/k^4$ dependence of the summand close to $k = 0$. As in the ideal Bose gas case we replace in the thermodynamical limit the summand by its low k approximation:

$$n_k \sim \frac{k_B T}{\hbar k c} \quad (7.62)$$

$$U_k \sim \frac{1}{2q^{1/2}} \quad (7.63)$$

$$V_k \sim -\frac{1}{2q^{1/2}} \quad (7.64)$$

and we keep in the summation the most diverging terms. We finally obtain [55, 56]

$$\text{Var}(\delta\hat{N})_{g>0} \simeq \frac{1}{2} \left(\frac{k_B T}{\Delta}\right)^2 \sum_{\vec{n} \neq \vec{0}} \frac{1}{n^4}. \quad (7.65)$$

Remarkably this result differs from the ideal Bose gas case equation (7.59) by a factor 1/2 only: fluctuations of N_0 remain large. The fact that equation (7.65) does not depend on the strength g of the interaction is valid only at the thermodynamical limit and indicates that the limit $g \rightarrow 0$ and the thermodynamical limit do not commute.

7.9 A simple reformulation of the thermodynamical stability condition

The thermodynamical stability condition simply requires that the Bogoliubov Hamiltonian $\hat{H}_{\text{quad}}$ is the sum of a constant (function of $\hat{N}$) and of a *positive* quadratic operator in the field variables. In the diagonal form (7.29) positivity is clearly equivalent to the requirement ϵ_k positive for all k in the $+$ family. How to express this condition from the non-diagonal form (7.24)? We simply have to rewrite equation (7.24) as

$$\hat{H}_{\text{quad}} = f(\hat{N}) + \frac{1}{2} \int d^3\vec{r} (\hat{\Lambda}^\dagger, \hat{\Lambda}) \eta \mathcal{L} \begin{pmatrix} \hat{\Lambda} \\ \hat{\Lambda}^\dagger \end{pmatrix} \quad (7.66)$$

where η is the operator

$$\eta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (7.67)$$

so that $\eta \mathcal{L}$ is an Hermitian operator.

The thermodynamical stability condition is therefore equivalent to the requirement that $\eta \mathcal{L}$ is positive:

$$\eta \mathcal{L} \geq 0. \quad (7.68)$$

More precisely, as $\hat{\Lambda}$ is orthogonal to ϕ_0 , $\eta \mathcal{L}$ has to be strictly positive in the subspace orthogonal to $(|\phi_0\rangle, 0)$ and $(0, |\phi_0^*\rangle)$.

We can give a simple physical interpretation of this condition: ϕ_0 has to be a local minimum of the Gross–Pitaevskii energy functional

$$E[\phi, \phi^*] = N \int d^3\vec{r} \left[\frac{\hbar^2}{2m} |\text{grad } \phi|^2 + U(\vec{r}) |\phi(\vec{r})|^2 + \frac{1}{2} N g |\phi(\vec{r})|^4 \right], \quad (7.69)$$

which is the expression of Section 5 with the approximation $N_0 \simeq N$. Let us consider indeed the variation δE of E from $E_0 \equiv E[\phi_0, \phi_0^*]$ up to second order in a small deviation $\delta\phi$ of ϕ from ϕ_0 .

The terms linear in $\delta\phi$ are given by:

$$\begin{aligned} \delta E^{(1)} &= N \int d^3\vec{r} \left[\frac{\hbar^2}{2m} \text{grad } \phi_0^* \cdot \text{grad } \delta\phi + U(\vec{r}) \phi_0^* \delta\phi \right. \\ &\quad \left. + N g \phi_0^{*2} \phi_0 \delta\phi + \text{c.c.} \right]. \end{aligned} \quad (7.70)$$

By integration by parts and using the fact that ϕ_0 solves the Gross–Pitaevskii equation (7.10) we rewrite this expression as

$$\delta E^{(1)} = N \mu [\langle \phi_0 | \delta\phi \rangle + \langle \delta\phi | \phi_0 \rangle]. \quad (7.71)$$

As both ϕ and ϕ_0 are normalized to unity $\delta\phi$ actually fulfills the identity

$$\langle\phi_0|\delta\phi\rangle + \langle\delta\phi|\phi_0\rangle = -\langle\delta\phi|\delta\phi\rangle. \quad (7.72)$$

The *a priori* first order energy change is *a posteriori* of second order:

$$\delta E^{(1)} = -N\mu\langle\delta\phi|\delta\phi\rangle! \quad (7.73)$$

The terms *a priori* quadratic in $\delta\phi$ are given by:

$$\begin{aligned} \delta E^{(2)} = & N \int d^3\vec{r} \left[\frac{\hbar^2}{2m} \text{grad } \delta\phi^* \cdot \text{grad } \delta\phi + U(\vec{r})\delta\phi^* \delta\phi + 2Ng|\phi_0|^2 \delta\phi^* \delta\phi \right. \\ & \left. + \frac{1}{2}Ng\phi_0^{*2} \delta\phi^2 + \frac{1}{2}Ng\phi_0^2 \delta\phi^{*2} \right]. \end{aligned} \quad (7.74)$$

We transform this expression by splitting $\delta\phi$ in a part parallel to ϕ_0 and a part orthogonal to ϕ_0 :

$$\delta\phi(\vec{r}) = \gamma\phi_0(\vec{r}) + \delta\phi_\perp(\vec{r}). \quad (7.75)$$

Using integration by parts, the Gross–Pitaevskii equation and the fact that operator $\mathcal{L}$ contains projectors orthogonally to ϕ_0, ϕ_0^* we are able to write $\delta E^{(2)}$ as

$$\begin{aligned} \delta E^{(2)} = & |\gamma|^2 N\mu + \frac{1}{2}(\gamma + \gamma^*)^2 N^2 g \int d^3\vec{r} |\phi_0|^4 \\ & + (\gamma + \gamma^*) N^2 g \int d^3\vec{r} |\phi_0|^2 (\phi_0^* \delta\phi_\perp + \text{c.c.}) \\ & + \frac{1}{2} N \int d^3\vec{r} (\delta\phi_\perp^*, \delta\phi_\perp) (\eta\mathcal{L} + \mu \text{Id}) \begin{pmatrix} \delta\phi_\perp \\ \delta\phi_\perp^* \end{pmatrix}. \end{aligned} \quad (7.76)$$

Note that we had to add μ times the identity matrix Id to $\eta\mathcal{L}$ as equation (7.74), contrarily to $\eta\mathcal{L}$, does not contain any term proportional to μ . From equation (7.72) we see that $\gamma + \gamma^*$ is actually of second order in $\delta\phi_\perp$ so that it can be set to zero in equation (7.76).

Summing the *a priori* first and second order energy changes we see that $\delta E^{(1)}$ exactly cancels the terms involving explicitly μ in equation (7.76) so that we arrive at

$$\delta E \simeq \frac{1}{2} N \int d^3\vec{r} (\delta\phi_\perp^*, \delta\phi_\perp) \eta\mathcal{L} \begin{pmatrix} \delta\phi_\perp \\ \delta\phi_\perp^* \end{pmatrix}. \quad (7.77)$$

Thermodynamical stability that is positivity of $\eta\mathcal{L}$ is therefore equivalent to the Gross–Pitaevskii energy functional having a local minimum in ϕ_0 .

7.10 Thermodynamical stability implies dynamical stability

As we show now the positivity of $\eta\mathcal{L}$ automatically leads to a purely real spectrum for $\mathcal{L}$, that is to dynamical stability. Consider an eigenvector (u, v) of $\mathcal{L}$ with the eigenvalue ϵ . Contracting the operator $\eta\mathcal{L}$ between the ket $(|u\rangle, |v\rangle)$ and the bra $(\langle u|, \langle v|)$ we get

$$(\langle u|, \langle v|)\eta\mathcal{L} \begin{pmatrix} |u\rangle \\ |v\rangle \end{pmatrix} = \epsilon [\langle u|u\rangle - \langle v|v\rangle]. \quad (7.78)$$

The matrix element of $\eta\mathcal{L}$ is real positive as $\eta\mathcal{L}$ is supposed to be a positive hermitian operator. We now face two possible cases for the real quantity $\langle u|u\rangle - \langle v|v\rangle$:

- $\langle u|u\rangle - \langle v|v\rangle = 0$. In this case $\eta\mathcal{L}$ has a vanishing expectation value in $(|u\rangle, |v\rangle)$; as $\eta\mathcal{L}$ is positive, $(|u\rangle, |v\rangle)$ has to be an eigenvector of $\eta\mathcal{L}$ with the eigenvalue zero; as η is invertible we find that $(|u\rangle, |v\rangle)$ is an eigenvector of $\mathcal{L}$ with the eigenvalue 0, so that $\epsilon = 0$ is a real number;
- $\langle u|u\rangle - \langle v|v\rangle > 0$: we get ϵ as the ratio of two real numbers, so that ϵ is real.

7.11 Examples of thermodynamical instability

7.11.1 Real condensate wavefunction with a node

Let us assume that the solution of the Gross–Pitaevskii equation is a real function $\phi_0(\vec{r})$. To decide if this solution is thermodynamically stable one has to check the positivity of the operator $\eta\mathcal{L}$. Consider an eigenvector of $\eta\mathcal{L}$ with eigenvalue ε :

$$\eta\mathcal{L} \begin{pmatrix} u \\ v \end{pmatrix} = \varepsilon \begin{pmatrix} u \\ v \end{pmatrix}. \quad (7.79)$$

This ε should not be confused with the quasi-particle energies as $\eta\mathcal{L}$ and $\mathcal{L}$ have different spectra. By performing the sum and the difference of the two lines of equation (7.79) we get decoupled equations for the sum $\psi_s = u + v$ and the difference $\psi_d = u - v$:

$$\varepsilon|\psi_s\rangle = \left[\frac{\vec{p}^2}{2m} + U(\vec{r}) + Ng\phi_0^2(\vec{r}) + 2NgQ\phi_0^2(\vec{r})Q - \mu \right] |\psi_s\rangle \quad (7.80)$$

$$\varepsilon|\psi_d\rangle = \left[\frac{\vec{p}^2}{2m} + U(\vec{r}) + Ng\phi_0^2(\vec{r}) - \mu \right] |\psi_d\rangle. \quad (7.81)$$

Both operators involved in these equations have to be positive to achieve thermodynamical stability. Note that for $g > 0$ the positivity of the second

operator equation (7.81) implies the positivity of the first one equation (7.80) as $gQ\phi_0^2(\vec{r})Q$ is positive.

We therefore concentrate on equation (7.81). It involves the Gross–Pitaevskii Hamiltonian

$$\mathcal{H}_{\text{GP}} = \frac{\vec{p}^2}{2m} + U(\vec{r}) + Ng\phi_0^2(\vec{r}) - \mu. \quad (7.82)$$

An obvious eigenvector of this Hamiltonian is $\psi_d = \phi_0$ with eigenvalue $\varepsilon = 0$, as ϕ_0 solves the Gross–Pitaevskii equation! The condition of a positive ε in equation (7.81) simply means that ϕ_0 should be the ground state of $\mathcal{H}_{\text{GP}}$!

We can then invoke a theorem claiming that the ground state of a potential has no node [58]. If $\phi_0(\vec{r})$ has a node it cannot be the ground state of $\mathcal{H}_{\text{GP}}$. The ground state of $\mathcal{H}_{\text{GP}}$ has therefore an eigenenergy ε lower than the one of ϕ_0 , that is lower than zero, so that the operator $\eta\mathcal{L}$ is not positive and there is no thermodynamical stability.

As an example consider in a harmonic trap with eigenaxis z , a solution of the Gross–Pitaevskii equation even along x and y but odd along z , so that it vanishes in the plane $z = 0$. Such a solution exists, for $g > 0$: within the class of *real* functions ϕ odd along z and even along x, y , the Gross–Pitaevskii energy $E[\phi, \phi]$, bounded from below, has a minimum, reached in ϕ_0 , and this ϕ_0 then solves the Gross–Pitaevskii equation. This solution however is no longer a local minimum of $E[\phi, \phi^*]$ when one includes all possible deviations of ϕ from ϕ_0 (complex and with no well defined parity along z).

7.11.2 Condensate with a vortex

Can we get a thermodynamically stable condensate wavefunction with a node? To beat the results of the previous subsection we now assume ϕ_0 to be complex.

A particular class of complex wavefunctions with a node are condensate wavefunctions with vortices. A vortex is characterized (i) by a nodal, not necessarily straight, line in ϕ_0 (the center of the so-called vortex core) and (ii) by the fact that the phase of ϕ_0 changes by $2q\pi$, q non-zero integer, along a closed path around the vortex core (q is the so-called charge of the vortex). This second property means that the circulation of the local velocity field (defined in Sect. 5.3.3) around the vortex core is $2\pi\hbar q/m$.

A condensate wavefunction can have several vortices; the change of the phase of ϕ_0 along a closed path is now $2\pi q_{\text{sum}}$ where q_{sum} is the algebraic sum of the charges of the vortex lines enclosed by the path.

It has been shown that a condensate wavefunction with a vortex in a harmonic trap is not thermodynamically stable [59]. In the limit of vanishing interaction between the particles ($g = 0$) this is clear indeed. Suppose that the trap is cylindrically symmetric with respect to z . $|\phi_0\rangle$ can be chosen as

$(|n_x = 1, n_y = 0, n_z = 0\rangle + i|n_x = 0, n_y = 1, n_z = 0\rangle)/\sqrt{2}$ where $|n_x, n_y, n_z\rangle$ is the eigenstate of the harmonic oscillator with quantum number n_α along axis α ($\alpha = x, y, z$). The chemical potential is simply $2\hbar\omega_{x,y} + \frac{1}{2}\hbar\omega_z$ where ω_α is the atomic oscillation frequency along axis α . One then finds that $(|u\rangle = |n_x = 0, n_y = 0, n_z = 0\rangle, |v\rangle = 0)$ is an eigenvector of $\eta\mathcal{L}$ with the strictly negative energy $\varepsilon = -\hbar\omega_{x,y}$.

What happens in the opposite Thomas–Fermi regime of strong interactions? An intuitive answer can be obtained in a 2D model of the Gross–Pitaevskii equation, assuming for simplicity a quasi-isotropic trapping potential and restricting to the following class of condensate wavefunctions:

$$\phi_0(x, y) = \phi_{\text{slow}}(x, y) \tanh[\kappa|\vec{r} - \vec{\alpha}R|]e^{i\theta_{\vec{\alpha}R}}. \quad (7.83)$$

In this ansatz $\phi_{\text{slow}}(x, y)$ is the usual square root of inverted parabola Thomas–Fermi approximation for a condensate wavefunction without vortex, with a radius R ; the $\tanh[\]$ represents the correction to the modulus of ϕ_0 due to the vortex core (of adjustable position $\vec{\alpha}R$ and inverse width κ); $\theta_{\vec{\alpha}R}$ is the polar angle of a system of Cartesian coordinates (X, Y) centered on the vortex core, and represents (approximately for $\vec{\alpha} \neq \vec{0}$) the phase of the unit-charge vortex.

One then calculates the mean energy of ϕ_0 , with the simplification that $\phi_{\text{slow}}(x, y)$ varies very slow at the scale of κ^{-1} , and one minimizes this energy over κ . This leads to the inverse size of the vortex core on the order of the local healing length of the condensate:

$$\frac{\hbar^2\kappa^2}{m} = 0.59 \left[\mu - \frac{1}{2}m\omega^2(\alpha R)^2 \right]. \quad (7.84)$$

The mean energy of ϕ_0 (7.69) is now a function of the position of the vortex core only,

$$E = E_{\text{no vortex}} + W(\vec{\alpha}) \quad (7.85)$$

where $E_{\text{no vortex}}$ is the energy of the condensate with no vortex and

$$W(\vec{\alpha}) = N \frac{(\hbar\omega)^2}{\mu_0} \left\{ \frac{1}{2} + (1 - \alpha^2) \left[\frac{2 \ln 2 + 1}{3} + \ln \frac{\nu\mu_0}{\hbar\omega} + \ln(1 - \alpha^2) \right] \right\} \quad (7.86)$$

with $\nu = 0.49312$ and μ_0 the chemical potential in the absence of vortex. This function W represents an effective potential seen by the vortex core. As shown in Figure 14a this potential is maximal at the center of the trap so that it is actually an expelling potential for the vortex core: shifting the vortex core away from the center of the trap lowers the condensate energy.

A method to stabilize the vortex is to rotate the harmonic trap around z at a frequency Ω (the trap is anisotropic in the $x - y$ plane otherwise

rotation would have no effect). Thermodynamical equilibrium will now be obtained in the frame rotating at the frequency Ω , where the harmonic trap is time independent. As this frame is non Galilean the Hamiltonian and therefore the Gross–Pitaevskii energy functional have to be supplemented by the inertial energy term $-\Omega L_z$ per atom, where L_z is the angular momentum operator along z . The effective potential $W(\vec{\alpha})$ gets an extra term:

$$W_\Omega(\vec{\alpha}) = W_{\Omega=0}(\vec{\alpha}) - N\hbar\Omega(1 - \alpha^2)^2 \quad (7.87)$$

where $W_{\Omega=0}$ is the result (7.86) in the absence of rotation. As shown in Figure 14b this extra term can trap the vortex core at the center of the harmonic trap if Ω is large enough.

What happens if Ω is increased significantly? It becomes favorable to put more vorticity in the condensate. As the vortices with charge larger than one are unstable the way out is to create several vortices with unit charge. This can be analyzed along the previous lines by a generalized multi-vortex ansatz, as discussed in [60]. A condensate with vortices has been recently obtained at the ENS in a rotating trap [61].

Another philosophy was followed at JILA: rather than relying on thermal equilibrium in a rotating trap to produce a vortex they used a “quantum engineering” technique [62] to directly induce the vortex by giving angular momentum to the atoms through coupling to electromagnetic fields [63]. It has also been suggested to imprint the phase of the vortex on the condensate through a lightshift induced by a laser beam whose spatial intensity profile has been conveniently tailored [64]. Such an imprinting technique has successfully led to the observation of dark and gray solitons in atomic condensates with repulsive interactions in Hannover [65] and in the group of Phillips at NIST. All these techniques illustrate again the powerfulness of atomic physics in its ability to manipulate a condensate.

8 Phase coherence properties of Bose–Einstein condensates

Consider two Bose–Einstein condensates prepared in spatially well separated traps and that have “never seen each other” (*e.g.* one rubidium condensate at JILA and one rubidium condensate at ENS). It is “natural” to assume that these two condensates do not have a well defined relative phase. However the trend in the literature on Bose condensates is to assume that the two condensates are in a *coherent* state with a well defined relative phase, the so-called “symmetry-breaking” point of view. So imagine that one lets the two condensates spatially overlap. Will interference fringes appear on the resulting atomic density or not?

One of the goals of this chapter is to answer this question and to reconcile the symmetry breaking point of view with the “natural” point of view.

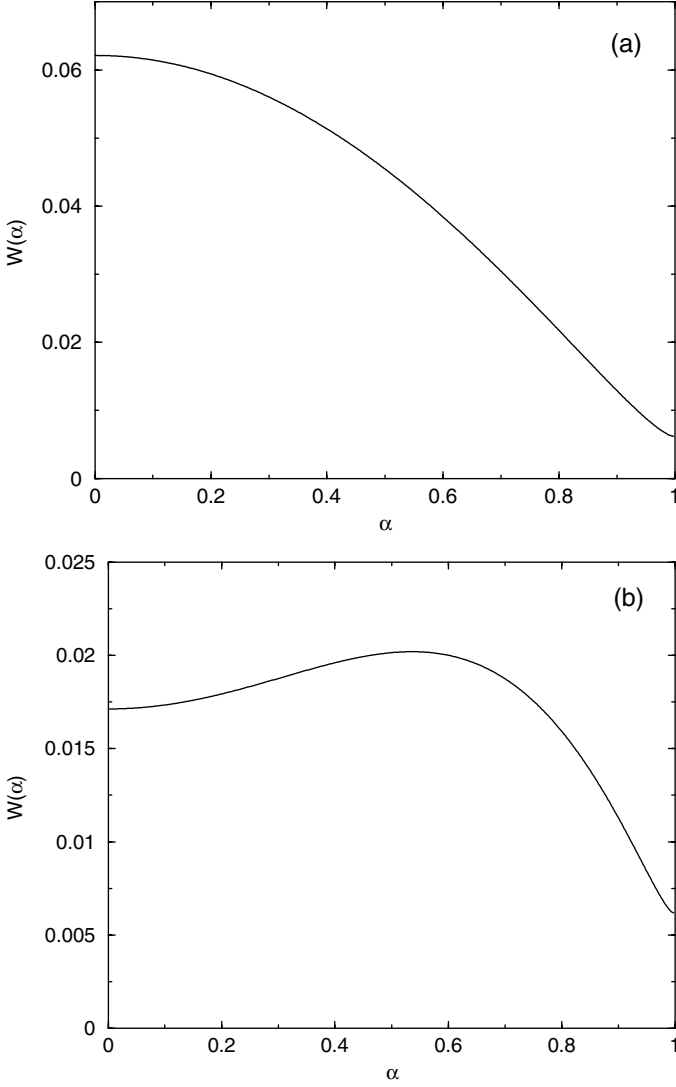


Fig. 14. In a 2D model, effective potential energy W of a vortex in a quasi-axisymmetric harmonic trap as function of the distance αR of the core from the trap center, for $\mu_0 = 80\hbar\omega$. (a) $\Omega = 0$ and (b) $\Omega = 0.045\omega$. The unit of energy is $N\hbar\omega$ where ω is the oscillation frequency of the atoms in the trap.

8.1 Interference between two BECs

At MIT a double well trapping potential was obtained by superimposing a sharp barrier induced with laser light on top of the usual harmonic trap

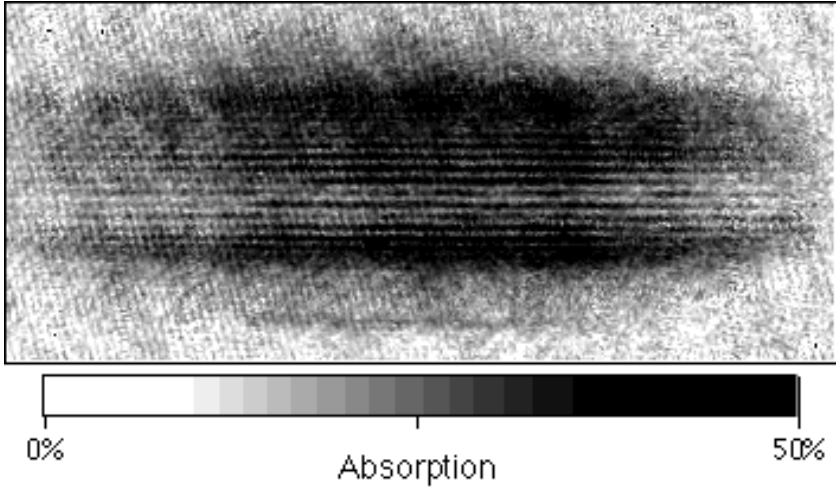


Fig. 15. Interference fringes between two condensates observed at MIT [66].

produced with a magnetic field. In this way one can produce two Bose–Einstein condensates, one on each side of the barrier. The height of the barrier can be made much larger than the chemical potential of the gas so that coupling between the two condensates *via* tunneling through the wall is very small. In this way one can consider the two condensates as independent.

One can then switch off the barrier and magnetic trap, let the two condensates ballistically expand and spatially overlap. One then measures the spatial density of the cloud by absorption imaging. This spatial density exhibits clearly fringes [66] (see Fig. 15). These fringes have to be interference fringes, as hydrodynamic effects (such as sound waves) are excluded at the very low densities of the ballistically expanded condensates. We show here on a simple model that we indeed expect to see interference fringes in such an experiment, even if the two condensates have initially no well defined relative phase.

8.1.1 A very simple model

In our simple modelization of an MIT-type interference experiment we will concentrate on the positions of the particles on an axis x connecting the two condensates so that we use a one-dimensional model enclosed in a box of size L with periodic boundary conditions. We assume that the system is

initially in the Fock state

$$|\Psi\rangle = \left| \frac{N}{2} : k_a, \frac{N}{2} : k_b \right\rangle \quad (8.1)$$

with $N/2$ particles in the plane wave of momentum $\hbar k_a$ and $N/2$ particles in the plane wave of momentum $\hbar k_b$:

$$\langle x | k_{a,b} \rangle = \frac{1}{\sqrt{L}} \exp[ik_{a,b}x] . \quad (8.2)$$

We assume that one detects the position of all the particles. What will be the outcome? As the numbers of particles are exactly defined in the two modes a and b the relative phase between the atomic fields in the two modes is totally undefined.

8.1.2 A trap to avoid

If we calculate the *mean density* in the state given by (8.1) we find a uniform result

$$\langle \hat{\psi}^\dagger(x) \hat{\psi}(x) \rangle = N/L \quad (8.3)$$

and we may be tempted to conclude that no interference fringes will appear in the beating of two Fock state condensates.

Actually this naive statement is wrong. Interference fringes appeared in a *single realization* of the experiment at MIT. We have therefore to consider the probability of the outcome of a particular density profile in a single realization of the measurement and not the average of the density profile over many realizations of the experiment. Indeed we will see that by interfering two independent Bose–Einstein condensates we get interference fringes on the density profile in each single realization of the experiment but the position of the interference pattern is random so that by averaging the density profile over many realizations we wash out the fringes.

We wish to emphasize the following crucial point of the quantum theory: Whatever single-time measurement is performed on the system all the information about the outcomes of a single realization of the measurement procedure is contained in the N -body density matrix, here

$$\hat{\rho} = |\Psi\rangle\langle\Psi|. \quad (8.4)$$

Indeed the only information we can get from quantum mechanics on a single realization outcome is its probability P , which can be obtained from $\hat{\rho}$ by

$$P = \text{Tr}[\hat{O}\hat{\rho}] \quad (8.5)$$

where the operator $\hat{O}$ depends on the considered outcome. *E.g.* in our gedanken experiment P is the probability density of finding the N particles at positions $x_1, x_2, \dots, x_N$ and the operator $\hat{O}$ is expressed in terms of the field operator as

$$\hat{O} = \frac{1}{N!} \hat{\psi}^\dagger(x_1) \dots \hat{\psi}^\dagger(x_N) \hat{\psi}(x_N) \dots \hat{\psi}(x_1). \quad (8.6)$$

In a first quantized picture this corresponds to the fact that the probability density P is equal to the modulus squared of the N -body wavefunction.

The complete calculation of the N -body distribution function $P(x_1, \dots, x_N)$ for the state $|\Psi\rangle$ in equation (8.1) is involved and we will see in the coming subsections how to circumvent the difficulty. But we can do a simple calculation of the pair distribution function of the atoms in state $|\Psi\rangle$:

$$\rho(x_1, x_2) = \langle \Psi | \hat{\psi}^\dagger(x_1) \hat{\psi}^\dagger(x_2) \hat{\psi}(x_2) \hat{\psi}(x_1) | \Psi \rangle \quad (8.7)$$

$$= ||\hat{\psi}(x_2) \hat{\psi}(x_1) | \Psi \rangle||^2. \quad (8.8)$$

We expand the field operator on the two modes $\phi_{a,b}$ and on other arbitrary orthogonal modes not relevant here as they are not populated in $|\Psi\rangle$:

$$\hat{\psi}(x) = \hat{a} \langle x | k_a \rangle + \hat{b} \langle x | k_b \rangle + \dots \quad (8.9)$$

where $\hat{a}$ and $\hat{b}$ annihilate a particle in state k_a and k_b respectively. We obtain

$$\begin{aligned} \hat{\psi}(x_2) \hat{\psi}(x_1) | \Psi \rangle &= \left[\frac{N}{2} \left(\frac{N}{2} - 1 \right) \right]^{1/2} \langle x_2 | k_a \rangle \langle x_1 | k_a \rangle | \frac{N}{2} - 2 : k_a, \frac{N}{2} : k_b \rangle \\ &+ \left[\frac{N}{2} \left(\frac{N}{2} - 1 \right) \right]^{1/2} \langle x_2 | k_b \rangle \langle x_1 | k_b \rangle | \frac{N}{2} : k_a, \frac{N}{2} - 2 : k_b \rangle \\ &+ \frac{N}{2} \left[\langle x_2 | k_a \rangle \langle x_1 | k_b \rangle + \langle x_2 | k_b \rangle \langle x_1 | k_a \rangle \right] | \frac{N}{2} - 1 : k_a, \frac{N}{2} - 1 : k_b \rangle. \end{aligned} \quad (8.10)$$

The last line of this expression exhibits an interference effect between two amplitudes, that could not appear in the previous naive reasoning on the one-body density operator equation (8.3)! In the limit $N \gg 1$ and using the fact that the populated modes are plane waves the pair distribution function simplifies to

$$\rho(x_1, x_2) \simeq \left(\frac{N}{L} \right)^2 \left\{ 1 + \frac{1}{2} \cos \left[(k_a - k_b)(x_1 - x_2) \right] \right\}. \quad (8.11)$$

This function exhibits oscillations around an average value equal to the square of the mean density. The oscillations are due to the interference

effect in equation (8.10): they favor detections of pairs of particles with a distance $|x_1 - x_2|$ equal to $2n\pi/|k_a - k_b|$ (n integer) and they rarefy detections of pairs of particles with a distance $(2n+1)\pi/|k_a - k_b|$. We therefore see on the pair distribution function a precursor of the interference fringes observed when the positions of all the particles are measured!

8.1.3 A Monte Carlo simulation

By sampling the N -body distribution function P with a Monte Carlo technique, Javanainen and Sung Mi Yoo in [67] made a numerical experiment with $N = 10^3$ particles and $k_b = -k_a$. By distributing the measured positions in a given realization $x_1, x_2, \dots, x_N$ among 30 position bins they obtained histograms like the ones in Figure 16. It turns out that the density in the outcome of each realization of the numerical experiment can be fitted by a cosine:

$$\frac{N}{2L} |e^{ik_a x} e^{i\theta_a} + e^{ik_b x} e^{i\theta_b}|^2 \quad (8.12)$$

where θ_a and θ_b are phases varying randomly from one realization to the other. In other words one has the impression that for each realization the system is in the state

$$|\theta\rangle_N = \frac{1}{\sqrt{N!}} \left[\frac{1}{\sqrt{2}} \left(a_{k_a}^\dagger e^{i\theta} + a_{k_b}^\dagger e^{-i\theta} \right) \right]^N |0\rangle \quad (8.13)$$

with the angle $\theta = (\theta_a - \theta_b)/2$ randomly distributed in $[-\pi/2, \pi/2]$. Such a state, corresponding to a well defined phase between the two modes a and b , is called a phase state [68].

8.1.4 Analytical solution

We wish to explain the result of the numerical experiment with an analytical argument. This has been done with slightly different points of view in [6, 69]. We give here what we think is the simplest possible presentation.

Let us allow Poissonian fluctuations in the number of particles N_a and N_b , corresponding to the distribution probabilities:

$$\mathcal{P}_\epsilon(N_\epsilon) = \frac{(\bar{N}_\epsilon)^{N_\epsilon}}{N_\epsilon!} e^{-\bar{N}_\epsilon} \quad \epsilon = a, b \quad (8.14)$$

with mean number of particles $\bar{N}_a = \bar{N}_b = \bar{N}/2$. These fluctuations become very small as compared to $\bar{N}$ when the number of particles becomes large:

$$\frac{\Delta N_\epsilon}{\bar{N}_\epsilon} = \frac{1}{\sqrt{\bar{N}_\epsilon}} \rightarrow 0 \quad \text{for} \quad \bar{N}_\epsilon \rightarrow \infty. \quad (8.15)$$

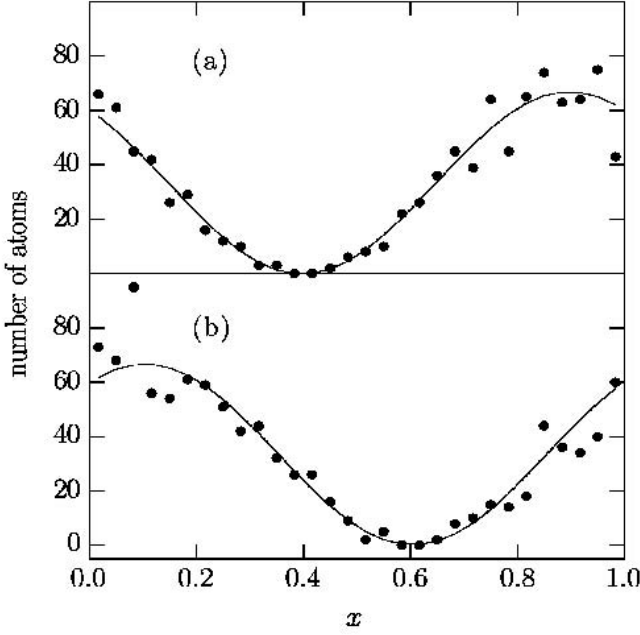


Fig. 16. For two different Monte Carlo realizations (a) and (b) of the gedanken experiment, histogram of the measured positions of $N = 1000$ particles for an initial Fock state with $N/2$ particles in plane wave k_a and $N/2$ particles in plane wave $k_b = -k_a$ [67]. The positions of the particles are expressed in units of $2\pi/(k_a - k_b)$ and are considered modulo $2\pi/(k_a - k_b)$.

The corresponding density operator is a statistical mixture of Fock states:

$$\hat{\rho} = \sum_{N_a, N_b=0}^{\infty} \mathcal{P}_a(N_a) \mathcal{P}_b(N_b) |N_a : k_a, N_b : k_b\rangle \langle N_a : k_a, N_b : k_b|. \quad (8.16)$$

From this form one can *imagine* that a single realization of the experiment is in a Fock state, provided that one keeps in mind that N_a and N_b vary in an unpredictable way from one experimental realization to the other. We known from the work [67] that there will be interference fringes in each experimental realization, but this fact is not intuitive.

The same density operator can also be written in terms of a statistical mixture of phase states:

$$\hat{\rho} = \sum_{N=0}^{\infty} \frac{(\bar{N})^N}{N!} e^{-\bar{N}} \int_{-\pi/2}^{\pi/2} \frac{d\theta}{\pi} |\theta\rangle_N \langle \theta|. \quad (8.17)$$

From this form one can *imagine* that a single realization of the experiment is in a phase state, provided that one keeps in mind that the total number of particles N and the relative phase θ vary in an unpredictable way from one realization to the other. This last form leads to the following algorithm to generate the positions of the particles according to the correct probability distribution:

1. generate an integer N according to the Poisson distribution of parameter $\bar{N}$;
2. generate θ according to a uniform probability distribution within $-\pi/2$ and $\pi/2$;
3. generate the positions $x_1, \dots, x_N$ *as if* the system was in the state $|\theta\rangle_N$, in which case all the particles are in the same single particle-state and the probability density $P(x_1, \dots, x_N)$ is factorized:

$$P(x_1, \dots, x_N) = \prod_{j=1}^N p(x_j) \quad (8.18)$$

where

$$p(x) = \frac{1}{2L} \left| e^{ik_a x} e^{i\theta} + e^{ik_b x} e^{-i\theta} \right|^2. \quad (8.19)$$

One then obtains interference fringes in each experimental realization, in a very explicit way.

One could also use a third form of the same density operator $\hat{\rho}$, that is a statistical mixture of Glauber coherent states:

$$\hat{\rho} = \int_0^{2\pi} \frac{d\theta_a}{2\pi} \int_0^{2\pi} \frac{d\theta_b}{2\pi} |\text{coh} : \bar{N}_a^{1/2} e^{i\theta_a}, \text{coh} : \bar{N}_b^{1/2} e^{i\theta_b}\rangle \langle \text{coh} : \bar{N}_a^{1/2} e^{i\theta_a}, \text{coh} : \bar{N}_b^{1/2} e^{i\theta_b}|. \quad (8.20)$$

This mathematical form is at the origin of the popular belief that condensates are in coherent states. From this form one can only *imagine* that a single realization of the experiment is in a coherent state, keeping in mind that the phases θ_a and θ_b vary in an unpredictable way from one realization to the other. In this representation the occurrence of interference fringes is straightforward.

There is an important difference between the coherent states and the Fock or phase states: as the number of particles is a conserved quantity in the non-relativistic Hamiltonian used to describe the experiments on atomic gases it seems difficult to produce a condensate in a coherent state in some

mode ψ , that is with $\hat{\rho}$ being a pure state $|\text{coh} : \alpha\rangle\langle\text{coh} : \alpha|$ where α is a complex number.

On the contrary one could imagine producing a condensate in a Fock state by measuring the number of particles in the condensate. One could then obtain a phase state by applying a $\pi/2$ Rabi pulse on the Fock state changing the internal atomic state a to a superposition $(|a\rangle + |b\rangle)/\sqrt{2}$ where b is another atomic internal state; such a Rabi pulse has been demonstrated at JILA and has allowed the measurement of the coherence time of the relative phase between the a and b condensates [70].

8.1.5 Moral of the story

- There is in general no unique way of writing the density operator $\hat{\rho}$ as a statistical mixture. The canonical form corresponding to the diagonalization of $\hat{\rho}$ is always a possibility but not always the most convenient one. *E.g.* in our simple model the eigenbasis (Fock states) is less convenient than the non-orthogonal family of phase states (symmetry breaking states);
- No measurement or no set of measurements performed *on the system* can distinguish between two different mathematical forms of the same density matrix as a statistical mixture;
- The symmetry breaking point of view consists in writing (usually in an approximate way) the N -body density operator as a statistical mixture of Hartree-Fock states. One can then imagine that a given experimental realization of the system is a Hartree-Fock state, whose physical properties are immediate to understand as all the particles are in the same quantum state;
- If the system is not in a state that is as simple as a Hartree-Fock state (*e.g.* in a Fock state for our simple model) it is dangerous to make reasonings on the single particle density operator (that is on the first order correlation function of the atomic field operator) to predict outcomes of single measurements on the system: the relevant information may be stored in higher order correlation functions of the field.

8.2 What is the time evolution of an initial phase state?

8.2.1 Physical motivation

Consider an interference experiment between two condensates A and B either in spatially separated traps or in different internal states (JILA-type configuration [70]). Assume that the two condensates have been prepared

initially in a state with a well defined relative phase θ ; this has actually been achieved at JILA. Let the system evolve freely for some time t . How long will the relative phase remain well defined? This question is probably not an easy one to answer. We present here a simple model including only two modes of the field. In real life the other modes of the field are not negligible (see for example [71] for a discussion of finite temperature effects) and phenomena neglected here such as losses of particles from the trap and fluctuations in the total number of particles may be important in a real experiment [7, 29].

We assume that the state of the system at time $t = 0$ is a phase state. More specifically, expanding the N -th power in equation (8.13) with the binomial formula, we take as initial state:

$$|\Psi(t=0)\rangle = 2^{-N/2} \sum_{N_a=0}^N \left(\frac{N!}{N_a!N_b!} \right)^{1/2} e^{i(N_a-N_b)\theta} |N_a : \phi_a, N_b : \phi_b\rangle \quad (8.21)$$

where $N_b = N - N_a$ and $\phi_{a,b}$ are the steady state condensate wavefunctions with $N_{a,b}$ particles in condensates A, B respectively. The time evolution during t is simple for each individual Fock states, as the system is then in a steady state with total energy $E(N_a, N_b)$:

$$|N_a : \phi_a, N_b : \phi_b\rangle \rightarrow e^{-iE(N_a, N_b)t/\hbar} |N_a : \phi_a, N_b : \phi_b\rangle. \quad (8.22)$$

The time evolution of the phase state equation (8.21) is much more complicated: the state vector $|\Psi(t)\rangle$ is a sum of many oscillating functions of time.

8.2.2 A quadratic approximation for the energy

The discussion can be greatly simplified if one uses the fact that the binomial factor in equation (8.21) for large N is a function of N_a and N_b sharply peaked around $N_a = N_b = N/2$ with a width $\sqrt{N}$: from Stirling's formula $n! \simeq (n/e)^n \sqrt{2\pi n}$ we obtain indeed

$$\begin{aligned} \frac{1}{2^N} \frac{N!}{N_a!N_b!} &\simeq \frac{1}{\sqrt{2\pi}2^N} \left(\frac{N}{N_a N_b} \right)^{1/2} e^{-N_a \log(N_a/N) - N_b \log(N_b/N)} \\ &\simeq \left(\frac{2}{\pi N} \right)^{1/2} e^{-(N_a - N_b)^2 / (2N)}. \end{aligned} \quad (8.23)$$

We therefore expand the energy E in powers of $N_a - N/2$ and $N_b - N/2$ up to second order.

$$\begin{aligned} E(N_a, N_b) &= E(N/2, N/2) + (N_a - N/2)\partial_{N_a} E + (N_b - N/2)\partial_{N_b} E \\ &\quad + \frac{1}{2}(N_a - N/2)^2 \partial_{N_a}^2 E + \frac{1}{2}(N_b - N/2)^2 \partial_{N_b}^2 E \\ &\quad + (N_a - N/2)(N_b - N/2)\partial_{N_a}\partial_{N_b} E + \dots, \end{aligned} \quad (8.24)$$

all the derivatives being taken in $(N_a, N_b) = (N/2, N/2)$. Note that the first derivatives of the energy are the chemical potentials $\mu_{a,b}$ of the two condensates; as the condensates are independent condensates (there is no mechanism locking the relative phase of the condensates) one has in general $\mu_a \neq \mu_b$. As we restrict to the set of occupation numbers such that $N_a + N_b = N$ we can rewrite the expansion of the energy using $N_a - N/2 = -(N_b - N/2) = (N_a - N_b)/2$:

$$E(N_a, N_b) \simeq E(N/2, N/2) + \frac{1}{2}(N_a - N_b)(\mu_a - \mu_b) + \frac{\hbar}{4}(N_a - N_b)^2 \chi \quad (8.25)$$

where we have introduced the quantity

$$\chi = \frac{1}{2\hbar} \left[(\partial_{N_a} - \partial_{N_b})^2 E \right]_{N_a=N_b=N/2}. \quad (8.26)$$

8.2.3 State vector at time t

If one uses the quadratic approximation of the energy the system evolves from the initial state equation (8.21) to the state

$$\begin{aligned} |\Psi(t)\rangle &= 2^{-N/2} \sum_{N_a=0}^N \left(\frac{N!}{N_a! N_b!} \right)^{1/2} \\ &\times e^{i(N_a - N_b)(\theta + vt)} e^{-i(N_a - N_b)^2 \chi t/4} |N_a : \phi_a, N_b : \phi_b\rangle. \end{aligned} \quad (8.27)$$

The contribution of the term linear in $N_a - N_b$ in equation (8.25) is contained in the quantity

$$v = \frac{1}{2\hbar} (\mu_b - \mu_a). \quad (8.28)$$

The resulting effect on the time evolution is simply to shift the relative phase between the condensate from θ to $\theta + vt$: this is a mere phase drift with a velocity v . This phase drift takes place only if the “frequencies” $\mu_a/\hbar$ and $\mu_b/\hbar$ of the atomic fields in A and in B are different.

The effect of the quadratic term in equation (8.25) is to spread the relative phase of the two condensates. This effect is formalized in [6], we give here the intuitive result. The spreading of the phase can be understood in analogy with the spreading of the wavepacket of a fictitious massive particle, with the relative phase θ being the position x of the particle and the occupation number difference $N_b - N_a$ being the wavevector k of the particle. The energy term proportional to χ plays the role of the kinetic energy of the particle responsible for the spreading in position. The effective mass of the fictitious particle is M such that

$$\frac{1}{4}(N_a - N_b)^2 \chi \longleftrightarrow \frac{\hbar k^2}{2M} \quad (8.29)$$

so that

$$M = \frac{2\hbar}{|\chi|}. \quad (8.30)$$

Replacing the discrete sum in equation (8.27) by an integral we formally obtain the expansion of the time dependent state vector of the fictitious particle over the plane waves in free space. In this case the variance of the position of the fictitious particle spreads as

$$\Delta x^2(t) = \Delta x^2(0) + \left(\frac{\hbar \Delta k}{M} \right)^2 t^2. \quad (8.31)$$

Within the approximation (8.23) the wavepacket of the fictitious particle is a Gaussian in momentum space, with a standard deviation $\Delta k = (N/2)^{1/2}$. Initially the position x is well defined with a spread $\sim 1/\Delta k \ll 1$. The relative phase of the condensates will start becoming undefined when the position spread Δx of the fictitious particle becomes on the order of unity. This happens after a time

$$t_{\text{spread}} \sim \frac{M}{\hbar \Delta k} = \frac{2\sqrt{2}}{|\chi| N^{1/2}}. \quad (8.32)$$

At times much longer than t_{spread} it is not correct to replace the discrete sum over $(N_a - N_b)/2$ by an integral. The discreteness of $N_a - N_b$ leads to reconstructions of a phase state (the so-called revivals) at times $t_q = q\pi/\chi$, q integer: one can check indeed from equation (8.27) that a phase state is reconstructed with a relative phase $\theta + vt_q + q\pi/2$ for N even and $\theta + vt_q$ for N odd. The observability of even the first revival at time t_1 is a non trivial question: the revivals are easily destroyed by decoherence phenomena such as the loss of a few particles out of the condensate due to inelastic atomic collisions [7], and effects of the non-condensed fraction also need to be investigated. This fragility of the revivals is not surprising if one realizes that the state vector $|\Psi(t)\rangle$ in equation (8.27) is a Schrödinger cat at time $t_1/2$, that is a coherent superposition of the N particles in some state ϕ_1 and of the N particles in some state ϕ_2 orthogonal to ϕ_1 : the revival at time t_1 is suppressed if the Schrödinger cat at time $t_1/2$ is transformed by decoherence into a statistical mixture of the states $|N : \phi_{1,2}\rangle$, which is difficult to avoid for large values of N (see the lecture notes of Brune in this volume).

8.2.4 An indicator of phase coherence

To characterize the degree of phase correlation between the two condensates it is natural to consider the average of $\langle \hat{a}^\dagger \hat{b} \rangle$ where $\hat{a}, \hat{b}$ annihilate a particle

in condensates A and B respectively. Consider indeed the average over many experimental realizations of some one-body observable $\hat{O}$ sensitive to the relative phase of the two condensates. This observable necessarily has a non-vanishing matrix element between the modes ϕ_a and ϕ_b so that in second quantized form the part of $\langle \hat{O} \rangle$ sensitive to the relative phase involves $\langle \hat{a}^\dagger \hat{b} \rangle$. *E.g.* in the case of spatially separated condensates one can beat on a 50–50 matter waves beam splitter atoms leaking out of the condensates and detect the atoms in the output channels of the beam splitter [6]; the number of counts in the + output channel averaged of many experimental realizations is proportional to the expectation value of

$$\hat{O} = \frac{\hat{a}^\dagger + \hat{b}^\dagger}{\sqrt{2}} \frac{\hat{a} + \hat{b}}{\sqrt{2}}. \quad (8.33)$$

Expanding this product of operators we get “diagonal” terms such as $\hat{a}^\dagger \hat{a}$ not sensitive to the relative phase, and crossed terms (actually interference terms!) such as $\hat{a}^\dagger \hat{b}$ sensitive to the phase. In the JILA-type configuration, where the condensates A and B are in different internal atomic states, an observable $\hat{O}$ similar to equation (8.33) has been achieved by mixing the internal states of the two condensates by a $\pi/2$ electromagnetic pulse and by measuring the mean density of atoms in A and B [70].

From the Schwartz inequality $|\langle u|v \rangle| \leq \|u\| \|v\|$ and setting $|u\rangle = \hat{a}|\Psi\rangle$, $|v\rangle = \hat{b}|\Psi\rangle$ we obtain an upper bound for the expectation value of $\hat{a}^\dagger \hat{b}$:

$$|\langle \Psi | \hat{a}^\dagger \hat{b} | \Psi \rangle| \leq \langle \Psi | \hat{a}^\dagger \hat{a} | \Psi \rangle^{1/2} \langle \Psi | \hat{b}^\dagger \hat{b} | \Psi \rangle^{1/2}. \quad (8.34)$$

The case of a maximally well defined relative phase corresponds to an equality in this inequality, obtained if $|u\rangle$ and $|v\rangle$ are proportional. In the present situation of equal mean numbers of particles $N/2$ in A and in B this corresponds to $|\Psi\rangle$ being a phase state.

For an initial phase state it is possible to calculate the expectation value of $\hat{a}^\dagger \hat{b}$ as function of time from the expansion (8.27). One obtains after simple transformations the sum

$$\langle \hat{a}^\dagger \hat{b} \rangle(t) = \frac{N}{2^N} e^{-2i(\theta+vt)} \sum_{N_a=0}^{N-1} \frac{(N-1)!}{N_a! (N_b-1)!} e^{i\chi t [N_a - (N_b-1)]} \quad (8.35)$$

with $N_b = N - N_a$ as in equation (8.27). After inspection one realizes that this sum is the binomial expansion of a $(N-1)$ -th power so that the final result is [72]:

$$\langle \hat{a}^\dagger \hat{b} \rangle(t) = \frac{N}{2} e^{-2i(\theta+vt)} \cos^{N-1} \chi t. \quad (8.36)$$

From this very simple expression one can calculate the time t_c after which the relative phase has experienced a significant spread. For short times

$\chi t \ll 1$ one can expand the cosine function in equation (8.36) to second order in t :

$$\cos^N \chi t = e^{N \log \cos \chi t} \simeq e^{-N(\chi t)^2/2}. \quad (8.37)$$

One obtains a Gaussian decay of phase coherence with a collapse time

$$t_c = \frac{1}{|\chi|N^{1/2}} \quad (8.38)$$

equivalent to the rougher estimate equation (8.32) up to a numerical factor. One can also easily see the revivals (reconstruction of $|\Psi\rangle$ to a phase state) at times $t_q = q\pi/\chi$ when the cosine function is equal to ± 1 in equation (8.36).

Formula (8.38) can be used to calculate the coherence time of the relative phase of the condensates in the present zero-temperature model. As an interesting application of this formula we now show that the spreading time of the relative phase can be significantly different for mutually interacting and non-mutually interacting condensates. Assume for simplicity that the two condensates are stored in cubic boxes of identical size L and with periodic boundary conditions. In the MIT-type configuration the two boxes are spatially separated and the atoms are in the same internal state; the energy of a configuration with N_a, N_b atoms in the condensates A, B is then

$$E = \frac{g}{2L^3} [N_a^2 + N_b^2]. \quad (8.39)$$

From equation (8.26) this form of E leads for an initial phase state to a collapse time of the relative phase

$$t_c = N^{1/2} \frac{\hbar}{2\rho g} \quad (8.40)$$

where $\rho = N/(2L^3)$ is the mean spatial density in each of the condensates. In the JILA-type configuration the atoms are in the same spatial box but in different internal states; the energy of a configuration with N_a, N_b atoms in the condensates A, B is given now by equation (6.76) if the two internal states are subject to spatial demixing, or by equation (6.77) if there is no demixing instability. The collapse time is then given by

$$t_c = N^{1/2} \frac{\hbar}{\rho[g_{aa} + g_{bb} - 2(g_{aa}g_{bb})^{1/2}]} \quad (8.41)$$

for a demixed condensates and by

$$t_c = N^{1/2} \frac{\hbar}{\rho[g_{aa} + g_{bb} - 2g_{ab}]} \quad (8.42)$$

for fully overlapping condensates. When the coupling constants among the various internal states are close to each other the denominator in equations (8.41, 8.42) can become small, which results in a relative phase coherence time t_c much larger than in the MIT-configuration equation (8.40). This fortunate feature of close coupling constants is present for rubidium in the JILA experiment [70]!

In real life the condensates are usually stored in harmonic traps; the simple formulas obtained for a cubic box have to be revisited. This has been done analytically for spatially separated condensates [73, 74] and numerically for mutually interacting condensates [29, 75].

9 Symmetry-breaking description of condensates

We have already seen in chapter 8 that it is very convenient, physically, to introduce phase states to understand the phenomenon of interference between two Bose–Einstein condensates: rather than assuming that two Bose–Einstein condensates that “have never seen each other” are in Fock states, one assumes that they are in a phase state with a relative phase varying in an unpredictable way for any new experimental realization. One can even suppose that the condensates are in coherent states of the atomic field; this description is said to “break the symmetry”, here the $U(1)$ symmetry associated to the invariance of the Hamiltonian by a change of the phase of the atomic field operator.

In this chapter we consider other examples of symmetry breaking descriptions: $SO(3)$ symmetry breaking (case of spinor condensates) and spatial translational symmetry breaking (case of one dimensional condensates with attractive interactions). In both cases the procedure is the same: the ground state of the system is symmetric, its mean-field approximation by Hartree–Fock states breaks the symmetry. In both cases we will consider Gedanken experiments whose single outcomes can be predicted from the exact ground state and from the Hartree–Fock state. This will illustrate the ability of the mean-field approximation to allow physical predictions in an easy and transparent way, correct in the limit of a large number of particles.

9.1 The ground state of spinor condensates

The alkali atoms used in the Bose–Einstein condensation experiments have an hyperfine structure in the ground state, each hyperfine level having several Zeeman sublevels. We have up to now ignored this structure in the lecture, as we were implicitly assuming that the atoms were polarized in a well defined Zeeman sublevel.

Consider for example ^{23}Na atoms used at MIT in the group of Wolfgang Ketterle. The ground state has an hyperfine splitting between the lower multiplicity of angular momentum $F = 1$ and the higher multiplicity of

angular momentum $F = 2$. All the three Zeeman sublevels $m_F = 0, \pm 1$ of the lower multiplicity $F = 1$ cannot be trapped in a magnetic trap (if $m_F = -1$ is trapped than $m_F = +1$ which experiences an opposite Zeeman shift is antitrapped). But they can all be trapped in an optical dipole trap, produced with a far off-resonance laser beam, as the Zeeman sublevels experience then all the same lightshift. This optical trapping was performed at MIT [76], opening the way to a series of interesting experiments with condensates of particles of spin one [77].

We concentrate here on a specific aspect, the ground state of the spinor condensate, assuming for simplicity that the atoms are stored in a cubic box with periodic boundary conditions.

9.1.1 A model interaction potential

We have to generalize the model scalar pseudo-potential (3.14) to the case of particles having a spin different from zero. As we want to keep the simplicity of a contact interaction potential we choose the simple form

$$V(1, 2) \equiv \mathcal{V}_{\text{spin}}(1, 2) \delta(\vec{r}_1 - \vec{r}_2) \left[\frac{\partial}{\partial r_{12}} (r_{12} \cdot) \right] \quad (9.1)$$

that is the product of an operator acting only on the spin of the particles 1 and 2, and of the usual regularized contact interaction acting only on the relative motion of the two particles. The interaction potential $V(1, 2)$ has to be invariant by a simultaneous rotation of the spin variables and of the position variables of the two particles. As the contact interaction is already rotationally invariant, the spin part of the interaction $\mathcal{V}_{\text{spin}}(1, 2)$ has to be invariant by any simultaneous rotation of the two spins.

This condition of rotational invariance of $\mathcal{V}_{\text{spin}}(1, 2)$ is easy to express in the coupled basis obtained by the addition of the two spins of particle 1 and particle 2: within each subspace of well defined total angular momentum $\mathcal{V}_{\text{spin}}(1, 2)$ has to be a scalar. Let us restrict to the case studied at MIT, with spin one particles. By addition of $F = 1$ and $F = 1$ we obtain a total angular momentum $F_{\text{tot}} = 2, 1$ or 0 , so that one can write

$$\mathcal{V}_{\text{spin}}(1, 2) = g_2 P_{F_{\text{tot}}=2}(1, 2) + g_1 P_{F_{\text{tot}}=1}(1, 2) + g_0 P_{F_{\text{tot}}=0}(1, 2) \quad (9.2)$$

where the g 's are coupling constants and the $P(1, 2)$'s are projectors on the subspace of particles 1 and 2 with a well defined total angular momentum F_{tot} . At this stage we can play a little trick, using the fact that the states of $F_{\text{tot}} = 1$ are antisymmetric by the exchange of particles 1 and 2 (whereas the other subspaces are symmetric). The regularized contact interaction scatters only in the s -wave, where the external wavefunction of atoms 1 and 2 is even by the exchange of the positions $\vec{r}_1$ and $\vec{r}_2$; as our atoms are bosons, the spin part has also to be symmetric by exchange of the spins

of atoms 1 and 2 so that the “fermionic” part of $\mathcal{V}_{\text{spin}}(1, 2)$, that is in the subspace $F_{\text{tot}} = 1$, has no effect. We can therefore change g_1 at will without affecting the interactions between bosons. The most convenient choice is to set $g_1 = g_2$ so that we obtain

$$\mathcal{V}_{\text{spin}}(1, 2) = g_2 \text{Id}(1, 2) + (g_0 - g_2) P_{F_{\text{tot}}=0}(1, 2) \quad (9.3)$$

where Id is the identity. The subspace $F_{\text{tot}} = 0$ is actually of dimension one, and it is spanned by the vanishing total angular momentum state $|\psi_0(1, 2)\rangle$. Using the standard basis $|m = -1, 0, +1\rangle$ of single particle angular momentum with z as quantization axis, one can write

$$|\psi_0(1, 2)\rangle = -\frac{1}{\sqrt{3}} [|+1, -1\rangle + |-1, +1\rangle - |0, 0\rangle] \quad (9.4)$$

A more symmetric writing is obtained in the single particle angular momentum basis $|x, y, z\rangle$ used in chemistry, defined by

$$|+1\rangle = -\frac{1}{\sqrt{2}} (|x\rangle + i|y\rangle) \quad (9.5)$$

$$|-1\rangle = +\frac{1}{\sqrt{2}} (|x\rangle - i|y\rangle) \quad (9.6)$$

$$|0\rangle = |z\rangle. \quad (9.7)$$

The vector $|\alpha\rangle$ in this basis ($\alpha = x, y, z$) is an eigenvector of angular momentum along axis α with the eigenvalue zero. One then obtains

$$|\psi_0(1, 2)\rangle = \frac{1}{\sqrt{3}} [|x, x\rangle + |y, y\rangle + |z, z\rangle] \quad (9.8)$$

To summarize the part of the Hamiltonian describing the interactions between the particles can be written, if one forgets for simplicity the regularizing operator in the pseudo-potential:

$$\begin{aligned} H_{\text{int}} &= \frac{g_2}{2} \int d^3\vec{r} \sum_{\alpha, \beta=x, y, z} \hat{\psi}_\alpha^\dagger \hat{\psi}_\beta^\dagger \hat{\psi}_\beta \hat{\psi}_\alpha \\ &+ \frac{g_0 - g_2}{6} \int d^3\vec{r} \sum_{\alpha, \beta=x, y, z} \hat{\psi}_\alpha^\dagger \hat{\psi}_\alpha^\dagger \hat{\psi}_\beta \hat{\psi}_\beta \end{aligned} \quad (9.9)$$

where $\hat{\psi}_\alpha(\vec{r})$ is the atomic field operator for the spin state $|\alpha\rangle$.

This model Hamiltonian has also been proposed by [78–80].

9.1.2 Ground state in the Hartree–Fock approximation

As we are mainly interested in the spin contribution to the energy we assume for simplicity that the condensate is in a cubic box of size L with periodic

boundary conditions. We assume that the interactions between the atoms are repulsive ($g_2, g_0 \geq 0$) and we suppose that there is no magnetic field applied to the sample.

We now minimize the energy of the condensate within the Hartree–Fock trial statevectors $|N_0 : \phi\rangle$ with the constraint that the number of particles N_0 is fixed ($|\phi\rangle$ is normalized to unity) but without any constraint on the total angular momentum of the spins. The external part of the condensate wavefunction is simply the plane wave with momentum $\vec{k} = \vec{0}$ whereas the spinor part of the wavefunction remains to be determined:

$$\langle \vec{r} | \phi \rangle = \frac{1}{L^{3/2}} \sum_{\alpha=x,y,z} c_\alpha |\alpha\rangle \quad \text{with} \quad \sum_{\alpha} |c_\alpha|^2 = 1. \quad (9.10)$$

Using the model interaction Hamiltonian equation (9.9) we find for the mean energy per particle in the condensate

$$\frac{E}{N_0} = \frac{N_0 - 1}{2L^3} g_2 + \frac{N_0 - 1}{6L^3} (g_0 - g_2) |A|^2 \quad (9.11)$$

where we have introduced the complex quantity

$$A = \sum_{\alpha=x,y,z} c_\alpha^2 = \vec{c}^2 \quad (9.12)$$

where $\vec{c}$ is the vector of components (c_x, c_y, c_z) . We have to minimize the mean energy over the state of the spinor.

- Case $g_2 > g_0$

This is the case of sodium [77]. As the coefficient $g_0 - g_2$ is negative in equation (9.11) we have to maximize the modulus of the complex quantity A . As the modulus of a sum is less than the sum of the moduli we immediately get the upper bound

$$|A| \leq \sum_{\alpha=x,y,z} |c_\alpha|^2 = 1 \quad (9.13)$$

leading to the minimal energy per particle

$$\frac{E}{N_0} = \frac{N_0 - 1}{2L^3} g_2 + \frac{N_0 - 1}{6L^3} (g_0 - g_2). \quad (9.14)$$

The upper bound for $|A|$ is reached only if all complex numbers c_α^2 have the same phase modulo 2π . This means that one can write

$$c_\alpha = e^{i\theta} n_\alpha \quad (9.15)$$

where θ is a constant phase and $\vec{n} = (n_x, n_y, n_z)$ is any unit vector with real components. Physically this corresponds to a spinor condensate wavefunction being the zero angular momentum state for a quantization axis pointing in the direction of $\vec{n}$. The direction of $\vec{n}$ is well defined in the Hartree–Fock ansatz, but it is arbitrary as no spin direction is privileged by the Hamiltonian. We are facing symmetry breaking, here a rotational $SO(3)$ symmetry breaking, as we shall see.

- Case $g_2 < g_0$

In this case we have to minimize $|A|$ to get the minimum of energy. The minimal value of $|A|$ is simply zero, corresponding to spin configurations such that

$$\vec{c}^2 \equiv \sum_{\alpha=x,y,z} c_\alpha^2 = 0 \quad (9.16)$$

with an energy per condensate particle

$$\frac{E}{N_0} = \frac{N_0 - 1}{2L^3} g_2. \quad (9.17)$$

To get more physical understanding we split the vector $\vec{c}$ as

$$\vec{c} = \vec{R} + i\vec{I} \quad (9.18)$$

where the vectors $\vec{R}$ and $\vec{I}$ have purely real components. Expressing the fact that the real part and imaginary part of $\vec{c}^2$ vanish, and using the normalization condition $\vec{c} \cdot \vec{c}^* = 1$ in equation (9.10) we finally obtain

$$\vec{R} \cdot \vec{I} = 0 \quad (9.19)$$

$$\vec{R}^2 = \vec{I}^2 = \frac{1}{2}. \quad (9.20)$$

This means that the complex vector $\vec{c}$ is circularly polarized with respect to the axis Z orthogonal to $\vec{I}$ and $\vec{R}$. Physically this corresponds to a spinor condensate wavefunction having an angular momentum $\pm\hbar$ along the axis Z . The direction of axis Z is well defined in the Hartree–Fock ansatz but it is arbitrary.

9.1.3 Exact ground state of the spinor part of the problem

Imagine that we perform some intermediate approximation, assuming that the particles are all in the ground state $\vec{k} = \vec{0}$ of the box but not assuming that they are all in the same spin state. We then have to diagonalize the model Hamiltonian

$$H_{\text{spin}} = \frac{g_2}{2L^3} \sum_{\alpha,\beta=x,y,z} \hat{a}_\alpha^\dagger \hat{a}_\beta^\dagger \hat{a}_\beta \hat{a}_\alpha + \frac{1}{6L^3} (g_0 - g_2) \hat{A}^\dagger \hat{A} \quad (9.21)$$

where $\hat{a}_\alpha$ annihilates a particle in state $|\vec{k} = 0\rangle|\alpha\rangle$ ($\alpha = x, y, z$) and where we have introduced

$$\hat{A} = \hat{a}_x^2 + \hat{a}_y^2 + \hat{a}_z^2. \quad (9.22)$$

Up to a numerical factor $\hat{A}$ annihilates a pair of particles in the two-particle spin state $|\psi_0(1, 2)\rangle$ of vanishing total angular momentum, as shown by equation (9.8).

The Hamiltonian equation (9.21) can be diagonalized exactly [81]. This is not surprising as (i) it is rotationally invariant and (ii) the bosonic N_0 -particle states with a well defined total angular momentum S_{N_0} can be calculated: one finds that $S_{N_0} = N_0, N_0 - 2, \dots$, leading to degenerate multiplicities of H_{spin} of degeneracy $2S_{N_0} + 1$.

In practice one may use the following tricks: The double sum proportional to g_2 in equation (9.21) can be expressed in terms of the operator number $\hat{N}_0$ of condensate particles only,

$$\hat{N}_0 = \sum_{\alpha} \hat{a}_{\alpha}^{\dagger} \hat{a}_{\alpha}. \quad (9.23)$$

So diagonalizing H_{spin} amounts to diagonalizing $\hat{A}^{\dagger} \hat{A}$!

Second the total momentum operator $\hat{\vec{S}}$ of the N_0 spins, defined as the sum of all the spin operators of the individual atoms in units of $\hbar$, can be checked to satisfy the identity

$$\hat{\vec{S}} \cdot \hat{\vec{S}} + \hat{A}^{\dagger} \hat{A} = \hat{N}_0(\hat{N}_0 + 1) \quad (9.24)$$

so that the Hamiltonian for N_0 particles becomes a function of $\hat{\vec{S}}$ [81]:

$$H_{\text{spin}} = \frac{g_2}{2L^3} \hat{N}_0(\hat{N}_0 - 1) + \frac{1}{6L^3} (g_0 - g_2) \left[\hat{N}_0(\hat{N}_0 + 1) - \hat{\vec{S}} \cdot \hat{\vec{S}} \right]. \quad (9.25)$$

We recall that $\hat{\vec{S}} \cdot \hat{\vec{S}} = S_{N_0}(S_{N_0} + 1)$ within the subspace of total spin S_{N_0} .

When $g_2 < g_0$ the ground state of H_{spin} corresponds to the multiplicity $S_{N_0} = N_0$, containing *e.g.* the state with all the spins in the state $|+\rangle$. In this case the N_0 -particle states obtained with the Hartree–Fock approximation are exact eigenstates of H_{spin} .

When $g_2 > g_0$ the ground state of H_{spin} corresponds to the multiplicity of minimal total angular momentum, $S_{N_0} = 1$ for N_0 odd or $S_{N_0} = 0$ for N_0 even. In this case the Hartree–Fock state is a symmetry breaking approximation of the exact ground state of H_{spin} . The error on the energy per particle tends to zero in the thermodynamical limit; for N_0 even one finds indeed

$$\frac{\delta E}{N_0} = -\frac{1}{3L^3} (g_0 - g_2). \quad (9.26)$$

But what happens if one restores the broken symmetry by summing up the Hartree–Fock ansatz over the direction $\vec{n}$ defined in equation (9.15)? Assume that N_0 is even; one has then to reconstruct from the Hartree–Fock ansatz a rotationally invariant state. This amounts to considering the following normalized state for the N_0 spins:

$$|\Psi\rangle = \sqrt{N_0 + 1} \int \frac{d^2\vec{n}}{4\pi} |N_0 : \vec{n}\rangle \quad (9.27)$$

where $d^2\vec{n}$ indicates the integration over the unit sphere (that is over all solid angles) and $|N_0 : \vec{n}\rangle$ is the state with N_0 particles in the single particle state

$$|\vec{n}\rangle = n_x|x\rangle + n_y|y\rangle + n_z|z\rangle. \quad (9.28)$$

The state vector $|\Psi\rangle$, being non zero and having a vanishing total angular momentum, is equal to the exact ground state of H_{spin} !

The expression (9.27) can be used as a starting point to obtain various forms of $|\Psi\rangle$. If one expresses the Hartree–Fock state as the N_0 -th power of the creation operator $\sum_{\alpha} \hat{a}_{\alpha}^{\dagger} n_{\alpha}$ acting on the vacuum $|\text{vac}\rangle$, and if one expands this power with the usual binomial formula, the integral over $\vec{n}$ can be calculated explicitly term by term and one obtains:

$$|\Psi\rangle = \mathcal{N} \left(\hat{A}^{\dagger} \right)^{N_0/2} |\text{vac}\rangle \quad (9.29)$$

where $\mathcal{N}$ is a normalization factor and the operator $\hat{A}$ is defined in equation (9.22). Formula (9.29) indicates that $|\Psi\rangle$ is simply a “condensate” of pairs in the pair state $|\psi_0(1, 2)\rangle$. It can be used to expand $|\Psi\rangle$ over Fock states with a well defined number of particles in the modes $m = 0, m = \pm 1$, reproducing equation (13) of [81].

To be complete we mention another way of constructing the exact eigenvectors and energy spectrum of H_{spin} . The idea is to diagonalize $\hat{A}^{\dagger} \hat{A}$ using the fact that $\hat{A}$ obeys a commutation relation that is reminiscent of that for an annihilation operator:

$$[\hat{A}, \hat{A}^{\dagger}] = 4\hat{N}_0 + 6. \quad (9.30)$$

In this way $\hat{A}^{\dagger}$ acts as a raising operator: acting on an eigenstate of $\hat{A}^{\dagger} \hat{A}$ with eigenvalue λ and N_0 particles, it gives an eigenstate of $\hat{A}^{\dagger} \hat{A}$ with eigenvalue $\lambda + 4N_0 + 6$ and with $N_0 + 2$ particles. One can also check from the identity (9.24) that the action of $\hat{A}^{\dagger}$ does not change the total spin:

$$[\hat{A}^{\dagger}, \hat{\vec{S}} \cdot \hat{\vec{S}}] = 0. \quad (9.31)$$

By repeated actions of $\hat{A}^{\dagger}$ starting from the vacuum one arrives at equation (9.29), creating the eigenstates with N_0 even and vanishing total spin $S = 0$. By repeated actions of $\hat{A}^{\dagger}$ starting from the eigenstates

with $N_0 = 2$ and total spin $S = 2$ (*e.g.* the state $|++\rangle$) one obtains all the states with N_0 even and total spin $S = 2$. More generally the eigenstate of H_{spin} with total spin S , a spin component $m = S$ along z and N_0 particles is:

$$||N_0, S, m = S\rangle \propto \left(\hat{A}^\dagger\right)^{(N_0-S)/2} |S : +1\rangle \quad (9.32)$$

where $|S : +1\rangle$ represents S particles in the state $|+1\rangle$. From equation (9.32) one can generate the states with spin components $m = S - 1, \dots, -S$ by repeated actions of the spin-lowering operator $\hat{S}_- = \hat{S}_x - i\hat{S}_y$ in the usual way. We note that formula (9.32) was derived independently in [82].

9.1.4 Advantage of a symmetry–breaking description

Imagine that we have prepared a condensate of sodium atoms ($g_2 > g_0$) in the collective ground spin state, and that we let the atoms leak one by one out of the trap, in a way that does not perturb their spin. We then measure the spin component along z of the outgoing atoms. Suppose that we have performed this measurement on k atoms, with $k \ll N_0$. We then raise the simple question: what is the probability p_k that all the k detections give a vanishing angular momentum along z ?

Let us start with a naive reasoning based on the one-body density matrix of the condensate (even if the reader has been warned already in Sect. 8.1.2 on the dangers of such an approach!). The mean occupation numbers of the single particle spin states $|m = -1\rangle$, $|m = 0\rangle$ and $|m = +1\rangle$ in the initial condensate are obviously all equal to $N_0/3$, as the condensate is initially in a rotationally symmetric state. The probability of detecting the first leaking atom in $|m = 0\rangle$ is therefore $1/3$. Naively we assume that since $k \ll N_0$ the detections have a very weak effect on the state of the condensate and the probability of detecting the n -th atom ($n \leq k$) in the $m = 0$ channel is nearly independent of the $n - 1$ previous detection results. The probability for k detections in the $m = 0$ channel should then be

$$p_k^{\text{naive}} = \frac{1}{3^k}. \quad (9.33)$$

Actually this naive reasoning is wrong (and by far) as soon as $k \geq 2$. The first detection of an atom in the $m = 0$ channel projects the spin state of the remaining atoms in

$$|\Psi_1\rangle = \mathcal{N}_1 \hat{a}_0 |\Psi\rangle \quad (9.34)$$

where $\hat{a}_0$ annihilates an atom in spin state $m = 0$, $|\Psi\rangle$ is the collective spin ground state (9.27) and $\mathcal{N}_1$ is a normalization factor. The probability

of detecting the second atom in $m = 0$ (knowing that the first atom was detected in $m = 0$) is then given by

$$\frac{p_2}{p_1} = \frac{\langle \Psi_1 | \hat{a}_0^\dagger \hat{a}_0 | \Psi_1 \rangle}{\langle \Psi_1 | \sum_{m=-1}^{+1} \hat{a}_m^\dagger \hat{a}_m | \Psi_1 \rangle}. \quad (9.35)$$

The denominator is simply equal to $N_0 - 1$ as $|\Psi_1\rangle$ is a state with $N_0 - 1$ particles. Using the integral form (9.27) and the simple effect of an annihilation operator on a Hartree–Fock state, *e.g.*

$$\hat{a}_0^2 |N_0 : \vec{n}\rangle = [N_0(N_0 - 1)]^{1/2} n_z^2 |N_0 - 2 : \vec{n}\rangle \quad (9.36)$$

we are able to express the probability in terms of integrals over solid angles:

$$\frac{p_2}{p_1} = \frac{\int d^2 \vec{n} \int d^2 \vec{n}' n_z^2 n_z'^2 (\vec{n} \cdot \vec{n}')^{N_0-2}}{\int d^2 \vec{n} \int d^2 \vec{n}' n_z n_z' (\vec{n} \cdot \vec{n}')^{N_0-1}}. \quad (9.37)$$

We suggest the following procedure to calculate these integrals. One first integrates over $\vec{n}'$ for a fixed $\vec{n}$, using spherical coordinates relative to the “vertical” axis directed along $\vec{n}$: the polar angle θ' is then the angle between $\vec{n}'$ and $\vec{n}$ so that one has simply $\vec{n} \cdot \vec{n}' = \cos \theta'$. The integral over θ' and over the azimuthal angle ϕ' can be performed, giving a result involving only n_z . The remaining integral over $\vec{n}$ is performed with the spherical coordinates of vertical axis z . This leads to

$$\frac{p_2}{p_1} = \frac{3}{5} + \frac{2}{5(N_0 - 1)}. \quad (9.38)$$

The ratio p_2/p_1 is therefore different from the naive (and wrong!) prediction (9.33). For $N_0 = 2$ one finds $p_2/p_1 = 1$ so that the second atom is surely in $m = 0$ if the first atom was detected in $m = 0$. As the two atoms were initially in the state with total angular momentum zero, this result could be expected from the expression (9.4) of the two-particle spin state. In the limit of large N_0 we find that once the first atom has been detected in the $m = 0$ channel, the probability for detecting the second atom in the same channel $m = 0$ is $3/5$. This somehow counter-intuitive result shows that the successive detection probabilities are strongly correlated in the case of the spin state (9.27).

The exact calculation of the ratio

$$\frac{p_{k+1}}{p_k} = \frac{\int d^2 \vec{n} \int d^2 \vec{n}' n_z^{k+1} n_z'^{k+1} (\vec{n} \cdot \vec{n}')^{N_0-(k+1)}}{\int d^2 \vec{n} \int d^2 \vec{n}' n_z^k n_z'^k (\vec{n} \cdot \vec{n}')^{N_0-k}} \quad (9.39)$$

is getting more difficult when k increases. The large N_0 limit for a fixed k is easier to obtain: in the integral over $\vec{n}'$ the function $(\vec{n} \cdot \vec{n}')^{N_0-(k+1)}$ is extremely peaked around $\vec{n}' = \vec{n}$ so that we can replace $n_z'^{k+1}$ by n_z^{k+1} . This leads to

$$\lim_{N_0 \rightarrow +\infty} \frac{p_{k+1}}{p_k} = \frac{2k+1}{2k+3}. \quad (9.40)$$

We now give the reasoning in the symmetry breaking point of view, which assumes that a single experimental realization of the condensate corresponds to a Hartree–Fock state $|N_0 : \vec{n}\rangle$ with the direction $\vec{n}$ being an unpredictable random variable with uniform distribution over the sphere. If the system is initially in the spin state $|N_0 : \vec{n}\rangle$ there is no correlation between the spins, and the probability of having k detections in the channel $m = 0$ is simply $(n_z^2)^k$. One has to average over the unknown direction $\vec{n}$ to obtain

$$p_k^{\text{sb}} = \int \frac{d^2\vec{n}}{4\pi} n_z^{2k} = \frac{1}{2k+1}. \quad (9.41)$$

One recovers in an easy calculation the large N_0 limit of the exact result, equation (9.40)! We note that the result (9.41) is much larger than the naive (and wrong) result (9.33) as soon as $k \gg 1$.

9.2 Solitonic condensates

We consider in this section a Bose–Einstein condensate with effective attractive interactions subject to a strong confinement in the $x - y$ plane so that it constitutes an approximate one-dimensional interacting Bose gas along z . Such a situation is interesting physically as it gives rise in free space to the formation of “bright” solitons well known in optics but not yet observed with atoms. Also the model of a one-dimensional Bose gas with a δ interaction potential has known exact solutions in free space, that can be used to test the translational symmetry breaking Hartree–Fock approximation.

9.2.1 How to make a solitonic condensate?

Consider a steady state condensate with effective attractive interactions in a three dimensional harmonic trap. The confinement in the $x - y$ plane is such that the transverse quanta of oscillation $\hbar\omega_{x,y}$ are much larger than the typical mean field energy per particle $N_0|g||\phi|^2$, where ϕ is the condensate wavefunction with N_0 particles. This confinement prevents the occurrence of a spatial collapse of the condensate (see Sect. 5.2.1). The confinement is however not strong enough to violate the validity condition of the Born approximation for the pseudo-potential, $k|a| \ll 1$ with $k \simeq (m\omega_{x,y}/\hbar)^{1/2}$.

In this case we face a quasi one-dimensional situation, where the condensate wavefunction is approximately factorized as

$$\phi(x, y, z) = \psi(z)\chi_x(x)\chi_y(y) \quad (9.42)$$

where χ_x and χ_y are the normalized ground states of the harmonic oscillator along x and along y respectively. By inserting the factorized form (9.42) in the Gross–Pitaevskii energy functional equation (5.6) and by integrating over the directions x and y we obtain an energy functional for ψ :

$$E[\psi, \psi^*] = N_0 \int dz \left[\frac{\hbar^2}{2m} \left| \frac{d\psi}{dz} \right|^2 + \frac{1}{2} m \omega_z^2 z^2 |\psi(z)|^2 + \frac{1}{2} N_0 g_{1d} |\psi(z)|^4 \right] \quad (9.43)$$

where we have dropped the zero-point energy of the transverse motion and we have called g_{1d} the quantity

$$g_{1d} = g \int dx \int dy |\chi_x(x)|^4 |\chi_y(y)|^4 = g \frac{m(\omega_x \omega_y)^{1/2}}{2\pi \hbar}. \quad (9.44)$$

The corresponding time independent Gross–Pitaevskii equation for ψ is

$$\mu \psi(z) = -\frac{\hbar^2}{2m} \frac{d^2 \psi}{dz^2} + \left[\frac{1}{2} m \omega_z^2 z^2 + N_0 g_{1d} |\psi(z)|^2 \right] \psi(z). \quad (9.45)$$

The energy functional equation (9.43) corresponds to a one-dimensional interacting Bose gas with an effective coupling constant between the atoms equal to g_{1d} , that is one can imagine that the particles have a binary contact interaction

$$V(z_1, z_2) = g_{1d} \delta(z_1 - z_2). \quad (9.46)$$

Note that such a Dirac interaction potential leads to a perfectly well defined scattering problem in one dimension, contrarily to the three dimensional case.

Imagine now that we slowly decrease the trap frequency along z while keeping intact the transverse trap frequencies, until ω_z vanishes. What will happen then? If g was positive the cloud would simply expand without limit along z . With attractive interaction the situation is dramatically different: due to the slow evolution of ω_z the condensate wavefunction will follow adiabatically the minimal energy solution of the Gross–Pitaevskii equation. For $\omega_z = 0$ this minimal energy solution is the so-called bright soliton, well known in non-linear optics. We recall the analytic form of the solitonic wavefunction:

$$\psi(z) = \frac{1}{(2l)^{1/2}} \frac{1}{\cosh(z/l)} \quad (9.47)$$

where l is the spatial radius of the soliton:

$$l = -\frac{2\hbar^2}{N_0 m g_{1d}}. \quad (9.48)$$

Note that this size l results of a compromise between minimization of kinetic energy by an increase of the size and minimization of interaction energy by a decrease of the size, so that the typical kinetic energy per particle $\hbar^2/(ml^2)$ is roughly opposite to the interaction energy per particle $N_0 g_{1d}/l$. We also give the corresponding chemical potential:

$$\mu = -\frac{1}{8} N_0^2 \frac{m g_{1d}^2}{\hbar^2}. \quad (9.49)$$

We briefly address the validity of the Gross–Pitaevskii solution (9.47). As we have pointed out in the three dimensional case (see for example Sect. 3.2.1) we wish that the Born approximation for the interaction potential be valid. In one dimension the δ interaction potential can be treated in the Born approximation only if the relative wavevector of the colliding particles is **high** enough (in contrast to the three-dimensional case):

$$\left| \frac{\hbar^2 k}{m g_{1d}} \right| \gg 1. \quad (9.50)$$

This condition can be obtained of course from a direct calculation, but also from a dimensionality argument ($m g_{1d}/\hbar^2$ is the **inverse** of a length) and from the fact that the Born approximation should apply in the limit $g_{1d} \rightarrow 0$ for a fixed k . If we use the estimate $k \simeq 1/l$ we obtain the condition

$$-\frac{\hbar^2}{m g_{1d} l} \simeq N_0 \gg 1, \quad (9.51)$$

implicitly valid here as we started from a condensate!

Another phenomenon neglected in the prediction (9.47) is the spreading of the center of mass coordinate during the switch-off of the trapping potential along z . Whereas equation (9.47) assumes that the abscissa of the center of the soliton z_0 is exactly 0 the spreading of the center of mass leads in real life to a finite width probability distribution for z_0 . This spreading can be calculated simply for an almost pure condensate $N_0 \simeq N$, using the fact that the center of mass coordinate operator $\hat{Z}$ and the total momentum operator $\hat{P}$ of the gas along z axis are decoupled from the relative coordinates of the particles in a harmonic potential, in presence of interactions depending only on the relative coordinates. To prove this assertion one expresses the operators $\hat{Z}$ and $\hat{P}$ in terms of the position and momentum

operators of each particle i of the gas:

$$\hat{Z} = \frac{1}{N} \sum_{i=1}^N z_i \quad (9.52)$$

$$\hat{P} = \sum_{i=1}^N p_i \quad (9.53)$$

and one derives the following equations of motion in Heisenberg point of view:

$$\frac{d\hat{Z}}{dt} = \frac{\hat{P}}{Nm} \quad (9.54)$$

$$\frac{d\hat{P}}{dt} = -Nm\omega_z^2(t)\hat{Z}. \quad (9.55)$$

The spreading acquired by $\hat{Z}$ is not negligible when it becomes comparable to the size l of the soliton.

The spreading of $\hat{Z}$ is interesting to calculate in the absence of harmonic confinement along z , $\omega_z \equiv 0$, with the simple assumption that all the particles of the gas are at time $t = 0$ in the soliton state $|\psi\rangle$ of equation (9.47). As $\hat{P}$ is a constant of motion for $\omega_z = 0$ one has simply

$$\hat{Z}(t) = \hat{Z}(0) + \frac{\hat{P}t}{Nm} \quad (9.56)$$

so that the variance of the center of mass coordinate at time t is

$$\text{Var}(\hat{Z})(t) = \text{Var}(\hat{Z})(0) + \frac{t}{Nm} \langle \hat{Z}(0)\hat{P} + \hat{P}\hat{Z}(0) \rangle + \frac{t^2}{N^2m^2} \text{Var}(\hat{P}). \quad (9.57)$$

One then replaces $\hat{Z}(0)$ and $\hat{P}$ by the sums (9.52, 9.53). As the single particle wavefunction ψ has vanishing mean position and mean momentum all the “crossed terms” expectation values involving two different particles vanish. As $\psi(z)$ is a real wavefunction one finds also $\langle \psi|zp + pz|\psi \rangle = 0$ so that the contribution linear in time vanishes. One is left with

$$\text{Var}(\hat{Z})(t) = \frac{1}{N} \langle \psi|z^2|\psi \rangle + \frac{t^2}{Nm^2} \langle \psi|p^2|\psi \rangle. \quad (9.58)$$

The variance of $\hat{Z}$, initially N times smaller than the single particle variance $\langle \psi|z^2|\psi \rangle$, becomes equal to the single particle variance after a time

$$t_c = \left(\frac{Nm^2 \langle \psi|z^2|\psi \rangle}{\langle \psi|p^2|\psi \rangle} \right)^{1/2} = N^{1/2} \frac{\pi m l^2}{2\hbar} \quad (9.59)$$

where we used the explicit expressions

$$\langle \psi | z^2 | \psi \rangle = \frac{\pi^2 l^2}{12} \quad (9.60)$$

$$\langle \psi | p^2 | \psi \rangle = \frac{\hbar^2}{3l^2}. \quad (9.61)$$

The spreading phenomenon of the position of the soliton is formally equivalent to the spreading of the relative phase of two condensates initially prepared in a phase state (see Sect. 8.2). The critical time t_c in (9.59) scales as $N^{1/2}\hbar/|\mu|$ as in equation (8.40).

9.2.2 Ground state of the one-dimensional attractive Bose gas

We consider here the model of the one-dimensional gas of N bosonic particles interacting with the contact potential equation (9.46) and in the absence of any confining potential.

It turns out that in this model with $g_{1d} > 0$ one can calculate exactly the eigenenergies and eigenstates of the Hamiltonian for N particles using the Bethe ansatz [83]. We consider here the less studied attractive case $g_{1d} < 0$, where several exact results are also available. In particular the exact expression for the ground state energy is known [84]:

$$E_0(N) = -\frac{1}{24} \frac{mg_{1d}^2}{\hbar^2} N(N^2 - 1) \quad (9.62)$$

and the corresponding N -particle wavefunction of the ground state is [85]:

$$\Psi(z_1, \dots, z_N) = \mathcal{N} \exp \left[\frac{mg_{1d}}{2\hbar^2} \sum_{1 \leq i < j \leq N} |z_i - z_j| \right]. \quad (9.63)$$

To determine the normalization factor $\mathcal{N}$ we enclose the gas in a fictitious box of size L tending to $+\infty$ ⁵:

$$|\mathcal{N}|^2 = \frac{(N-1)!}{NL} \left(\frac{m|g_{1d}|}{\hbar^2} \right)^{N-1}. \quad (9.64)$$

⁵The center of mass of the gas corresponds to a fictitious particle of wavevector K , where $\hbar K$ is the total momentum of the gas, and of position Z , where Z is the centroid of the gas. In the ground state $|\Psi\rangle$ the center of mass is completely delocalized with $K = 0$. The factor $1/L$ in $|\mathcal{N}|^2$ originates from the normalization of the fictitious particle plane wave in the fictitious box of size L , $\langle Z|K\rangle = e^{iKZ}/\sqrt{L}$. The more correct mathematical way (not used here) is to normalize in free space (no box) using the closure relation $\int dK |K\rangle\langle K| = \text{Id}$, which amounts to replace L by 2π .

To what extent can we recover these results using a Hartree–Fock ansatz $|N : \psi\rangle$ for the ground state wavefunction? As discussed around equation (5.18) we get a mean energy for the Hartree–Fock state very similar to equation (9.43):

$$E[\psi, \psi^*] = N \int dz \left[\frac{\hbar^2}{2m} \left| \frac{d\psi}{dz} \right|^2 + \frac{1}{2} (N-1) g_{1d} |\psi(z)|^4 \right]. \quad (9.65)$$

We minimize this functional using the results of Section 9.2.1, replacing N_0 by $N-1$, and we obtain

$$E_0^{\text{hf}}(N) = -\frac{1}{24} \frac{m g_{1d}^2}{\hbar^2} N(N-1)^2. \quad (9.66)$$

The deviation of the Hartree–Fock result from the exact result is a fraction $1/N$ of the energy and is small indeed in the large N limit, as expected from the validity condition (9.51)!

There is a notable difference of translational properties however. Whereas the exact ground state (9.63) is invariant by a global translation of the positions of the particles, as it should be, the Hartree–Fock ansatz leads to condensate wavefunctions ψ localized within the length l around some arbitrary point z_0 (around $z_0 = 0$ in equation (9.47)):

$$\psi_{z_0}(z) = \frac{1}{(2l)^{1/2}} \frac{1}{\cosh[(z - z_0)/l]} \quad (9.67)$$

with a spatial radius

$$l = -\frac{2\hbar^2}{(N-1)m g_{1d}}. \quad (9.68)$$

The Hartree–Fock ansatz $|N : \psi\rangle$ therefore breaks the translational symmetry of the system.

Breaking a symmetry of the system costs energy, and this can be checked for the present translational symmetry breaking. As the center of mass coordinates Z, P of the N particles are decoupled from the relative coordinates of the particles we can write the total energy of the gas as the sum of the kinetic energy of the center of mass and an “internal” energy including the kinetic energy of the relative motion of the particles and the interaction energy. Whereas the exact ground state wavefunction has a vanishing center of mass kinetic energy, the symmetry breaking ansatz $|N : \psi\rangle$ contains a center of mass kinetic energy:

$$E_{\text{c.o.m.}} = \left\langle N : \psi \left| \frac{\hat{P}^2}{2mN} \right| N : \psi \right\rangle \quad (9.69)$$

where mN is the total mass of the gas and $\hat{P}$ is the total momentum operator. Using the definition (9.53), expanding the square of $\hat{P}$, and using the fact that the soliton wavefunction ψ has a vanishing mean momentum we obtain

$$E_{\text{c.o.m.}} = \left\langle \psi \left| \frac{p^2}{2m} \right| \psi \right\rangle \quad (9.70)$$

$$= \frac{1}{24} \frac{mg_{1d}^2}{\hbar^2} (N-1)^2. \quad (9.71)$$

We see that $E_{\text{c.o.m.}}$ accounts for half the energy difference between the exact ground state energy (9.62) and the Hartree–Fock energy (9.66).

9.2.3 Physical advantage of the symmetry–breaking description

We now raise the question: is there a Bose–Einstein condensate in the one-dimensional free Bose gas with attractive interaction? To make things simple we assume that the gas is at zero temperature so that the N -particle wavefunction is known exactly, see equation (9.63).

We start with a reasoning in terms of the one-body density operator (even if we know from the previous physical examples that this may be dangerous). Paraphrasing the usual three dimensional definition of a Bose–Einstein condensate in free space we put the one-dimensional gas in a fictitious box of size L and we calculate the mean number of particles n_0 in the plane wave with vanishing momentum $p = 0$ in the limit $L \rightarrow +\infty$.

The calculation with the exact ground state wavefunction has been done [85]. One finds that n_0 is going to zero as $1/L$:

$$\lim_{L \rightarrow +\infty} n_0 L = C(N) \frac{2\hbar^2}{m|g_{1d}|}. \quad (9.72)$$

The factor $C(N)$ is given by

$$C(N) = \sum_{i=1}^N \sum_{j=i}^N \frac{(j-1)!}{(i-1)!} \frac{(N-i)!}{(N-j)!} \prod_{k=i}^j \left[k(N+1-k) - \frac{1}{2}(N+1) \right]^{-1} \quad (9.73)$$

and converges to $\pi^2/2$ in the large N limit, so that n_0 no longer depends on N in this limit. There is therefore no macroscopic population in the $p = 0$ momentum state. One may then be tempted to conclude that there is no Bose–Einstein condensate, even at zero temperature, in the one-dimensional Bose gas with attractive contact interactions. However we have learned that a reasoning based on the one-body density matrix may miss crucial correlations between the particles, and that the symmetry breaking point of view may be illuminating in this respect.

The translational symmetry breaking point of view approximates the state of the gas by the N -body density operator:

$$\hat{\rho}^{\text{sb}} = \lim_{L \rightarrow +\infty} \int_{-L/2}^{L/2} \frac{dz_0}{L} |N : \psi_{z_0}\rangle \langle N : \psi_{z_0}|. \quad (9.74)$$

In the large N limit we expect this prescription to be valid for few-body observables. Of course for a N -body observable such as the kinetic energy of the center of mass of the gas, the results will be different, equation (9.71) for the symmetry breaking point of view *vs.* a vanishing value for the exact result.

Let us test this expectation by calculating in the Hartree–Fock approximation the mean number of particles in the plane wave $\langle z|k\rangle = \exp(ikz)/L^{1/2}$. Using the following action of the annihilation operator $\hat{a}_k$ of a particle with wavevector k on the Hartree–Fock state:

$$\hat{a}_k |N : \psi_{z_0}\rangle = N^{1/2} \langle k|\psi_{z_0}\rangle |N-1 : \psi_{z_0}\rangle \quad (9.75)$$

we obtain

$$n_k^{\text{hf}} = N |\langle k|\psi\rangle|^2. \quad (9.76)$$

The momentum distribution of the particles in the gas in this approximation is simply proportional to the momentum distribution of a single particle in the solitonic wavefunction ψ ! It turns out that the Fourier transform of the $1/\cosh$ function can be calculated exactly, and it is also a $1/\cosh$ function. We finally obtain:

$$n_k^{\text{hf}} \simeq \frac{1}{L} \frac{\pi^2 \hbar^2}{m |g_{1d}|} \frac{1}{\cosh^2\left(\frac{\pi k l}{2}\right)} \quad (9.77)$$

where l is the soliton size given in equation (9.68). For $k=0$ one recovers the large N limit of the exact result (9.72).

In more physical terms, one can imagine from equation (9.74) that a given experimental realization of the Bose gas corresponds to a condensate of N particles in the solitonic wavefunction (9.67), with a central position z_0 being a random variable varying in an unpredictable way for any new realization of the experiment. There is therefore a Bose–Einstein condensate in the one-dimensional attractive Bose gas!

An illustrative gedanken experiment would be to measure the positions along z of all the particles of the gas. In the symmetry breaking point of view the positions $z_1, \dots, z_N$ obtained in a single measurement are randomly distributed according to the density $|\psi_{z_0}^2|(z) = |\psi(z - z_0)|^2$ where z_0 varies from shot to shot as the relative phase of the two condensates did in the MIT interference experiment. As we know the exact ground state (9.63) we

also know the exact N -body distribution function, $|\Psi(z_1, \dots, z_N)|^2$. This is however not so easy to use!

So we suggest instead to consider the mean spatial density of the particles *knowing* that the center of mass of the cloud has a position Z . In the exact formalism this gives [85]:

$$\begin{aligned} \rho(z|Z) &= \int dz_1 \dots \int dz_N |\Psi(z_1, \dots, z_N)|^2 \left(\sum_{j=1}^N \delta(z - z_j) \right) \\ &\quad \times L \delta \left(Z - \frac{1}{N} \sum_{n=1}^N z_n \right) \\ &= \frac{2N}{l} \sum_{k=0}^{N-2} \frac{(N-2)!}{(N-k-2)!} \frac{N!}{(N+k)!} (-1)^k (k+1) \\ &\quad \times \exp \left[-(k+1) \frac{2N}{N-1} \frac{|z-Z|}{l} \right] \end{aligned} \quad (9.78)$$

where l is the N -dependent length of the soliton (9.68), the integrals are taken in the range $[-L/2, L/2]$ and $L \rightarrow +\infty$; the factor L , compensating the one in the normalization factor of Ψ , ensures that the integral of $\rho(z|Z)$ over z is equal to N .

In the symmetry breaking point of view the definition of $\rho(z|Z)$ is similar to equation (9.78); the factor L cancels with the $1/L$ factor of equation (9.74). This leads to

$$\begin{aligned} \rho^{\text{sb}}(z|Z) &= \int dz_0 \int dz_1 \dots \int dz_N \left(\prod_{k=1}^N |\psi(z_k - z_0)|^2 \right) \\ &\quad \times \left(\sum_{j=1}^N \delta(z - z_j) \right) \delta \left(Z - \frac{1}{N} \sum_{n=1}^N z_n \right) \\ &= N \int dz_1 \dots \int dz_N \left(\prod_{k=1}^N |\psi(z_k)|^2 \right) \delta \left(Z - z + z_1 - \frac{1}{N} \sum_{n=1}^N z_n \right) \end{aligned} \quad (9.79)$$

where we have made the change of variables $z_k \rightarrow z_k + z_0$ (which allows to integrate over z_0) and we have replaced the sum over the indiscernible particles j by N times the contribution of particle $j = 1$. The multiple integral over the positions $z_1, \dots, z_N$ can be turned into a single integral over a wavevector q by using the identity $\delta(X) = \int dq / (2\pi) \exp(iqX)$, allowing a numerical calculation of $\rho^{\text{sb}}(z|Z)$.

Does the approximate result (9.79) get close to the exact result for large N ? We compare numerically in Figure 17 the exact density $\rho(z|Z)$ to the

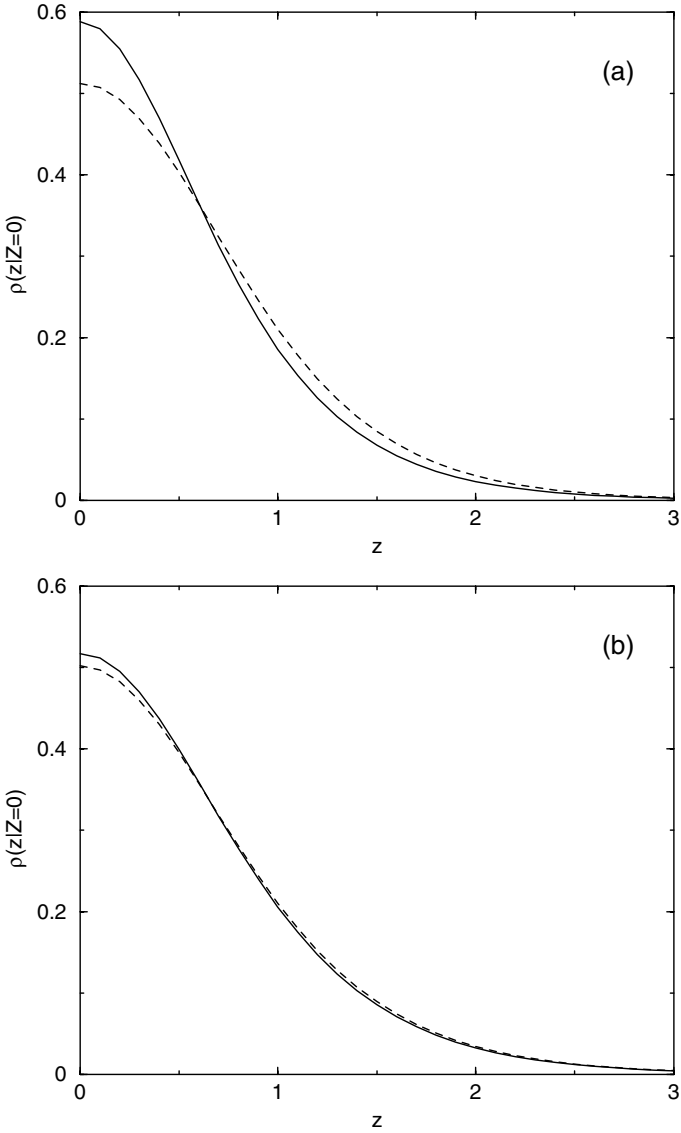


Fig. 17. For the ground state of the one-dimensional attractive Bose gas, position dependence of the mean density of particles knowing that the center-of-mass of the gas is in $Z = 0$. Solid line: exact result $\rho(z|Z = 0)$. Dashed line: mean-field approximation $\rho^{\text{sb}}(z|Z = 0)$. The position z is expressed in units of the “soliton” radius l given in equation (9.68), and the linear density in units of N/l . The number of particles is (a) $N = 10$ and (b) $N = 45$.

symmetry breaking mean-field prediction $\rho^{\text{sb}}(z|Z)$: modestly large values of N give already good agreement between the two densities. This validates the symmetry breaking approach for the considered gedanken experiment.

What happens in the large N limit? In equation (9.79) each variable z_k explores an interval of size $\sim l$ so that the quantity $(z_1 + \dots + z_N)/N$ has a standard deviation $\sim l/\sqrt{N}$ much smaller than l and can be neglected as compared to z_1 inside the δ distribution. This leads to

$$\rho^{\text{sb}}(z|Z) \simeq N |\psi_{z_0=Z}(z)|^2 \quad \text{for} \quad \sqrt{N} \gg 1 \quad (9.80)$$

where the solitonic wavefunction $\psi_{z_0=Z}$ is given in equation (9.67). Numerical calculation of $\rho^{\text{sb}}(z|Z)$ shows that equation (9.80) is a good approximation over the range $|z - Z| \simeq l$ for $N = 10$ already!

Acknowledgements

I warmly thank all my colleagues of the École normale supérieure and all my coworkers for their contribution to my understanding and knowledge of Bose–Einstein condensates; in particular the lectures of Claude Cohen-Tannoudji at the Collège de France have been an illuminating example and the notes taken by David Guéry-Odelin at an early version of this course have been useful. I am very indebted to Franck Laloë for useful comments on the manuscript. I am immensely grateful to my wife Alice for her invaluable help in the production of these lecture notes; her careful notes taken in Les Houches and her help in typing the manuscript have been crucial.

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COURSE 2

SPINOR CONDENSATES AND LIGHT SCATTERING FROM BOSE-EINSTEIN CONDENSATES

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SPINOR CONDENSATES AND LIGHT SCATTERING FROM BOSE–EINSTEIN CONDENSATES

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Abstract

These notes discuss two aspects of the physics of atomic Bose–Einstein condensates: optical properties and spinor condensates. The first topic includes light scattering experiments which probe the excitations of a condensate in both the free-particle and phonon regime. At higher light intensity, a new form of superradiance and phase-coherent matter wave amplification were observed. We also discuss properties of spinor condensates and describe studies of ground-state spin domain structures and dynamical studies which revealed metastable excited states and quantum tunneling.

1 Introduction

The possibility of creating optical fields with many photons in a single mode of a resonator was realized with the creation of the laser in 1960. The possibility of creating a matter-wave field with many atoms in a single mode of an atom trap (which is the atomic equivalent of an optical resonator) was realized with the achievement of Bose–Einstein condensation (BEC) in 1995. Because of the wealth of new phenomena which the condensates display, and the precision and flexibility with which they can be manipulated, interest in them has grown explosively in the communities of atomic physics, quantum optics, and many-body physics. At least twenty groups have created condensates, and the publication rate on Bose–Einstein condensation has soared following the discovery of the gaseous condensates.

Although atomic condensates and laser light share many properties, they also differ fundamentally: atoms interact readily, while photons do not.

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As a result, the atomic condensates constitute a novel class of many-body systems that provide a new laboratory for many-body physics. They have already yielded discoveries such as stability and collapse of condensates with attractive interactions, multi-component condensates, Feshbach resonances and novel optical properties, and have led to advances in many-body theory. Furthermore, because atoms interact, atom optics is inherently non-linear optics. Consequently, nonlinear effects such as four-wave mixing that were first achieved with light only with difficulty, occur almost automatically with coherent matter waves.

These lecture notes will focus on two aspects of Bose–Einstein condensation: light scattering from a Bose–Einstein condensate and spinor condensates. Our lectures at Les Houches covered a broader range of topics, including trapping techniques, methods to probe the condensate and studies of sound and condensate formation. For those topics we refer to our Varenna Summer School Notes which give a comprehensive discussion of experimental techniques, static and dynamic properties, coherence and optical trapping of condensates [1]. This paper and some other recent review papers summarize the state of the field [2–4].

Research on gaseous BEC can be divided into two areas: in the first, which could be labeled “the atomic condensate as a coherent gas” or “atom lasers,” one would like to have as little interaction as possible between atoms — almost like photons in an optical laser. Thus the experiments are preferentially done at low densities. The Bose–Einstein condensate serves as an intense source of ultracold coherent atoms for experiments in atom optics, in precision studies or for explorations of basic aspects of quantum mechanics. The second area could be labeled as “BEC as a new quantum fluid” or “BEC as a many-body system.” The focus here is on the interactions between the atoms which are most pronounced at high densities.

The topics covered in these notes illustrate both aspects of BEC. Spinor condensates realize a new class of quantum fluids. Coherent matter wave amplification is at the heart of atom lasers. Our studies of light scattering from a Bose condensate link both aspects together: light scattering was used to imprint phonons into the condensate, but also to measure the coherence of an atom laser and to realize a matter wave amplifier.

Chapters 2 and 4 of this review are based on the thesis of one of the authors [5]. An abbreviated version of Chapter 2 will appear in reference [6].

2 Optical properties of a Bose–Einstein condensate

What does a trapped Bose–Einstein condensate look like? More precisely, how does it interact with light, and does this differ fundamentally from what one would naively expect from a similar collection of very cold atoms? In the early 1990s, before Bose–Einstein condensation was realized in atomic

gases, there were lively debates about how a condensate could be observed. Some researchers thought it would absorb all light and would therefore be “pitch black”, some predicted it would be “transparent” (due to superradiant line-broadening [7]), others predicted that it would reflect light due to polaritons [8, 9] and be “shiny” like a mirror.

All the observations of Bose condensates have employed scattering or absorption of laser light. These observations were either done on ballistically expanding dilute clouds or with far-off-resonant light. Under those circumstances, a Bose condensate scatters light as ordinary atoms do. On resonance, the condensate strongly absorbs the light, giving rise to the well-known “shadow pictures” of expanding condensates where the condensate appears black. For off-resonant light, the absorption can be made negligibly small, and the condensate acts as a dispersive medium bending the light like a glass sphere. This regime has been used for non-destructive *in situ* imaging of Bose–Einstein condensates.

Our group has recently looked more closely at how coherent, weakly-interacting atoms interact with coherent light. Light scattering imparts momentum to the condensate and creates an excitation in a many-body system (Fig. 1). Consequently, the collective nature of excitations and the coherence of the condensate can affect its optical properties. Thus light scattering can be used to illuminate properties of the condensate.

2.1 Light scattering from a Bose–Einstein condensate

2.1.1 Elastic and inelastic light scattering

Let us begin by considering the effect on a single atom of a single light scattering event. The initial state of the atom–light system is $|N_k, \dots 0_l \dots; i\rangle$ where N_k photons are in an incident beam with wavevector k , no photons are in other photon modes (such as mode l), and the atom is in state $|i\rangle$ which can be either a trapped or untrapped state. After adiabatically eliminating the excited atomic state, the coupling between the atom and the light is described by the operator

$$\mathcal{H}' = C \sum_{k,l,m,n} \hat{c}_l^\dagger \hat{a}_n^\dagger \hat{c}_k \hat{a}_m \delta_{l+n-k-m}. \quad (2.1)$$

Here $\hat{c}_k$ ($\hat{c}_k^\dagger$) is the destruction (creation) operator for optical waves, and $\hat{a}_k$ ($\hat{a}_k^\dagger$) is the destruction (creation) operator for atomic waves of wavevector k . The strength of atomic resonances and the detuning of the light determines the strength of the coupling, summarized in the coefficient C .

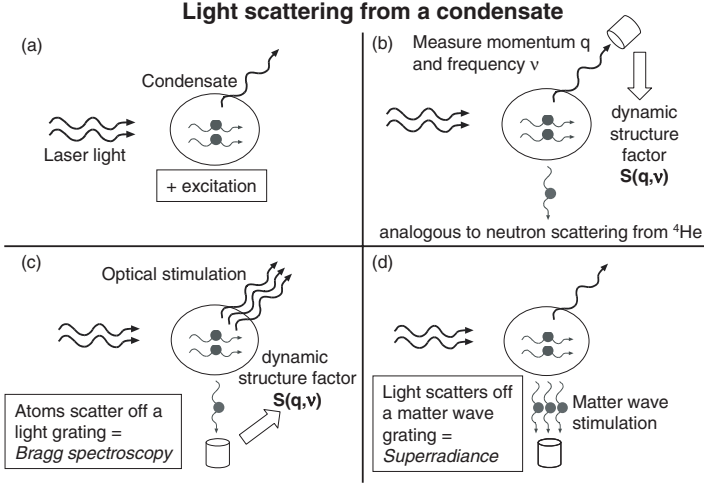


Fig. 1. Light scattering from a Bose–Einstein condensate. When a photon is scattered, it transfers momentum to the condensate and creates an excitation (a). Therefore, an analysis of the scattered light allows the determination of the dynamic structure factor, in close analogy to neutron scattering experiments with superfluid helium (b). For sufficiently large momentum transfer the excitation leads to an atom scattered out of the condensate. The signal is greatly increased by stimulating the light scattering by a second laser beam and detecting the scattered atoms (c)—this is the scheme for Bragg spectroscopy. Light scattering can also be stimulated by adding a coherent atomic field (d). This led to superradiant scattering of light and atoms.

Due to the coupling, light is scattered from the incident beam to wavevector $l = k - q$ with a cross-section proportional to¹

$$\begin{aligned} \frac{d\sigma}{d\Omega} \propto |C|^2 & \left(\left| \langle N_k - 1, \dots, 1_l \dots ; i | \sum_m \hat{c}_{k-q}^\dagger \hat{a}_{m+q}^\dagger \hat{c}_k \hat{a}_m | N_k, \dots, 0_l \dots ; i \rangle \right|^2 \right. \\ & \left. + \sum_{j \neq i} \left| \langle N_k - 1, \dots, 1_l \dots ; j | \sum_m \hat{c}_{k-q}^\dagger \hat{a}_{m+q}^\dagger \hat{c}_k \hat{a}_m | N_k, \dots, 0_l \dots ; i \rangle \right|^2 \right). \end{aligned} \quad (2.2)$$

Two contributions to the light scattering are separated in the above expression. The first part describes “coherent” light scattering, *i.e.* diffraction and

¹Our discussion is limited to low intensity of the probe light, allowing us to neglect the Mollow triplet fluorescence spectrum observed at high intensities.

refraction, in which the atomic system is left in its original state, and the scattered light has the same frequency as the incident light. The coupling shifts the phase of the elastically scattered light by an amount proportional to $\langle N_k - 1, \dots, 1_l \dots; i | \mathcal{H}' | N_k, \dots, 0_l \dots; i \rangle$. This phase shift can be used to spatially image an atomic cloud by a dispersive imaging technique, such as dark-ground or phase-contrast imaging. For a dilute cloud of size d , the coherent scattering is limited to the diffraction angle λ/d . When the cloud is much larger than an optical wavelength λ , only small-angle forward scattering is coherent.

The second part of the scattering cross-section describes “incoherent” light scattering in which the state of the atom is changed. For the case considered here, $d \gg \lambda$, this occurs when light is scattered outside the diffraction angle. Incoherent, or inelastic light scattering is used for absorption imaging where the light which is transmitted by the cloud is collected, and the amount of probe light scattered out of the imaging system is determined.

One can learn more from inelastic scattering than just by observing absorption, *i.e.* counting the total sum of scattered photons. An inelastically scattered photon is shifted in frequency from the incident photon. Further, the outgoing angle of the scattered photon determines the momentum $\hbar\vec{q}$ which is imparted to the sample. Thus, a spectroscopic analysis of inelastically scattered photons at a given angle from the incident light beam determines the response of the atomic sample to a given energy and momentum transfer (Fig. 1).

Analyzing photons scattered by a Bose–Einstein condensate from a single beam would be a difficult task. Alkali Bose–Einstein condensates are currently produced with $\lesssim 10^7$ atoms. If one would scatter light from a small fraction of these over a 4π solid angle, only a few photons would be collected and one would need to determine their frequency amidst a large background of incident and scattered light.

Instead, we have adopted a different approach. Rather than detecting *spontaneous* scattering from a single beam, we study light scattering as a *stimulated* process, called Bragg scattering, induced by two laser beams which illuminate the atomic sample (Fig. 1). The momentum and energy transfer is *pre-determined* by the angle and frequency difference between the incident beams, respectively, rather than *post-determined* by the position of a photo-detector and by a difficult frequency measurement. The quantities of interest are matrix elements which characterize the response of the condensate, and they are the same for spontaneous and stimulated scattering. Furthermore, since the momentum transfer can be much greater than the momentum spread of the sub-recoil atomic sample, and since stimulated light scattering can be made to dominate over spontaneous scattering,

the response of the system can be assessed by the nearly background-free detection of recoiling atoms.

We have studied Bose–Einstein condensates by the spectroscopic measurement of the Bragg scattering resonance. In this paper, we describe two applications of Bragg spectroscopy to study excitations of a Bose–Einstein condensate in either the free-particle [10] (large momentum transfer) or the phonon [11] (small momentum transfer) regime. The discussion includes a description of the dynamic structure factor of a Bose–Einstein condensate which leads to the interpretation of our measurements as an observation of the zero-point momentum distribution of trapped condensates, as a measurement of the energies of free-particle and phonon excitations, and as evidence for correlations in the many-body condensate wavefunction introduced by interatomic interactions.

2.1.2 Light scattering from atomic beams and atoms at rest

The interaction of a neutral atomic beam with an optical standing wave was studied by several groups in the early 1980's. Quantitative studies which focused on the effect of conservative optical potentials were performed by Pritchard *et al.* [12, 13]. In two different experiments, a collimated atomic beam of sodium was incident upon a standing light wave formed by a retro-reflected laser beam. Two regimes of scattering were identified: Kapitza–Dirac scattering from a thin optical grating (tightly focused beams) which is non-specific in the angle between the incident atomic beam and the standing wave [12], and Bragg scattering from a thick grating (loosely focused beams) which occurs only at specific resonant angles [13]. In these atomic beam experiments, the kinetic energy of the atoms, and thus the magnitude of their momentum, is unchanged by scattering off the stationary optical field. Thus, scattering can occur only if the optical field contains photons propagating in a direction so that the atomic momentum can be rotated by the absorption and stimulated emission of photons from the standing wave. A thin optical grating contains photons propagating over a wide angular range, and thus scattering is not limited to specific angles. In the case of a broad focus, the angular divergence of the photons is too small to allow scattering except at specific incident angles of the atomic beam to the standing wave (the so-called Bragg angles).

Kapitza–Dirac [14] and Bragg [15] scattering of Bose–Einstein condensates have also been demonstrated. These experiments were performed by exposing the nearly stationary atomic sources to a pulse of two intersecting laser beams which had a variable differential detuning ω . Such an experimental situation is identical to the aforementioned atomic beam experiments when viewed in the frame of reference of the atoms: the duration of the optical pulse corresponds to the width of the optical grating, and a differential detuning between the optical beams is equivalent to an atom crossing an

optical grating at an angle which introduces opposite Doppler shifts to the two counter-propagating laser beams. Kapitza-Dirac scattering occurs for short pulses which contain frequency components necessary to excite the atom to an energy of $\hbar\omega_q^0 = \hbar^2 q^2/2m$ where $\hbar q$ is the momentum recoil due to a single scattering event. Similarly, the condition for Bragg scattering becomes a resonance condition for exciting an atom to an excited momentum state: $\omega = \omega_q^0$ (for first order scattering).

The Bragg resonance condition is sensitive to the motion of the atom with respect to the optical standing wave orientation. By simple energy and momentum conservation, the energy transferred to an atom with initial velocity $\vec{v}_i$ by a momentum kick of $\hbar\vec{q}$ is

$$\hbar\omega = \frac{(\hbar\vec{q} + m\vec{v}_i)^2}{2m} - \frac{mv_i^2}{2} = \frac{\hbar^2 q^2}{2m} + \hbar\vec{q} \cdot \vec{v}_i. \quad (2.3)$$

Thus, the Bragg resonance is Doppler sensitive and can be used to determine spectroscopically the velocity distribution of an atomic sample. It has been used previously to determine the temperature of laser-cooled atoms [16]. Our work has extended the method to the determination of the zero-point motion and many-body effects in a condensate.

2.1.3 Relation to the dynamic structure factor of a many-body system

Inelastic scattering has long been used to probe the properties of condensed-matter systems. In the case of liquid helium, both neutron and light scattering were used to determine the elementary excitations of this system [17–21]. A theoretical discussion of the spectrum of inelastically scattered light from a Bose-Einstein condensate has been presented by a number of authors [22–24]. The dilute atomic condensates are particularly simple examples for the general scattering theory since the scattering can be treated in an atomic basis. Following the experimental studies of inelastic light scattering which are summarized in this review, a thorough interpretation of light scattering from an inhomogeneous Bose-Einstein condensate was presented [25].

Let us discuss how Bragg scattering is used to probe the properties of a many-body system. An atomic sample is exposed to two laser beams, with wavevectors $\vec{k}_1$ and $\vec{k}_2$ and a frequency difference ω which is generally much smaller than the detuning Δ of the beams from an atomic resonance. The two laser beams interfere to form a “walking” wave intensity modulation $I_{\text{mod}}(\vec{r}, t) = I \cos(\vec{q} \cdot \vec{r} - \omega t)$ where $\vec{q} = \vec{k}_1 - \vec{k}_2$. Due to the ac Stark effect [26], atoms exposed to this intensity modulation experience a conservative optical potential with a spatial modulation of $V_{\text{mod}} = (\hbar\Gamma^2/8\Delta) \cdot (I_{\text{mod}}/I_{\text{sat}})$ where Γ is the line width of the atomic resonance and I_{sat} the saturation intensity.

To determine the Bragg scattering response of a many-body system, we express the modulated potential in second quantized notation as

$$V_{\text{mod}} = \frac{V}{2} (\hat{\rho}^\dagger(\vec{q})e^{-i\omega t} + \hat{\rho}^\dagger(-\vec{q})e^{+i\omega t}) \quad (2.4)$$

where $\hat{\rho}(\vec{q}) = \sum_m \hat{a}_{m+\vec{q}}^\dagger \hat{a}_m$ is the Fourier transform of the atomic density operator at wavevector $\vec{q}$. Equivalently, V_{mod} is found by isolating those terms in $\mathcal{H}'$ (Eq. (2.1)) which involve the macroscopically occupied optical modes at wavevectors $\vec{k}_1$ and $\vec{k}_2$, and replacing the photon creation and destruction operators with c -numbers proportional to the electric field strength of the Bragg scattering laser beams.

We may then determine the Bragg scattering rate using Fermi's golden rule. Considering scattering out of the many-body ground state $|g\rangle$, we neglect the counter-rotating term in V_{mod} and obtain the excitation rate per particle as

$$\frac{W}{N} = \frac{2\pi}{N\hbar} \left(\frac{V}{2}\right)^2 \sum_f |\langle f | \hat{\rho}^\dagger(\vec{q}) | g \rangle|^2 \delta(\hbar\omega - (E_f - E_g)) \equiv 2\pi\omega_R^2 S(\vec{q}, \omega). \quad (2.5)$$

Here N is the number of atoms in the system, and the sum is performed over all final excited states $|f\rangle$ with energy E_f . We have introduced the dynamic structure factor $S(\vec{q}, \omega)$ which is the Fourier transform of density-density fluctuations in state $|g\rangle$ with spatial and temporal frequencies of $\vec{q}$ and ω , respectively [20, 21]. The dynamic structure factor generally characterizes the response of the system to longitudinal perturbations of any source, not solely to optical excitation. The density fluctuation spectrum is directly determined by the Bragg scattering response, normalized by the two-photon Rabi frequency $\omega_R = V/2\hbar$. Integrating over all frequencies ω one obtains the static structure factor $S(\vec{q}) = \langle g | \hat{\rho}(\vec{q}) \hat{\rho}^\dagger(\vec{q}) | g \rangle / N$ which is equivalent to the line strength of the Bragg resonance.

2.2 The dynamic structure factor of a Bose-Einstein condensate

In this section, we use the theory of the weakly-interacting Bose-Einstein condensate to predict the dynamic structure factor, first for a homogeneous condensate and then for the situation of experimental relevance, an inhomogeneous condensate confined by a harmonic trapping potential.

2.2.1 The homogeneous condensate

A Bose-Einstein condensate is quite different from other fluids in that the *microscopic* (*i.e.* single-atom) excitations of the system become manifest as

macroscopic density fluctuations due to interference with the macroscopic wavefunction. Considering density fluctuations in a homogeneous Bose-Einstein condensate, we may approximate

$$\begin{aligned} |e\rangle &= \frac{1}{\sqrt{N}} \hat{\rho}^\dagger(\vec{q}) |g\rangle \\ &= \frac{1}{\sqrt{N}} \sum_m \hat{a}_{m+q}^\dagger \hat{a}_m |g\rangle \simeq \frac{(\hat{a}_q^\dagger \hat{a}_0 + \hat{a}_0^\dagger \hat{a}_{-q}) |g\rangle}{\sqrt{N}} = |e^+\rangle + |e^-\rangle. \end{aligned} \quad (2.6)$$

Here, the macroscopic occupation of the zero-momentum state picks out two terms in the sum. Following Bogoliubov [27], we identify $\hat{a}_0^\dagger = \hat{a}_0 = \sqrt{N_0}$ and transform to Bogoliubov operators by substituting $\hat{a}_k = u_k \hat{b}_k - v_k \hat{b}_{-k}^\dagger$. The operators $\hat{b}_k^\dagger$ and $\hat{b}_k$ are creation and destruction operators for the proper microscopic quasi-particle excitations of the condensate, with $u_k = \cosh \phi_k$, $v_k = \sinh \phi_k$ and $\tanh 2\phi_k = \mu/(\hbar\omega_k^0 + \mu)$. Here, μ is the chemical potential, and, again, $\hbar\omega_k^0 = \hbar^2 k^2/2m$ is the free recoil energy at wavevector $\vec{k}$. The Bogoliubov quasi-particle spectrum is given as $\hbar\omega_k^B = \sqrt{\hbar\omega_k^0(\hbar\omega_k^0 + 2\mu)}$ (see Fig. 2).

The many-body wavefunction of the condensate $|g\rangle$ corresponds to the quasi-particle vacuum defined by the relations $\hat{b}_k |g\rangle = 0, \forall k$. Thus, we find

$$\hat{\rho}^\dagger(\vec{q}) |g\rangle \simeq \sqrt{N_0} (u_q - v_q) \hat{b}_q^\dagger |g\rangle. \quad (2.7)$$

From this, it follows that for a homogeneous Bose-Einstein condensate $S(\vec{q}, \omega) \simeq (u_q - v_q)^2 \delta(\omega - \omega_q^B)$, and $S(\vec{q}) = (u_q - v_q)^2 = \omega_q^0/\omega_q^B$.

Thus, we expect Bragg scattering from an interacting, homogeneous Bose-Einstein condensate to differ from the Bragg scattering of a non-interacting condensate in two ways. First, the Bragg resonance occurs at the Bogoliubov quasi-particle energy which is higher than the free-particle recoil energy, *i.e.* the Bragg resonance line at a momentum transfer of $\hbar\vec{q}$ is shifted upwards in frequency from the free particle resonance by $\Delta\omega = \omega_q^B - \omega_q^0$. Second, the Bragg scattering response is weakened relative to that of free particles by a factor $S(\vec{q}) = (u_q - v_q)^2 < 1$. In other words, light scattering from a Bose-Einstein condensate is suppressed by the presence of repulsive interatomic interactions. Indeed, these two statements are equivalent: by the f -sum rule which states that $\int \omega S(\vec{q}, \omega) d\omega = \omega_q^0$, an increase in the resonance frequency implies a decrease in the excitation strength [20].

Let us evaluate the structure factor in two limits of the Bragg scattering wavevector $\vec{q}$. The wavevector which corresponds to the interaction energy is the inverse healing length $\xi^{-1} = \sqrt{2}mc/\hbar$ where c is the speed of Bogoliubov sound. For large scattering wavevectors ($q \gg \xi^{-1}$), Bragg scattering occurs in the free-particle regime. The Bragg resonance is shifted

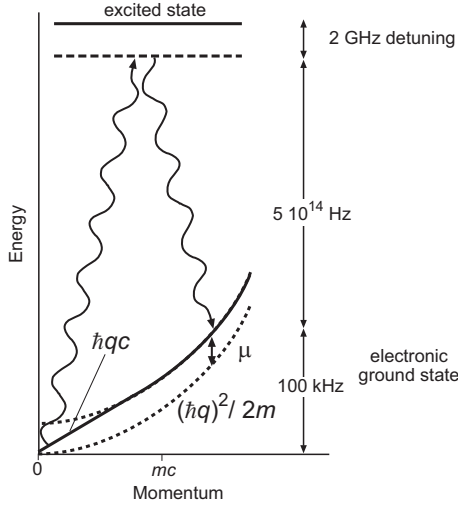


Fig. 2. Probing the dispersion relation of a Bose–Einstein condensate by off-resonant light scattering. The microscopic excitation spectrum in a homogeneous weakly-interacting Bose–Einstein condensate is given by the Bogoliubov dispersion relation (solid line). For small momenta $\hbar q$, such that $\hbar q \ll mc$ the dispersion relation is phonon-like (linear). Here m is the mass, and the speed of sound c is related to the interaction energy μ by $\mu = mc^2$. For large momenta ($\hbar q \gg mc$) it is particle-like (quadratic) offset from the energy of a free-particle excitation by a mean-field shift of μ (≈ 5 kHz for our experiments). Excitations can be created optically by stimulated light scattering using two laser beams which are both far detuned (about 2 GHz) from the atomic resonance. Momentum and energy are provided by absorption of one photon to a virtual excited level, followed by stimulated emission of a second, lower energy photon.

upwards by the chemical potential $\Delta\omega \simeq \mu/\hbar$, and the line strength tends to $S(\vec{q}) \rightarrow 1 - \mu/\hbar\omega_q^0$. Thus, by measuring the frequency shift of the Bragg scattering resonance in the free-particle regime, one can directly measure the chemical potential [10]. For small wavevectors ($q \ll \xi^{-1}$), the Bose–Einstein condensate responds to optical excitation collectively with the creation of phonons. The static structure factor tends to $S(\vec{q}) \rightarrow \hbar q/2mc$ and vanishes in the long wavelength limit, as required of a zero-temperature system with finite compressibility [28].

2.2.2 Bragg scattering as a probe of pair correlations in the condensate

It is interesting to re-examine these modifications to light scattering from a Bose–Einstein condensate in terms of the structure of the many-body

condensate wavefunction. What is it about a dilute, weakly-interacting Bose–Einstein condensate that suppresses light scattering compared to non-interacting atoms? As discussed above, the static structure factor $S(\vec{q})$ is the magnitude of the state vector $|e\rangle \simeq |e^+\rangle + |e^-\rangle$ (Eq. (2.6)). The states $|e^+\rangle$ and $|e^-\rangle$ represent two means by which momentum is imparted to the condensate: either by promoting a zero-momentum particle to momentum $\hbar\vec{q}$, or else by demoting a particle from momentum $-\hbar\vec{q}$ to zero momentum.

If correlations could be neglected, the total rate of excitation would simply be the sum of the independent rates for these two processes, proportional to $\langle e^+|e^+\rangle = \langle N_q^0 \rangle + 1 = u_q^2$ and $\langle e^-|e^-\rangle = \langle N_{-q}^0 \rangle = v_q^2$ where $\langle N_k^0 \rangle$ is the expected number of atoms of momentum $\hbar\vec{k}$ in the condensate. Indeed, a simple-minded rate equation leads to an expression for the total scattering rate which is proportional to $N_0(\langle N_q^0 \rangle + 1) + \langle N_{-q}^0 \rangle(N_0 + 1)$. This expression is the sum of the rates of the two processes which can transfer momentum $\hbar\vec{q}$ to the system and scatter particles into or out of the condensate. Each rate is proportional to the number of particles in the initial state and, because of bosonic stimulation, to the number of atoms in the final state plus one. This would apply, for example, to a condensate in a pure number state, or to an ideal gas condensate with a thermal admixture of atoms with momenta $\pm\hbar\vec{q}$, and would always lead to $S(\vec{q}) > 1$.

Yet, for the many-body ground state of the interacting Bose gas, the behavior is dramatically different. Interactions between zero-momentum atoms admix into the condensate pairs of atoms at momenta $\pm\hbar\vec{q}$ the population of which comprises the quantum depletion [29]. As a result, the two momentum transfer mechanisms described above produce indistinguishable final states, and the total rate of momentum transfer is given by the interference of two amplitudes, not by the sum of two rates. Pair excitations in the condensate are correlated so as to minimize the total energy, and this results in a relative phase between the two amplitudes which produces destructive interference: $S(\vec{q}) = (u_q - v_q)^2 < 1$. For high momentum, $\langle N_q^0 \rangle \ll 1$ and the interference plays a minor role. In the phonon regime, while the independent rates u_q^2 and v_q^2 (and hence $\langle N_{\pm q}^0 \rangle$) diverge as $1/q$, the correlated quantum depletion extinguishes the rate of Bragg excitation.

It is interesting to note that the extinction of Bragg scattering at low momentum, *i.e.* the minus sign in the amplitude $u_q - v_q$ of state $|e\rangle$, arises from minimizing the energy of an interacting Bose gas with positive scattering length. One might wonder whether a negative sign of the scattering length would lead to an enhancement of scattering. However, homogeneous condensates with negative scattering length are unstable. In a trap, they are only stable when their size is smaller than the healing length, effectively cutting off the long-wavelength phonon modes. Therefore, a condensate with negative scattering length should show essentially the same behavior as a similar-sized condensate of non-interacting atoms.

2.2.3 Mean-field theory determination of $S(\vec{q}, \omega)$

These same results are obtained also in a self-consistent mean-field approach. Considering again the homogeneous case, we introduce the perturbation

$$V_{\text{mod}} = \frac{V}{2} (e^{i\vec{q}\cdot\vec{r}-i\omega t} + e^{-i\vec{q}\cdot\vec{r}+i\omega t}) \quad (2.8)$$

to the time-dependent Gross-Pitaevskii equation [30, 31], and use a condensate wavefunction of the form

$$\psi(\vec{r}, t) = e^{-i\mu t/\hbar} (\psi_0(\vec{r}, t) + u(t)e^{i\vec{q}\cdot\vec{r}-i\omega t} + v^*(t)e^{-i\vec{q}\cdot\vec{r}+i\omega t}). \quad (2.9)$$

Here, $\mu = ng$ is the chemical potential where n is the condensate density, $g = 4\pi\hbar^2 a/m$ and a is the s -wave scattering length. In the absence of the perturbation, the ground-state condensate wavefunction is $\psi_0(\vec{r}, t) = \sqrt{n}$.

The weak potential V_{mod} introduces the small perturbations $u(t)e^{i\vec{q}\cdot\vec{r}-i\omega t}$ and $v(t)e^{-i\vec{q}\cdot\vec{r}+i\omega t}$ where the amplitudes $u(t)$ and $v(t)$ are slowly varying functions of time. Using the Gross-Pitaevskii equation and isolating terms proportional to $e^{i\vec{q}\cdot\vec{r}-i\omega t}$ and $e^{-i\vec{q}\cdot\vec{r}+i\omega t}$, we obtain the set of equations

$$\hbar\omega u + i\hbar \frac{du}{dt} = \left(\frac{\hbar^2 q^2}{2m} + ng \right) u + ngv + \frac{V}{2} \psi_0 \quad (2.10)$$

$$-\hbar\omega v - i\hbar \frac{dv}{dt} = \left(\frac{\hbar^2 q^2}{2m} + ng \right) v + ngu + \frac{V}{2} \psi_0. \quad (2.11)$$

Let us now apply the Bogoliubov transformation, and write

$$\begin{pmatrix} u(t) \\ v(t) \end{pmatrix} = \alpha(t) \begin{pmatrix} u_q \\ -v_q \end{pmatrix} + \beta(t) \begin{pmatrix} v_q \\ -u_q \end{pmatrix}. \quad (2.12)$$

The two component vectors $\begin{pmatrix} u_q \\ -v_q \end{pmatrix}$ and $\begin{pmatrix} v_q \\ -u_q \end{pmatrix}$ are solutions of the equations [27, 31]

$$\begin{bmatrix} (\hbar\omega_q^0 + \mu) & \mu \\ -\mu & -(\hbar\omega_q^0 + \mu) \end{bmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = \hbar\tilde{\omega} \begin{pmatrix} u \\ v \end{pmatrix} \quad (2.13)$$

with frequencies $\tilde{\omega} = \omega_q^B$ and $\tilde{\omega} = -\omega_q^B$, respectively. The negative frequency solution corresponds to excitations in the $-\vec{q}$ direction. With this substitution, equations (2.10) and (2.11) are decoupled:

$$\hbar\omega\alpha + i\hbar \frac{d\alpha}{dt} = \hbar\omega_q^B \alpha + (u_q - v_q) \frac{V}{2} \psi_0 \quad (2.14)$$

$$\hbar\omega\beta + i\hbar \frac{d\beta}{dt} = -\hbar\omega_q^B \beta + (u_q - v_q) \frac{V}{2} \psi_0. \quad (2.15)$$

These equations are identical to those of first-order perturbation theory for a single-particle Schrödinger equation, and thus the rates of growth of $|\alpha|^2$ and $|\beta|^2$ can be evaluated using Fermi's golden rule. $|\alpha|^2$ and $|\beta|^2$ are the probabilities for creating quasiparticles with momentum $\hbar\vec{q}$ and $-\hbar\vec{q}$, respectively.

The response of the condensate to Bragg scattering can be evaluated by calculating the momentum imparted to the condensate

$$\langle \psi(\vec{r}, t) | \hat{p} | \psi(\vec{r}, t) \rangle = \hbar\vec{q} \times (|\alpha|^2 - |\beta|^2) = \hbar\vec{q} \times (|u|^2 - |v|^2). \quad (2.16)$$

Normalizing by the Bragg scattering momentum $\hbar q$, we obtain the Bragg excitation rate per particle as

$$\begin{aligned} \frac{d}{dt} \left(\frac{\langle \psi(\vec{r}, t) | \hat{p} | \psi(\vec{r}, t) \rangle}{\hbar q N_0} \right) &= 2\pi\omega_R^2 (u_q - v_q)^2 [\delta(\hbar\omega - \hbar\omega_q^B) - \delta(\hbar\omega + \hbar\omega_q^B)] \\ &= 2\pi\omega_R^2 [S(\vec{q}, \omega) - S(-\vec{q}, -\omega)] \end{aligned} \quad (2.17)$$

where, again, ω_R is the two-photon Rabi frequency.

This treatment reveals two important points. First, the mean-field treatment reproduces the suppression of the structure factor, even though, as discussed in Section 2.2.2, this suppression is indicative of correlations in the many-body condensate wavefunction. In the mean-field theory, correlations in the condensate wavefunction are explicitly neglected by the use of a Hartree wavefunction. Nevertheless, when the excitation of the condensate is also treated in a Hartree approximation (*i.e.* assuming all particles to be in the same, albeit time-varying, single-particle wavefunction), the dynamic response is correctly obtained.

Second, this treatment takes into account both the positive and negative frequency terms in V_{mod} , unlike in Section 2.1.3 where we chose to consider only the positive frequency part for simplicity. One finds that the momentum imparted by stimulated scattering from the two Bragg beams measures the difference $S(\vec{q}, \omega) - S(-\vec{q}, -\omega)$. This is important when one considers Bragg scattering from a non-zero temperature system which has thermally excited states and undergo anti-Stokes scattering. The dynamic structure factor for a non-zero temperature Bose-Einstein condensate is given as [20, 21]

$$S(\vec{q}, \omega) = (u_q - v_q)^2 [(\langle N_q^B \rangle + 1)\delta(\omega - \omega_q^B) + \langle N_{-q}^B \rangle \delta(\omega + \omega_q^B)] \quad (2.18)$$

where $\langle N_q^B \rangle$ is the thermal population of *quasi-particles*. Light scattering is thus quite sensitive to the presence of excitations in the condensate, as confirmed by the recent observation of superradiant light scattering from a condensate which is due to the buildup of excited particles in a preferred mode [32]. However, inserting equation (2.18) into equation (2.17) shows

that the effects of thermally-excited particles are cancelled out in the Bragg scattering response, and thus one measures the zero-temperature structure factor even in a finite-temperature sample.

2.2.4 The inhomogeneous condensate

The Bose-Einstein condensates realized experimentally differ from the homogeneous condensates considered above due to their confinement. This confinement changes the Bragg scattering resonance from that predicted for a homogeneous Bose-Einstein condensate by introducing an inhomogeneous density distribution and by introducing Doppler broadening due to the zero-point momentum distribution.

The confining potential of magnetic or even optical traps is typically harmonic, taking the form $V(\vec{r}) = (m/2)(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2)$, where ω_x , ω_y , and ω_z are the trap frequencies. The condensate wavefunction $\psi(\vec{r})$ can be determined by the mean-field Gross-Pitaevskii equation [30, 31]. For large condensates for which the interaction energy is much larger than the kinetic energy, the wavefunction is given by the Thomas-Fermi solution as [3]

$$|\psi(\vec{r})|^2 = n \max \left(1 - \left(\frac{x}{x_c} \right)^2 - \left(\frac{y}{y_c} \right)^2 - \left(\frac{z}{z_c} \right)^2, 0 \right) \quad (2.19)$$

where the Thomas-Fermi radii are defined as $x_c^2 = 2\mu/m\omega_x^2$ (similar for y_c and z_c), and $\mu = gn$ where n is the maximum condensate density and $g = 4\pi\hbar^2 a/m$ with a being the s -wave scattering length.

Let us first consider the two effects of confinement separately:

- a) **Mean-field shift and broadening:** the effects of interactions on Bragg scattering from an inhomogeneous density distribution can be accounted for using a local density approximation (discussed further in [25]). Using the density distribution of a condensate in the Thomas-Fermi regime (Eq. (2.19)) and the predicted $S(\vec{q}, \omega)$ for a homogeneous condensate at the local value of the density, the Bragg resonance line shape is calculated to be [11]

$$I_\mu(\omega) d\omega = \frac{15}{8} \frac{\omega^2 - \omega_q^{02}}{\omega_q^0(\mu/\hbar)^2} \sqrt{1 - \frac{\omega^2 - \omega_q^{02}}{2\omega_q^0\mu/\hbar}} d\omega. \quad (2.20)$$

The line strength $S(\vec{q})$ and center frequency can be obtained from equation (2.20) by integration. Explicitly, the static structure factor of a harmonically-confined Bose-Einstein condensate is given by

$$S(\vec{q}) = \frac{15\eta}{64} (y + 4\eta - 2y\eta^2 + 12\eta^3 - 3y\eta^4) \quad (2.21)$$

where $\eta^2 = \hbar\omega_q^0/2\mu$ and $y = \pi - 2 \arctan((\eta^2 - 1)/2\eta)$. The line strength has the limiting values of $S(\vec{q}) \rightarrow 15\pi/32 (\hbar\omega_q^0/2\mu)^{1/2}$ in the phonon regime and $S(\vec{q}) \rightarrow 1 - 4\mu/7\hbar\omega_q^0$ in the free-particle regime. In accordance with the f -sum rule, the center frequency $\bar{\omega}$ is given as $\omega_q^0/S(\vec{q})$. In the free-particle regime ($\hbar\omega_q^0 \gg \mu$), the line center is shifted upwards from the free-particle resonance frequency by $4\mu/7\hbar$, and broadened to an rms-width of

$$\Delta\omega_\mu = \sqrt{\frac{8}{147}} \frac{\mu}{\hbar}. \quad (2.22)$$

- b) **Doppler broadening:** doppler broadening arises due to the initial momentum distribution of the condensate. The momentum distribution of a trapped Bose-Einstein condensate, assuming its full coherence, is given by the Fourier transform of the condensate wavefunction (Eq. (2.19)). Thus, neglecting the mean-field shift (the impulse approximation as discussed in [25]), the Bragg excitation rate $I_D(\omega)$ from a Bose-Einstein condensate at a frequency difference of ω between the two Bragg beams is

$$\begin{aligned} I_D(\omega)d\omega & \quad (2.23) \\ & \propto \int d^3\vec{k} \, \delta\left(\frac{\hbar\vec{k} \cdot \vec{q}}{m} - (\omega - \omega_q^0)\right) \left| \int d^3\vec{r} \, e^{-i\vec{k} \cdot \vec{r}} \psi(\vec{r}) \right|^2 d\omega \\ & \propto \int dx_1 dx_2 e^{-ik(\omega) \cdot (x_2 - x_1)} \int dy dz \, \psi^*(x_1, y, z) \psi(x_2, y, z) d\omega \end{aligned}$$

where $\hbar\vec{q}$ is the Bragg scattering momentum and $\psi(\vec{r})$ is the condensate wave function. In the last line, a coordinate system is chosen so that $\hbar\vec{q}$ lies in the $\hat{x}$ -direction, and $k(\omega) = m(\omega - \omega_q^0)/\hbar q$. In the Thomas-Fermi regime, for Bragg scattering along one of the principal axes of the harmonic trap, the Doppler line shape is then

$$\begin{aligned} I_D(\omega)d\omega & \propto \quad (2.24) \\ & \frac{2(4 + \kappa^2)J_1(\kappa)J_2(\kappa) + \kappa J_0(\kappa)[5\kappa J_1(\kappa) - 16J_2(\kappa) + 3\kappa J_3(\kappa)]}{\kappa^3} d\omega \end{aligned}$$

where $\kappa = k(\omega)x_c$, and J_i are Bessel functions. This line shape is similar to a Gaussian, but its rms-width is undefined. We therefore fitted a Gaussian function to the line shape and extracted an effective rms-width of

$$\Delta\omega_D \simeq 1.58 \frac{\hbar q}{m x_c}. \quad (2.25)$$

2.2.5 Relevance of Doppler broadening

Thus, the Bragg scattering resonance for a trapped Bose–Einstein condensate is sensitive both to the velocity (Doppler shift) and the density (mean–field shift) of the atomic sample. The above treatments, in which we considered the effects of each of these shifts separately, are valid predictions in two limiting cases: for large condensates so that $\mu/\hbar \gg \hbar q/mx_c$ one can neglect Doppler broadening, while for small condensates where $\mu/\hbar \ll \hbar q/mx_c$ one can neglect mean–field broadening. However, in our experiments on Bragg scattering in the free–particle regime [10], the Doppler and mean–field widths were comparable, and one must consider both effects simultaneously.

We now show with the aid of simple sum rules that it is correct to add the Doppler broadening (Eq. (2.25)) and the mean–field broadening (Eq. (2.22)) in quadrature to obtain the total rms line width which can then be compared to experiments. A unified approach toward determining fully the dynamic structure factor in the presence of both Doppler and mean–field shifts has been presented recently by Zambelli *et al.* and was compared favorably with experimental data [25].

The condensate wavefunction $|g\rangle$ determined by the Gross–Pitaevskii equation is a solution of the equation $\mathcal{H}_0|g\rangle = \mu|g\rangle$ where

$$\mathcal{H}_0 = \frac{\hat{p}^2}{2m} + U(\vec{r}) + gn(\vec{r}). \quad (2.26)$$

In the regime $\hbar\omega_q^0 \gg \mu$, the excitations relevant to Bragg scattering are well described as free–particle excitations which obey

$$\hbar\omega_f|f\rangle = \left(\frac{\hat{p}^2}{2m} + U(\vec{r}) + 2gn(\vec{r}) \right) |f\rangle = \mathcal{H}_{\text{exc}}|f\rangle. \quad (2.27)$$

This can be seen, for example, by considering equation (2.13) in the free–particle regime where $v_q \rightarrow 0$. Thus, the excitations are eigenfunctions of the Hamiltonian $\mathcal{H}_{\text{exc}} = \mathcal{H}_0 + gn(\vec{r})$ which is different from the Hamiltonian $\mathcal{H}_0$ which gives the condensate wavefunction [33]. The extra term $gn(\vec{r})$ represents the repulsion of excitations from the condensate which gives rise to the mean–field shift in the free–particle regime.

An exact determination of the resonance line shape using Fermi’s golden rule requires detailed knowledge of the excitation wavefunctions. Such an explicit calculation has been performed [34] in the context of the two–photon optical excitation from the $1S$ to the $2S$ state in hydrogen which has been employed to probe properties of a hydrogen Bose–Einstein condensate [35, 36]. However, even without this exact description, moments of the spectral line can be easily determined. The first moment of the spectral line is

given by

$$\hbar\bar{\omega} = \frac{\int_0^\infty d\omega \omega S(\vec{q}, \omega)}{\int_0^\infty d\omega S(\vec{q}, \omega)} \quad (2.28)$$

$$= \langle e^{i\vec{q}\cdot\vec{r}} \mathcal{H}_{\text{exc}} e^{-i\vec{q}\cdot\vec{r}} - \mathcal{H}_0 \rangle_c \quad (2.29)$$

$$= \frac{\hbar^2 q^2}{2m} + g\langle n \rangle_c \quad (2.30)$$

where $\langle X \rangle_c = \langle g | X | g \rangle$, and $\langle \vec{p} \rangle_c = 0$ in the ground state. Thus the Bragg resonance line for a harmonically trapped condensate is shifted from the free-particle resonance by $g\langle n \rangle_c = 4\mu/7\hbar$.

The rms-width of the line $\Delta\omega = \sqrt{\overline{\omega^2} - \bar{\omega}^2}$ is calculated using

$$\hbar^2 \overline{\omega^2} = \langle e^{i\vec{q}\cdot\vec{r}} \mathcal{H}_{\text{exc}}^2 e^{-i\vec{q}\cdot\vec{r}} - \mathcal{H}_0^2 \rangle_c \quad (2.31)$$

by which one obtains

$$\hbar^2 (\Delta\omega)^2 = \left\langle \left(\frac{\hbar \vec{q} \cdot \vec{p}}{m} \right)^2 \right\rangle_c + g^2 (\langle n^2 \rangle_c - \langle n \rangle_c^2). \quad (2.32)$$

Thus the total rms-width of the line is the sum of two widths in quadrature: the Doppler width due to the finite size of the condensate, and the line broadening due to the inhomogeneous condensate density.

2.3 Experimental aspects of Bragg spectroscopy

For the experimental studies of light scattering from Bose-Einstein condensates, condensates of atomic sodium were produced as in our previous experiments [1, 37]. These condensates typically contained 10^7 atoms, and were held in a magnetic trap which provided a cylindrically-symmetric cigar-shaped harmonic confinement. The strength of the confining field could be easily modified by adjusting the currents through the magnetic trapping coils, allowing us to vary the peak condensate density in the range $(0.5-6) \times 10^{14} \text{ cm}^{-3}$ and the radial half-width of the condensate (x_c) between 7 and 15 μm .

The two laser beams used for Bragg scattering were derived from a common source, and had a detuning to the red of the $3S_{1/2}, |F=1\rangle \rightarrow 3P_{3/2}, |F'=0, 1, 2\rangle$ optical transitions of about $\Delta = 1.7 \text{ GHz}$ (similar parameters were used for experiments at NIST, Gaithersburg [14, 15, 38, 39]). A small frequency difference ω between the counter-propagating beams,

on the order of $2\pi \times 100$ kHz, was introduced by using two independently-controlled acousto-optic modulators (AOM's) to control the frequency of two independent beams².

To determine the Bragg scattering response, the laser beams were pulsed on for about $400 \mu\text{s}$. After the optical excitation, the Bose-Einstein condensate was allowed to freely expand for 20–70 ms time of flight, after which the atoms were imaged by absorption imaging. Bragg scattered atoms were clearly distinguished by their displacement in the time-of-flight images (see Figs. 3, 8). The Bragg resonance spectrum for both trapped and untrapped Bose-Einstein condensates was determined by scanning the frequency difference ω and determining the fraction of Bragg scattered atoms.

As discussed above, there are two different regimes of excitations described by the Bogoliubov theory for the zero-temperature, weakly-interacting Bose-Einstein condensate: the phonon and the free-particle regimes. These two regimes can be distinguished in a number of equivalent ways. In the phonon regime, the wavevector of the excitation q is smaller than the inverse healing length $q \ll \xi^{-1} = \sqrt{2m\mu/\hbar^2}$. Equivalently, the free recoil velocity $\hbar q/m$ is smaller than the speed of sound c . One can also distinguish the free-particle from the phonon regime by comparing the free recoil energy $\hbar^2 q^2/2m = \hbar\omega_q^0$ to the condensate interaction energy μ : $\hbar\omega_q^0 \ll \mu$ in the phonon regime, and $\hbar\omega_q^0 \gg \mu$ in the free-particle regime.

Either of these types of excitations can be accessed by Bragg scattering. In an N -th order Bragg scattering event induced by laser beams of wavevectors $\vec{k}_1$ and $\vec{k}_2$ ($|\vec{k}_1| \simeq |\vec{k}_2| = k$), N photons are transferred from one incident beam to another, imparting a momentum $\hbar q = 2N\hbar k \sin(\theta/2)$, where θ is the angle between $\vec{k}_1$ and $\vec{k}_2$. Thus, small-angle Bragg scattering can be used to excite low-momentum phonon excitations, while large-angle or high-order Bragg scattering can excite high-momentum free-particle excitations.

The conditions in our two experiments are shown in Table 1. In our first experimental study of Bragg scattering, excitations in the free-particle regime were studied by using two counter-propagating Bragg beams [10]. As shown in Table 1, the recoil velocity and energy for an excitation with a momentum of two photon recoils ($\hbar q = 2\hbar k$) were clearly in the free-particle regime. In a second experiment, we accessed the phonon regime by using Bragg beams which were inclined at a small angle of about 14° with respect to one another. This yielded a recoil velocity and energy which implied that

²In our study of the free-particle regime using counter-propagating Bragg beams, we alternately used a single AOM to generate a single beam with two different frequencies which was retro-reflected. This was done to minimize the deleterious effects of vibrations of optical components.

Table 1. Conditions for Bragg scattering in the phonon and the free-particle regimes. The two regimes can be distinguished by comparing the Bragg scattering velocity $\hbar q/m$ to the speed of Bogoliubov sound $c = \sqrt{\mu/m}$, or, similarly, the Bragg scattering kinetic energy $\hbar\omega_q^0 = \hbar^2 q^2/2m$ to the chemical potential μ . Bragg scattering using beams inclined by 14° to one another accessed the phonon regime, while the use of counter-propagating beams accessed the free-particle regime.

	Phonon [11]	BEC	Free-particle [10]
Velocity	$\hbar q/m = 7 \text{ mm/s}$	$c = 10 \text{ mm/s}$	$\hbar q/m = 60 \text{ mm/s}$
Energy	$\hbar\omega_q^0 = h \times 1.5 \text{ kHz}$	$\mu = h \times 6 \text{ kHz}$	$\hbar\omega_q^0 = h \times 100 \text{ kHz}$

Bragg scattering in a trapped Bose–Einstein condensate would occur in the phonon regime.

2.4 Light scattering in the free-particle regime

2.4.1 Measurement of line shift and line broadening

Figure 3 illustrates our experimental method for probing the free-particle regime. Counter-propagating Bragg beams were incident along a radial direction (vertical in image) of the cigar-shaped condensate. After probing, the condensate was allowed to freely expand, allowing Bragg scattered atoms to separate spatially from the unscattered atoms, as shown in the figure. During free expansion, a cigar-shaped condensate expands primarily radially, with a maximum radial velocity of $v_r = \sqrt{2\mu/m} = \sqrt{2}c$. Thus, since the Bragg scattered atoms are clearly separated from the remaining condensate during the time of flight, $\hbar q/m \gg c$ and thus Bragg scattering at a momentum of $\hbar q = 2\hbar k$ produces free-particle excitations.

The use of Bragg spectroscopy allowed the true momentum distribution of a gaseous Bose–Einstein condensate to be observed for the first time. Previous to this work, the onset of Bose–Einstein condensation had been observed by the observation of a bimodal density distribution either *in situ*, or else in time-of-flight. In both cases, the condensate can be distinguished from the thermal cloud because its energy μ , which is typically dominated by interaction energy, is smaller than the thermal energy $k_B T$. *In situ*, a separation between the two components of the gas occurs due to the inhomogeneous quadratic trapping potential, while in time-of-flight images, the separation is seen in velocity space after the explosive conversion of the interaction energy of the condensate to kinetic energy of ballistic expansion; in both cases, the spatial extent of the gas scales as the square root of its energy. As a result, both in time-of-flight and in the spatial domain, the onset of BEC is indicated by a narrowing of the density distribution

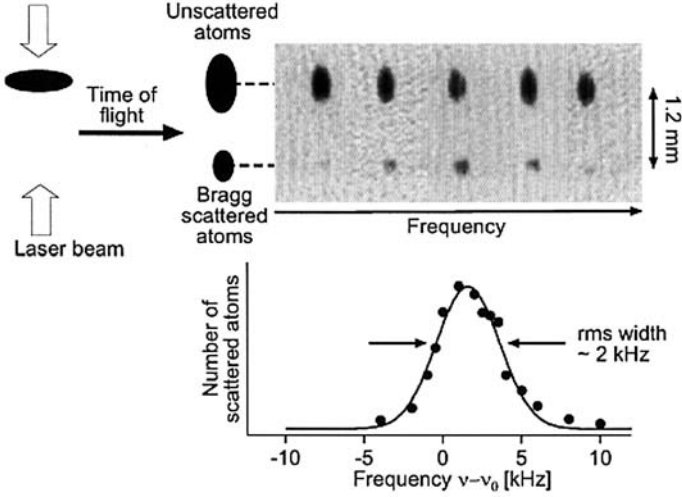


Fig. 3. Measuring the momentum distribution of a condensate [10]. Atoms were stimulated by two counter-propagating laser beams to absorb a photon from one beam and emit it into the other beam, resulting in momentum transfer to the atoms, as observed in ballistic expansion after 20 ms time of flight. The number of Bragg scattered atoms showed a narrow resonance when the difference frequency between the two laser beams was varied.

Table 2. Scaling of spatial and momentum widths of thermal clouds and Bose–Einstein condensates in an isotropic harmonic trap with frequency ω . The parameter $\xi = \sqrt{\mu/\hbar\omega}$ denotes the strength of the mean-field interaction, and $a_{\text{osc}} = \sqrt{\hbar/m\omega}$ the oscillator length.

	thermal cloud	ideal BEC	interacting BEC	time-of- flight
Δx	$a_{\text{osc}} \sqrt{k_B T / \hbar \omega}$	a_{osc}	$a_{\text{osc}} \xi$	
Δp	$(\hbar / a_{\text{osc}}) \sqrt{k_B T / \hbar \omega}$	$\hbar / a_{\text{osc}}$	$(\hbar / a_{\text{osc}}) (1 / \xi)$	$(\hbar / a_{\text{osc}}) \xi$
$\Delta x \Delta p / \hbar$	$k_B T / \hbar \omega$	1	1	

relative to that of the thermal component by a factor of $\sqrt{\mu/k_B T}$ (Tab. 2). Indeed, we used Bragg spectroscopy to observe the expanding condensate in momentum space *after* its interaction energy had been converted to kinetic energy during its time of flight (Fig. 4). In a time-of-flight analysis, the condensate distribution is just ≈ 3 times narrower than that of the

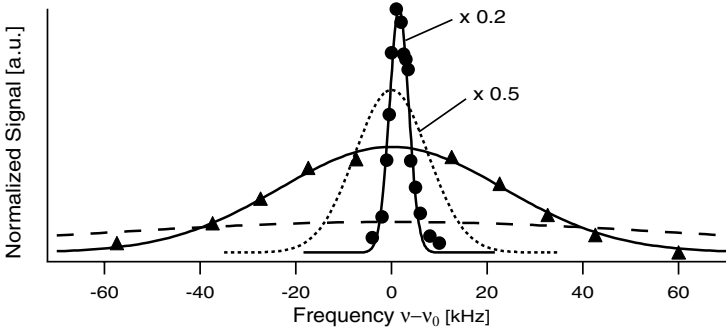


Fig. 4. Bragg resonances for a trapped condensate (circles) and after 3 ms time of flight (triangles). For comparison, the momentum distributions of the ground state of the trapping potential (dots) and of a 1 μK cold, thermal cloud (dashes) are indicated. Figure taken from reference [10].

thermal cloud (corresponding to the factor $\sqrt{\mu/k_B T}$), but wider than the momentum distribution of the harmonic oscillator ground state.

However, the *in situ* momentum distribution of the trapped condensate is much narrower than in ballistic expansion, by a factor $\xi^2 = \mu/\hbar\omega$ (Tab. 2). It is also narrower than the momentum distribution of the harmonic oscillator ground state. This could be directly determined by the use of Bragg spectroscopy *before* releasing the condensate from its trap. As shown in Figure 4, the momentum distribution of a trapped Bose–Einstein condensate is significantly narrower than that observed in time-of-flight; for the data shown, the *in situ* momentum width is 10 times narrower than in time-of-flight. Thus, the distinction between the thermal cloud and the condensate in momentum space is much more stark than in coordinate space and emphasizes the original description by Einstein of Bose–Einstein condensation as a condensation in momentum space.

We obtained Bragg resonance spectra for trapped condensates over a range of condensate densities and radial widths, and determined the shifts of the line center (Fig. 10) and the rms-widths (Fig. 5) of the resonances. The shifts of the line center for trapped condensates from the free-particle resonance frequency were compared with measurements of the chemical potential determined from the width of condensates in time-of-flight images [1]. The measured shift of $(0.54 \pm 0.07)\mu/\hbar$ was in agreement with the predicted $0.57\mu/\hbar$. In related work, mean-field line shifts measured by two-photon spectroscopy of atomic hydrogen were used as a measurement of the $a_{1S,2S}$ scattering length for collisions between atoms in the 1S and 2S states [35].

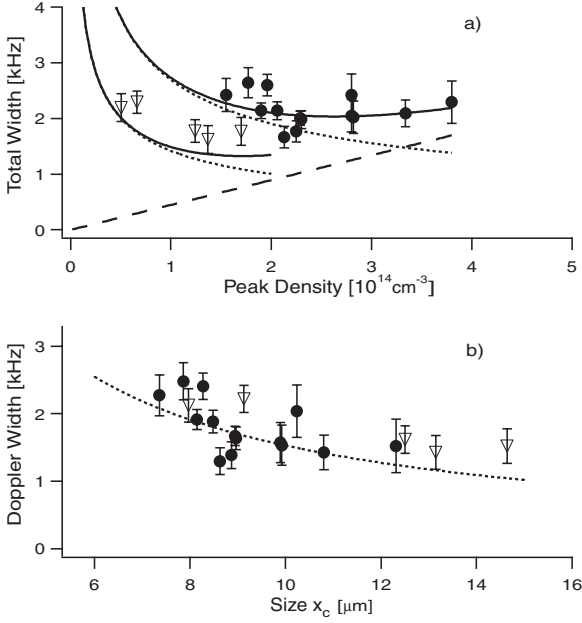


Fig. 5. Line width in Bragg spectroscopy. The widths are shown for various densities and sizes of the condensate using two different radial trapping frequencies, $\nu_r = (195 \pm 20) \text{ Hz}$ (circles), and $\nu_r = (95 \pm 20) \text{ Hz}$ (triangles). The lines in a) show the contributions of the mean-field energy (dashed), due to the finite size (dotted, for both trapping frequencies), and their quadrature sum (solid lines). Figure b) displays the Doppler width, obtained by subtracting the contributions of the mean-field and the finite pulse duration from the total width. The observed Doppler width of the resonance is proportional to the condensate's momentum uncertainty Δp , and was consistent with the Heisenberg limit $\Delta p \approx \hbar/x_c$ as the condensate radius x_c was varied. Thus, the coherence length of the condensate is equal to its physical size, *i.e.* the condensate is one “coherent matter wave.” An analogous measurement in the time domain has been done in Gaithersburg [38]. The error bars are 1σ errors of the Gaussian fits to the data. Figure taken from reference [10].

The rms line widths showed effects of both mean-field broadening and Doppler broadening: mean-field broadening caused the line width to increase as the condensate number, and hence its size and density, were increased, while Doppler-broadening caused the rms-width to increase as the radial width of the condensate was decreased. Experimental Bragg spectra for conditions at the cross-over between mean-field dominated (local density approximation) and Doppler dominated (impulse approximation)

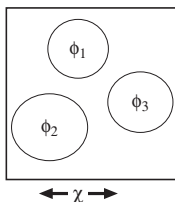


Fig. 6. A quasi-condensate can be depicted pictorially as being composed of many smaller condensates, each with a well-defined phase which is unrelated to the phase of the other small condensates. The range of phase coherence is the coherence length χ .

behaviour are shown in Figure 5. These were analyzed in reference [25] and compared with a theoretical treatment based on an eikonal approximation which accounts for both effects.

The Doppler line widths were extracted from Bragg spectra by subtracting the broadening due to the mean-field and the finite pulse duration. Doppler widths were determined for both trapped condensates and condensates released from the trap. The width for freely-expanding condensates during the conversion of their interaction energy into kinetic energy was in full agreement with mean-field theory [40]. Thus, both in momentum space and in coordinate space [1], the predicted behaviour of freely-expanding Bose-Einstein condensates has been quantitatively verified, nicely confirming the mean-field description of large-amplitude dynamics of a condensate.

2.4.2 A measurement of the coherence length of a Bose-Einstein condensate

The Doppler width of the Bragg scattering resonance of trapped Bose-Einstein condensates measured their momentum distribution and thus measured their coherence length. By observing momentum distributions which were equal to the Heisenberg-limited momentum distribution determined by the condensate size (Fig. 5), our measurements showed that the coherence length of the condensate was no smaller than the radial width of the condensate, or simply that condensates can be described by a single macroscopic wavefunction.

To make this statement more quantitative, consider the possibility that the condensate is not fully coherent. As shown pictorially in Figure 6, consider a situation in which the trapped Bose-Einstein condensate is actually composed of many smaller coherent condensates of typical size χ with no phase relation between them. Formally, one considers

$$\langle \hat{\Psi}^\dagger(\vec{r}_1) \hat{\Psi}(\vec{r}_2) \rangle = \langle \hat{\Psi}^\dagger(\vec{r}_1) \rangle \langle \hat{\Psi}(\vec{r}_2) \rangle g^{(1)}(|\vec{r}_1 - \vec{r}_2|) \quad (2.33)$$

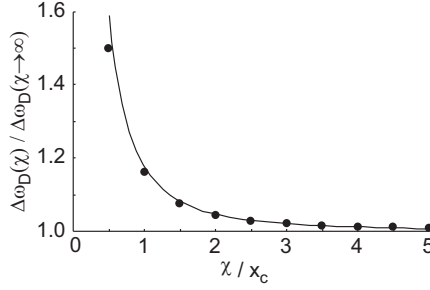


Fig. 7. Doppler width of the Bragg resonance as a function of the coherence length χ . Shown is the ratio of the Doppler width of a partly coherent condensate to that of a fully coherent condensate, *i.e.* one for which $\chi \rightarrow \infty$. The coherence length is given in units of the Thomas–Fermi radius x_c . The results of a numerical calculation of equation (2.34) using a Thomas–Fermi wavefunction and $g^{(1)}(r) = \exp(-r^2/2\chi^2)$ (points) are well-described by the approximation of equation (2.35) (line).

where $g^{(1)}(r)$ is the first-order coherence function which decays from $g^{(1)}(0) = 1$ to $g^{(1)}(r \gg \chi) = 0$. The Doppler line shape of the Bragg resonance, shown in equation (2.23) for the case of full coherence, now becomes

$$\begin{aligned}
 I_D(\omega) d\omega &\propto \int dx_1 dx_2 e^{-ik(\omega)(x_2-x_1)} \int dy dz \left\langle \hat{\Psi}^\dagger(x_1, y, z) \hat{\Psi}(x_2, y, z) \right\rangle d\omega \\
 &= \int dx_1 dx_2 e^{-ik(\omega)(x_2-x_1)} g^{(1)}(|x_1 - x_2|) \int dy dz \psi^*(x_1, y, z) \psi(x_2, y, z) d\omega.
 \end{aligned} \tag{2.34}$$

The effect of a limited coherence length is to increase the momentum distribution and thereby broaden the Doppler width of the Bragg resonance. For example, consider a condensate wavefunction which is Gaussian $\psi(\vec{r}) = \exp(-\sum x_i^2/2\sigma_i^2)$ with rms-widths of σ_i , ($i = x, y, z$), and a first-order correlation function of the form $g^{(1)}(r) = e^{-r^2/2\chi^2}$. For Bragg scattering along the $\hat{x}$ -direction, the Doppler line width becomes $\Delta\omega_D(\chi) = \hbar q/m \times \sqrt{\sigma_x^{-2} + \chi^{-2}}$. Figure 7 shows the Doppler line width $\Delta\omega_D(\chi)$ calculated using the Thomas–Fermi condensate wavefunction for different values of the coherence length χ . The calculations agree well with an approximation of the form

$$\Delta\omega_D(\chi) \simeq \sqrt{[\Delta\omega_D(\chi \rightarrow \infty)]^2 + \left[\frac{\hbar q}{m\chi}\right]^2}. \tag{2.35}$$

This relation can be used to extract a coherence length from the Doppler widths for trapped Bose–Einstein condensates. Taking the average for all

data points shown in Figure 5b (assuming the ratio of the coherence length to the condensate size is constant), one finds an average value for the ratio of the measured Doppler width to that predicted for a fully coherent condensate of $\Delta\omega_D(\chi)/\Delta\omega_D(\chi \rightarrow \infty) = 1.09 \pm 0.11$. This corresponds to a determination of the coherence length in the range $\chi = 1.4_{-0.5}^{+\infty} \times x_c$, *i.e.* the measurements place a lower bound on the coherence length of $\chi \simeq x_c$ and are consistent with full coherence ($\chi \rightarrow \infty$).

The coherence of a condensate was first demonstrated by Andrews *et al.* by the observation of matter-wave interference when two independent Bose-Einstein condensates were overlapped [41]. The regular high-contrast fringes indicated, at least qualitatively, that the condensates possessed long-range first-order coherence. Our measurements using Bragg scattering provide a more quantitative measure of this property. Recently, two other groups have made measurements of the coherence length [38, 42]. These measurements give evidence of a decay of the coherence length over two length scales. In particular, the Munich group ascribes the short-range decay of the first-order coherence function to the presence of thermal excitations. Instead of light, one could also use the scattering of fast atoms to determine the coherence length of a condensate, as suggested recently [43].

2.5 Light scattering in the phonon regime

2.5.1 Experimental study

A second experiment explored the use of Bragg spectroscopy of a Bose-Einstein condensate in the phonon regime [11]. Laser beams separated by an angle of about 14° were directed at a condensate so that the Bragg scattering momentum $\hbar\vec{q}$ was directed along the condensate axis (Fig. 8). Orienting the Bragg scattering momentum in the axial direction was necessary to allow for a clear distinction between the Bragg scattered atoms and the unscattered condensate in time-of-flight images, since the condensate expands radially at a velocity $v_r = \sqrt{2}c$ which is greater than the recoil velocity $\hbar q/m$ in the phonon regime ($c > \hbar q/m$). The axial expansion is slower than the radial expansion by a factor which is $2/\pi$ times the aspect ratio of the cylindrical condensate [40], and was negligible for our experimental conditions.

We could directly compare Bragg scattering in the phonon and free-particle regimes by using the identical optical setup to optically excite either a trapped Bose-Einstein condensate, or a condensate that had been allowed to freely expand for 5 ms before the Bragg excitation. As discussed above, excitation in the trapped condensate occurred in the phonon regime. As for the expanded cloud, its density was reduced by a factor of 23 and thus the speed of sound by a factor of 5 from that of a trapped Bose-Einstein condensate. Therefore, excitations in expanded cloud occurred in the free-particle regime.

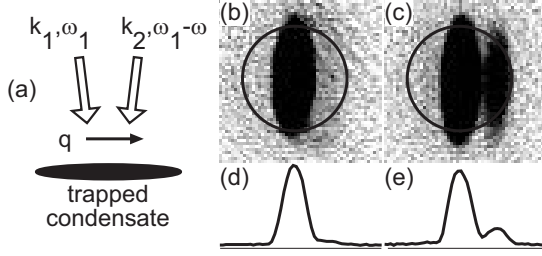


Fig. 8. Observation of momentum transfer by Bragg scattering. (a) Atoms were exposed to laser beams with wavevectors $\vec{k}_1$ and $\vec{k}_2$ and frequency difference ω , imparting momentum $\hbar\vec{q}$ along the axis of the trapped condensate. The Bragg scattering response of trapped condensates (b,d) was much weaker than that of condensates after a 5 ms free expansion (c,e). Absorption images (b,c) after 70 ms time of flight show scattered atoms distinguished from the denser unscattered cloud by their axial displacement. Curves (d,e) show radially averaged (vertically in image) profiles of the optical density after subtraction of the thermal distribution. The Bragg scattering velocity is smaller than the speed of sound in the condensate (position indicated by circle). Images are 3.3×3.3 mm. Figure taken from reference [11].

As shown in Figures 8 and 9, the Bragg scattering response in the phonon regime was significantly weaker in strength and shifted upwards in frequency from that of free particles as predicted by Bogoliubov theory (Sect. 2.2). The line strength and center shift were measured for condensates at various densities, as presented in Figure 10. As the condensate density is increased, the speed of sound increases and, at a constant Bragg scattering momentum $\hbar q$, one pushes further into the phonon regime where the line strength decreases. We could directly compare our experimental results to the predictions of the local density approximation (Eq. (2.20)) since the Doppler shift was negligible at small momentum transfer. The striking difference from the free-particle regime demonstrates the collective nature of low momentum excitations.

The results summarized in Figure 10 show that we have confirmed the Bogoliubov dispersion relation (Fig. 2) in both the small- and large-momentum regime. Data were taken at only two values of the momentum transfer, but by varying the condensate density, the ratio of the recoil energy to the mean-field energy could be smoothly varied.

2.5.2 Suppression of light scattering from a Bose-Einstein condensate

The diminished line strength for stimulated light scattering observed in the phonon regime shows that inelastic spontaneous light scattering (Rayleigh

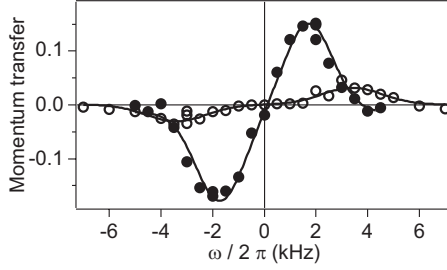


Fig. 9. Bragg scattering of phonons and of free particles. Momentum transfer per particle, in units of $\hbar q$, is shown *vs.* the frequency difference $\omega/2\pi$ between the two Bragg beams. Open symbols represent the phonon excitation spectrum for a trapped condensate at a chemical potential $\mu/h = 9.2$ kHz (compared to the free recoil shift of ≈ 1.4 kHz). Closed symbols show the free-particle response of an expanded cloud. Lines are fits to the difference of two Gaussian line shapes representing excitation in the forward and backward directions. Figure taken from reference [11].

scattering) from a Bose–Einstein condensate is different from the light scattering from an equal number of non-interacting atoms. Consider Rayleigh scattering from a homogeneous Bose–Einstein condensate with a chemical potential μ . Light scattered at an angle θ from an incident beam of light with wavevector $\vec{k}$ imparts a momentum of magnitude $\hbar q = 2\hbar k \sin(\theta/2)$. The intensity of light scattered at this angle is diminished by $S(q) = \omega_q^0/\omega_q^B$. Integrating over all possible scattering angles θ and accounting for the dipolar emission pattern, we find that Rayleigh scattering from a homogeneous interacting Bose–Einstein condensate is suppressed by a factor

$$\begin{aligned}
 F &= \frac{3}{8\pi} \int d\Omega (\cos^2 \theta + \sin^2 \theta \sin^2 \phi) \frac{2k \sin(\theta/2)}{\sqrt{(2k \sin(\theta/2))^2 + 2\xi^{-2}}} \\
 &= \frac{1}{64x^3 \sqrt{1+2x}} \left[\sqrt{2x} (15 + 46x + 64x^2 + 64x^3) \right. \\
 &\quad \left. - 3\sqrt{1+2x} (5 + 12x + 16x^2) \tanh^{-1} \left(\sqrt{\frac{2x}{1+2x}} \right) \right] \quad (2.36)
 \end{aligned}$$

where $x = \hbar\omega_k^0/\mu$.

This suppression in Rayleigh scattering should be observable in current Bose–Einstein condensation experiments (Fig. 11). For example, Rayleigh scattering of near-resonant light from a sodium condensate at a density of $3 \times 10^{15} \text{ cm}^{-3}$, which is the maximum density of condensates which has been obtained in optical traps [44], should be reduced by a factor of two. It would also be interesting to measure this suppression of light scattering

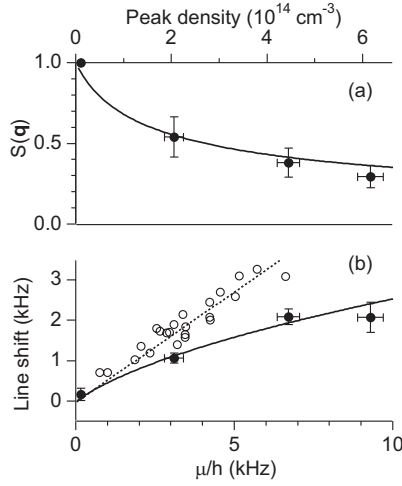


Fig. 10. Line strengths and line shifts of Bragg resonances. Shown are (a) the static structure factor $S(\vec{q})$ and (b) the shift of the line center from the free-particle resonance. $S(\vec{q})$ is the ratio of the line strength at a given chemical potential μ to that observed for free particles. As the density and μ increase, the structure factor is reduced, and the Bragg resonance is shifted upward in frequency. Solid lines are predictions of a local-density approximation for light scattering by 14° . The dotted line indicates a mean-field shift of $4\mu/7h$ as measured in the free-particle regime using a scattering angle of 180 degrees. Data from experiments with large (Ref. [10]) and small momentum transfer are indicated by open and closed circles, respectively. Figure taken from reference [11].

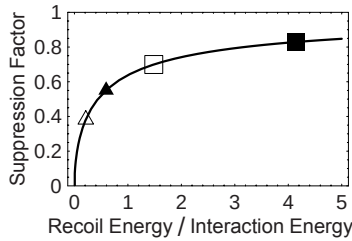


Fig. 11. Rayleigh scattering from a homogeneous interacting Bose–Einstein condensate is suppressed with respect to scattering from free atoms. The suppression factor is plotted against the ratio of the recoil energy $\hbar\omega_k^0 = \hbar^2 k^2/2m$ to the interaction energy μ , where k the wavevector of the incident light. Points indicate the factor by which the scattering of near-resonant light at $\lambda = 589 \text{ nm}$ (closed symbols) and infrared light at $\lambda = 985 \text{ nm}$ (open symbols) is suppressed at typical condensate densities attained in our magnetic ($n = 4 \times 10^{14} \text{ cm}^{-3}$, squares) and optical ($n = 3 \times 10^{15} \text{ cm}^{-3}$, triangles) traps.

at a Feshbach resonance [45], where the chemical potential can be made quite large by tuning the scattering length a using magnetic fields. In such experiments, light scattering may allow one to study dynamically how the pair correlations in a condensate are established in response to a sudden increase in the interaction strength.

3 Amplified scattering of light

3.1 Introduction

In the previous section, we discussed the elementary process in which a photon is inelastically scattered from a condensate and creates a quasi-particle. We focused on the limit of low intensity of the probe light which means that each photon is assumed to probe the “original condensate”. This is valid as long as the quasi-particles created by photon scattering decay or decohere fast enough so that the optical properties of the condensate don’t change.

However, the low temperature and coherent nature of the condensate imply very long decoherence times, leading to long-lived quasi-particles which can affect the scattering of subsequent photons. The presence of long-lived excitations introduces strong correlations between successive Rayleigh scattering events [46]. This provides a positive feedback mechanism and leads to directional amplified Rayleigh scattering.

This non-linear behavior happens already at very low laser intensity. The amplification of the scattering process is stimulated by the matter-wave field analogous to stimulated emission in the optical laser. When this amplification process starts spontaneously, a new form of superradiance is realized (Sect. 3.2). When it is initiated by seeding the condensate with an input matter wave, it leads to coherent atom amplification (Sect. 3.3).

3.2 Superradiant Rayleigh scattering

3.2.1 Semiclassical derivation of the gain mechanism

The gain mechanism for Rayleigh scattering from a condensate can be derived semi-classically. When a condensate of N_0 atoms is exposed to a laser beam with wavevector $\vec{k}_0$ and scatters a photon with wavevector $\vec{k}_i$, an atom (or quasi-particle, also called momentum side-mode in [47]) with recoil momentum $\hbar\vec{K}_j = \hbar(\vec{k}_0 - \vec{k}_i)$ is generated. Since light propagates at a velocity about ten orders of magnitude greater than the atomic recoil velocity (3 cm/s for sodium), the recoiling atoms remain within the volume of the condensate long after the photons have left and affect subsequent scattering events. They interfere with the condensate at rest to form a moving matter wave grating of wavevector $\vec{K}_j$, which diffracts the laser

beam into the phase-matching direction $\vec{k}_i$ ($= \vec{k}_0 - \vec{K}_j$). This diffraction is a self-amplifying process because every diffracted photon creates another recoiling atom which further increases the amplitude of the matter wave grating.

When N_j recoiling atoms interfere with N_0 condensate atoms, the density modulation comprises $N_{\text{mod}} = 2\sqrt{N_0 N_j}$ atoms. The light scattered by these atoms interferes constructively in the phase-matching direction with a total power P of

$$P = \hbar\omega f_j R \frac{N_{\text{mod}}^2}{4}, \quad (3.1)$$

$$f_j = \frac{\sin^2 \theta_j}{8\pi/3} \Omega_j. \quad (3.2)$$

Here, R is the rate for single-atom Rayleigh scattering which is proportional to the laser intensity, and ω is the frequency of the radiation. The angular term in equation (3.2) reflects the dipolar emission pattern with θ_j being the angle between the polarization of the incident light and the direction of emission. Due to the finite size of the sample, the phase matching condition is fulfilled over the solid angle $\Omega_j \sim \lambda^2/A$, where A is the cross-sectional area of the condensate perpendicular to the direction of the light emission and λ the optical wavelength. More rigorously, Ω_j is given by the usual phase-matching integral for superradiance in extended samples [48]:

$$\Omega_j = \int d\Omega(\vec{k}) \left| \int \tilde{\rho}(\vec{r}) \exp^{i(\vec{k}_i - \vec{k}) \cdot \vec{r}} d\vec{r} \right|^2, \quad (3.3)$$

where $|\vec{k}| = |\vec{k}_i|$, and $\tilde{\rho}(\vec{r})$ is the normalized density distribution of the condensate ($\int \tilde{\rho}(\vec{r}) d\vec{r} = 1$).

Since each scattered photon creates a recoiling atom, we obtain the growth rate for N_j from $P/\hbar\omega$:

$$\dot{N}_j = G_j N_j. \quad (3.4)$$

This equation predicts exponential growth of N_j with the small-signal gain $G_j = RN_0 f_j \sim R \sin^2 \theta_j D_j$, where $D_j \sim \rho_0 \lambda^2 l_j$ is the resonant optical density for a condensate with an atomic density ρ_0 and a length l_j along the axis of emission. Therefore, for an anisotropic Bose condensate, the gain is largest when the light is emitted along its longest axis (the “end-fire mode” [49]). Equation (3.4) is valid in the absence of decoherence and predicts the build-up of highly anisotropic Rayleigh scattering from a non-spherical sample of atoms.

The built-up of a matter-wave grating dramatically changes the optical properties of the condensate — the condensate becomes “reflective”.

This property is only due to the coherent nature of the condensate. This phenomenon is completely different from the reflectivity caused by polaritons which depends on the dipole-dipole interaction of excited atoms and requires high atomic densities [8, 9].

3.2.2 Four-wave mixing of light and atoms

Further insight is obtained by describing the scattering process fully quantum-mechanically. As discussed in Section 2.1.1, the Hamiltonian $\mathcal{H}'$ describes light scattering as a coupling (*i.e.* a four-wave mixing) between two Schrödinger (matter) waves and two electromagnetic waves. It is convenient to rewrite $\mathcal{H}'$ by choosing to quantize the recoiling atoms in the volume of the condensate and use plane waves for the light. The important terms in $\mathcal{H}'$ include the macroscopically occupied initial atom field $\hat{a}_0$ (the condensate) and electromagnetic field $\hat{c}_0$ (the incident laser beam with wavevector $\vec{k}_0$), *i.e.* $\mathcal{H}' \simeq C_{i,j} \hat{c}_i^\dagger \hat{a}_j^\dagger \hat{c}_0 \hat{a}_0$ where $\vec{k}_i$ is the wavevector of the outgoing light, and $\hat{a}_j^\dagger$ is the creation operator for an atom in the final state j .

The square of the matrix element which describes the creation of recoiling atoms is proportional to $N_j + 1$ reflecting bosonic stimulation in the atomic field, where N_j is the number of atoms in the final state j . We use Fermi's Golden Rule to sum over all final states of the electromagnetic field which are assumed to be initially empty (spontaneous scattering) and obtain the growth rate of N_j as

$$\dot{N}_j = G_j(N_j + 1) = R N_0 \frac{\sin^2 \theta_j}{8\pi/3} \Omega_j (N_j + 1), \quad (3.5)$$

which is identical to the classical treatment of Section 3.2.1 except that N_j is replaced by $N_j + 1$. The solid angle factor Ω_j now reflects the number of electromagnetic plane wave modes i which are excited together with a quasiparticle in state j localized in the volume of the condensate. Energy conservation requires that the frequency of the scattered light be red-shifted with respect to the incident radiation by the kinetic energy of the recoiling atoms. Equation (3.5) describes both normal Rayleigh scattering at a constant total rate $\Sigma \dot{N}_j = R N_0$ when $N_j \ll 1$, and exponential gain of the j -th recoil mode due to bosonic stimulation once N_j becomes non-negligible. Initially, the angular distribution of the scattered light follows the single-atom spontaneous (dipolar) emission pattern, but can become highly anisotropic when stimulation by the atomic field becomes important.

The choice of plane waves for the scattered light is arbitrary. Another basis set are spherical waves [49]. For the situation considered here it is more convenient to choose orthogonal modes for the different directions of light emission which have diffraction limited beam waists A_j identical to the cross section of the condensate perpendicular to the axis of light

emission (see Ref. [49], p. 45). Therefore, for scattering into a specific direction, one has to consider only the longitudinal “beam waist modes” along the direction of scattering, and their wavevector is determined by energy conservation. Of course, the final result is the same (Eq. (3.5)). The solid angle factor $\Omega_j \propto 1/A_j$ appears in this derivation because the energy density of a single photon in the beam waist is inversely proportional to A_j .

One can account for decoherence and losses by adding a damping term to equation (3.5).

$$\dot{N}_j = G_j(N_j + 1) - D_j N_j. \quad (3.6)$$

As we discuss below, this damping term reflects the finite linewidth of the Bragg resonance and is necessary to account for the observed threshold behavior.

3.2.3 Bosonic stimulation by scattered atoms or scattered light?

In the previous discussion, we evaluated coupling matrix elements assuming that the atoms scatter light always into empty modes of the electromagnetic field, and thus found that bosonic stimulation by the occupied atomic recoil mode was responsible for superradiant light scattering. If the time between light scattering events from the condensate is much longer than the time it takes the scattered photons to leave the condensate, this assumption is clearly justified. But suppose that the Rayleigh scattering rate were increased so that the mean number of scattered photons in the condensate were non-zero. What effect would this have on the observed superradiance? Does the number of photons occupying the scattered light mode lead to additional bosonic stimulation?

To answer this question and, in particular, to clarify the importance of the decay times of the atom and optical modes, let us consider light scattering into just one selected electromagnetic mode which is defined as the mode of a cavity built around the condensate. In the so-called bad cavity limit, we will obtain the results of the previous section.

The two modes of the light and the atoms are labeled as before and coupled by the operator

$$\mathcal{H}' = C \hat{c}_i^\dagger \hat{a}_j^\dagger \hat{c}_0 \hat{a}_0 + \text{h.c.} \quad (3.7)$$

where C denotes the strength of the coupling. In the interaction picture, we obtain coupled equations of motion for the mode operators

$$\frac{d\hat{a}_j}{dt} = -\frac{D_a}{2} \hat{a}_j - (iC\hat{a}_0\hat{c}_0)\hat{c}_i^\dagger \quad (3.8)$$

$$\frac{d\hat{c}_i^\dagger}{dt} = (iC\hat{a}_0^\dagger\hat{c}_0^\dagger)\hat{a}_j - \frac{D_c}{2} \hat{c}_i^\dagger \quad (3.9)$$

D_a and D_c are the damping rates for the number of atoms in mode j and for the number of photons in mode i . Similar coupled equations were considered in references [47, 50]. If the scattered light is strongly damped we can adiabatically eliminate it by setting the l.h.s. of equation (3.9) to zero

$$\hat{c}_i^\dagger = \frac{2iC}{D_c} \hat{a}_0^\dagger \hat{c}_0^\dagger \hat{a}_j. \quad (3.10)$$

Inserting this expression into equation (3.8) leads to a gain equation for the atomic field operator

$$\frac{d\hat{a}_j}{dt} = \frac{1}{2} \left[\frac{4|C|^2}{D_c} N_0 n_0 - D_a \right] \hat{a}_j. \quad (3.11)$$

The field operators for the initial states were replaced by the square root of the occupation numbers N_0 and n_0 for the atoms in the condensate and the photons in the laser beam which leads to an expression for the gain $G = 4(|C|^2/D_c)N_0n_0$.

Alternatively, we can find the eigenvalues $\lambda_{1,2}$ of the matrix in equations (3.8) and (3.9) as

$$\lambda_{1,2} = -\frac{D_a + D_c}{4} \pm \sqrt{\left(\frac{D_a - D_c}{4}\right)^2 + C^2 N_0 n_0}. \quad (3.12)$$

For $C = 0$, the two eigenvalues are $-D_a/2$ and $-D_c/2$. When $D_c \gg D_a$, G , the two eigenvalues are $-D_c/2$ and $\frac{1}{2}[(4|C|^2/D_c)N_0n_0 - D_a]$; this is the result obtained in equation (3.11).

Equations (3.8) and (3.9) can be applied to the free-space situation discussed in the previous section where the optical modes i are the beam-waist modes quantized in a longitudinal box of length L and mode density L/c . The rate of spontaneous emission into the beam waist mode is given by Fermi's golden rule and is proportional to the square of the matrix element times the mode density $|C|^2 N_0 n_0 (L/c)$ and is equivalent to equation (3.5).

On resonance, a cavity of finesse F enhances the density of states by the factor $8F/\pi$ [51]. The cavity walls create mirror images of the radiating atoms which enhance the scattering rate. The number of effective mirror images is proportional to the finesse of the cavity. Therefore, the gain in equation (3.11) is proportional to the rate of spontaneous emission into the solid angle Ω_j and to the finesse of the cavity.

$$G = R N_0 \frac{\sin^2 \theta_j}{8\pi/3} \Omega_j \frac{8F}{\pi}. \quad (3.13)$$

The free-space limit is retrieved by setting the finesse to about unity ($F = \pi/8$) which cancels the last factor in equation (3.13). Or equivalently, free space corresponds to the limit of a cavity with a damping time of about L/c .

This result is useful to discuss bosonic stimulation by the matter wave field and the optical field. The operator describing light scattering (Eq. (3.7)) has a matrix element squared of $|C|^2(N_j + 1)(n_i + 1)N_0n_0$. Since this expectation value is proportional to $(N_j + 1)(n_i + 1)$, it seems that there is bosonic stimulation by both the final atomic state (occupied by N_j atoms) and the final optical state (occupied by n_i photons). However, equations (3.11) and (3.13) show that this notion is incorrect. After adiabatic elimination of the rapidly-damped scattered light we have only stimulation by the atomic field. The superradiant gain G is increased by increasing the finesse of the optical cavity, thus increasing the decay time of the scattered light. However, the gain does not explicitly depend on the number of photons in this mode.

Since the coupled equations have complete symmetry between light and atoms, one can also discuss the complementary case where the atoms are rapidly damped and are adiabatically eliminated. In this case, one obtains a gain equation for the scattered light showing optical stimulation, but not stimulation by the matter wave field in the final state. This situation applies to the optical laser and also to stimulated Brillouin scattering (see also Sect. 3.2.5).

On first sight it appears counterintuitive that bosonic stimulation is not multiplicative if we have a large occupation in both the final photon state and the final atomic state. However, when we have occupancy in all final states, the scattering can go both ways. Thus, let us consider the situation in which there are N_j recoiling atoms and n_i scattered photons in the volume of the condensate, and look at time scales much longer than the coherence time, *i.e.* a situation in which rate equations apply. The process $|n_0, n_i; N_0, N_j\rangle \rightarrow |n_0 - 1, n_i + 1; N_0 - 1, N_j + 1\rangle$ by which atoms scatter out of the condensate into the recoil mode j occurs with a rate proportional to the square of the matrix element $|C|^2(N_j + 1)(n_i + 1)N_0n_0$. The process $|n_0, n_i; N_0, N_j\rangle \rightarrow |n_0 + 1, n_i - 1; N_0 + 1, N_j - 1\rangle$ by which atoms scatter *back into* the condensate has a rate proportional to $|C|^2N_jn_i(N_0 + 1)(n_0 + 1)$. The *net* rate of scattering atoms from the condensate into mode j is the difference of the two partial rates. If we assume $N_0, N_j, n_0 \gg 1$ and also much larger than n_i , since the scattered light was assumed to suffer the strongest damping, we obtain the leading term in the net scattering rate to be proportional to $|C|^2N_jN_0n_0$ as before. The bosonic stimulation by the *least* populated field (mode i) in the matrix element dropped out when the net rate was calculated.

This finding should be generally applicable. For example, when two condensed atoms form molecules by photoassociation or near a Feshbach resonance, the coupled equations involve a matter wave field for the atoms and for the molecules [52,53] which leads to bosonic stimulation in the coupling matrix element and therefore in the partial rate. However, molecules

are the most rapidly damped mode. Therefore the net rate of molecule formation is independent of bosonic stimulation by the particles in the final state and can not distinguish between a coherent molecular matter wave field and an incoherent classical ensemble of molecules in the final state.

Equation (3.8) also describes Bragg scattering where a condensate is exposed to two strong laser beams in modes 0 and i . This results in Rabi oscillations of the atoms between states 0 and j . For short times t , one has $N_j \propto N_0 n_0 n_i t^2$. The scattering rate $\dot{N}_j$ is now proportional to $N_j^{1/2}$ which is incompatible with the simple concept of bosonic stimulation. The simple picture of bosonic stimulation is only obtained when we are in the regime where rate equations apply. This example shows that one has to be careful not to over-interpret the intuitive concept of bosonic stimulation. It can be misleading to use this concept in the case of coherently coupled fields. It can be applied to the situation where one of the fields (either the atomic or the optical one) is strongly damped, but then there is bosonic stimulation of the net scattering rate *only* by the long-lived field.

3.2.4 Observation of directional emission of light and atoms

For the experimental study of directional Rayleigh scattering, elongated Bose–Einstein condensates were prepared in a magnetic trap [37]. The trapped condensates were approximately $20\,\mu\text{m}$ in diameter d and $200\,\mu\text{m}$ in length l and contained several million sodium atoms in the $F = 1$ hyperfine ground state. The condensate was exposed to a single off-resonant laser pulse which was red-detuned by 1.7 GHz from the $3S_{1/2}, F = 1 \rightarrow 3P_{3/2}, F = 0, 1, 2$ transition. The beam had a diameter of a few millimeters, propagated at an angle of 45 degrees to the vertical axis and intersected the elongated condensate perpendicular to its long axis (Fig. 12). Typical laser intensities were between 1 and $100\,\text{mW}/\text{cm}^2$ corresponding to Rayleigh scattering rates of 45 to $4500\,\text{s}^{-1}$, and the pulse duration between 10 and $800\,\mu\text{s}$. In order to probe the momentum distribution of scattered atoms, the magnetic trap was suddenly turned off immediately after the light pulse, and the ballistically expanding cloud was imaged after 20 to 50 ms time-of-flight using resonant probe light propagating vertically onto a CCD camera.

The momentum distributions of atoms after light scattering (Fig. 12B–G) showed a dramatic dependence on the polarization of the incident laser beam. For polarization parallel to the long axis of the elongated condensate ($\theta_j = 0$), light emission into the end-fire mode was suppressed, and the distribution of atoms followed the dipolar pattern of normal Rayleigh scattering. For perpendicular polarization ($\theta_j = \pi/2$), photons were predominantly emitted along the long axis of the condensate where the superradiant gain was the largest. The recoiling atoms appeared as highly directional beams propagating at an angle of 45 degrees with respect to this axis.

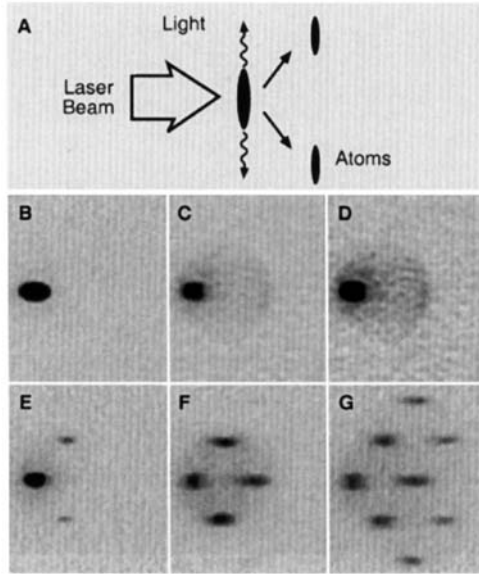


Fig. 12. Observation of superradiant Rayleigh scattering. (A) An elongated condensate is illuminated with a single off-resonant laser beam. Collective scattering leads to photons scattered predominantly along the axial direction, and atoms at 45 degrees. (B–G) Absorption images after 20 ms time-of-flight show the atomic momentum distribution after their exposure to a laser pulse of variable duration. When the polarization was parallel to the long axis, superradiance was suppressed, and normal Rayleigh scattering was observed (B–D). For perpendicular polarization, directional superradiant scattering of atoms was observed (E–G), and evolved to repeated scattering for longer laser pulses (F,G). The pulse durations were 25 (B), 100 (C,D), 35 (E), 75 (F), 100 μ s (G). The field of view of each image is 2.8×3.3 mm. The scattering angle appears larger than 45 degrees due to the angle of observation. All images use the same gray scale except for (D), which enhances the small signal of Rayleigh scattered atoms in (C). Reprinted with permission from reference [32], copyright 1999 American Association for the Advancement of Science.

A characteristic feature of superradiance is an accelerated decay of the initial state. In our experiment, normal exponential decay and the superradiant decay could be directly compared by tracing the number of atoms remaining in the condensate at rest after exposure to light of different polarizations. For parallel polarization, we observed a simple exponential decay with the expected Rayleigh scattering rate (Fig. 13). For perpendicular

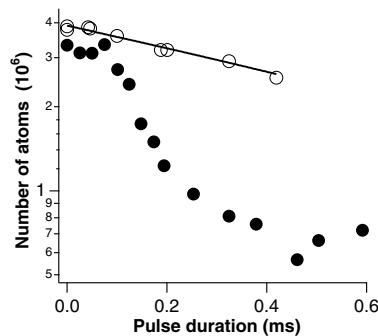


Fig. 13. Exponential and superradiant decay. The decay of atoms in the condensate at rest showed the normal exponential decay for parallel polarization (open circles) and faster superradiant decay for perpendicular polarization (full circles). The laser intensities (13 mW/cm^2) and oscillator strengths were equal in both cases. Reprinted with permission from reference [32], copyright 1999 American Association for the Advancement of Science.

polarization, the end-fire mode was active and the condensate decayed non-exponentially with a strongly accelerated superradiant rate.

The directional scattering of atoms implies that the light is scattered preferentially into the axial direction. This was verified by observing the scattered light with a CCD camera (Fig. 14A). The camera was positioned out of focus of the imaging system, so that the images represent the angular distribution of photons emitted around the axial direction. The images consisted of bright spots with angular widths equal to the diffraction limit for a source with a diameter $\sim 14 \mu\text{m}$. Typical images showed more than one such spot, and their pattern changed randomly under the same experimental conditions. The observation of a few spots is consistent with a Fresnel number $F = \pi d^2 / 4\lambda l$ slightly larger than one, implying that the geometric angle d/l is larger than the diffraction angle λ/d . $F > 1$ leads to multimode superradiance [54] since there is now more than one end-fire mode.

By replacing the camera with a photomultiplier, a time-resolved measurement of the scattered light intensity was obtained (Fig. 14B). Simple Rayleigh scattering would give a constant signal during the square-shaped laser pulse. Instead, we observed a fast rise and a subsequent decay consistent with a stimulated process. Measurements at variable laser intensities showed a threshold for the onset of superradiance, and a shorter rise time for higher laser intensities. This behavior can be accounted for by equation (3.6).

We determined the exponential rate ($G_j - D_j$) by fitting the initial rise in the light intensity. At early times the depletion of the condensate

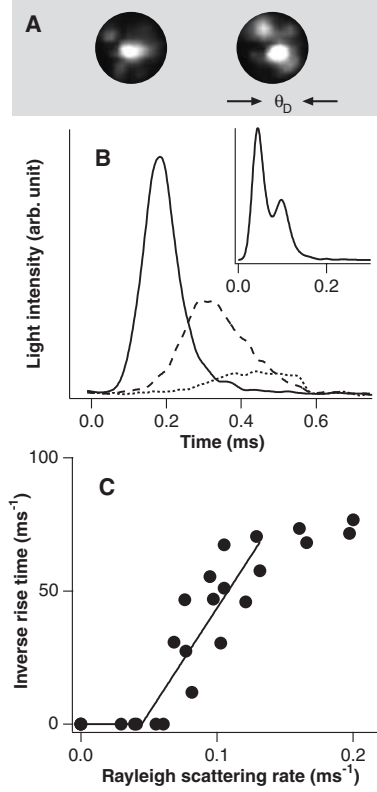


Fig. 14. Observation of directional emission of light. (A) The angular pattern of the emitted light along the axial direction showed a few bright spots with an angular width θ_D ($1/e^2$ diameter) of 107 ± 20 mrad, corresponding to the diffraction limited angle of an object of $\sim 14 \mu\text{m}$ in diameter. The images were integrated over the entire duration of the light pulse. (B) The temporal evolution of the light intensity showed a strong initial increase characteristic of a stimulated process. For higher laser power, the pulse was shorter and more intense. The laser intensities were 3.8 (solid line), 2.4 (dashed line), and 1.4 mW/cm^2 (dotted line), and the duration was $550 \mu\text{s}$. The inset shows a double-peak in the temporal signal when the laser intensity was about 15 mW/cm^2 , which was above the threshold for sequential superradiant scattering. The photomultiplier recorded the light over an angle of 200 mrad around the axial direction. (C) The dependence of the inverse initial rise time on the Rayleigh scattering rate shows a threshold for the stimulated process. The solid curve is a straight-line fit. Reprinted with permission from reference [32], copyright 1999 American Association for the Advancement of Science.

is negligible and G_j and D_j are constants. Figure 14C shows the inverse rise time $\dot{N}/N$ *vs.* the Rayleigh scattering rate R , which was measured by “switching off” the superradiance using parallel polarization. The slope gives G_j/R and the offset determines the loss L_j . The agreement between the calculated value for $G_j/R \sim 890$ (using $\Omega_j \sim 1.9 \times 10^{-4}$ and $N_0 = 4.7 \times 10^6$) and the result of the simple linear fit (790) is better than the uncertainty in the Rayleigh scattering rate (40%). The offset in Figure 14C determines the threshold for superradiance and yields $1/D_j = 35 \mu\text{s}$.

The rate of decoherence D_j for the superradiance indicates the decay of the matter wave interference. This has been studied separately using stimulated Rayleigh scattering (or Bragg spectroscopy) [10], where the linewidth of the Bragg resonance resulted from Doppler and mean-field broadening. The observed FWHM of approximately 5 kHz yields a decoherence time of 32 μs , in good agreement with the value shown above.

For higher laser powers, a distinct change in both the momentum pattern of the atoms (Figs. 12F,G) and in the photomultiplier traces (Fig. 14B) was observed. The atomic pattern showed additional momentum peaks which can be explained as a sequential scattering process where atoms in the initial momentum peak undergo further superradiant scattering. These processes are time-delayed with respect to the primary process, and showed up as a second peak in the time-resolved photomultiplier traces (Fig. 14B). Those higher-order peaks may also be affected by stimulated Raman scattering and four-wave mixing between matter waves [39] which couple the different recoil modes.

3.2.5 Relation to other non-linear phenomena

The directional emission of light and atoms described in the previous sections is analogous to the superradiance discussed by Dicke [49]. He considered an elongated radiating system of incoherently electronically excited atoms, and showed that this system realizes “a laser which does not employ mirrors in order to produce feedback amplification”. The amplification of this “Coherence brightened laser” is provided by electronic coherence: “the memory of the previously emitted electromagnetic field is burned into the radiating system rather than being sent back into the radiating system by the use of mirrors [49]”. The key feature of superradiance (or superfluorescence) [54–58] is that spontaneous emission is not a single-atom process, but a collective process of all atoms, leaving the atoms in a coherent superposition of ground and excited states [59]. The condensate at rest “pumped” by the off-resonant laser corresponds to the electronically excited state in the Dicke case. It can decay by a spontaneous Raman process to a state with photon recoil (corresponding to the ground state). The rate of superradiant emission in Dicke’s treatment is proportional to the square of an oscillating macroscopic dipole moment. In the present case, the radiated intensity is

proportional to the square of the contrast of the matter wave interference pattern between the condensate and the recoiling atoms, which then gives a spatially periodic electric polarization in the presence of the driving laser field. In both cases, the initial emission of light shows the single atom dipole pattern. Quantum noise and spontaneous emission create spatial coherence and lead to directional emission different from forward scattering.

The situation of an atom cloud with a small excited state admixture (“dressed” condensate) nicely demonstrates the analogy between the optical laser and the atom laser. If the emitted light is allowed to build up in a cavity, an optical laser is realized (called the Coherent Atomic Recoil Laser (CARL) [60–62]). If the matter wave field builds up in a cavity, it realizes an atom laser by optical pumping [63–65]. In our experiment, the matter wave field builds up in a traveling wave even without a cavity because of the slow motion of the recoiling atoms.

For smaller momentum transfer, the nature of the quasi-particles in the condensate will change from recoiling atoms to phonons. The observed phenomenon is therefore related to stimulated Brillouin scattering which was called “phonon maser action” [66] due to the amplification of sound waves. However, the analogy is closest when the roles of light and atoms are exchanged. In Brillouin scattering, the optical field builds up, whereas the phonon field generated by the momentum transfer is usually rapidly damped and adiabatically eliminated from the equations. In our case, the matter wave field builds up and the optical field can be eliminated due to the fact that light propagates at a velocity which is ten orders of magnitude faster than the atomic recoil velocity.

The observed phenomenon differs from other stimulated processes like Brillouin scattering and Dicke superradiance in two regards. In those cases, the electromagnetic field is treated either classically, or spontaneous emission (“quantum noise”) is needed only to initiate the process, which then evolves classically after many photons have been accumulated. In our case, all of the light is emitted spontaneously, *i.e.* without *optical* stimulation. Furthermore, our system gives rise to a “cascade” of superradiant scattering processes which does not exist in the two-level superradiance systems studied so far.

More generally, one can regard the observed superradiance as an instability against spatial pattern formation triggered by noise. The spatial pattern is the periodic density modulation, the noise is the quantum noise which leads to spontaneous scattering. Spontaneous pattern formation is an interesting non-linear phenomenon studied in fluid mechanics, optics and chemical reactions [67].

Superradiance is based on the coherence of the emitting system, but it does not require quantum degeneracy. The condition for superradiance is that the gain exceed the losses, or that the superradiant decay time

be shorter than any decoherence time. Above the BEC transition temperature T_c , thermal Doppler broadening results in a thirty times shorter decoherence time than for a condensate. Further, the larger size of the thermal cloud reduces the solid angle Ω_j and therefore the gain by another factor of ten. Therefore, the threshold for superradiance in a thermal cloud is several orders of magnitude higher than for a condensate. No signs of superradiant scattering were observed above T_c ; rather, the sudden appearance of superradiant emission was a sensitive indicator for reaching the phase transition.

3.3 Phase-coherent amplification of matter waves

Atom amplification differs from light amplification in one important aspect. Since the total number of atoms is conserved (in contrast to photons), the active medium of a matter wave amplifier has to include a reservoir of atoms. One also needs a coupling mechanism which transfers atoms from the reservoir to an input mode while conserving energy and momentum. The gain mechanism which was explained above can act as a matter wave amplifier. The momentum required to transfer atoms from the condensate at rest to the input mode is provided by light scattering. References [47, 50] discussed that a condensate pumped by an off-resonant laser beam acts as a matter wave amplifier which can amplify input matter waves within the momentum range which can be reached by scattering a single pump photon.

The inversion in this matter wave amplifier is most apparent in the dressed atom picture where the condensate at rest and the pump light field are treated as one system. An atom in the dressed condensate can now spontaneously decay into a recoiling atom and a scattered photon which escapes. Inversion is maintained since the photons escape and thus the inverse process of combining recoiling atom and emitted photon into a dressed atom at rest is not possible. Thus, in principle, a complete transfer of the condensate atoms into the recoil mode can occur.

Our observation of superradiance can be regarded as the observation of matter wave amplification of noise, *i.e.* of spontaneously scattered atoms. To examine this amplification mechanism further, we performed an experiment in which, rather than examine the amplification of noise, we amplify a well-defined input signal, *i.e.* a matter wave of well-defined momentum which was generated by Bragg scattering. By comparing the input and output waves, we could characterize the amplification process.

The input atoms were generated by exposing the condensate to a pulsed optical standing wave which transferred a small fraction of the atoms (between 10^{-4} and 10^{-2}) into a recoil mode by Bragg diffraction [10, 15]. Both laser beams were red-detuned by 1.7 GHz from the $3S_{1/2}, |F=1\rangle \rightarrow 3P_{3/2}, |F=0, 1, 2\rangle$ transition to suppress normal Rayleigh scattering. The geometry of the light beams is shown in Figure 15. The beam which was

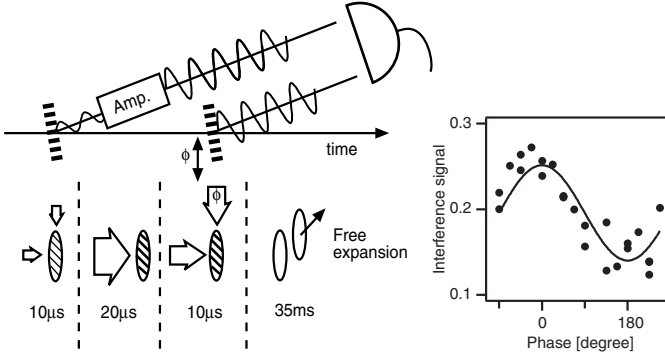


Fig. 15. Experimental scheme for observing phase coherent matter wave amplification. A small-amplitude matter wave was split off the condensate by applying a pulse of two off-resonant laser beams (Bragg pulse). This input matter wave was amplified by passing it through the condensate pumped by a laser beam. The coherence of the amplified wave was verified by observing its interference with a reference matter wave, which was produced by applying a second (reference) Bragg pulse to the condensate. The interference signal was observed after 35 ms of ballistic expansion. The fringes on the right side show the interference between the amplified input and the reference matter wave. Reprinted by permission from Nature, reference [68], copyright 1999 Macmillan Magazines Ltd.

perpendicular to the long axis of the condensate (radial beam) was blue detuned by 50 kHz relative to the axial beam. This detuning fulfilled the Bragg resonance condition.

Amplification of the input matter wave was realized by applying an intense radial pump pulse for the next 20 μs with a typical intensity of 40 mW/cm^2 . The number of atoms in the recoil mode was determined by suddenly switching off the trap and observing the ballistically expanding atoms after 35 ms of time-of-flight using resonant absorption imaging. After the expansion, the condensate and the recoiling atoms were fully separated (Fig. 16c).

Figure 16 shows the input-output characteristics of the amplifier. The number of input atoms was below the detection limit of our absorption imaging (Fig. 16a) and was determined from a calibration of the Bragg process at high laser powers, where the diffracted atoms were clearly visible in the images. The amplification pulse alone, although above the threshold for superradiance [32], did not generate a discernible signal of atoms in the recoil mode (Fig. 16b). When the weak input matter wave was added, the amplified signal was clearly visible (Fig. 16c). The gain was controlled by the intensity of the pump pulse (see Eq. (3.11)) and typically varied

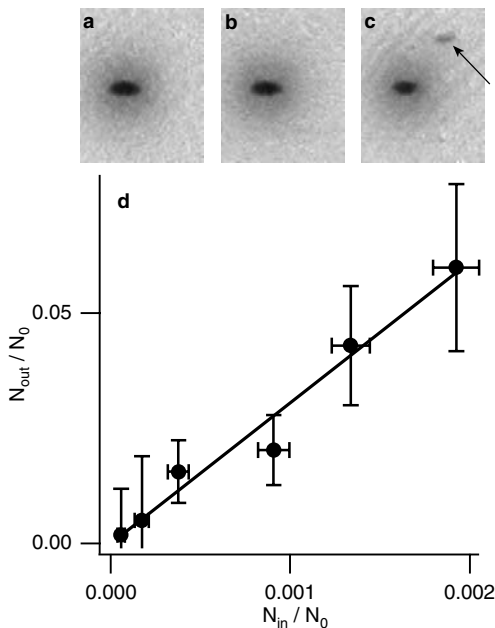


Fig. 16. Input–output characteristic of the matter-wave amplifier. (a–c) Typical time-of-flight absorption images demonstrating matter wave amplification. The output of the seeded amplifier (c) is clearly visible, whereas no recoiling atoms are discernible in the case without amplification (a) or amplification without the input (b). The size of the images is 2.8 mm $\times$ 2.3 mm. (d) Output of the amplifier as a function of the number of atoms at the input. A straight line fit shows a number gain of 30. Reprinted by permission from Nature, reference [68], copyright 1999 Macmillan Magazines Ltd.

between 10 and 100. Figure 16d shows the observed linear relationship between the atom numbers in the input and the amplified output with a number gain of 30.

The phase of the amplified matter wave was determined with an interferometric technique (Fig. 15). For this, a reference matter wave was split off the condensate in the same way as the first (input) wave. The phase of the reference matter wave was scanned by shifting the phase of the radio-frequency signal that drove the acousto-optic modulator generating the axial Bragg beam. We then observed the interference between the reference and the amplified matter waves by measuring the number of atoms in the recoil mode.

When the input was comparable in intensity to the reference matter wave, high contrast fringes were observed even without amplification.

Fringes were barely visible when the input was about 40 times weaker in population. After amplification, we regained a large visibility (Fig. 15). This increase in visibility proved the coherent nature of the matter wave amplification process. The increase in visibility of the interference fringes was a factor of two, less than the expected square root of the total gain of thirty. This might be due to a distortion of the matter wave during the amplification, but this effect requires further study. A similar experiment with rubidium atoms was done at the University of Tokyo [69].

This experiment can be regarded as a demonstration of an active atom interferometer. It realizes a two-pulse atom interferometer with phase-coherent amplification in one of the arms. Such active interferometers may be advantageous for precise measurements of phase shifts in highly absorptive media, *e.g.* for measurements of the index of (matter wave) refraction when a condensate passes through a gas of atoms or molecules [70]. Since the most accurate optical gyroscopes are active interferometers [71], atom amplification might also play a role in future matter-wave gyroscopes [72].

4 Spinor Bose–Einstein condensates

The experiments described in the previous sections explored the nature of Bose–Einstein condensates of atomic gases in which all the atoms were in the same internal state, in particular, the $|F = 1, m_F = -1\rangle$ hyperfine state of sodium. The Bose–Einstein condensation phase transition leads to a non-zero value of a *scalar* order parameter, the condensate wavefunction $\psi(\vec{r}) = \langle \hat{\Psi}(\vec{r}) \rangle$. As such, a single-component gaseous condensate can be considered as a simple, tractable model of the more complicated spinless superfluid ^4He . Many experiments in recent years have explored aspects of this connection between the two quantum fluids [1].

However, unlike ^4He , alkali atoms can have a non-zero spin and therefore numerous internal hyperfine states which are stable electronic ground states. Thus, there exists the possibility of creating a quantum fluid simultaneously composed of several, distinguishable components by Bose condensing a gas of atoms in several hyperfine states.

The study of multi-component superfluid systems has been a tantalizing goal of low-temperature physics for decades. The earliest discussion focused on $^4\text{He} - ^6\text{He}$ mixtures. ^6He is radioactive with a half-life of 1 second. An ambitious experiment by Guttman and Arnold [73] in 1953 sought evidence for the superfluid flow of ^6He mixed with ^4He to no avail. Nevertheless, this pursuit touched off a series of theoretical works on two-component superfluid hydrodynamics ([74], and others since). In 1978, Colson and Fetter [75] considered such mixtures in the context of mean-field theories which apply directly to current experiments, and discussed the criterion for interactions between the superfluids to cause miscibility or

phase-separation. After progress in the stabilization of a spin-polarized atomic hydrogen gas, Siggia and Ruckenstein [76] considered the use of different hyperfine states to achieve a mixture of superfluids. Since the observation of gaseous Bose condensates, the interest in multi-component condensates has been revived with a flurry of theoretical attention [77–80, for example].

For atomic gases in magnetic traps, the availability of hyperfine states is restricted by the requirement that the trapped atoms remain in weak-field seeking states. For example, alkali atoms with a nuclear spin of $I = 3/2$, such as ^{87}Rb and ^{23}Na , have three weak-field seeking states at zero-field: one in the lower hyperfine manifold ($|F = 1, m_F = -1\rangle$), and two in the upper hyperfine manifold ($|F = 2, m_F = 1, 2\rangle$). Generally, the simultaneous confinement of more than one of these states is unstable against exothermic hyperfine state changing collisions.

However, it was recently found that magnetically-trapped multi-component gases of ^{87}Rb are quite long lived due to a fortunate near-equality of the singlet and triplet scattering lengths which greatly suppresses the spin exchange collision rate [81–84]. This allowed for the creation of multi-component condensates by the simultaneous magnetic confinement of ^{87}Rb atoms in the $|F = 1, m_F = -1\rangle$ and $|F = 2, m_F = 2\rangle$ [81] (and, in later work, $|F = 2, m_F = 1\rangle$) states. The Boulder group has used magnetically trapped multi-component condensates for a remarkable series of experiments. Studies have probed the spatial separation of a two-component Bose–Einstein condensate [81, 85] and the stability of a relative phase between the two components even in the presence of dissipation [86]. The Boulder group has also explored the nature of multi-component condensates in the presence of continuous resonant and non-resonant rf coupling between the components. Such coupling links the external center-of-mass and the internal degrees of freedom of the condensed gas and gives rise to a rich variety of dynamical effects such as Josephson-type oscillations [87] and spin-wave excitations [88, 89], as well as new techniques for manipulating the phase of the condensate wavefunction [90, 91]. Some of this work is reviewed in references [92, 93].

In contrast, a far-off-resonant optical trap confines atoms regardless of their hyperfine state [44]. Thus, the atomic spin is liberated from the requirements of magnetic trapping and becomes a new degree of freedom. In particular, all atoms in the lower hyperfine manifold, for example the $F = 1$ hyperfine manifold of sodium, can be stably trapped simultaneously without suffering from hyperfine manifold changing collisions. Such multi-component optically trapped condensates are represented by an order parameter which is a *vector* in hyperfine spin space, and are thus called spinor Bose–Einstein condensates. A variety of new phenomena are

predicted for this new quantum fluid such as spin textures, spin waves, and coupling between atomic spin and superfluid flow [94–96].

Spinor Bose condensates differ from other multi-component Bose condensates, such as the experimentally realized ^{87}Rb mixtures or the proposed mixtures of several atomic species, in important ways stemming from symmetries under rotations of the vectorial order parameter. Furthermore, spin relaxation collisions within the lower $F = 1$ hyperfine manifold

$$|m_F = 0\rangle + |m_F = 0\rangle \leftrightarrow |m_F = +1\rangle + |m_F = -1\rangle \quad (4.1)$$

allow for population mixing among the different hyperfine states without trap loss. In contrast, spin relaxation is the major limitation to the lifetime (about a second) of the ^{87}Rb mixtures.

Since the realization of an optical trap for Bose–Einstein condensates [44], our group has performed several experimental studies of this new quantum fluid. In three different experiments we explored the ground-state spin structure of spinor condensates in external magnetic fields [97], the formation and persistence of metastable spin domain configurations [98], and the transport across spin domain boundaries by quantum tunneling [99]. In this section, we summarize our current understanding of this fluid as derived from our experiments and from a growing number of theoretical works. While a portion of this work has been reviewed in references [1, 100], this section is the first comprehensive review on spinor Bose–Einstein condensates.

4.1 *The implications of rotational symmetry*

An $F = 1$ spinor Bose–Einstein condensate is described by a three-component order parameter

$$\vec{\psi}(\vec{r}) = \begin{pmatrix} \psi_1(\vec{r}) \\ \psi_0(\vec{r}) \\ \psi_{-1}(\vec{r}) \end{pmatrix} \quad (4.2)$$

and can thus be regarded as a particular instance of a multi-component condensate. Here, the subscripts refer to the spin projection on the quantization axis, $m_F = -1, 0, +1$. However, the spinor Bose–Einstein condensate is distinguished from a general, multi-component quantum fluid by the fact that the order parameter $\vec{\psi}$ transforms as a vector. The vectorial character of the order parameter has a pronounced effect on interatomic interactions, and defines important features of the spinor condensate at zero magnetic field, where the rotational symmetry of the system is preserved.

In second-quantized notation, the Hamiltonian for a multi-component gas has the general form

$$\hat{\mathcal{H}} = \int d^3\vec{r} \left\{ \hat{\Psi}_i^\dagger(\vec{r}) \left(-\frac{\hbar^2 \nabla^2}{2m} \delta_{ij} + U_{ij}(\vec{r}) \right) \hat{\Psi}_j(\vec{r}) + \frac{g_{ij,kl}}{2} \int d^3\vec{r}_1 d^3\vec{r}_2 \hat{\Psi}_i^\dagger(\vec{r}_1) \hat{\Psi}_j^\dagger(\vec{r}_2) \hat{\Psi}_k(\vec{r}_2) \hat{\Psi}_l(\vec{r}_1) \delta(\vec{r}_1 - \vec{r}_2) \right\} \quad (4.3)$$

where the indices i, j, k, l correspond to the N components of the gas, and repeated indices are summed. The general form of the external potential $U_{ij}(\vec{r})$ allows for a potential which is not diagonal in the hyperfine spin basis, in which case it can represent a Josephson-type coupling between spin components. The $U_{ij}(\vec{r})$ terms also contain the effects of magnetic fields which are discussed in later sections.

The interatomic interaction (second line of the above expression) has been approximated as a contact interaction in which the coefficients $g_{ij,kl}$ describe the strength of the various elastic and inelastic (state converting) collisions. These generally constitute a large number of free parameters. Particle exchange ($g_{ij,kl} = g_{ji,kl}$) and time-reversal ($g_{ij,kl} = g_{kl,ij}$) symmetries reduce the number of free parameters from N^4 to $[(N^2 + N + 2)(N^2 + N)]/8$ but still a large number of interaction parameters remain³. For a three-component condensate, the number of interaction parameters is 21.

This situation is greatly simplified in the case of spinor condensates due to rotational symmetry. The rotationally symmetric characterization of two-body collisions among atoms of hyperfine spin F_1 and F_2 can only depend on their total spin $f = F_1 + F_2$ and not on its orientation. Thus, in the s -wave limit, the interatomic interaction $V_{\text{int}}(\vec{r}_1 - \vec{r}_2)$ is reduced to the form [94, 95]

$$V_{\text{int}}(\vec{r}_1 - \vec{r}_2) = \frac{4\pi\hbar^2}{m} \delta(\vec{r}_1 - \vec{r}_2) \sum_f a_f \tilde{\mathcal{P}}_f \quad (4.4)$$

where a_f is the scattering length for collisions between atoms with total spin f , and $\tilde{\mathcal{P}}_f$ is the projection operator for the total spin. For colliding bosons of spin F , f can take the values $f = 0, 2, \dots, 2F$. Therefore, the interaction parameters $g_{ij,kl}$ describing collisions among the $N = 2F + 1$ different components of a spinor condensate of spin F depend only on $F + 1 = (N + 1)/2$ scattering lengths.

³Due to particle exchange symmetry, we may denote the interaction parameter as $g_{\mathcal{A},\mathcal{B}}$ where $\mathcal{A}$ and $\mathcal{B}$ are elements of the set $\mathbb{P}$ of distinct unordered pairs of indices i, j . There are $Z = N(N + 1)/2$ such pairs. Due to time-reversal symmetry, the interaction parameters are enumerated as g_Z where Z is an unordered pair of elements from $\mathbb{P}$. Thus, the number of free interaction parameters is $Z(Z + 1)/2 = [(N^2 + N + 2)(N^2 + N)]/8$.

Table 3. Interaction parameters $g_{ij,kl}$ describing elastic collisions in the $F = 1$ spinor system. The interaction Hamiltonian is defined as in equation (4.3). The interaction parameter responsible for spin relaxation is $g_{00,-1+1} = g_2$. The cross-species scattering length discussed in Section 4.6 is given as $g_{\text{AB,AB}} = 2\pi\hbar^2 a_{\text{AB}}/m$.

$g_{\text{AB,AB}}$	$m_F = +1$	$m_F = 0$	$m_F = -1$
$m_F = +1$	$g_0 + g_2$	$\frac{g_0 + g_2}{2}$	$\frac{g_0 - g_2}{2}$
$m_F = 0$	$\frac{g_0 + g_2}{2}$	g_0	$\frac{g_0 + g_2}{2}$
$m_F = -1$	$\frac{g_0 - g_2}{2}$	$\frac{g_0 + g_2}{2}$	$g_0 + g_2$

In particular, for the $F = 1$ spinor system which was realized in gaseous sodium, interactions are described fully by just two parameters, the scattering lengths $a_{f=0}$ and $a_{f=2}$. The interaction potential can then be written as

$$V_{\text{int}}(\vec{r}_1 - \vec{r}_2) = \left(g_0 + g_2 \vec{F}_1 \cdot \vec{F}_2 \right) \delta(\vec{r}_1 - \vec{r}_2) \quad (4.5)$$

where the parameters g_0 and g_2 are defined as

$$g_0 = \frac{4\pi\hbar^2}{m} \frac{2a_{f=2} + a_{f=0}}{3} \quad (4.6)$$

$$g_2 = \frac{4\pi\hbar^2}{m} \frac{a_{f=2} - a_{f=0}}{3} \quad (4.7)$$

and $\vec{F}_1$ and $\vec{F}_2$ are the spin operators for the two colliding particles. The spin-dependence of the interatomic interaction is thereby isolated in the rotationally-symmetric term $g_2 \vec{F}_1 \cdot \vec{F}_2 \delta(\vec{r}_1 - \vec{r}_2)$. The Hamiltonian describing a weakly-interacting Bose gas of spin $F = 1$ now becomes [94,95]

$$\begin{aligned} \hat{\mathcal{H}} = \int d^3\vec{r} \left\{ \hat{\Psi}_i^\dagger(\vec{r}) \left(-\frac{\hbar^2 \nabla^2}{2m} \delta_{ij} + V_{ij}(\vec{r}) \right) \hat{\Psi}_j(\vec{r}) \right. \\ \left. + \frac{1}{2} \left[g_0 \hat{\Psi}_i^\dagger(\vec{r}) \hat{\Psi}_j^\dagger(\vec{r}) \hat{\Psi}_i(\vec{r}) \hat{\Psi}_j(\vec{r}) \right. \right. \\ \left. \left. + g_2 \left(\hat{\Psi}_i^\dagger(\vec{r}) (F_\eta)_{ij} \hat{\Psi}_j(\vec{r}) \right) \cdot \left(\hat{\Psi}_k^\dagger(\vec{r}) (F_\eta)_{kl} \hat{\Psi}_l(\vec{r}) \right) \right] \right\} \quad (4.8) \end{aligned}$$

where the index η runs over the three coordinate axes x, y, z .

Equivalently, the Hamiltonian can be written in the form of equation (4.3), where all non-zero $g_{ij,kl}$ are determined by g_0 and g_2 as shown in Table 3. Taking into account particle exchange symmetries and

gathering similar terms, the interaction Hamiltonian can be written as

$$\begin{aligned} \mathcal{H}_{\text{int}} = & \frac{1}{2} \int d^3\vec{r} \left[(g_0 + g_2) \hat{\Psi}_1^\dagger \hat{\Psi}_1^\dagger \hat{\Psi}_1 \hat{\Psi}_1 + g_0 \hat{\Psi}_0^\dagger \hat{\Psi}_0^\dagger \hat{\Psi}_0 \hat{\Psi}_0 \right. \\ & + (g_0 + g_2) \hat{\Psi}_{-1}^\dagger \hat{\Psi}_{-1}^\dagger \hat{\Psi}_{-1} \hat{\Psi}_{-1} + 2(g_0 + g_2) \hat{\Psi}_1^\dagger \hat{\Psi}_0^\dagger \hat{\Psi}_1 \hat{\Psi}_0 \\ & + 2(g_0 + g_2) \hat{\Psi}_{-1}^\dagger \hat{\Psi}_0^\dagger \hat{\Psi}_{-1} \hat{\Psi}_0 + 2(g_0 - g_2) \hat{\Psi}_1^\dagger \hat{\Psi}_{-1}^\dagger \hat{\Psi}_1 \hat{\Psi}_{-1} \\ & \left. + 2g_2 (\hat{\Psi}_0^\dagger \hat{\Psi}_0^\dagger \hat{\Psi}_1 \hat{\Psi}_{-1} + \hat{\Psi}_1^\dagger \hat{\Psi}_{-1}^\dagger \hat{\Psi}_0 \hat{\Psi}_0) \right]. \end{aligned} \quad (4.9)$$

The first three terms are the self-scattering terms, the following three the cross-scattering terms, and the last line contains the spin relaxation terms.

It is important to note that this simplification of the interaction term is only strictly valid in the absence of magnetic fields. As the magnetic field is increased, the hyperfine spin F is no longer a good quantum number for describing the atomic states, and thus collisional properties deviate from the relations imposed by rotational symmetry. Dramatic deviations from rotational symmetry can be seen, for example, at a Feshbach resonance where the scattering length for one particular collisional channel is greatly varied. Nonetheless, away from Feshbach resonances and at low magnetic fields for which the Zeeman shifts are much smaller than the hyperfine splitting, one can expect the zero-field description of collisional interactions to remain valid.

The properties of spinor Bose-Einstein condensates at zero-magnetic field have been recently discussed by a number of authors. Ho [94] and Ohmi and Machida [95] considered the ground state of a spinor condensate by an extension of mean-field theory (see also [101]). The N -particle condensate ground state is found by replacing the field operators $\hat{\Psi}_i$ in equation (4.8) with c -number order parameters ψ_i . It is convenient to express the order parameter as $\vec{\psi} = \sqrt{n} \vec{\zeta}$ where n is the atomic density and $\vec{\zeta}$ is a three-component spinor of normalization $|\vec{\zeta}| = 1$, obtaining the energy functional

$$E = \int d^3\vec{r} \left[\psi_i^*(\vec{r}) \left(-\frac{\hbar^2 \nabla^2}{2m} \right) \psi_i(\vec{r}) + (U(\vec{r}) - \mu) n(\vec{r}) + \frac{n^2}{2} (g_0 + g_2 \langle \vec{F} \rangle^2) \right]. \quad (4.10)$$

Here it is assumed that the external potential is scalar, *i.e.* diagonal in the hyperfine spin basis and equal for each of the spin components. The chemical potential μ determines the number of atoms in the condensate.

The ground-state spinor $\vec{\zeta}$ is determined by minimizing the spin-dependent interaction energy, $n^2 g_2 \langle \vec{F} \rangle^2 / 2$, which is expressed in terms of the average condensate spin $\langle \vec{F} \rangle_\eta = \zeta_i^* (F_\eta)_{ij} \zeta_j$. There are two distinct

solutions depending on the sign of the spin-dependent interaction parameter g_2 :

- $g_2 > 0$: the collisional coupling is anti-ferromagnetic as the condensate lowers its energy by minimizing its average spin, *i.e.* by making $|\langle \vec{F} \rangle| = 0$. The ground state spinor is then one of a degenerate set of spinors, the “polar” states, corresponding to all possible rotations of the hyperfine state $|m_F = 0\rangle$.
- $g_2 < 0$: the collisional coupling is ferromagnetic as the condensate lowers its energy by maximizing its average spin, *i.e.* by making $|\langle \vec{F} \rangle| = 1$. In this case the ground state spinors correspond to all rotations of the hyperfine state $|m_F = +1\rangle$.

Law *et al.* [96] explicitly calculated the many-body state of a homogeneous spinor Bose–Einstein condensate without assuming a Hartree form. They describe an elegant transformation of the spinor Hamiltonian in terms of operators which obey an angular momentum algebra, and thus immediately yield eigenstates of the many-body Hamiltonian and their energy spectrum. Anti-ferromagnetic coupling leads to a unique ground-state which cannot be represented in the Hartree form and which has super-Poissonian fluctuations in the population of each spin state. Ferromagnetic coupling yields a degenerate family of ground states with sub-Poissonian fluctuations. The Hartree solution with all atoms in the $|m_F = +1\rangle$ state is included in the family of ferromagnetic ground states obtained by Law *et al.*

The highly entangled ground state of Law *et al.* for the anti-ferromagnetic case differs in energy from the ground state in the mean-field formalism (all atoms in the $|m_F = 0\rangle$ state) only by a term which is proportional to N , the number of atoms. This energy is N times smaller than the mean-field energy which scales as N^2 . Therefore, it will be difficult to observe this highly correlated state. For example, several authors have extended the treatment to finite magnetic fields and shown that the singlet state of reference [96] is only the ground state at very small magnetic fields; otherwise the ground state approaches the Hartree form [102, 103].

The scattering lengths $a_{f=0}$ and $a_{f=2}$ can be calculated by incorporating data from a variety of experiments into models of the interparticle potentials. For sodium, it is predicted that $a_{f=2} = 2.75$ nm [104] and $a_{f=2} - a_{f=0} = 0.29$ nm [105]. Thus, an $F = 1$ spinor condensate of sodium should be anti-ferromagnetic. For ^{87}Rb , it appears that $a_{f=2} - a_{f=0} < 0$ and thus an $F = 1$ spinor condensate of ^{87}Rb should be ferromagnetic [94].

4.2 Tailoring the ground-state structure with magnetic fields

These theoretical considerations differ from the conditions in our experiment in two major regards: the imposition of spin conservation, and the effects

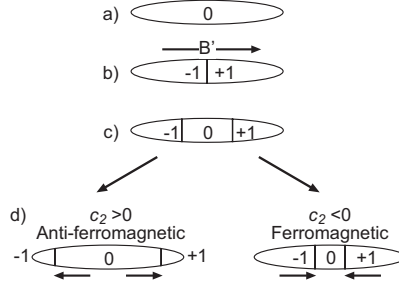


Fig. 17. Constructing the ground-state $\langle F_z \rangle = 0$ spinor in a trap. In each step (a–d), another contribution to the Hamiltonian is considered (see text): a) linear Zeeman shift from homogeneous field, b) linear Zeeman shift from field gradient, c) quadratic Zeeman shift, d) spin-dependent mean-field interaction.

of field inhomogeneities and quadratic Zeeman shifts. These differences are exemplified by considering the outcome of an experiment we performed, in which an optically-trapped Bose condensed cloud was prepared with all atoms in the $|m_F = 0\rangle$ state. The cloud was then allowed to equilibrate to the ground state by spin relaxation and by spatial redistribution [97]. For simplicity, consider only variations in the condensate wavefunction in one dimension, the $\hat{z}$ -direction, and define the coordinate z to give the distance from the center of the condensate. This corresponds to the experimental situation in which the spinor condensates were held in the highly anisotropic, cigar-shaped potential of an optical trap.

Let us consider the evolution of the pure $m_F = 0$ condensate as we slowly add the effects of magnetic fields and mean-field interactions and construct the relevant energy functional (Fig. 17).

- a) *Linear Zeeman shift from homogeneous field.* In a homogeneous magnetic field of strength B_0 , the linear Zeeman energy

$$E_{\text{lin}} = -p \int d^3r n \langle F_z \rangle \quad (4.11)$$

is minimized by placing all atoms in the strong-field seeking $|m_F = +1\rangle$ state (a ferromagnetic state)⁴. Here, $p = g\mu_B B_0$ where g is the Landé g -factor and μ_B is the Bohr magneton.

However, spin non-conserving collisions (dipolar relaxation), which would be necessary to transform the $m_F = 0$ condensate to the

⁴The operator F_z gives the component of the spin along the direction of the magnetic field. This direction need not be the same as the long axis of the trapped condensate.

$m_F = +1$ ground state, are negligible over the lifetime of the condensate. Thus, the total spin is a conserved quantity, and rather than considering the global ground state of the system, one must consider the lowest energy state under the restriction of spin conservation. Formally, one minimizes the restricted energy functional

$$K_{\text{tot}} = E_{\text{tot}} + \tilde{p} \int d^3\vec{r} n \langle F_z \rangle \quad (4.12)$$

where $\tilde{p}$ is a Lagrange parameter determined by the given value of the total spin. For the case where $\int \langle F_z \rangle n d^3\vec{r} = 0$, the linear Zeeman shift of a homogeneous magnetic field (E_{1Z}) is exactly canceled ($p_0 = \tilde{p}$).

This is an important point: spin conservation allows one to study the effects of the small spin-dependent interaction energies even at magnetic fields for which the linear Zeeman energy would otherwise be dominant. For example, in the case of sodium, the spin-dependent mean-field energy is just $c_2 n \simeq h \times 50$ Hz for a typical density of $n = 3 \times 10^{14} \text{ cm}^{-3}$. Thus, without the restriction of spin conservation, the ground-state spinor would trivially consist of all atoms in the $|m_F = +1\rangle$ state at a magnetic field of just $70 \mu\text{G}$, and any interesting structure, correlations or dynamics due to the anti-ferromagnetic coupling would be obscured. However, due to spin conservation, many of these effects can be studied even in the absence of such demanding field stability.

- b) *Linear Zeeman shift from field gradient.* A field gradient B' along the long axis of the condensate introduces an energy term

$$E_{\text{grad}} = - \int d^3\vec{r} p(z) n \langle F_z \rangle \quad (4.13)$$

with $p(z) = g\mu_B B' z$, which makes it energetically favorable for two $m_F = 0$ atoms to collide and produce a $m_F = +1$ atom on the high-field end of the cloud, and a $m_F = -1$ atom on the low-field end. Thus, the condensate is magnetically polarized into two pure spin domains.

- c) *Quadratic Zeeman shift from homogeneous field.* The quadratic Zeeman shift at a field B_0 introduces an energy term of the form

$$E_{\text{quad}} = q \int d^3\vec{r} n \langle F_z^2 \rangle \quad (4.14)$$

which causes the energy of a $m_F = 0$ atom to be lower than the average energy of a $m_F = +1$ and $m_F = -1$ atom by an amount $q = \hat{q} B_0^2$. For sodium, $\hat{q} = h \times 390 \text{ Hz/G}^2$. The quadratic Zeeman energy favors

population in the $|m_F = 0\rangle$ state, and thus introduces an $m_F = 0$ domain at the center of the cloud with boundaries at $q = |p(z)|$ (see Fig. 17c).

- d) *Spin-dependent mean-field interaction.* As discussed previously, the collisional interactions give a spin-dependent energy term of the form

$$E_{\text{int}} = \frac{1}{2} \int d^3\vec{r} g_2 n^2 \langle \vec{F} \rangle^2. \quad (4.15)$$

Anti-ferromagnetic coupling ($g_2 > 0$) favors the polar state, and thus makes the central $m_F = 0$ domain larger. Ferromagnetic coupling ($g_2 < 0$) favors the ferromagnetic states $|m_F = +1\rangle$ and $|m_F = -1\rangle$ at the ends of the cloud, and thus the $m_F = 0$ domain shrinks (see Fig. 17d).

Collecting spin-dependent energy terms, we now have the restricted energy functional

$$K_{\text{tot}} = \int d^3\vec{r} (K_0 + K_{\text{spin}}) \quad (4.16)$$

$$K_0 = \vec{\psi}^\dagger \left(-\frac{\hbar^2 \nabla^2}{2m} \right) \vec{\psi} + \left(U(\vec{r}) - \mu + \frac{g_0}{2} n \right) n \quad (4.17)$$

$$K_{\text{spin}} = \left(-p(z) \langle F_z \rangle + q \langle F_z^2 \rangle + c \langle \vec{F} \rangle^2 \right) n \quad (4.18)$$

where $c = g_2 n/2$. The ground-state spin structure of a spinor condensate is found by minimizing K_{tot} .

4.3 Spin-domain diagrams: A local density approximation to the spin structure of spinor condensates

Focusing on the spin-dependent part, K_{spin} has a simple and elegant form. Let us step away from the specific experimental considerations and consider a homogeneous spinor condensate with some arbitrary, uniform values of the parameters p , q and c . The ground-state spinors obtained by minimizing the energy functional K_{spin} are indicated in the three diagrams of Figure 18 for three conditions on the parameter c [97]. For a non-interacting gas ($c = 0$), the ground-state spinor is determined by the effects of magnetic fields alone.

In the case of anti-ferromagnetic coupling ($c > 0$), the spinor diagram changes in two significant ways. First, since the anti-ferromagnetic energy favors the $|m_F = 0\rangle$ polar state, the region in which the $|m_F = 0\rangle$ state is the ground state is enlarged. Second, at low values of q , in addition to the region of pure hyperfine states, a region is introduced in which the ground-state spinor is a superposition of the $|m_F = \pm 1\rangle$ states. While admixing the

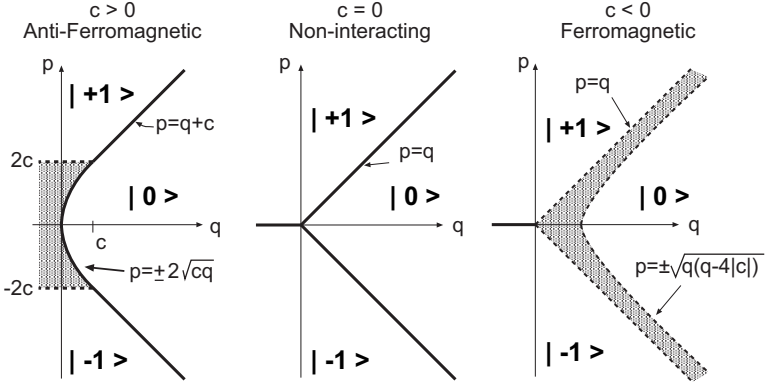


Fig. 18. Spin-domain diagrams for $F = 1$ spinor condensates for the three cases $c > 0$ (anti-ferromagnetic collisional coupling), $c = 0$ (no spin-dependent interactions), and $c < 0$ (ferromagnetic coupling). The ground-state spinors which minimize K_{spin} for the given values of p , q , and c are shown. Regions in which the ground state contains just one component are labeled by the magnetic hyperfine sublevel. Regions of mixed components are shaded. The ground-state spin-domain structure of a spinor condensate in the presence of a magnetic bias field and field gradient is indicated by a vertical line across the relevant domain diagram (see Fig. 22). Reprinted by permission from Nature [97], copyright 1999 Macmillan Magazines Ltd.

$|m_F = -1\rangle$ ($|m_F = +1\rangle$) state for $p > 0$ ($p < 0$) increases the linear Zeeman energy, it reduces the interaction energy by making the superposition state more polar in character. Explicitly, in the shaded region, $\langle F_z \rangle = p/2c$ independent of q . The effect of the linear Zeeman energy on anti-ferromagnetic condensates was considered also by Ohmi and Machida [95] whose work did not include the quadratic Zeeman energy, and thus concerned the $q = 0$ axis of the spin-domain diagram.

In the case of ferromagnetic coupling ($c < 0$), the situation is different. The higher interaction energy for the polar state diminishes the region in which the ground state is the $|m_F = 0\rangle$ state. In between the regions of single-component ground-state spinors there is a region in which *all three* hyperfine states are generally mixed. In these regions, the $|m_F = 0\rangle$ state is mixed predominantly with a large population of only one of the $|m_F = \pm 1\rangle$ states and with a small population of the other.

Returning now to the experimental situation, the spin-domain diagram is used to describe the ground-state spin structure of a spinor condensate through a local density approximation. The values of q and c (but not its sign) are determined by the magnetic bias field and by the condensate density, which we assume for now to be constant across the condensate.

The coefficient p varies across the condensate due to the presence of a magnetic field gradient; thus, the variations in the condensate spin structure across the length of the condensate are determined by scanning along a vertical line in the spin-domain diagrams. The length of this line is determined by the condensate length and the field gradient B' . The center of this vertical line is determined by the total spin in the condensate: it moves upwards (larger p) as $\langle F_z \rangle$ is increased and moves downwards (smaller p) as $\langle F_z \rangle$ is decreased. Thus, by adjusting the condensate density, the magnetic bias field, and the total spin of the cloud, all regions of the spin-domain diagrams are accessible.

4.4 *Experimental methods for the study of spinor condensates*

Having introduced this new quantum fluid, let us describe how we made it, and how we probed it. First, magnetically-trapped Bose-Einstein condensates were produced in the $|F = 1, m_F = -1\rangle$ hyperfine state and transferred to an optical trap [44]. Then, we pulsed on rf fields of variable strength which were swept in frequency to distribute the optically-trapped atoms among the $F = 1$ hyperfine sublevels by the method of adiabatic rapid passage [106]. High amplitudes or slow sweep rates transferred all the atoms from one hyperfine state to another, while low amplitudes or fast sweep rates transferred just a fraction of the atoms. To achieve an arbitrary hyperfine distribution, it was necessary to make these rf-transitions at large (15–30 G) bias fields, separating the $|m_F = +1\rangle \rightarrow |m_F = 0\rangle$ and $|m_F = 0\rangle \rightarrow |m_F = -1\rangle$ transition frequencies by about 1 MHz due to the quadratic Zeeman shift. Otherwise, at low fields where level spacings between the hyperfine sublevels are equal, rf fields can only be used to rotate the atomic spin vector and cannot, for example, change the atoms from the ferromagnetic $|m_F = +1\rangle$ state to the polar $|m_F = 0\rangle$ state.

After state preparation, the optically-trapped spinor condensates were allowed to evolve in the presence of variable magnetic bias fields and field gradients. After a variable dwell time in the optical trap, the spinor condensates were probed by time-of-flight imaging combined with a Stern-Gerlach spin separation (Fig. 19). The optical trap was suddenly switched off, allowing the atoms to expand primarily radially from the highly anisotropic optical trap. Then, after allowing about 5 ms for the interaction energy to be completely converted to kinetic energy, a magnetic field gradient was applied which separated the spin state populations without distorting them. Finally, after 15–30 ms, the atoms were optically pumped to the $|F = 2\rangle$ hyperfine manifold. This gave the same optical cross-section for all the atoms in the subsequent absorption probing on the $|F = 2, m_F = 2\rangle \rightarrow |F' = 3, m_{F'} = 3\rangle$

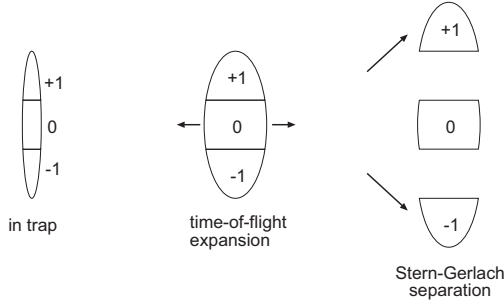


Fig. 19. Probing spinor condensates. After release from the elongated optical trap, the trapped spinor condensate expands primarily radially while maintaining the axial hyperfine distribution. A magnetic field gradient is then used to separate out the different components while preserving their shape. A subsequent absorption probe reveals the spatial and hyperfine distributions in the trap.

cycling transition. This probing method obtained both the spatial and hyperfine distributions along the axis of the optical trap in a single image.

4.5 The formation of ground-state spin domains

In reference [97] we explored the ground-state structure of spinor Bose–Einstein condensates with an average spin of $\langle F_z \rangle = 0$. Condensates were prepared either with all atoms in the $|m_F = 0\rangle$ state or in an equal mixture of the $|m_F = \pm 1\rangle$ states. The atoms were then allowed to relax to their equilibrium distribution in the presence of a variable magnetic bias field and field gradient. Probing at variable times after the state preparation revealed that the condensates relaxed to the same spin structure from either of the initial conditions, and remained thereafter in the same equilibrium state (Fig. 20).

Figure 21 shows three examples of the spin structures which were observed. The corresponding representations of these structures in the anti-ferromagnetic spin–domain diagram are indicated in Figure 22.

Figure 21b shows the equilibrium structure of a spinor condensate for which the quadratic Zeeman energy is larger than the interaction energy ($q > c$). The magnetic field gradient is sufficiently strong so that $|p| > q + c$ at the ends of the cloud, and thus the condensate consists of three pure spin domains with a $m_F = +1$ domain on the high-field end of the cloud, a $m_F = 0$ domain in the center, and a $m_F = -1$ domain at the low-field end.

In Figure 21a, the magnetic field is weaker, and thus the central $m_F = 0$ domain is now flanked by regions in which the $m_F = \pm 1$ components are mixed. The appearance of a large population of the $m_F = 1$ ($m_F = -1$) component on the low-field (high-field) end of the cloud provides a

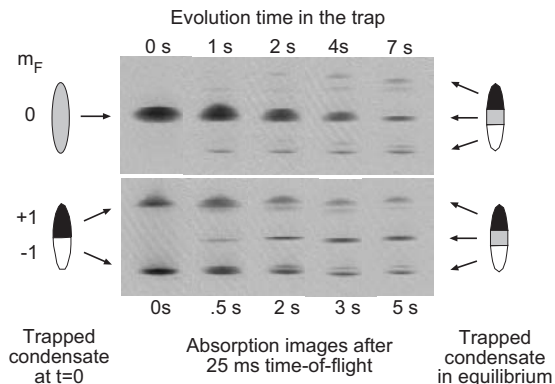


Fig. 20. Formation of ground state spin domains. Absorption images of ballistically expanding spinor condensates show both the spatial and hyperfine distributions. The images of clouds with various dwell times in the trap show the evolution to the same equilibrium for condensates prepared in either a pure $|m_F = 0\rangle$ state (upper row) or in equally populated $|m_F = \pm 1\rangle$ states (lower row). The bias field and field gradient during the dwell time was $B_0 = 20$ mG and $B' = 11$ mG/cm. The image size for each spinor condensate is 1.7×2.7 mm.

qualitative confirmation of the anti-ferromagnetic collisional coupling in the $F = 1$ hyperfine manifold of sodium. The division between the $m_F = 0$ domain and the domains containing the $m_F = \pm 1$ components indicates the immiscibility of the $m_F = 0$ component with the others.

Finally, in Figure 21c, a condensate is shown for which the total spin is greater than zero. The magnetic field gradient is about zero, and thus the condensate corresponds to a point on the spin-domain diagram in which the $m_F = \pm 1$ components are mixed. This situation nicely demonstrates the miscibility of the $m_F = \pm 1$ components with each other. The different widths of the two components may be due to the curvature of stray magnetic fields, which has opposite effects on the $|m_F = \pm 1\rangle$ states due to their different magnetic moments. Another explanation was recently given by Huang and Gou [107] who ascribe the different widths to the inhomogeneous density of the condensate.

There were some apparent discrepancies between our observations and the local density description (Sect. 4.3). For instance, as shown in Figures 21a and b, the separation between the central $m_F = 0$ domain and the neighboring $m_F = \pm 1$ domains was not sharp, as would have been predicted by the spin-domain diagram which neglects the kinetic energy. Including the kinetic energy requires that the condensate spinor vary gradually between the domains. As discussed in Sections 4.7 and 4.8, the condensate spinor should change over a length scale given by $\xi_s = \sqrt{\hbar^2/2m\Delta E}$,

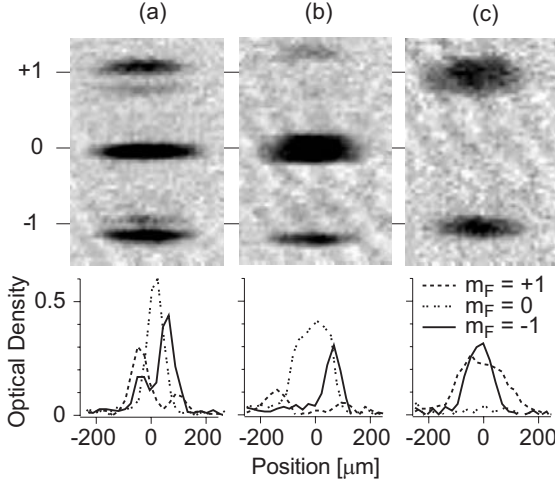


Fig. 21. Ground state spin domains in $F = 1$ spinor Bose-Einstein condensates. Time-of-flight images after Stern-Gerlach separation are shown, along with the indicated axial density profiles in the optical trap, for which the Stern-Gerlach separation was “undone”. Images (a) and (b) show spin domains of all three components. Image (c) shows a miscible $m_F = \pm 1$ component condensate. Conditions are: (a) $B = 20$ mG, $B' = 11$ mG/cm; (b) $B = 100$ mG, $B' = 11$ mG/cm; (c) $B = 20$ mG, $B' \simeq 0$, $\langle F_z \rangle > 0$.

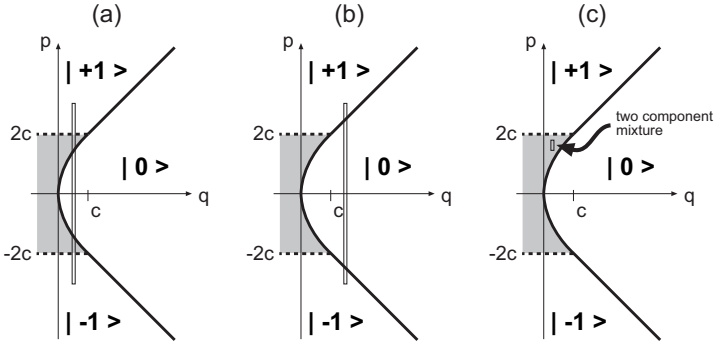


Fig. 22. Representation of ground-state spin-domain structures of Figure 21 on the spin-domain diagram. The spin structures shown in Figures 21a and b correspond to long vertical lines through the spin-domain diagram, centered at $p = 0$ to correspond to an average spin $\langle F_z \rangle = 0$. (a) At low magnetic field $q < c$ and mixed-spin domains are introduced. (b) At higher fields, they are absent. (c) Lowering the gradient focuses on a small portion of the diagram in which a cloud of non-zero spin consists of overlapping $m_F = \pm 1$ components.

where

$$\Delta E = \mu_0 \left(\sqrt{\frac{g_0 + g_2}{g_0}} - 1 \right) \simeq 0.018\mu_0 \quad (4.19)$$

is the height of the interaction energy barrier which expels $m_F = 0$ atoms from $m_F = 1$ spin domains, and $\mu_0 = g_0 n$ is the chemical potential of the $m_F = 0$ atoms at a condensate density of n . This width ξ_s can be called a “spin healing length” in analogy with the healing length $\xi = \sqrt{\hbar^2/2m\mu}$ which is the minimum length for density variations. For typical conditions, $\xi_s \simeq 1 - 2 \mu\text{m}$.

In our time-of-flight images (Fig. 21), the overlap between the components appears to be much larger, on the order of tens of microns. This discrepancy may just be an artifact of the indirect probing technique from which the spin structure of the trapped condensate is inferred. During the expansion of the condensate, the kinetic energy at the spin-domain boundaries is released axially, imparting velocities of $\sqrt{2\Delta E/m} \simeq 2 \text{ mm/s}$. During the 25 ms time of flight, this would cause a sharp boundary between spin components to be smeared out by $\simeq 50 \mu\text{m}$, consistent with the observed width of the overlap between the $m_F = 0$ and $m_F = \pm 1$ components. Thus, our time-of-flight imaging technique cannot properly characterize the boundary between neighboring spin domains. In future work, it would be interesting to examine such boundaries with an *in situ* imaging technique, perhaps to observe the spatial structures recently predicted by Isoshima *et al.* [108]. It is interesting to note that the radial expansion of the cigar-shaped condensate occurs at a velocity near the speed of Bogoliubov sound, which describes the propagation of density waves, while the axial expansion of a spin domain boundary occurs at a “spin sound velocity” which would describe the propagation of spin waves.

4.6 Miscibility and immiscibility of spinor condensate components

As discussed above, the spin-domain diagram and the observed ground-state spin structures showed evidence for the miscibility of the $m_F = -1$ and $m_F = +1$ components and the immiscibility of $m_F = \pm 1$ and $m_F = 0$ components. The bulk miscibility or immiscibility of two-component condensate mixtures is predicted by mean-field theory [75, 77–79, 109]. The interaction energy density of such condensates is given by

$$E = \frac{1}{2}(n_a^2 g_a + n_b^2 g_b + 2n_a n_b g_{ab}) \quad (4.20)$$

where m is the common atomic mass, and n_a and n_b are the densities of each of the components. The interaction parameters are given generally as $g = 4\pi\hbar^2 a/m$ where a_a and a_b are the same-species scattering lengths,

and a_{ab} is the scattering length for interspecies collisions. Consider a two-component mixture in a box of volume V with N atoms in each component. If the condensates overlap, their total mean-field energy is

$$E_O = \frac{N^2}{2V} (g_a + g_b + 2g_{ab}). \quad (4.21)$$

If they phase separate, their energy is

$$E_S = \frac{N^2}{2} \left(\frac{g_a}{V_a} + \frac{g_b}{V_b} \right). \quad (4.22)$$

The volumes V_a and V_b occupied by each of the separated condensates are determined by the condition of equal pressure:

$$g_a \left(\frac{N}{V_a} \right)^2 = g_b \left(\frac{N}{V_b} \right)^2. \quad (4.23)$$

Comparing the energies E_O and E_S the condensates will phase-separate if $g_{ab} > \sqrt{g_a g_b}$, and will mix if $g_{ab} < \sqrt{g_a g_b}$.

In the $F = 1$ three-component spinor system, the scattering lengths are determined by $a_{f=0}$ and $a_{f=2}$. Defining $\bar{a} = (2a_{f=2} + a_{f=0})/3$ and $\Delta a = (a_{f=2} - a_{f=0})/3$, the scattering lengths for the $m_F = 1, 0$ two-component system (or equivalently the $m_F = -1, 0$ system) are given by $a_0 = \bar{a}$, and $a_1 = a_{0,1} = \bar{a} + \Delta a$. Since Δa is positive for sodium, the condition $a_{0,1} > \sqrt{a_0 a_1}$ applies and the components should phase-separate, as we have observed [97,98]. Interestingly, this phase-separation should not occur in the non-condensed cloud because the same-species mean-field interaction energies are doubled due to exchange terms.

In the $m_F = \pm 1$ two component system, the scattering lengths are $a_1 = a_{-1} = \bar{a} + \Delta a$ and $a_{1,-1} = \bar{a} - \Delta a$. Thus, $a_{1,-1} < \sqrt{a_1 a_{-1}}$, and these two components should mix. Indeed, as shown in Figure 21c, an equilibrium spinor condensate with $\langle F_z \rangle \neq 0$, small field gradient, and near-zero field consists of an overlapping mixture of atoms in the $m_F = \pm 1$ states. This particular miscible two-component system has an important advantage. If the trapping potential varies across a two-component condensate, the lowest energy state may be a phase-separated state if $a_a \neq a_b$ even though the condition $a_{ab} < \sqrt{a_a a_b}$ is fulfilled [110]. In this case, the atoms with the smaller scattering length concentrate near the trap center, making it harder to observe miscibility. However, in the $m_F = \pm 1$ system, the two scattering lengths a_1 and a_{-1} are equal by rotational symmetry, so the components mix completely even in a trapping potential.

4.7 Metastable states of spinor Bose-Einstein condensates

Having observed and explained ground state spin-domain structures, we began to explore dynamical properties of spinor Bose-Einstein

condensates. Reference [98] discusses the observation of long-lived excited states of spinor Bose–Einstein condensates. We observed two complementary types of metastable states: one type in which a two-component condensate was stable in spin composition but which persisted in a non-equilibrium structure of spin domains, and another in which a spatially uniform condensate was metastable with respect to spin relaxation to an equilibrium spin composition. In each case, the energy barriers to relaxation to the ground state (the activation energy) were identified and found to be much smaller than the thermal energies of the metastable gases; thus, such states would not be metastable in a non-condensed cloud. However, in a Bose condensed cloud with a large condensate fraction, the thermal energy is only available to the scarce thermal component and thus thermal relaxation is considerably slowed. In other words, Bose–Einstein condensation allows the study of weak effects in an energy regime which is much lower than the temperature of the gas.

4.7.1 Metastable spin-domain structures

The first type of metastability was observed in spinor Bose–Einstein condensates in a high magnetic field (15 G) which caused a two-component $m_F = 0, 1$ cloud to be stable in spin composition. This occurs because the large quadratic Zeeman shift makes $|m_F = 0\rangle + |m_F = 0\rangle \rightarrow |m_F = +1\rangle + |m_F = -1\rangle$ collisions endothermic, even if the $|m_F = \pm 1\rangle$ atoms would move to the ends of the condensate. We prepared clouds in an equal superposition of the two hyperfine states using a brief rf pulse, and then allowed the system to equilibrate.

Because of the immiscibility of the $m_F = 0$ and $m_F = 1$ components, the ground-state spin structure in this case consists of two phase-separated spin domains, one for each of the components, on opposite sides of the elongated trap with a domain boundary in the middle. What we observed was dramatically different: a spontaneously formed, metastable arrangement of alternating $m_F = 0$ and $m_F = 1$ spin domains (Fig. 23).

These spin striations began forming within about 50 ms of the initial preparation of two overlapping, immiscible components. The striations were initially angled due to radial excitations in the narrow spinor condensates which soon damped out, leaving strictly horizontal striations. The observed width of the spin domains grew to an equilibrium value of about $40\ \mu\text{m}$ within about 100 ms (Fig. 24). Thereafter, the clouds were essentially unchanged, remaining in the metastable state for 10 or more seconds as the number of trapped atoms slowly decayed due to three-body trap losses.

To understand the reason for the metastability, let us consider two adjacent spin domains of the $m_F = 0$ and $m_F = 1$ components, as shown in Figure 25. Suppose that, in order for the condensate to decay to its ground state, the atoms of each spin domain must somehow be transported across

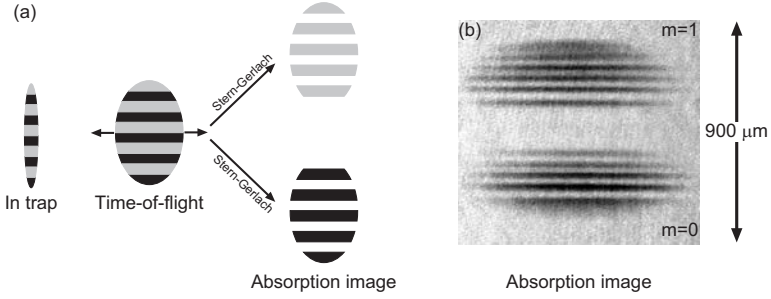


Fig. 23. Quantum “bubbles”: a metastable arrangement of alternating spin domains in a two-component condensate. (a) A two-component optically-trapped condensate composed of atoms in the $|m_F = 0\rangle$ (black) and $|m_F = 1\rangle$ (grey) hyperfine states expands primarily radially once the trap is switched off. A magnetic field gradient is used to separate the two spin states before imaging, allowing a determination of the axial distribution of the two components in the trap. (b) The observed density striations indicate that the trapped condensate was composed of alternating $m_F = 0$ and $m_F = 1$ spin domains.

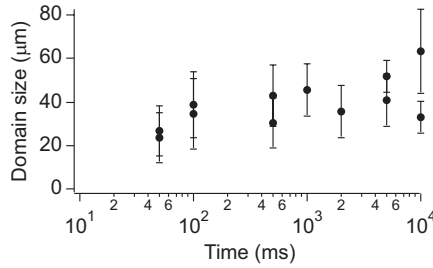


Fig. 24. Evolution of metastable domain sizes. Shown is the average size (points) and standard deviation (one sigma error bars) of the spin domains observed at various time after the initial state preparation at a bias field of 15 G. Each point corresponds to measurements made on a different condensate.

the spin-domain boundary. For this to occur, the atoms of one component must either pass around or through the other component.

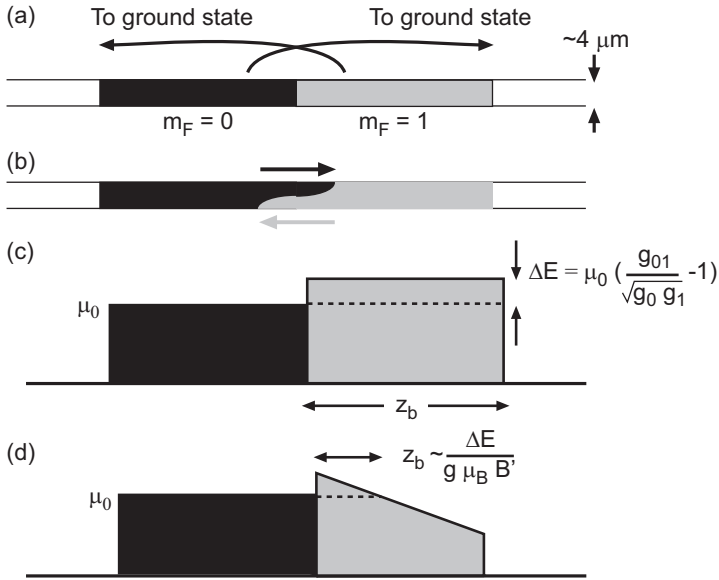


Fig. 25. Energy barriers responsible for the metastability of spin domains in a two-component $m_F = 0, 1$ condensate. (a) Metastable domains of the $m_F = 0$ (black) and $m_F = 1$ (gray) components are held in a narrow optical trap. For the population in these domains to decay to the ground state they must either pass each other without overlapping, or pass through each other. (b) The former is prohibited due to the kinetic energy barrier of modifying the condensate wavefunction on a radial length scale. (c) The latter is prohibited due to an interaction energy barrier ΔE , shown here for the passage of an $m_F = 0$ domain of chemical potential μ_0 through the neighboring $m_F = 1$ domain. (d) If a magnetic field gradient B' is imposed, the width of the classically forbidden region for the passage of $m_F = 0$ atoms through the $m_F = 1$ domain is reduced to $z_b = \Delta E / g \mu_B B'$, and the tunneling rate which governs the decay of the metastable domains is increased.

If one component passes around the other, the condensate wavefunction must be varied spatially in the radial direction. This gives a kinetic energy barrier to decay of about $\hbar^2/2mr^2 \simeq k_B \times 3$ nK where $r \simeq 2 \mu\text{m}$ is the condensate radius. The passage of one component through the other is limited by an interaction barrier since the components are immiscible. As explained in reference [99], the interaction energy barrier for atoms in the $|m_F = 0\rangle$ state to pass through a $m_F = 1$ domain is (see Eq. (4.19)) $\Delta E \simeq g_2/2g_0 \times \mu_0 = c$ where μ_0 is the chemical potential of atoms in the $m_F = 0$ spin domain, and c is the spin-dependent interaction energy introduced in Section 4.1. At a chemical potential $\mu_0 = k_B \times 300$ nK,

the interaction energy barrier height is $c \simeq k_B \times 5$ nK. The probability of tunneling through the spin domains is exceedingly small because the axial length of the domains of $\simeq 40$ μm is much larger than the spin healing length $\xi_s \simeq 1.4$ μm . Thus, because of these two energy barriers, the non-equilibrium arrangement of spin-domains is metastable.

The formation of these metastable spin-domains was considered recently by Chui and Ao [111] as a spinodal decomposition in a binary system. Equilibration occurs on two time scales. First, on a short time scale determined by the spin-dependent interaction energy c as $t \simeq \hbar/c$, the homogeneous initial state begins to phase separate into small domains of length scale $\xi_s = \sqrt{\hbar^2/2m\Delta E}$. Thereafter, the domains grow by the coalescence of small spin domains on the long time scales required for quantum tunneling. This work supports the physical picture which we suggested in reference [98]. A similar picture emerges from the work of Pu *et al.* [112] who consider the quantum dynamics (without dissipation) of a trapped condensate composed of two overlapping components which tend to phase separate. In their calculations, they observe the evolution of fine spatial features which exemplify the instability of such a system against spin domain formation.

4.7.2 Metastable spin composition

Another type of metastability was discovered in the studies of ground-state spin domains of a $\langle F_z \rangle = 0$ condensate discussed in Section 4.5. Condensates were prepared either with all atoms in the $|m_F = 0\rangle$ state or in an equal mixture of the $|m_F = \pm 1\rangle$ states. While the ground state reached from either starting condition was the same (Fig. 20), equilibration occurred on much different time scales. When starting from the $|m_F = 0\rangle$ state, the condensate remained unchanged for several seconds before evolving over the next few seconds to the ground state. When starting from the $|m_F = \pm 1\rangle$ superposition, the fraction of atoms in the $|m_F = 0\rangle$ state grew without delay, arriving at equilibrium within less than a second (Fig. 26).

This difference can be understood by considering a spin-relaxation collision, in which two $|m_F = 0\rangle$ atoms collide to produce a $|m_F = 1\rangle$ and a $|m_F = -1\rangle$ atom. In the presence of a magnetic field B_0 , quadratic Zeeman shifts cause the energy of the two $|m_F = 0\rangle$ atoms to be lower than that of the $|m_F = 1\rangle$ and $|m_F = -1\rangle$ atoms. Due to this activation energy, condensate atoms in the $|m_F = 0\rangle$ state could not undergo spin-relaxation collisions. Thus, even though the creation of $m_F = 1$ and $m_F = -1$ spin domains at the ends of the condensate is energetically favored *globally* in the presence of a magnetic field gradient, the $m_F = 0$ condensate cannot overcome the *local* energy barrier for spin-relaxation. In contrast, condensate atoms in the $|m_F = 1\rangle$ and $|m_F = -1\rangle$ states can directly lower their energy through such collisions, and equilibrate quickly.

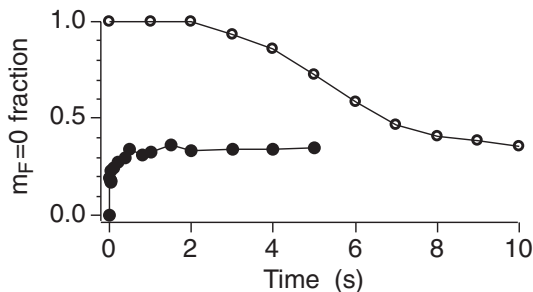


Fig. 26. Metastability of the pure $|m_F = 0\rangle$ state in the presence of a magnetic bias field (250 mG), and gradient (44 mG/cm). The evolution toward equilibrium of an initially pure $|m_F = 0\rangle$ condensate (open symbols), and a mixture of $|m_F = 1\rangle$ and $|m_F = -1\rangle$ (closed symbols) is shown by plotting the fraction of atoms in the $|m_F = 0\rangle$ state *vs.* dwell time in the optical trap. Figure taken from reference [98].

In support of this explanation, the metastability time was found to depend strongly on the quadratic Zeeman energy which was varied by changing the magnetic bias field. Importantly, the equilibration time changed significantly when q was varied by less than a nanokelvin; this dependence excludes thermal spin relaxation (in a gas at a temperature $T \sim 100$ nK $\gg q/k_B$) as the equilibration mechanism, and suggests that the metastable condensate decays to the ground state via quantum tunneling. In such tunneling, a pair of atoms in the $|m_F = \pm 1\rangle$ states would be produced in a classically forbidden collision, and would then tunnel to opposite ends of the cloud where their energy is lowered due to the magnetic field gradient. It would be interesting to study this process further in the future.

4.8 Quantum tunneling

Metastable states can generally overcome the activation energy barrier for decay to the ground state in two ways. Classically, the system can decay by acquiring thermal energy larger than the activation energy. However, even without this thermal energy, the system can decay to the ground state by quantum tunneling. Tunneling describes a wide range of phenomena such as nuclear decay, field ionization of neutral atoms, and scanning tunneling microscopy. In macroscopic quantum systems, coherent tunneling can lead to a variety of Josephson effects [113] which have been observed in superconductors and quantum fluids. As exemplified by the observation of metastable states which persist in spite of temperatures higher than the activation energy, gaseous Bose–Einstein condensates are an appealing new system to study tunneling and Josephson oscillations [114–117].

In our study of optically trapped spinor Bose–Einstein condensates, we looked at the decay of metastable spin domains via quantum tunneling through the spin domain boundaries [99]. Tunneling barriers were formed not by an external potential, but rather by the intrinsic repulsion between two immiscible components of a quantum fluid. Tunneling across spin domain boundaries is a spin transport mechanism inherent to such a fluid (emphasized in [111]), and the tunneling rates are sensitive probes of the structure of the domain boundaries. From a practical viewpoint, the use of phase-separated spin domains rather than externally imposed potentials is an attractive option for future studies of tunneling in Bose condensates since the energy barriers for tunneling are naturally of nanokelvin-scale height and micron-scale width.

The system we chose for our study was a simple, well-characterized metastable arrangement of spin domains in a spinor condensate composed of the $m_F = 1$ and $m_F = 0$ components. Such a state was obtained by first preparing a spinor condensate in a superposition of the $|m_F = 0, 1\rangle$ states. A strong field gradient (several G/cm) was applied to break up the many-domain metastable state (discussed in the previous section) and separate the spin components into the two-domain ground state. Then, a weak gradient was applied in the opposite direction, which energetically favored the rearrangement of the spin domains on opposite ends of the optical trap, and thus yielded a two-domain metastable state. This simple system allowed for the characterization of the decay of metastable states by the easy identification of atoms in the metastable and ground-state spin domains of each component (Fig. 27).

To ascribe the decay of these metastable spin domains to quantum tunneling, it was first necessary to rule out thermal relaxation as a decay mechanism. Figure 28 shows a series of time-of-flight images reflecting the state of the two-domain metastable state at various times after the state was initially prepared and held under a 0.1 G/cm gradient.

One can identify two stages in the decay of this metastable cloud to the ground state: a slow decay over the first 12 seconds, followed by a rapid decay to the ground state within less than one second. The slow decay was found to be rather insensitive to changes in the condensate density and field gradient, and was thus consistent with thermal relaxation wherein condensate atoms from the metastable state are thermally excited, and then re-condense into the ground state domains. The number of atoms which accumulated in the ground-state domains reached a nearly constant value of about 5×10^4 , perhaps due to a dynamic equilibrium between the growth of the domain *via* re-condensation and its depletion *via* inelastic losses. We also observed that the total population in the $|m_F = 0\rangle$ spin state decreases more rapidly than that in the $|m_F = 1\rangle$ state, indicating higher inelastic collision rates for the $|m_F = 0\rangle$ state.

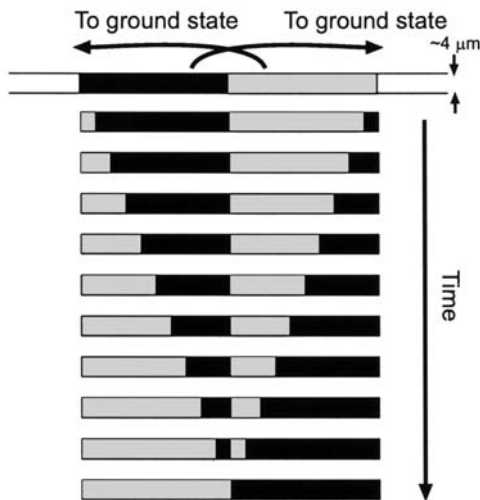


Fig. 27. Evolution from a metastable state to the ground state. The ground state domain structure is formed by tunneling of the two components through each other. The intermediate state is characterized by outer ground state domains and inner metastable domains.

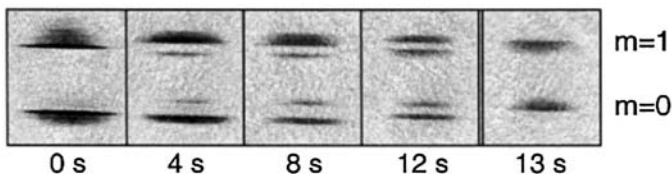


Fig. 28. Decay of a metastable state by thermal relaxation and quantum tunneling. A two-domain metastable state was prepared at a 15 G axial bias field and a 0.1 G/cm gradient. Images show metastable (outer parts in the time-of-flight picture) and ground state (inner parts) spin domains of $|m_F = 1\rangle$ and $|m_F = 0\rangle$ atoms, probed at various times after state preparation. The height of each image is 1.3 mm. The number of atoms in the ground state domains grew slowly over the first 12 s, after which the atoms tunneled quickly to the ground state. The total number of atoms (and thus the condensate density) decreased during the dwell time due to inelastic three-body collisions. Thus, the slow thermal relaxation gave way to a rapid tunneling once the density fell below a threshold value. Figure taken from reference [98].

The rapid decay which ensued (after 12 s) was due to quantum tunneling. As discussed below, the tunneling rate is acutely sensitive to the condensate density. While the condensate is stored in the optical trap, its

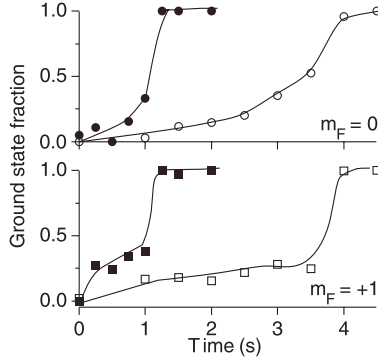


Fig. 29. A comparison of the decay of metastable states at different densities. Shown is the fraction of $m_F = 0$ and $m_F = 1$ atoms found in the ground-state domains after a variable delay time at a constant field gradient of 0.35 G/cm and a 2 G bias field. The evolution is shown for condensates prepared with different populations in the initial state, either 1×10^6 (open symbols) or 2.5×10^5 atoms (closed symbols). The rapid tunneling in the denser condensate occurred at a later time. The solid lines are guides to the eye.

density decreases as atoms are lost from the trap due to three-body inelastic collisions. Thus, as time progressed, the density of the metastable condensate in Figure 28 decreased until the tunneling rate was fast enough to cause a rapid (within about 1 second) relaxation to the ground state.

The dependence of the relaxation time on the condensate density is also shown in Figure 29. Metastable condensates were prepared with different initial numbers of atoms, and held in a constant magnetic field gradient. The metastable lifetimes for the two starting conditions were different, with the denser condensate decaying to the ground state at a later time.

A mean-field description of the tunneling rates was developed [99]. We considered the one-dimensional motion of a Bose-Einstein condensate composed of two immiscible components of atoms in states $|a\rangle$ and $|b\rangle$ and atomic mass m , as in Figure 25 for the experimental realization of the $m_F = 1$ and $m_F = 0$ components. The chemical potentials of the two components $\mu_i = g_i n_i$ are related by the condition of constant pressure $\mu_a^2/g_a = \mu_b^2/g_b$ where $g_i = 4\pi\hbar^2 a_i/m$, a_i is the same-species scattering length, and $i \in a, b$ labels the component. The mean-field interaction energy for each component is $U_i = g_i n_i + g_{ab} n_j$ ($i \neq j$) where g_{ab} is determined by the cross-species scattering length a_{ab} .

If we assume the boundary between the spin domains to be sharp, component a is excluded from the domain of component b by an energy barrier

ΔE given by

$$\Delta E = g_{ab}n_b - g_a n_a = \left(\frac{g_{ab}}{\sqrt{g_a g_b}} - 1 \right) \mu_a. \quad (4.24)$$

This energy barrier is responsible for the metastability of spin domains which have an axial length which is much larger than the spin healing length $\xi_s = \sqrt{\hbar^2/2m\Delta E}$.

In the presence of a state-selective force F , which was experimentally applied in our experiments using a magnetic field gradient B' , the energy barrier decreases away from the domain boundary as $\Delta E(z) = \Delta E - Fz$. Thus the width of the energy barrier is reduced to $z_b = \Delta E/F$, and tunneling can occur when $z_b \sim \xi_s$. More precisely, the tunneling rate across the barrier is given by the Fowler–Nordheim (WKB) equation

$$\frac{dN_a}{dt} = \gamma \exp \left(-2\sqrt{\frac{2m}{\hbar^2}} \int_0^{z_b} \sqrt{\Delta E(z)} dz \right) \quad (4.25)$$

$$= \gamma \exp \left(-\frac{4}{3} \sqrt{\frac{2m}{\hbar^2}} \frac{\Delta E^{3/2}}{F} \right) \quad (4.26)$$

$$= \gamma \exp \left(-\frac{4}{3} \frac{z_b}{\xi_s} \right) \quad (4.27)$$

which also describes the analogous phenomenon of the field emission of electrons from cold metals [118]. Here γ is the total tunneling attempt rate (*i.e.* not the rate per particle), and the exponential is the tunneling probability. This relation explains the strong dependence of the tunneling rate on the condensate density n , which causes the density threshold behaviour observed in Figure 28.

This mean-field description was tested experimentally by measuring the tunneling rate across barriers of constant height and variable width. For this, metastable condensates were prepared at a constant density (giving a constant barrier height of ≈ 5 nK), exposed to a variable gradient (giving barrier widths between 4 and 20 μm), and allowed to decay for a period $\tau = 2$ s which was short enough that the condensate density did not vary appreciably due to trap losses. We then measured the number of atoms of each component in the metastable and ground-state spin domains by time-of-flight absorption imaging (Fig. 30). When the barrier was wide (small field gradients), the tunneling rate was small and only a small fraction of atoms were observed in the ground-state domains. When the barrier was narrow (large field gradients), the tunneling rate was large and a large fraction of atoms were observed in the ground-state domains. The data were in quantitative agreement with our mean-field approach using the scattering lengths calculated by Burke *et al.* [105].

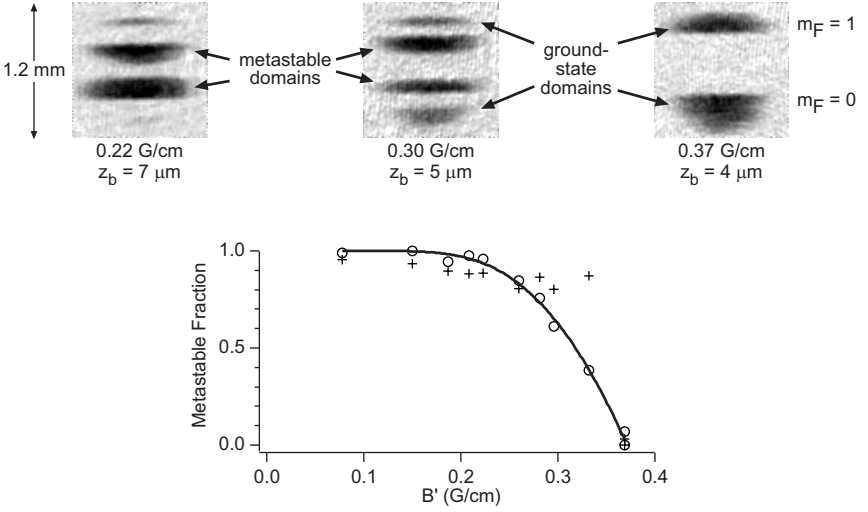


Fig. 30. Tunneling across barriers of constant height and variable width z_b . Condensates at constant density were probed after 2 seconds of tunneling at a variable field gradient B' . The population of atoms in the metastable and ground-state domains of each spin state were easily identified in time-of-flight images (see Fig. 27). Also shown is the fraction of atoms of each spin state in their metastable domain. Circles represent the $m_F = 0$ atoms, and pluses the $m_F = 1$ atoms. The energy barrier height was ≈ 5 nK at the chemical potential of $\mu_0 \approx 300$ nK. The tunneling rate depended strongly on the width of the energy barrier $z_b = \Delta E / g\mu_B B'$: at $z_b = 7$ μ m ($B' = 0.22$ G/cm) little tunneling was observed, while at $z_b = 4$ μ m ($B' = 0.37$ G/cm) the atoms had completely tunneled to the ground state in 2 s. The barrier attempt rate and tunneling probability were determined by a fit to the $m_F = 0$ data (solid line), and found to agree with a mean-field model. The data indicate that the tunneling rate for $m_F = 0$ atoms is larger than that for $m_F = 1$ atoms (see Ref. [99]).

4.9 Magnetic field dependence of spin-domain boundaries

While the tunneling rates measured at high magnetic fields (15 G) agreed with a model of tunneling in a two-component Bose condensate, at lower magnetic fields, a dramatic increase in the tunneling rate was observed indicating the breakdown of the two-component description. As described in our paper (see Fig 4 of reference [99]), the threshold chemical potential for tunneling at a constant field gradient dramatically increased at magnetic fields below about 1 G. Figure 31 shows similar data. This strong increase in the tunneling rate at low fields reveals that the structure of the domain boundary is changed by the presence of the third spin component, the $|m_F = -1\rangle$ state.

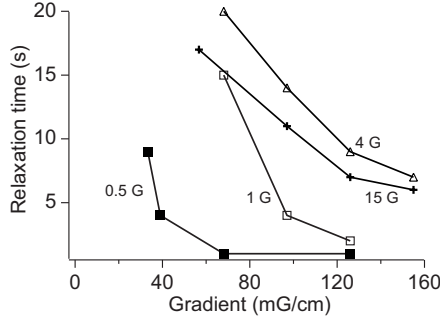


Fig. 31. Variation of the metastable state lifetime with magnetic field and field gradient. Metastable condensates at a constant initial chemical potential of $\mu_0 \simeq 600$ nK were allowed to decay at a variable bias field and field gradient. Shown is the time at which the condensates were observed to have relaxed completely to the ground state. The dependence of the lifetime on the field gradient at 15 G and 4 G was similar. At fields of 1 G or lower, the lifetime was dramatically shortened, indicating a substantially higher tunneling rate at low magnetic fields.

The introduction of the third spin component to the barrier has the effect of reducing the energy barrier for the tunneling of $m_F = 0$ atoms. This can be seen by considering a mixture of components a and b where $|a\rangle = |m_F = 0\rangle$ and $|b\rangle = \cos\theta|m_F = 1\rangle - \sin\theta|m_F = -1\rangle$ ($0 \leq \theta \leq \pi/2$). The interaction energy density of this system can be written in the form of equation (4.20) with the definitions

$$g_a = g_0 \quad (4.28)$$

$$g_b = g_0 + \Delta g \cos^2 2\theta \quad (4.29)$$

$$g_{ab} = g_0 + \Delta g(1 - \sin 2\theta) \quad (4.30)$$

where $\Delta g = g_2$. Using these interaction parameters, the energy barrier height which governs the tunneling of the $m_F = 0$ component becomes

$$\Delta E(\theta) = \left(\frac{g_0 + \Delta g(1 - \sin 2\theta)}{\sqrt{g_0(g_0 + \Delta g \cos^2 2\theta)}} - 1 \right) \mu_0 \simeq \frac{\Delta g}{g_0} \left(1 - \sin 2\theta - \frac{\cos^2 2\theta}{2} \right) \mu_0 \quad (4.31)$$

for $\Delta g \ll g_0$. For $\theta = 0$ or $\theta = \pi/2$, one recovers the energy barrier for tunneling through a pure $m_F = 1$ or $m_F = -1$ barrier. For intermediate values, the height of the energy barrier is reduced. Indeed, at $\theta = \pi/4$, the energy barrier disappears completely. In this case, $|b\rangle = \frac{1}{\sqrt{2}}(|m_F = 1\rangle - |m_F = -1\rangle)$ describes a polar state obtained by rotating the $|m_F = 0\rangle$ state. The condensate spinor can thus evolve continuously from state

$|a\rangle$ to $|b\rangle$ by a gradual rotation which is associated with a gap-less (*i.e.* no barrier) Goldstone excitation mode. Recent calculations by Isoshima, Machida and Ohmi [108] confirm the disappearance of the energy barrier when the populations in the $|m_F = \pm 1\rangle$ states become equal. These changes of effective interaction parameters in the presence of the $|m_F = -1\rangle$ state provide a mechanism for the variation of the tunneling rates with magnetic fields.

The local density approximation discussed in Section 4.3 indicates that, indeed, the $m_F = -1$ component should be introduced to the spin domain boundaries at low magnetic fields. According to this approximation, the boundaries studied in our experiment between an $m_F = 0$ domain and a region of $\langle F_z \rangle > 0$ are described in the spin domain diagram (Fig. 22) by a short vertical line at constant q (determined by the magnetic field) which straddles the border of the $m_F = 0$ region in the $p > 0$ half-plane. The diagram thus suggests that a pure two-component description of the boundary is correct for magnetic fields at which the quadratic Zeeman energy is larger than the spin-dependent interaction energy ($q > c$). Taking a typical value of the chemical potential of $\mu_0 = 300$ nK, this condition indicates that the two-component description of tunneling should be valid for magnetic fields greater than 500 mG⁵. Below this magnetic field, the $m_F = 0$ component is bordered not by a pure $m_F = 1$ domain, but rather by a region in which the $|m_F = 1\rangle$ and $|m_F = -1\rangle$ states are mixed.

However, the local density approach fails to explain why the tunneling rates should increase even at magnetic fields for which $q > c$, as we observed. This failure stems from the incomplete description of the spin domain boundary due to the neglect of kinetic energy in the local density approximation. As discussed above, $\langle F_z \rangle$ must vary continuously at the boundary between spin domains. One may approximate the spin composition of the boundary region by explicitly minimizing the energy of a spinor with a given value of $\langle F_z \rangle$, and then applying a local density approximation in which we assume that the spinor at each location in the boundary is determined by the local value of $\langle F_z \rangle$. We can write a spinor for which $\langle F_z \rangle > 0$ as

$$\vec{\zeta} = \begin{pmatrix} \sqrt{\langle F_z \rangle + \epsilon^2} \\ \sqrt{1 - \langle F_z \rangle - 2\epsilon^2} \\ -\epsilon \end{pmatrix} \quad (4.32)$$

where a choice of complex phases has already been made which reduces the anti-ferromagnetic interaction energy. The spin-dependent energy K_{spin} is

⁵Unlike in reference [97], we do not apply here a one-dimensional approximation to reduce the effective interaction energy by averaging over the radial directions.

then

$$c \left(\langle F_z \rangle^2 + 2(1 - 2\epsilon^2 - \langle F_z \rangle)(\sqrt{\epsilon^2 + \langle F_z \rangle} - \epsilon)^2 \right) + q(2\epsilon^2 + \langle F_z \rangle) \quad (4.33)$$

which is minimized to determine the fractional population ϵ^2 in the $|m_F = -1\rangle$ state.

At high magnetic fields ($q \gg c$) one finds the approximate solution

$$\epsilon^2 \simeq \frac{1}{(q/c)^2} \langle F_z \rangle (1 - \langle F_z \rangle)^2 \quad (4.34)$$

which indicates that atoms in the $|m_F = -1\rangle$ state are *always* energetically favored to reside in the domain boundary⁶. Their population scales with the magnetic field B_0 as $q^{-2} \propto B_0^{-4}$. At a magnetic field of 15 G where $q/c \approx 400$, the fraction of atoms in the $|m_F = -1\rangle$ state is exceedingly small and thus the two-component approximation to the domain boundary should be quite accurate, as indicated by our data. At lower magnetic fields, the population in the $|m_F = -1\rangle$ state plays an increasingly important role.

Guided by these simple approximate treatment, one can also explicitly calculate the spinor wavefunction at the domain boundary which minimizes the total energy. Such calculations were presented in reference [5], and the results are summarized in Figures 32 and 33. One finds indeed that the fractional population of atoms in the $|m_F = -1\rangle$ state is non-zero at all magnetic fields and scales as B_0^{-4} at high magnetic fields. The introduction of $m_F = -1$ atoms in the boundary layer increases the penetration depth of $m_F = 0$ atoms in the boundary region, and thus should increase the rate of tunneling across the domain boundary. The magnetic field at which this effect becomes significant, according to these calculations, is about 1 G for our experimental conditions and agrees with the magnetic field value below which an increased tunneling rate was observed.

Conclusions

These notes have reviewed advances in atomic BEC in two areas, spinor condensates and light scattering. Many further advances are described in other contributions to this volume. This rapid pace of developments during the last few years has taken the community by surprise. After decades of an elusive search nobody expected that condensates would be so robust and relatively easy to manipulate. Also, nobody imagined that such a simple system would pose so many challenges, not only to experimentalists, but also to our fundamental understanding of physics. The list of future challenges

⁶In our paper, an incorrect solution was given which indicated a high-field scaling of $\epsilon^2 \propto B_0^{-2}$ [99].

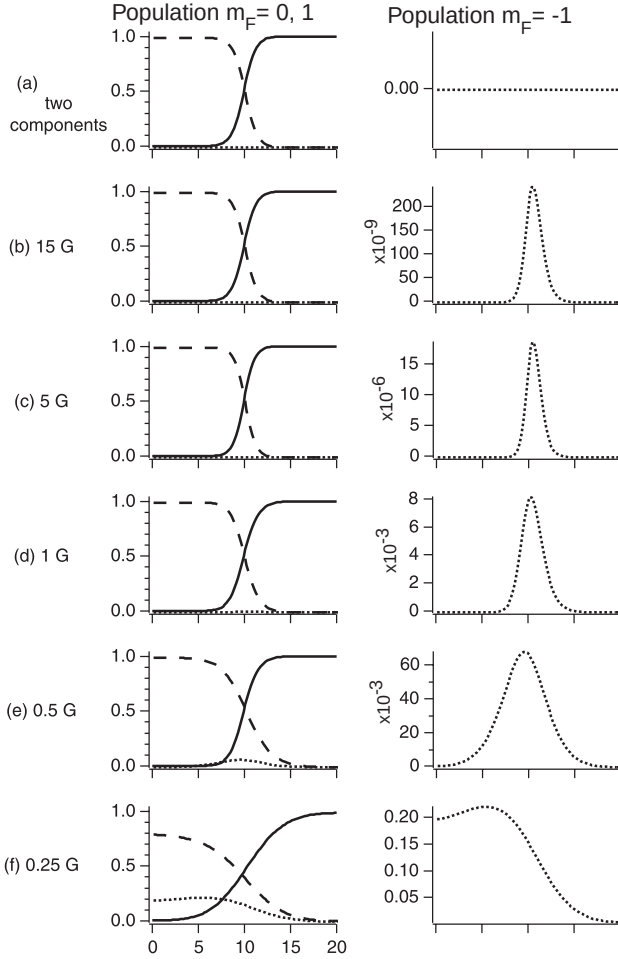


Fig. 32. Numerical calculation of the spin structure at the domain boundaries at different magnetic fields. Shown are the fractional population in the $|m_F = 1\rangle$ (dashed line), $|m_F = 0\rangle$ (solid line), and $|m_F = -1\rangle$ (dotted line) states, with the $|m_F = -1\rangle$ population shown at right on an expanded scale. In (a), the calculation was restricted to just the $m_F = 0$ and $m_F = 1$ components, and hence the results are magnetic field independent. In the remaining graphs, all three components were considered at magnetic fields of (b) 15 G, (c) 5 G, (d) 1 G, (e) 0.5 G, and (f) 0.25 G. As the magnetic field is decreased, the population in the $|m_F = -1\rangle$ state increases, and the boundary region becomes wider. Further details are found in reference [5].

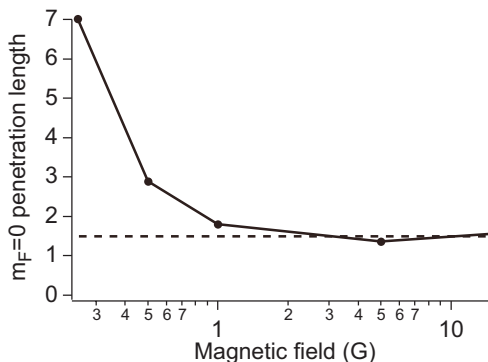


Fig. 33. Variation of the spin-domain boundary width with magnetic field. The calculated spatial variation of the fractional population of atoms in the $|m_F = 0\rangle$ state was fitted to the function $f(z) = [1 - \text{Erf}((z - z_0)/\xi_0)]/2$, where ξ_0 characterizes the penetration length of the $m_F = 0$ component in the boundary region. The points correspond to graphs (b–f) of Figure 32, while the dashed line shows the penetration length calculated for the two-component case. The penetration length is close to the two-component limit at high magnetic fields, and then increases sharply at lower fields beginning at about 1 G, in agreement with our experimental observation of an increased tunneling rate below this magnetic field value.

is long and includes the complete characterization of elastic and inelastic collisions at ultralow temperatures, the exploration of superfluidity, vortices, and second sound in Bose gases, the study of quantum-degenerate molecules and Fermi gases, the development of practical “high-power” atom lasers, and their application in atom optics and precision measurements.

Acknowledgements

We are grateful to Chris Westbrook and Robin Kaiser for organizing a stimulating summer school, to Shin Inouye for valuable discussions, to Chandra Raman and Ananth Chikkatur for comments on the manuscript. The BEC work at MIT was done in collaboration with M.R. Andrews, A.P. Chikkatur, K.B. Davis, D.S. Durfee, A. Görlitz, S. Gupta, Z. Hadzibabic, S. Inouye, M. Köhl, C.E. Kulewicz, M.-O. Mewes, H.-J. Miesner, R. Onofrio, T. Pfau, D.E. Pritchard, C. Raman, D.M. Stamper-Kurn, J. Stenger, C.G. Townsend, N.J. van Druten, and J. Vogels. This work was supported by NSF, ONR, JSEP, ARO, NASA, and the David and Lucile Packard Foundation. D.M.S.-K. acknowledges additional support from JSEP, and is presently supported by a Millikan Prize Postdoctoral Fellowship.

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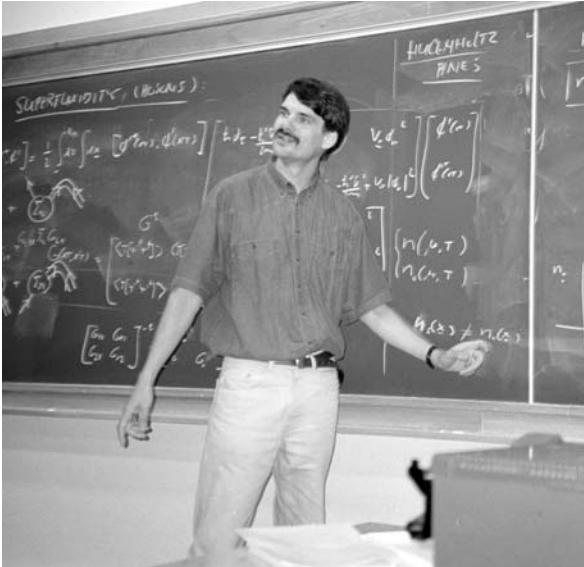
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COURSE 3

FIELD THEORY FOR TRAPPED ATOMIC GASES

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FIELD THEORY FOR TRAPPED ATOMIC GASES

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Abstract

In this course we give a selfcontained introduction to the quantum field theory for trapped atomic gases, using functional methods throughout. We consider both equilibrium and nonequilibrium phenomena. In the equilibrium case, we first derive the appropriate Hartree–Fock theory for the properties of the gas in the normal phase. We then turn our attention to the properties of the gas in the superfluid phase, and present a microscopic derivation of the Bogoliubov and Popov theories of Bose–Einstein condensation and the Bardeen–Cooper–Schrieffer theory of superconductivity. The former are applicable to trapped bosonic gases such as rubidium, lithium, sodium and hydrogen, and the latter in particular to the fermionic isotope of atomic lithium. In the nonequilibrium case, we discuss various topics for which a field-theoretical approach is especially suited, because they involve physics that is not contained in the Gross-Pitaevskii equation. Examples are quantum kinetic theory, the growth and collapse of a Bose condensate, the phase dynamics of bosonic and fermionic superfluids, and the collisionless collective modes of a Bose gas below the critical temperature.

1 Introduction

An important trend in the condensed matter physics of the last two decades, has been the use of advanced field-theoretical methods to discuss various subtle and fundamental properties of interacting many-particle systems at low temperatures. There are several reasons for this trend. The first reason is of course, that a traditional topic in statistical and condensed matter physics is the study of phase transitions and critical phenomena, for which the universal properties are independent of the microscopic details of the system and can therefore be determined by a field theory describing only the large-scale properties of the system of interest. Since the latter are usually solely determined by symmetry considerations, this has led to the important concept of spontaneous symmetry breaking, which has turned out to be not

only highly successful in condensed matter physics, but also in high-energy physics and in particular in the Standard Model of elementary particles [1].

A second reason is that soon after the development of the renormalization group methods for critical phenomena [2], it was realized that the same methods can in fact be used to describe the large-scale properties of many-particle systems at any temperature and not only near the critical one. Moreover, application of the renormalization group ideas does not only lead to an understanding of the static behaviour but also of the dynamical properties [3]. As a result quantum field theories can be used to conveniently determine the dynamics of many-particle systems close to equilibrium, *i.e.*, for example the linear hydrodynamical equations of motion. In addition, it can even be used in highly nonequilibrium situations where in general also nonlinearities play an important role. This feature, that also the dynamics of the system can be captured by a quantum field theory, has for instance led in recent years to the study of so-called quantum phase transitions [4].

Finally, the importance of field-theoretical methods in condensed matter physics is associated with the observation that also the effects of imperfections, *i.e.*, disorder, can be treated in this way [5]. Apart from the technological importance of disorder, for example for superconducting magnets, disorder leads also to fundamentally new physics such as the phenomenon of localization [6]. In quantum Hall systems, a combination of disorder and interaction effects give rise to the realization of various peculiar quantum fluids with fractionally charged excitations [7]. The application of field theories has proven to be highly successful in this case and has led to a theory of the quantum Hall effect in terms of edge states that form a chiral Luttinger liquid [8]. In mesoscopic physics, the study of disorder in small electronic structures has resulted in the so-called random matrix theory [9], which has also been of much use in the study of the quantization of classically chaotic systems.

In this course we aim to show that quantum field theory is also very convenient for obtaining a detailed understanding of the equilibrium and nonequilibrium properties of trapped atomic gases. After the first observations of Bose-Einstein condensation in 1995 [10–12], degenerate atomic gases have received again a great deal of attention and are presently the main subject of study of a large number of experimental and theoretical groups around the world. The reason for all this excitement is, first of all, that Bose-Einstein condensation has never before been observed experimentally in a clear-cut manner, even though this phenomenon was already predicted by Einstein in 1925 [13]. Second, it is of fundamental interest because it is the only phase transition that occurs also in the absence of interactions and is, therefore, the textbook example for the use of statistical-physics methods. Finally, the goal of achieving Bose-Einstein condensation turned out to be much more difficult than anticipated at first. Just before the

breakthrough in 1995, it had even acquired the nature of a “quest for the holy grail”, since the pioneering experiments were already performed in 1980 [14].

From a theoretical point of view, a quantitative understanding of the experiments with cold atomic gases requires that we take into account the following two effects. First, the gas is magnetically trapped in an, usually axially symmetric, harmonic oscillator potential. This is necessary because, in order to obtain the required record low temperatures of 1 – 100 nK, the gas cannot be allowed to have any contact with material walls. Second, the atoms of the gas interact with each other, which in general dramatically affects the behaviour of the condensed gas, even at the relevant low densities of $10^{12} - 10^{14} \text{ cm}^{-3}$. An accurate description of these degenerate gases thus requires the solution of a highly inhomogeneous many-body problem. The theoretical challenge posed by these new quantum systems lies therein that the density of the gas is sufficiently small that it should be possible to accurately solve this many-body problem from first principles and to compare the outcome of the theory directly with experiment, *i.e.*, without any adjustable parameters. In our opinion, quantum field theory is the most simple way in which we are able to meet this challenge.

2 Equilibrium field theory

We start our development of the quantum field theory of trapped atomic gases by considering first the equilibrium properties of these gases. We consider both Bose and Fermi gases, and the ultimate aim of this section is to arrive, for both cases, at an accurate description of the normal and superfluid phases of the gas. Although mixtures of Bose and Fermi gases are also of current interest, we do not consider them explicitly here, because they can be treated by a straightforward generalization of the theory. In Section 3 we then turn to the nonequilibrium properties, which are perhaps the most interesting and certainly the least understood at present. The reason for organizing the course in this way, is that the development of the equilibrium theory gives us an opportunity to introduce all the necessary tools that are required for a treatment of the more complicated nonequilibrium case. In particular, we present in detail the way in which we can make use of functional methods. To make also a connection with the more familiar operator language, however, we first briefly summarize the outcome of the second quantization formalism.

2.1 Second quantization

The atoms of interest to us have internal degrees of freedom due to the electron and nuclear spins. In principle this is very important, because it gives the atom a magnetic moment, which is used to trap the atoms in a

magnetic field minimum. During this course, however, we restrict ourselves to atomic gases that are a mixture of at most two hyperfine states. Without loss of generality, we can then suppose to have N identical atoms with mass m and effective spin $\mathbf{s}$ in an external potential $V^{\text{ex}}(\mathbf{x})$. As a result, the time-dependent Schrödinger equation we have to solve is

$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = \hat{H} |\Psi(t)\rangle, \quad (2.1)$$

where the hamiltonian is

$$\hat{H} = \sum_{i=1}^N \left\{ \frac{\hat{\mathbf{p}}_i^2}{2m} + V^{\text{ex}}(\hat{\mathbf{x}}_i) - \gamma \hat{\mathbf{s}}_i \cdot \mathbf{B}^{\text{eff}} \right\} + \frac{1}{2} \sum_{i \neq j=1}^N V(\hat{\mathbf{x}}_i - \hat{\mathbf{x}}_j), \quad (2.2)$$

$[\hat{\mathbf{x}}_j, \hat{\mathbf{p}}_j]_- = i\hbar$, and all other commutators of the positions and momenta vanish. The first term in the right-hand side is the sum of the one-particle hamiltonians, which includes an effective Zeeman interaction that accounts for a possible difference in the hyperfine energies. The second term represents the interactions. For simplicity, we have assumed that the interaction $V(\hat{\mathbf{x}}_i - \hat{\mathbf{x}}_j)$ is independent of the hyperfine states of the atoms i and j . This is in general not justified for realistic atomic gases, but is valid for the specific applications that we have in mind. Moreover, in Section 2.6 we also discuss the general case. Finally, we have also neglected possible three-body forces. This is a result of the fact that we are interested in dilute quantum gases, for which it is highly improbable for three atoms to simultaneously interact with each other.

Without interactions the eigenstates are, of course, given by the states $\{|\mathbf{n}_1, \alpha_1\rangle_1 \otimes |\mathbf{n}_2, \alpha_2\rangle_2 \otimes \cdots \otimes |\mathbf{n}_N, \alpha_N\rangle_N\}$, where the specific quantum state for each atom is exactly known. Here $\mathbf{n} = (n_x, n_y, n_z)$ and the nonnegative integers n_x , n_y , and n_z denote the three quantum numbers that are required to specify the one-particle eigenstates in the external potential. The wave functions and energies of these eigenstates are $\chi_{\mathbf{n}}(\mathbf{x}) \equiv \langle \mathbf{x} | \mathbf{n} \rangle$ and $\epsilon_{\mathbf{n}}$, respectively, and are found from the time-independent Schrödinger equation

$$\left\{ -\frac{\hbar^2 \nabla^2}{2m} + V^{\text{ex}}(\mathbf{x}) - \epsilon_{\mathbf{n}} \right\} \chi_{\mathbf{n}}(\mathbf{x}) = 0. \quad (2.3)$$

In addition, the internal state $|\alpha\rangle$ is a shorthand notation for $|s, m_s\rangle$. The many-body wave function $|\Psi(t)\rangle$, however, has to be symmetric or antisymmetric under permutations for bosonic or fermionic atoms, respectively. Therefore it is more convenient to use a properly (anti)symmetrized version of the above basis, *i.e.*, the states $|\{N_{\mathbf{n},\alpha}\}\rangle$ with the occupation numbers $N_{\mathbf{n},\alpha} = 0, 1, 2, \dots, \infty$ for bosons and $N_{\mathbf{n},\alpha} = 0, 1$ for fermions. The Hilbert space of all these states, without the constraint $N = \sum_{\mathbf{n},\alpha} N_{\mathbf{n},\alpha}$, is known as the Fock space.

Clearly, the many-body wave function $|\Psi(t)\rangle$ can be expanded in this basis as

$$|\Psi(t)\rangle = \sum_{\{N_{\mathbf{n},\alpha}\}} \Psi(\{N_{\mathbf{n},\alpha}\}, t) |\{N_{\mathbf{n},\alpha}\}\rangle, \quad (2.4)$$

where $\Psi(\{N_{\mathbf{n},\alpha}\}, t)$ is the amplitude for the gas to be in state $|\{N_{\mathbf{n},\alpha}\}\rangle$ at time t . In this basis the Schrödinger equation becomes

$$i\hbar \frac{\partial}{\partial t} \Psi(\{N_{\mathbf{n},\alpha}\}, t) = \sum_{\{N'_{\mathbf{n},\alpha}\}} \langle \{N_{\mathbf{n},\alpha}\} | \hat{H} | \{N'_{\mathbf{n},\alpha}\} \rangle \Psi(\{N'_{\mathbf{n},\alpha}\}, t), \quad (2.5)$$

which shows that we need the matrix elements of the hamiltonian between different states in the Fock space. To calculate these most easily we introduce so-called annihilation operators $\hat{\psi}_{\mathbf{n},\alpha}$ by

$$\hat{\psi}_{\mathbf{n},\alpha} |\dots, N_{\mathbf{n},\alpha}, \dots\rangle = \sqrt{N_{\mathbf{n},\alpha}} |\dots, N_{\mathbf{n},\alpha} - 1, \dots\rangle, \quad (2.6)$$

from which it follows that the creation operators $\hat{\psi}_{\mathbf{n},\alpha}^\dagger$ obey

$$\hat{\psi}_{\mathbf{n},\alpha}^\dagger |\dots, N_{\mathbf{n},\alpha}, \dots\rangle = \sqrt{1 \pm N_{\mathbf{n},\alpha}} |\dots, N_{\mathbf{n},\alpha} + 1, \dots\rangle. \quad (2.7)$$

As a result, we see that the operator $\hat{\psi}_{\mathbf{n},\alpha}^\dagger \hat{\psi}_{\mathbf{n},\alpha}$ counts the number of atoms in the state $|\mathbf{n}, \alpha\rangle$, *i.e.*,

$$\hat{\psi}_{\mathbf{n},\alpha}^\dagger \hat{\psi}_{\mathbf{n},\alpha} |\dots, N_{\mathbf{n},\alpha}, \dots\rangle = N_{\mathbf{n},\alpha} |\dots, N_{\mathbf{n},\alpha}, \dots\rangle. \quad (2.8)$$

We have also that $[\hat{\psi}_{\mathbf{n},\alpha}, \hat{\psi}_{\mathbf{n}',\alpha'}]_{\mp} = [\hat{\psi}_{\mathbf{n},\alpha}^\dagger, \hat{\psi}_{\mathbf{n}',\alpha'}^\dagger]_{\mp} = 0$ and most importantly that

$$[\hat{\psi}_{\mathbf{n},\alpha}, \hat{\psi}_{\mathbf{n}',\alpha'}^\dagger]_{\mp} = \delta_{\mathbf{n},\mathbf{n}'} \delta_{\alpha,\alpha'}. \quad (2.9)$$

In equations (2.7) and (2.9) the upper sign refers to bosons and the lower to fermions. This will be true throughout the course.

From these results we can now easily show, first of all, that the basis in the Fock space is given by

$$|\{N_{\mathbf{n},\alpha}\}\rangle = \prod_{\mathbf{n},\alpha} \frac{(\hat{\psi}_{\mathbf{n},\alpha}^\dagger)^{N_{\mathbf{n},\alpha}}}{\sqrt{N_{\mathbf{n},\alpha}!}} |0\rangle, \quad (2.10)$$

with $|0\rangle$ the vacuum state containing no atoms. Second, the hamiltonian is

$$\begin{aligned} \hat{H} = & \sum_{\mathbf{n},\alpha} \epsilon_{\mathbf{n},\alpha} \hat{\psi}_{\mathbf{n},\alpha}^\dagger \hat{\psi}_{\mathbf{n},\alpha} \\ & + \frac{1}{2} \sum_{\alpha,\alpha'} \sum_{\mathbf{n},\mathbf{n}',\mathbf{m},\mathbf{m}'} V_{\mathbf{n},\mathbf{n}';\mathbf{m},\mathbf{m}'} \hat{\psi}_{\mathbf{n},\alpha}^\dagger \hat{\psi}_{\mathbf{n}',\alpha'}^\dagger \hat{\psi}_{\mathbf{m}',\alpha'} \hat{\psi}_{\mathbf{m},\alpha}, \end{aligned} \quad (2.11)$$

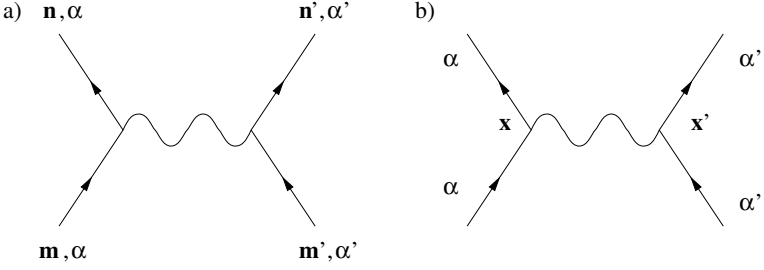


Fig. 1. Diagrammatic representation of the interaction terms in a) equation (2.11) and b) equation (2.13).

with $\epsilon_{n,\alpha} = \epsilon_n - \gamma m_s B^{\text{eff}} \equiv \epsilon_n + \epsilon_\alpha$ the one-particle energies. Furthermore,

$$V_{n,n';m,m'} = \int d\mathbf{x} \int d\mathbf{x}' \chi_n^*(\mathbf{x}) \chi_{n'}^*(\mathbf{x}') V(\mathbf{x} - \mathbf{x}') \chi_m(\mathbf{x}) \chi_{m'}(\mathbf{x}') \quad (2.12)$$

is the amplitude for a collision which scatters two atoms out of the states $|m, \alpha\rangle$ and $|m', \alpha'\rangle$ into the states $|n, \alpha\rangle$ and $|n', \alpha'\rangle$, as schematically shown in Figure 1(a).

Introducing the field operators $\hat{\psi}_\alpha(\mathbf{x}) = \sum_n \hat{\psi}_{n,\alpha} \chi_n(\mathbf{x})$ and $\hat{\psi}_\alpha^\dagger(\mathbf{x}) = \sum_n \hat{\psi}_{n,\alpha}^\dagger \chi_n^*(\mathbf{x})$, that annihilate and create atoms in the spin state $|\alpha\rangle$ at position $\mathbf{x}$ respectively, we can rewrite this result into

$$\begin{aligned} \hat{H} = & \sum_\alpha \int d\mathbf{x} \hat{\psi}_\alpha^\dagger(\mathbf{x}) \left\{ -\frac{\hbar^2 \nabla^2}{2m} + V^{\text{ex}}(\mathbf{x}) + \epsilon_\alpha \right\} \hat{\psi}_\alpha(\mathbf{x}) \\ & + \frac{1}{2} \sum_{\alpha, \alpha'} \int d\mathbf{x} \int d\mathbf{x}' \hat{\psi}_\alpha^\dagger(\mathbf{x}) \hat{\psi}_{\alpha'}^\dagger(\mathbf{x}') V(\mathbf{x} - \mathbf{x}') \hat{\psi}_{\alpha'}(\mathbf{x}') \hat{\psi}_\alpha(\mathbf{x}). \end{aligned} \quad (2.13)$$

Note that, due to the (anti)commutation relations of the creation and annihilation operators and the orthogonality of the wave functions $\chi_n(\mathbf{x})$, the field operators obey $[\hat{\psi}_\alpha(\mathbf{x}), \hat{\psi}_{\alpha'}(\mathbf{x}')]_{\mp} = [\hat{\psi}_\alpha^\dagger(\mathbf{x}), \hat{\psi}_{\alpha'}^\dagger(\mathbf{x}')]_{\mp} = 0$ and $[\hat{\psi}_\alpha(\mathbf{x}), \hat{\psi}_{\alpha'}^\dagger(\mathbf{x}')]_{\mp} = \delta(\mathbf{x} - \mathbf{x}') \delta_{\alpha, \alpha'}$. Moreover, it is also important for the following to note that the number operator is

$$\hat{N} = \sum_{n,\alpha} \hat{\psi}_{n,\alpha}^\dagger \hat{\psi}_{n,\alpha} = \sum_\alpha \int d\mathbf{x} \hat{\psi}_\alpha^\dagger(\mathbf{x}) \hat{\psi}_\alpha(\mathbf{x}) \quad (2.14)$$

and, similarly, that the effective total spin operator is

$$\hat{\mathbf{S}} = \sum_{n,\alpha,\alpha'} \hat{\psi}_{n,\alpha}^\dagger \langle \alpha | \hat{\mathbf{S}} | \alpha' \rangle \hat{\psi}_{n,\alpha'} = \sum_{\alpha,\alpha'} \int d\mathbf{x} \hat{\psi}_\alpha^\dagger(\mathbf{x}) \langle \alpha | \hat{\mathbf{S}} | \alpha' \rangle \hat{\psi}_{\alpha'}(\mathbf{x}). \quad (2.15)$$

The density of atoms in the state $|\alpha\rangle$ is thus simply $\hat{n}_\alpha(\mathbf{x}) = \hat{\psi}_\alpha^\dagger(\mathbf{x})\hat{\psi}_\alpha(\mathbf{x})$.

This completes our brief discussion of the second quantization formalism. In principle, we could now proceed to develop an operator formulation of the quantum field theory of interest to us. Since the experimentally most important observables can be expressed as appropriate products of the field operators, as we have just seen, this would essentially amount to the study of the (imaginary) time evolution of the Heisenberg operator $\hat{\psi}(\mathbf{x}, \tau) = e^{(\hat{H} - \mu\hat{N})\tau/\hbar} \hat{\psi}_\alpha(\mathbf{x}) e^{-(\hat{H} - \mu\hat{N})\tau/\hbar}$ at a fixed chemical potential μ [15]. Put differently, the desired quantum field theory would be defined by the Heisenberg equation of motion

$$\hbar \frac{\partial}{\partial \tau} \hat{\psi}_\alpha(\mathbf{x}, \tau) = [\hat{H} - \mu\hat{N}, \hat{\psi}_\alpha(\mathbf{x}, \tau)]_-, \quad (2.16)$$

and we would need to solve this equation in a sufficiently accurate approximation. As mentioned previously, however, we here want to develop Feynman's "path-integral" formulation of the problem, which will turn out to be much more convenient for our purposes. To do so in a manner that is the same for both bosonic and fermionic atomic gases, we first need to introduce some mathematical background.

2.2 Grassmann variables and coherent states

We have seen that in the case of fermions, we need to make use of anticommuting creation and annihilation operators. This automatically builds in the Pauli principle in the theory, because it implies that $(\hat{\psi}_{\mathbf{n},\alpha}^\dagger)^2|0\rangle = 0$ and thus that the occupation numbers $N_{\mathbf{n},\alpha}$ are restricted to be either 0 or 1. For reasons that will become clear in a moment, it is in that case also convenient to introduce anticommuting complex numbers or Grassmann variables. The simplest example is to have two such Grassmann variables, say ϕ and ϕ^* . The set $\{1, \phi, \phi^*, \phi^*\phi\}$, and linear combinations thereof with complex coefficients, form then a so-called Grassmann algebra.

By definition we have $[\phi, \phi]_+ = [\phi, \phi^*]_+ = [\phi^*, \phi^*]_+ = 0$ and thus in particular $\phi^2 = \phi^{*2} = 0$. Therefore, the above set is indeed complete. The complex conjugation in this algebra is defined by $(\phi)^* = \phi^*$, $(\phi^*)^* = \phi$, and $(\phi^*\phi)^* = (\phi)^*(\phi^*)^* = \phi^*\phi$. Moreover, we can also define an analytic function on this algebra by

$$A(\phi^*, \phi) = a_{11} + a_{12}\phi + a_{21}\phi^* + a_{22}\phi^*\phi. \quad (2.17)$$

As a result, it is natural to define also a differentiation by

$$\frac{\partial}{\partial \phi} A(\phi^*, \phi) = a_{12} - a_{22}\phi^*. \quad (2.18)$$

To be more precise this is in fact a left differentiation and the minus sign occurs, because we need to permute ϕ^* and ϕ before we can differentiate with respect to ϕ . So, similarly, we have

$$\frac{\partial}{\partial \phi^*} A(\phi^*, \phi) = a_{21} + a_{22} \phi \quad (2.19)$$

and

$$\frac{\partial^2}{\partial \phi^* \partial \phi} A(\phi^*, \phi) = -\frac{\partial^2}{\partial \phi \partial \phi^*} A(\phi^*, \phi) = -a_{22}. \quad (2.20)$$

Next we also need integrations over these Grassmann variables. Note that since $\phi^2 = 0$ we have only two possible integrals, namely $\int d\phi \, 1$ and $\int d\phi \, \phi$. We define these by

$$\int d\phi \, 1 = 0 \quad (2.21)$$

and

$$\int d\phi \, \phi = 1. \quad (2.22)$$

This means that integration is equivalent to differentiation. The main reason for the above definition is that we want the integration to obey the usual rules of partial integration. In particular, this implies that

$$\int d\phi \, \frac{\partial F(\phi)}{\partial \phi} = 0, \quad (2.23)$$

for any function $F(\phi) = f_1 + f_2 \phi$. It is clear that this condition requires that $\int d\phi \, 1 = 0$. The result of $\int d\phi \, \phi$ is then solely a question of normalization. It turns out that we are primarily interested in integrals of the form

$$\int d\phi^* d\phi \, A(\phi^*, \phi) = \int d\phi^* d\phi \, (a_{11} + a_{12} \phi + a_{21} \phi^* + a_{22} \phi^* \phi) = -a_{22} \quad (2.24)$$

as we will see in Section 2.3.

Clearly, we can now also consider the Grassmann algebra based on the variables ϕ_n and ϕ_n^* with $n = 1, 2, \dots, \infty$. What we will need in the following are gaussian integrals over these variables. It is not difficult to show with the above definitions that

$$\int \left(\prod_n d\phi_n^* d\phi_n \right) \exp \left\{ - \sum_{n,n'} \phi_n^* A_{n,n'} \phi_{n'} \right\} = \det A = e^{\text{Tr}[\ln A]}. \quad (2.25)$$

If the variables ϕ_n and ϕ_n^* were just ordinary complex numbers we would in contrast have the result

$$\int \left(\prod_n \frac{d\phi_n^* d\phi_n}{2\pi i} \right) \exp \left\{ - \sum_{n,n'} \phi_n^* A_{n,n'} \phi_{n'} \right\} = \frac{1}{\det A} = e^{-\text{Tr}[\ln A]}. \quad (2.26)$$

These last two results will be used many times in the following.

One immediate use of these Grassmann variables is that we can now consider eigenstates of the annihilation operator $\hat{\psi}_{\mathbf{n},\alpha}$, also when we are dealing with fermions. These eigenstates are called coherent states. Consider the state

$$|\phi_{\mathbf{n},\alpha}\rangle \equiv (1 - \phi_{\mathbf{n},\alpha} \hat{\psi}_{\mathbf{n},\alpha}^\dagger) |0\rangle = \exp \left\{ -\phi_{\mathbf{n},\alpha} \hat{\psi}_{\mathbf{n},\alpha}^\dagger \right\} |0\rangle, \quad (2.27)$$

where $\phi_{\mathbf{n},\alpha}$ is a Grassmann variable that also anticommutes with the creation and annihilation operators in our Fock space. Clearly we have that

$$\begin{aligned} \hat{\psi}_{\mathbf{n},\alpha} |\phi_{\mathbf{n},\alpha}\rangle &= \hat{\psi}_{\mathbf{n},\alpha} |0\rangle + \phi_{\mathbf{n},\alpha} \hat{\psi}_{\mathbf{n},\alpha} \hat{\psi}_{\mathbf{n},\alpha}^\dagger |0\rangle \\ &= \phi_{\mathbf{n},\alpha} |0\rangle = \phi_{\mathbf{n},\alpha} (1 - \phi_{\mathbf{n},\alpha} \hat{\psi}_{\mathbf{n},\alpha}^\dagger) |0\rangle = \phi_{\mathbf{n},\alpha} |\phi_{\mathbf{n},\alpha}\rangle, \end{aligned} \quad (2.28)$$

so $|\phi_{\mathbf{n},\alpha}\rangle$ is indeed an eigenstate of $\hat{\psi}_{\mathbf{n},\alpha}$ with eigenvalue $\phi_{\mathbf{n},\alpha}$. In general we can now make the states

$$|\phi\rangle = \exp \left\{ - \sum_{\mathbf{n},\alpha} \phi_{\mathbf{n},\alpha} \hat{\psi}_{\mathbf{n},\alpha}^\dagger \right\} |0\rangle \quad (2.29)$$

that obey $\hat{\psi}_{\mathbf{n},\alpha} |\phi\rangle = \phi_{\mathbf{n},\alpha} |\phi\rangle$. Introducing the Grassmann-valued field $\phi_\alpha(\mathbf{x}) = \sum_{\mathbf{n}} \phi_{\mathbf{n},\alpha} \chi_{\mathbf{n}}(\mathbf{x})$, the latter two relations can be rewritten as

$$|\phi\rangle = \exp \left\{ - \sum_{\alpha} \int d\mathbf{x} \phi_{\alpha}(\mathbf{x}) \hat{\psi}_{\alpha}^\dagger(\mathbf{x}) \right\} |0\rangle \quad (2.30)$$

and $\hat{\psi}_{\alpha}(\mathbf{x}) |\phi\rangle = \phi_{\alpha}(\mathbf{x}) |\phi\rangle$.

It is important to note that these coherent states are not orthonormal. In contrast, we find that

$$\begin{aligned} \langle \phi | \phi' \rangle &= \prod_{\mathbf{n},\alpha} \langle 0 | (1 - \hat{\psi}_{\mathbf{n},\alpha} \phi_{\mathbf{n},\alpha}^*) (1 - \phi'_{\mathbf{n},\alpha} \hat{\psi}_{\mathbf{n},\alpha}^\dagger) | 0 \rangle \\ &= \prod_{\mathbf{n},\alpha} (1 + \phi_{\mathbf{n},\alpha}^* \phi'_{\mathbf{n},\alpha}) = \exp \left\{ \sum_{\mathbf{n},\alpha} \phi_{\mathbf{n},\alpha}^* \phi'_{\mathbf{n},\alpha} \right\} \\ &= \exp \left\{ \sum_{\alpha} \int d\mathbf{x} \phi_{\alpha}^*(\mathbf{x}) \phi'_{\alpha}(\mathbf{x}) \right\} \equiv e^{(\phi|\phi')}. \end{aligned} \quad (2.31)$$

Nevertheless they obey a closure relation, as can be seen explicitly from

$$\begin{aligned}
 & \int \left(\prod_{\mathbf{n}, \alpha} d\phi_{\mathbf{n}, \alpha}^* d\phi_{\mathbf{n}, \alpha} \right) \exp \left\{ - \sum_{\mathbf{n}, \alpha} \phi_{\mathbf{n}, \alpha}^* \phi_{\mathbf{n}, \alpha} \right\} |\phi\rangle \langle \phi| \\
 &= \prod_{\mathbf{n}, \alpha} \int d\phi_{\mathbf{n}, \alpha}^* d\phi_{\mathbf{n}, \alpha} (1 - \phi_{\mathbf{n}, \alpha}^* \phi_{\mathbf{n}, \alpha}) (1 - \phi_{\mathbf{n}, \alpha} \hat{\psi}_{\mathbf{n}, \alpha}^\dagger) |0\rangle \langle 0| (1 - \hat{\psi}_{\mathbf{n}, \alpha} \phi_{\mathbf{n}, \alpha}^*) \\
 &= \prod_{\mathbf{n}, \alpha} (|0\rangle \langle 0| + |1\rangle \langle 1|) = \hat{1}.
 \end{aligned} \tag{2.32}$$

We write this from now on simply as

$$\int d[\phi^*] d[\phi] e^{-(\phi|\phi)} |\phi\rangle \langle \phi| = \hat{1}. \tag{2.33}$$

The interesting observation at this point is that essentially the same formulae also hold for bosons [16, 17]. We have only a minus sign difference in

$$|\phi\rangle = \exp \left\{ \sum_{\alpha} \int d\mathbf{x} \phi_{\alpha}(\mathbf{x}) \hat{\psi}_{\alpha}^{\dagger}(\mathbf{x}) \right\} |0\rangle, \tag{2.34}$$

but then it can still be easily shown that $\hat{\psi}_{\alpha}(\mathbf{x})|\phi\rangle = \phi_{\alpha}(\mathbf{x})|\phi\rangle$. A convenient way to do so is, for instance, by noting that the commutation relation $[\hat{\psi}_{\alpha}(\mathbf{x}), \hat{\psi}_{\alpha'}^{\dagger}(\mathbf{x}')]_{-} = \delta(\mathbf{x} - \mathbf{x}')\delta_{\alpha, \alpha'}$ implies that $\hat{\psi}_{\alpha}(\mathbf{x})$ acts as $\delta/\delta\hat{\psi}_{\alpha}^{\dagger}(\mathbf{x})$ on these states. Furthermore, the same expressions hold for the overlap $\langle\phi|\phi'\rangle$ and the closure relation, if we define the integration measure by $\int d[\phi^*]d[\phi] \equiv \int \prod_{\mathbf{n}, \alpha} d\phi_{\mathbf{n}, \alpha}^* d\phi_{\mathbf{n}, \alpha} / (2\pi i)$ in this case.

Summarizing, we have thus found for bosons and fermions that

$$|\phi\rangle = \exp \left\{ \pm \sum_{\alpha} \int d\mathbf{x} \phi_{\alpha}(\mathbf{x}) \hat{\psi}_{\alpha}^{\dagger}(\mathbf{x}) \right\} |0\rangle, \tag{2.35}$$

$$\langle\phi|\phi'\rangle = e^{(\phi|\phi')}, \tag{2.36}$$

and

$$\int d[\phi^*] d[\phi] e^{-(\phi|\phi)} |\phi\rangle \langle \phi| = \hat{1}. \tag{2.37}$$

The last ingredient we need is that in terms of these coherent states the trace of an operator $\hat{O}$ over the Fock space can be expressed as

$$\text{Tr}[\hat{O}] = \int d[\phi^*] d[\phi] e^{-(\phi|\phi)} \langle \pm \phi | \hat{O} | \phi \rangle. \tag{2.38}$$

The minus sign in the fermionic case is easily understood from the fact that we then have $\langle \{N_{\mathbf{n},\alpha}\} | \phi \rangle \langle \phi | \{N_{\mathbf{n},\alpha}\} \rangle = \langle -\phi | \{N_{\mathbf{n},\alpha}\} \rangle \langle \{N_{\mathbf{n},\alpha}\} | \phi \rangle$, due to the anticommuting nature of the Grassmann variables. After this mathematical interlude we can now return to physics and to our goal of arriving at a unified treatment of bosonic and fermionic atomic gases.

2.3 Functional integrals

We are interested in determining the equilibrium properties of a trapped atomic gas at some temperature T . From statistical physics we know that all these properties can be obtained from the grand-canonical partition function

$$Z = \text{Tr} \left[e^{-\beta(\hat{H} - \mu\hat{N})} \right], \quad (2.39)$$

where $\beta = 1/k_B T$ and μ the chemical potential. We thus need to evaluate this quantity. As mentioned previously, we want to do so by making use of quantum field theory and, in addition, of Feynman's path-integral approach to quantum mechanics. We thus want to write the partition function as a functional integral over time-dependent fields $\phi_\alpha(\mathbf{x}, \tau)$, just like the partition function of a single particle in an external potential can be written as a functional integral over all time-dependent paths $\mathbf{x}(\tau)$. This can indeed be achieved with the coherent states that we have introduced in the previous section.

We start with using our formula (2.38) for the trace of an operator,

$$Z = \int d[\phi^*] d[\phi] e^{-(\phi|\phi)} \langle \pm\phi | e^{-\beta(\hat{H} - \mu\hat{N})} | \phi \rangle, \quad (2.40)$$

and observe that we are thus faced with the task of calculating the matrix elements $\langle \phi_M | e^{-\beta(\hat{H} - \mu\hat{N})} | \phi_0 \rangle$ with $\phi_0(\mathbf{x}) = \phi(\mathbf{x})$ and $\phi_M^*(\mathbf{x}) = \pm\phi^*(\mathbf{x})$. This is difficult in general but can be simplified in the following way. We first realize that the operator $e^{-\beta(\hat{H} - \mu\hat{N})}$ is identical to the quantum mechanical evolution operator $U(t, 0) = e^{-i(\hat{H} - \mu\hat{N})t/\hbar}$ evaluated at $t = -i\hbar\beta$. Put differently, we thus want to calculate the matrix elements of the imaginary-time evolution operator $U(-i\tau, 0)$ for $\tau = \hbar\beta$. To do so, we next split the time interval $[0, \hbar\beta]$ into M pieces, with $\tau_m = m\hbar\beta/M$ and $m = 0, 1, \dots, M$. So $\Delta\tau = \hbar\beta/M$. The procedure is summarized in Figure 2.

At each intermediate time τ_m we then apply a closure relation of the coherent states. This gives

$$\begin{aligned} & \langle \phi_M | e^{-\beta(\hat{H} - \mu\hat{N})} | \phi_0 \rangle \\ &= \int \left(\prod_{m=1}^{M-1} d[\phi_m^*] d[\phi_m] e^{-(\phi_m|\phi_m)} \right) \prod_{m=1}^M \langle \phi_m | e^{-\Delta\tau(\hat{H} - \mu\hat{N})/\hbar} | \phi_{m-1} \rangle. \end{aligned} \quad (2.41)$$



Fig. 2. Illustration of the slicing of the imaginary time interval $[0, \hbar\beta]$ needed for Feynman's path-integral formulation of the partition function.

Now we can use that in the limit $M \rightarrow \infty$ we only need to know the latter matrix elements up to order $\Delta\tau$, because terms of order $(\Delta\tau)^2$ lead to corrections of order $M(\Delta\tau)^2 \propto 1/M$, which vanish in that limit. Hence

$$\begin{aligned} \langle \phi_m | e^{-\Delta\tau(\hat{H} - \mu\hat{N})/\hbar} | \phi_{m-1} \rangle &\simeq \langle \phi_m | 1 - \Delta\tau(\hat{H} - \mu\hat{N})/\hbar | \phi_{m-1} \rangle \quad (2.42) \\ &\equiv \langle \phi_m | \phi_{m-1} \rangle (1 - \Delta\tau H[\phi_m^*, \phi_{m-1}]/\hbar), \end{aligned}$$

with the grand-canonical hamiltonian functional resulting from equations (2.13) and (2.14) equal to

$$\begin{aligned} H[\phi^*, \phi] &= \sum_{\alpha} \int d\mathbf{x} \, \phi_{\alpha}^*(\mathbf{x}) \left\{ -\frac{\hbar^2 \nabla^2}{2m} + V^{\text{ex}}(\mathbf{x}) + \epsilon_{\alpha} - \mu \right\} \phi_{\alpha}(\mathbf{x}) \\ &+ \frac{1}{2} \sum_{\alpha, \alpha'} \int d\mathbf{x} \int d\mathbf{x}' \, \phi_{\alpha}^*(\mathbf{x}) \phi_{\alpha'}^*(\mathbf{x}') V(\mathbf{x} - \mathbf{x}') \phi_{\alpha'}(\mathbf{x}') \phi_{\alpha}(\mathbf{x}), \quad (2.43) \end{aligned}$$

since $\psi_{\alpha}(\mathbf{x})|\phi\rangle = \phi_{\alpha}(\mathbf{x})|\phi\rangle$ and $\langle\phi|\psi_{\alpha}^{\dagger}(\mathbf{x}) = \langle\phi|\phi_{\alpha}^*(\mathbf{x})$.

Thus, neglecting terms of order $(\Delta\tau)^2$, we can again exponentiate the right-hand side of equation (2.42), which leads in first instance to

$$\langle \phi_m | e^{-\Delta\tau(\hat{H} - \mu\hat{N})/\hbar} | \phi_{m-1} \rangle = e^{(\phi_m | \phi_{m-1}) - \Delta\tau H[\phi_m^*, \phi_{m-1}]/\hbar}, \quad (2.44)$$

and therefore for the desired matrix element of the imaginary-time evolution operator to

$$\begin{aligned} \langle \phi_M | e^{-\beta(\hat{H} - \mu\hat{N})} | \phi_0 \rangle &= \int \left(\prod_{m=1}^{M-1} d[\phi_m^*] d[\phi_m] e^{-(\phi_m | \phi_m)} \right) \quad (2.45) \\ &\times \exp \left\{ \sum_{m=1}^M ((\phi_m | \phi_{m-1}) - \Delta\tau H[\phi_m^*, \phi_{m-1}]/\hbar) \right\}. \end{aligned}$$

This can then be manipulated into the suggestive form

$$\begin{aligned} \langle \phi_M | e^{-\beta(\hat{H}-\mu\hat{N})} | \phi_0 \rangle &= e^{(\phi_M|\phi_M)} \int \left(\prod_{m=1}^{M-1} d[\phi_m^*] d[\phi_m] \right) \\ &\times \exp \left\{ -\frac{1}{\hbar} \sum_{m=1}^M \Delta\tau \left(\hbar \frac{(\phi_m|\phi_m) - (\phi_m|\phi_{m-1})}{\Delta\tau} + H[\phi_m^*, \phi_{m-1}] \right) \right\}. \end{aligned} \quad (2.46)$$

Taking now the continuum limit $M \rightarrow \infty$ and putting $\phi_m \equiv \phi(\tau_m)$, we find that

$$\begin{aligned} \langle \phi_M | e^{-\beta(\hat{H}-\mu\hat{N})} | \phi_0 \rangle &= \\ &e^{(\phi(\hbar\beta)|\phi(\hbar\beta))} \int_{\phi(0)=\phi_0}^{\phi^*(\hbar\beta)=\phi_M^*} d[\phi^*] d[\phi] e^{-S[\phi^*, \phi]/\hbar}, \end{aligned} \quad (2.47)$$

where the so-called Euclidean action is

$$\begin{aligned} S[\phi^*, \phi] &= \\ &\int_0^{\hbar\beta} d\tau \left\{ \sum_{\alpha} \int d\mathbf{x} \phi_{\alpha}^*(\mathbf{x}, \tau) \hbar \frac{\partial}{\partial \tau} \phi_{\alpha}(\mathbf{x}, \tau) + H[\phi^*(\tau), \phi(\tau)] \right\}. \end{aligned} \quad (2.48)$$

This is essentially the desired functional integral over the complex fields $\phi_{\alpha}(\mathbf{x}, \tau)$ with the boundary conditions $\phi_{\alpha}(\mathbf{x}, 0) = \phi_{0;\alpha}(\mathbf{x})$ and $\phi_{\alpha}^*(\mathbf{x}, \hbar\beta) = \phi_{M;\alpha}^*(\mathbf{x})$. It is precisely the field theory analogue of the Feynman path integral. To obtain the partition function we only need to put $\phi_0(\mathbf{x})$ equal to $\pm\phi_M(\mathbf{x})$ and perform a last integration over $\phi_M(\mathbf{x})$ and $\phi_M^*(\mathbf{x})$. It then finally becomes

$$Z = \int d[\phi^*] d[\phi] e^{-S[\phi^*, \phi]/\hbar} \quad (2.49)$$

with the boundary conditions $\phi_{\alpha}(\mathbf{x}, \hbar\beta) = \pm\phi_{\alpha}(\mathbf{x}, 0)$, *i.e.*, the fields are periodic in $[0, \hbar\beta]$ for bosons and antiperiodic for fermions. Note that in equation (2.47) we have used the same notation for the integration measure as in equation (2.49), although there is in principle one more integration in the expression for the partition function. The difference is in the continuum limit accounted for in the boundary conditions, which are in practice usually left implicit. Having arrived at an exact identity between the partition function and a functional integral, we are now going to familiarize ourselves with this identity, and with how to perform functional integrals in general, by considering the ideal quantum gases.

2.4 Ideal quantum gases

Since the partition functions Z_0 of the ideal quantum gases are known exactly, they are ideal test cases for our field-theoretical methods. Moreover, a thorough knowledge of the ideal quantum gases is also an important first step in understanding experiments with trapped atomic gases, because the effects of the interatomic interaction can essentially be included perturbatively. How this perturbation theory is performed is discussed in detail in Section 2.5, but before we can do that we need to understand the noninteracting gases first. In that case, we have

$$S_0[\phi^*, \phi] = \sum_{\alpha} \int_0^{\hbar\beta} d\tau \int d\mathbf{x} \quad (2.50)$$

$$\times \phi_{\alpha}^*(\mathbf{x}, \tau) \left\{ \hbar \frac{\partial}{\partial \tau} - \frac{\hbar^2 \nabla^2}{2m} + V^{\text{ex}}(\mathbf{x}) + \epsilon_{\alpha} - \mu \right\} \phi_{\alpha}(\mathbf{x}, \tau)$$

and the partition function is a Gaussian integral, which explains why we were interested in Gaussian integrals in Section 2.2. It will be illustrative to evaluate this partition function in three different ways.

2.4.1 Semiclassical method

In the first way, we perform the evaluation of the trace involved in the definition of the partition function at the end of the calculation, and start by considering the matrix element $\langle \pm \phi | e^{-\beta(\hat{H} - \mu \hat{N})} | \phi \rangle$ as the functional integral

$$\int_{\phi(0)=\phi}^{\phi^*(\hbar\beta)=\pm\phi^*} \left(\prod_{\mathbf{n}, \alpha} d[\phi_{\mathbf{n}, \alpha}^*] d[\phi_{\mathbf{n}, \alpha}] \right) \exp \left\{ \sum_{\mathbf{n}, \alpha} \phi_{\mathbf{n}, \alpha}^*(\hbar\beta) \phi_{\mathbf{n}, \alpha}(\hbar\beta) \right\}$$

$$\times \exp \left\{ -\frac{1}{\hbar} \int_0^{\hbar\beta} d\tau \sum_{\mathbf{n}, \alpha} \phi_{\mathbf{n}, \alpha}^*(\tau) \left(\hbar \frac{\partial}{\partial \tau} + \epsilon_{\mathbf{n}, \alpha} - \mu \right) \phi_{\mathbf{n}, \alpha}(\tau) \right\},$$

which is the product for each $\mathbf{n}$ and α of the path integral

$$\int d[\phi^*] d[\phi] \exp \left\{ \phi^*(\hbar\beta) \phi(\hbar\beta) - \frac{1}{\hbar} \int_0^{\hbar\beta} d\tau \phi^*(\tau) \left(\hbar \frac{\partial}{\partial \tau} + \epsilon - \mu \right) \phi(\tau) \right\}$$

with the boundary conditions $\phi(0) = \phi$ and $\phi(\hbar\beta) = \pm \phi^*$. It clearly corresponds to the matrix element $\langle \pm \phi | e^{-\beta(\epsilon - \mu) \hat{\psi}^\dagger \hat{\psi}} | \phi \rangle$ for one particular value of $\mathbf{n}$ and α . We calculate this matrix element by performing a shift in the integration variables, *i.e.*, $\phi(\tau) = \phi_{\text{cl}}(\tau) + \xi(\tau)$ and $\phi^*(\tau) = \phi_{\text{cl}}^*(\tau) + \xi^*(\tau)$, where $\phi_{\text{cl}}(\tau)$ obeys the “classical” equations of motion

$$\left. \frac{\delta S_0[\phi^*, \phi]}{\delta \phi^*(\tau)} \right|_{\phi=\phi_{\text{cl}}} = \left(\hbar \frac{\partial}{\partial \tau} + \epsilon - \mu \right) \phi_{\text{cl}}(\tau) = 0 \quad (2.51)$$

and similarly for $\phi_{\text{cl}}^*(\tau)$. The solutions with the correct boundary solutions are $\phi_{\text{cl}}(\tau) = \phi e^{-(\epsilon-\mu)\tau/\hbar}$ and $\phi_{\text{cl}}^*(\tau) = \pm \phi^* e^{(\epsilon-\mu)(\tau-\hbar\beta)/\hbar}$, leading to the path integral

$$\exp \left\{ \pm e^{-\beta(\epsilon-\mu)} \phi^* \phi \right\} \\ \times \int d[\xi^*] d[\xi] \exp \left\{ -\frac{1}{\hbar} \int_0^{\hbar\beta} d\tau \xi^*(\tau) \left(\hbar \frac{\partial}{\partial \tau} + \epsilon - \mu \right) \xi(\tau) \right\}$$

with the boundary conditions $\xi^*(\hbar\beta) = \xi(0) = 0$. This means that the last path integral is just equal to $\langle 0 | e^{-\beta(\epsilon-\mu)\hat{\psi}^\dagger \hat{\psi}} | 0 \rangle = 1$ and that the desired result is just the prefactor.

Substituting this for each value of $\mathbf{n}$ and α , we apparently have

$$\langle \pm \phi | e^{-\beta(\hat{H}-\mu\hat{N})} | \phi \rangle = \exp \left\{ \pm \sum_{\mathbf{n},\alpha} e^{-\beta(\epsilon_{\mathbf{n},\alpha}-\mu)} \phi_{\mathbf{n},\alpha}^* \phi_{\mathbf{n},\alpha} \right\} \quad (2.52)$$

and the partition function becomes the product

$$Z_0 = \prod_{\mathbf{n},\alpha} \int \frac{d\phi_{\mathbf{n},\alpha}^* d\phi_{\mathbf{n},\alpha}}{(2\pi i)^{(1\pm 1)/2}} \exp \left\{ -(1 \mp e^{-\beta(\epsilon_{\mathbf{n},\alpha}-\mu)}) \phi_{\mathbf{n},\alpha}^* \phi_{\mathbf{n},\alpha} \right\} \quad (2.53) \\ = \prod_{\mathbf{n},\alpha} (1 \mp e^{-\beta(\epsilon_{\mathbf{n},\alpha}-\mu)})^{\mp 1} = \exp \left\{ \mp \sum_{\mathbf{n},\alpha} \ln(1 \mp e^{-\beta(\epsilon_{\mathbf{n},\alpha}-\mu)}) \right\}.$$

This is the correct result, because from the usual thermodynamic identity $\langle \hat{N} \rangle = \partial \ln Z_0 / \partial(\beta\mu)$ we find

$$\langle \hat{N} \rangle = \sum_{\mathbf{n},\alpha} \frac{1}{e^{\beta(\epsilon_{\mathbf{n},\alpha}-\mu)} \mp 1}, \quad (2.54)$$

as desired.

2.4.2 Matsubara expansion

The second way is easier and more common in practice. We immediately start with

$$Z_0 = \int d[\phi^*] d[\phi] e^{-S_0[\phi^*, \phi]/\hbar} \quad (2.55)$$

and incorporate the boundary conditions by expanding the fields as

$$\phi_\alpha(\mathbf{x}, \tau) = \sum_{\mathbf{n},n} \phi_{\mathbf{n},n,\alpha} \chi_{\mathbf{n}}(\mathbf{x}) \frac{e^{-i\omega_n \tau}}{\sqrt{\hbar\beta}} \quad (2.56)$$

where $\omega_n = \pi(2n)/\hbar\beta$ for bosons and $\omega_n = \pi(2n+1)/\hbar\beta$ for fermions. These are known as the even and odd Matsubara frequencies, respectively. Using this expansion we have

$$Z_0 = \int \left(\prod_{\mathbf{n}, n, \alpha} \frac{d\phi_{\mathbf{n}, n, \alpha}^* d\phi_{\mathbf{n}, n, \alpha}}{(2\pi i)^{(1\pm 1)/2}} \frac{1}{(\hbar\beta)^{\pm 1}} \right) \times \exp \left\{ -\frac{1}{\hbar} \sum_{\mathbf{n}, n, \alpha} \phi_{\mathbf{n}, n, \alpha}^* (-i\hbar\omega_n + \epsilon_{\mathbf{n}, \alpha} - \mu) \phi_{\mathbf{n}, n, \alpha} \right\}, \quad (2.57)$$

if we also take account of the jacobian involved in the change of integration variables. Note that the difference between the jacobians in the bosonic and fermionic case, is a consequence of the fact that for Grassmann variables we have that $\int d\phi f_2 \phi = f_2 = \int d(f_2 \phi) f_2(f_2 \phi)$ instead of the result $\int d(f_2 \phi) (1/f_2) (f_2 \phi)$ that we expect on the basis of ordinary complex integration. Note also that these are all again gaussian integrals, so we find in first instance

$$Z_0 = \prod_{\mathbf{n}, n, \alpha} (\beta(-i\hbar\omega_n + \epsilon_{\mathbf{n}, \alpha} - \mu))^{\mp 1} = \exp \left\{ \mp \sum_{\mathbf{n}, n, \alpha} \ln(\beta(-i\hbar\omega_n + \epsilon_{\mathbf{n}, \alpha} - \mu)) \right\}. \quad (2.58)$$

To evaluate the sum over Matsubara frequencies we need to add a convergence factor $e^{i\omega_n \eta}$ and finally take the limit $\eta \downarrow 0$. The precise reason for this particular procedure cannot be fully understood at this point but is explained in Section 2.5. However, doing so we indeed find that

$$\lim_{\eta \downarrow 0} \sum_n \ln(\beta(-i\hbar\omega_n + \epsilon - \mu)) e^{i\omega_n \eta} = \ln(1 \mp e^{-\beta(\epsilon - \mu)}). \quad (2.59)$$

To see that this is correct, we differentiate the latter equation with respect to $\beta\mu$. This gives us

$$\lim_{\eta \downarrow 0} \frac{1}{\hbar\beta} \sum_n \frac{e^{i\omega_n \eta}}{i\omega_n - (\epsilon - \mu)/\hbar} = \mp \frac{1}{e^{\beta(\epsilon - \mu)} \mp 1}, \quad (2.60)$$

which can be proved by contour integration in the following way. The function $\hbar\beta/(e^{\hbar\beta z} \mp 1)$ has poles at the even and odd Matsubara frequencies with residu ± 1 . Hence, by Cauchy's theorem the left-hand side is equal to

$$\lim_{\eta \downarrow 0} \frac{1}{2\pi i} \int_C dz \frac{e^{\eta z}}{z - (\epsilon - \mu)/\hbar} \frac{\pm 1}{e^{\hbar\beta z} \mp 1}$$

with C a contour that fully encloses the imaginary axis in the direction shown in Figure 3. Adding to the contour C the contour C' , which gives no

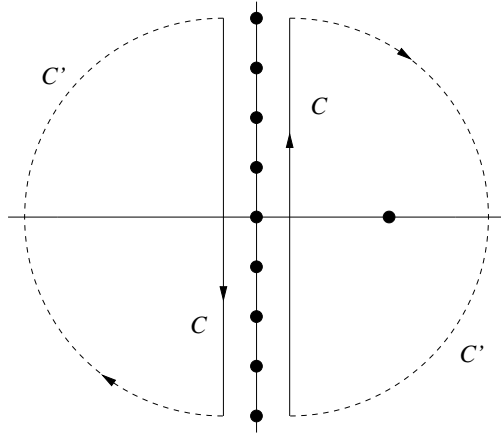


Fig. 3. Illustration of the contour integration that is required to perform the summation over the Matsubara frequencies. The black dots indicate the position of the poles in the integrant.

contribution to the integral, we can again apply Cauchy's theorem to obtain the desired result. Why does the integration over the contour C' vanish? The reason for this is that the integrant behaves as $\pm e^{-(\hbar\beta-\eta)\text{Re}(z)}/|z|$ for $\text{Re}(z) \rightarrow \infty$ and as $-e^{\eta\text{Re}(z)}/|z|$ for $\text{Re}(z) \rightarrow -\infty$. The integrant thus always vanishes much faster than $1/|z|$ on the contour C' for any $0 < \eta < \hbar\beta$.

2.4.3 Green's function method

The third and last method is simplest and, therefore, most common in practice. We first rewrite the partition function as

$$Z_0 = \int d[\phi^*]d[\phi] \exp \left\{ \sum_{\alpha} \int_0^{\hbar\beta} d\tau \int d\mathbf{x} \right. \quad (2.61)$$

$$\left. \times \sum_{\alpha'} \int_0^{\hbar\beta} d\tau' \int d\mathbf{x}' \phi_{\alpha}^*(\mathbf{x}, \tau) G_{\alpha, \alpha'}^{-1}(\mathbf{x}, \tau; \mathbf{x}', \tau') \phi_{\alpha'}(\mathbf{x}', \tau') \right\}$$

and see G^{-1} as a “matrix” both in spin space as in coordinate space. We then know that this gaussian integral is just

$$Z_0 = [\det(-G^{-1})]^{\mp 1} = \exp \{ \mp \text{Tr}[\ln(-G^{-1})] \}. \quad (2.62)$$

Clearly, we have from the action $S_0[\phi^*, \phi]$ that

$$G_{\alpha, \alpha'}^{-1}(\mathbf{x}, \tau; \mathbf{x}', \tau') = -\frac{1}{\hbar} \left\{ \hbar \frac{\partial}{\partial \tau} - \frac{\hbar^2 \nabla^2}{2m} + V^{\text{ex}}(\mathbf{x}) + \epsilon_\alpha - \mu \right\} \delta(\mathbf{x} - \mathbf{x}') \delta(\tau - \tau') \delta_{\alpha, \alpha'} \quad (2.63)$$

or equivalently that

$$\left\{ \hbar \frac{\partial}{\partial \tau} - \frac{\hbar^2 \nabla^2}{2m} + V^{\text{ex}}(\mathbf{x}) + \epsilon_\alpha - \mu \right\} G_{\alpha, \alpha'}(\mathbf{x}, \tau; \mathbf{x}', \tau') = -\hbar \delta(\mathbf{x} - \mathbf{x}') \delta(\tau - \tau') \delta_{\alpha, \alpha'}, \quad (2.64)$$

which means that $G_{\alpha, \alpha'}(\mathbf{x}, \tau; \mathbf{x}', \tau')$ is a Green's function. We come back to its physical meaning shortly. For now we only need to see that the last equation is solved by

$$G_{\alpha, \alpha'}(\mathbf{x}, \tau; \mathbf{x}', \tau') = \delta_{\alpha, \alpha'} \sum_{\mathbf{n}, n} \frac{-\hbar}{-i\hbar\omega_n + \epsilon_{\mathbf{n}, \alpha} - \mu} \chi_{\mathbf{n}}(\mathbf{x}) \chi_{\mathbf{n}}^*(\mathbf{x}') \frac{e^{-i\omega_n(\tau - \tau')}}{\hbar\beta} \quad (2.65)$$

thus again

$$\begin{aligned} Z_0 &= \exp \left\{ \mp \sum_{\mathbf{n}, n, \alpha} \ln(\beta(-i\hbar\omega_n + \epsilon_{\mathbf{n}, \alpha} - \mu)) \right\} \\ &= \exp \left\{ \mp \sum_{\mathbf{n}, \alpha} \ln(1 \mp e^{-\beta(\epsilon_{\mathbf{n}, \alpha} - \mu)}) \right\}. \end{aligned} \quad (2.66)$$

In principle, we have slightly cheated in the last step of this derivation, because equation (2.65) shows that

$$G_{\mathbf{n}, n, \alpha; \mathbf{n}', n', \alpha'} = \delta_{\mathbf{n}, \mathbf{n}'} \delta_{n, n'} \delta_{\alpha, \alpha'} \frac{-\hbar}{-i\hbar\omega_n + \epsilon_{\mathbf{n}, \alpha} - \mu}. \quad (2.67)$$

The problem with this last way of calculating the functional integral is that it does not correctly account for the jacobian involved in the change of variables from imaginary time τ to the Matsubara frequencies ω_n . However, this problem can be avoided by calculating never a single determinant, but always the ratio of two determinants. In this manner the effect of the jacobian is exactly cancelled. We will see some examples of how this works in Sections 2.6 and 2.8.3.

We now return to the physical meaning of the above Green's function. To see its meaning, we first consider the time-ordered expectation value

$$\begin{aligned} \langle T[\hat{\psi}_\alpha(\mathbf{x}, \tau) \hat{\psi}_{\alpha'}^\dagger(\mathbf{x}', \tau')] \rangle \\ \equiv \theta(\tau - \tau') \langle \hat{\psi}_\alpha(\mathbf{x}, \tau) \hat{\psi}_{\alpha'}^\dagger(\mathbf{x}', \tau') \rangle \pm \theta(\tau' - \tau) \langle \hat{\psi}_{\alpha'}^\dagger(\mathbf{x}', \tau') \hat{\psi}_\alpha(\mathbf{x}, \tau) \rangle. \end{aligned} \quad (2.68)$$

Here the expectation value is taken in the grand-canonical ensemble and $\hat{\psi}_\alpha(\mathbf{x}, \tau)$ is the imaginary time Heisenberg operator, which is defined by $e^{(\hat{H} - \mu \hat{N})\tau/\hbar} \hat{\psi}_\alpha(\mathbf{x}) e^{-(\hat{H} - \mu \hat{N})\tau/\hbar}$ and therefore obeys the Heisenberg equation of motion $\hbar \partial_\tau \hat{\psi}_\alpha(\mathbf{x}, \tau) = [\hat{H} - \mu \hat{N}, \hat{\psi}_\alpha(\mathbf{x}, \tau)]_-$. For the noninteracting case it reads

$$\hbar \frac{\partial}{\partial \tau} \hat{\psi}_\alpha(\mathbf{x}, \tau) = \left(\frac{\hbar^2 \nabla^2}{2m} - V^{\text{ex}}(\mathbf{x}) - \epsilon_\alpha + \mu \right) \hat{\psi}_\alpha(\mathbf{x}, \tau). \quad (2.69)$$

As a result

$$\begin{aligned} \hbar \frac{\partial}{\partial \tau} \langle T[\hat{\psi}_\alpha(\mathbf{x}, \tau) \hat{\psi}_{\alpha'}^\dagger(\mathbf{x}', \tau')] \rangle &= \hbar \delta(\tau - \tau') \langle [\hat{\psi}_\alpha(\mathbf{x}, \tau), \hat{\psi}_{\alpha'}^\dagger(\mathbf{x}', \tau')]_{\mp} \rangle \\ &+ \left(\frac{\hbar^2 \nabla^2}{2m} - V^{\text{ex}}(\mathbf{x}) - \epsilon_\alpha + \mu \right) \langle T[\hat{\psi}_\alpha(\mathbf{x}, \tau) \hat{\psi}_{\alpha'}^\dagger(\mathbf{x}', \tau')] \rangle. \end{aligned} \quad (2.70)$$

Substituting the equal-time relations that we derived in Section 2.1, *i.e.*, $[\hat{\psi}_\alpha(\mathbf{x}, \tau), \hat{\psi}_{\alpha'}^\dagger(\mathbf{x}', \tau)]_{\mp} = \delta(\mathbf{x} - \mathbf{x}') \delta_{\alpha, \alpha'}$, thus suggests that

$$G_{\alpha, \alpha'}(\mathbf{x}, \tau; \mathbf{x}', \tau') = -\langle T[\hat{\psi}_\alpha(\mathbf{x}, \tau) \hat{\psi}_{\alpha'}^\dagger(\mathbf{x}', \tau')] \rangle. \quad (2.71)$$

We can actually also prove this important relation, that bridges the gap between the functional formulation of quantum field theory used here and the more familiar operator formalism. First of all, it is clear from the slicing procedure used in our derivation of the functional integral in Section 2.3, that it automatically leads to time-ordered expectation values. We should, therefore, only be able to prove that

$$\begin{aligned} -G_{\alpha, \alpha'}(\mathbf{x}, \tau; \mathbf{x}', \tau') &= \langle \phi_\alpha(\mathbf{x}, \tau) \phi_{\alpha'}^*(\mathbf{x}', \tau') \rangle \\ &\equiv \frac{1}{Z_0} \int d[\phi^*] d[\phi] \phi_\alpha(\mathbf{x}, \tau) \phi_{\alpha'}^*(\mathbf{x}', \tau') e^{-S_0[\phi^*, \phi]/\hbar}. \end{aligned} \quad (2.72)$$

This is most easily achieved in the following way. We introduce a partition function in the presence of external currents $J_\alpha(\mathbf{x}, \tau)$ and $J_\alpha^*(\mathbf{x}, \tau)$, where in the fermionic case these currents are also Grassmann variables. The partition function is taken to be

$$\begin{aligned} Z_0[J, J^*] &= \int d[\phi^*] d[\phi] \exp \left\{ -\frac{1}{\hbar} S_0[\phi^*, \phi] \right. \\ &\quad \left. + \sum_\alpha \int_0^{\hbar\beta} d\tau \int d\mathbf{x} (\phi_\alpha^*(\mathbf{x}, \tau) J_\alpha(\mathbf{x}, \tau) + J_\alpha^*(\mathbf{x}, \tau) \phi_\alpha(\mathbf{x}, \tau)) \right\}, \end{aligned} \quad (2.73)$$

since then we must simply prove that

$$-G_{\alpha,\alpha'}(\mathbf{x}, \tau; \mathbf{x}', \tau') = \frac{\pm 1}{Z_0} \frac{\delta^2 Z_0}{\delta J_{\alpha}^*(\mathbf{x}, \tau) \delta J_{\alpha'}(\mathbf{x}', \tau')} \Big|_{J, J^*=0}. \quad (2.74)$$

Using a short-hand notation we have

$$Z_0[J, J^*] = \int d[\phi^*] d[\phi] \exp \{ (\phi | G^{-1} | \phi) + (\phi | J) + (J | \phi) \}. \quad (2.75)$$

The terms in the exponent can be rewritten as $(\phi + JG|G^{-1}|\phi + GJ) - (J|G|J)$, which is usually called completing the square. Performing a shift in the integration variables, we then easily see that

$$\begin{aligned} Z_0[J, J^*] &= Z_0[0, 0] e^{-(J|G|J)} = Z_0[0, 0] \exp \left\{ - \sum_{\alpha} \int_0^{\hbar\beta} d\tau \int d\mathbf{x} \right. \\ &\quad \times \left. \sum_{\alpha'} \int_0^{\hbar\beta} d\tau' \int d\mathbf{x}' J_{\alpha}^*(\mathbf{x}, \tau) G_{\alpha,\alpha'}(\mathbf{x}, \tau; \mathbf{x}', \tau') J_{\alpha'}(\mathbf{x}', \tau') \right\}, \end{aligned} \quad (2.76)$$

which after differentiation indeed leads to the desired result. We can now in fact calculate the expectation value of the time-ordered product of any number of operators. With the above expression for $Z_0[J, J^*]$ one can easily prove that this results in the sum of all possible products of time-ordered expectation values of two operators. For instance

$$\begin{aligned} &\langle \phi_{\alpha}^*(\mathbf{x}, \tau) \phi_{\alpha'}^*(\mathbf{x}', \tau') \phi_{\alpha''}(\mathbf{x}'', \tau'') \phi_{\alpha'''}(\mathbf{x}''', \tau''') \rangle \\ &= \langle \phi_{\alpha}^*(\mathbf{x}, \tau) \phi_{\alpha'''}(\mathbf{x}''', \tau''') \rangle \langle \phi_{\alpha'}^*(\mathbf{x}', \tau') \phi_{\alpha''}(\mathbf{x}'', \tau'') \rangle \\ &\quad \pm \langle \phi_{\alpha}^*(\mathbf{x}, \tau) \phi_{\alpha''}(\mathbf{x}'', \tau'') \rangle \langle \phi_{\alpha'}^*(\mathbf{x}', \tau') \phi_{\alpha'''}(\mathbf{x}''', \tau''') \rangle. \end{aligned} \quad (2.77)$$

This is the famous Wick's theorem, which plays a crucial role in the next section where we start to discuss the profound effects that interactions can have on the results obtained thusfar.

2.5 Interactions and Feynmann diagrams

The Green's function, or one-particle propagator, $G_{\alpha,\alpha'}(\mathbf{x}, \tau; \mathbf{x}', \tau')$ is one of the most important quantities that we want to determine theoretically, because it gives us the possibility to calculate in principle the expectation value of any one-particle observable. It also gives us the elementary excitations of our system of interest. For example, the average density of the spin state $|\alpha\rangle$ is in an ideal gas given by

$$\begin{aligned} \langle \hat{\psi}_{\alpha}^{\dagger}(\mathbf{x}, \tau) \hat{\psi}_{\alpha}(\mathbf{x}, \tau) \rangle &= \mp G_{\alpha,\alpha}(\mathbf{x}, \tau; \mathbf{x}, \tau^{+}) \\ &= \lim_{\eta \downarrow 0} \sum_{\mathbf{n}, n} \frac{\pm e^{i\omega_n \eta}}{\beta(-i\hbar\omega_n + \epsilon_{\mathbf{n},\alpha} - \mu)} |\chi_{\mathbf{n}}(\mathbf{x})|^2 = \sum_{\mathbf{n}} \frac{1}{e^{\beta(\epsilon_{\mathbf{n},\alpha} - \mu)} \mp 1} |\chi_{\mathbf{n}}(\mathbf{x})|^2, \end{aligned} \quad (2.78)$$

where we introduced the notation τ^+ for the limit $\eta \downarrow 0$ of $\tau + \eta$. Note that this procedure is necessary due to the time-ordering involved in the definition of the Green's function and the fact that the field operators do not commute at equal times. It also gives a natural explanation for our previous use of the convergence factor $e^{i\omega_n\eta}$. Moreover, from the argument of the Bose or Fermi distribution function, we see that the elementary excitations have an energy of $\epsilon_{\mathbf{n},\alpha} - \mu$. If we replace in the Fourier transform of the Green's function, *i.e.*, in

$$G_{\alpha,\alpha'}(\mathbf{x}, \mathbf{x}'; i\omega_n) = -\hbar\delta_{\alpha,\alpha'} \sum_{\mathbf{n}} \frac{1}{-i\hbar\omega_n + \epsilon_{\mathbf{n},\alpha} - \mu} \chi_{\mathbf{n}}(\mathbf{x}) \chi_{\mathbf{n}}^*(\mathbf{x}'), \quad (2.79)$$

$i\omega_n$ by ω we also see that $G_{\alpha,\alpha'}(\mathbf{x}, \mathbf{x}'; \omega)$ has a pole at $\hbar\omega = \epsilon_{\mathbf{n},\alpha} - \mu$. This is a general result: Poles in $G_{\alpha,\alpha'}(\mathbf{x}, \mathbf{x}'; \omega)$ correspond to the energies of the elementary excitations. These energies in general can also have a negative imaginary components, which then correspond to the lifetime of the excitation. The question that arises, therefore, is how to determine also the Green's function for an interacting system.

This can be done in perturbation theory, as follows. We want to calculate the expectation value

$$\begin{aligned} -\langle \phi_{\alpha}(\mathbf{x}, \tau) \phi_{\alpha'}^*(\mathbf{x}', \tau') \rangle = \\ -\frac{1}{Z} \int d[\phi^*] d[\phi] \phi_{\alpha}(\mathbf{x}, \tau) \phi_{\alpha'}^*(\mathbf{x}', \tau') e^{-S[\phi^*, \phi]/\hbar} \end{aligned} \quad (2.80)$$

with the action $S[\phi^*, \phi] = S_0[\phi^*, \phi] + S_{\text{int}}[\phi^*, \phi]$. We now expand both the numerator and the denominator in powers of S_{int} . Up to first order we find for the partition function

$$\begin{aligned} Z &= \int d[\phi^*] d[\phi] e^{-S_0[\phi^*, \phi]/\hbar} \left(1 - \frac{S_{\text{int}}[\phi^*, \phi]}{\hbar} \right) \\ &\equiv Z_0 \left(1 - \frac{1}{\hbar} \langle S_{\text{int}}[\phi^*, \phi] \rangle_0 \right). \end{aligned} \quad (2.81)$$

Using Wick's theorem, we thus have

$$\begin{aligned} -\frac{1}{\hbar} \langle S_{\text{int}}[\phi^*, \phi] \rangle_0 &= \frac{1}{2} \sum_{\alpha,\alpha'} \int_0^{\hbar\beta} d\tau \int d\mathbf{x} \int d\mathbf{x}' G_{0;\alpha,\alpha}(\mathbf{x}, \tau; \mathbf{x}, \tau^+) \\ &\quad \times \frac{-V(\mathbf{x} - \mathbf{x}')}{\hbar} G_{0;\alpha',\alpha'}(\mathbf{x}', \tau; \mathbf{x}', \tau^+) \\ &\quad \pm \frac{1}{2} \sum_{\alpha} \int_0^{\hbar\beta} d\tau \int d\mathbf{x} \int d\mathbf{x}' G_{0;\alpha,\alpha}(\mathbf{x}', \tau; \mathbf{x}, \tau^+) \\ &\quad \times \frac{-V(\mathbf{x} - \mathbf{x}')}{\hbar} G_{0;\alpha,\alpha}(\mathbf{x}, \tau; \mathbf{x}', \tau^+). \end{aligned} \quad (2.82)$$

$$Z = Z_0 \left(1 + \frac{1}{2} \text{diagram 1} + \frac{1}{2} \text{diagram 2} \right)$$

Fig. 4. Diagrammatic representation of the partition function up to first order in the interaction.

$$Z_0 \left(\begin{array}{l} \text{diagram 3} + \frac{1}{2} \text{diagram 4} + \frac{1}{2} \text{diagram 5} \\ + \text{diagram 6} + \text{diagram 7} \end{array} \right)$$

Fig. 5. Diagrammatic representation of the numerator of equation (2.80) up to first order in the interaction.

To understand the general structure of the perturbation expansion, it is very convenient to represent equations (2.81) and (2.82) in terms of Feynman diagrams. The final result is shown in Figure 4, where a wiggly line corresponds to the factor $-V(\mathbf{x} - \mathbf{x}')/\hbar$ and a thin arrowed line pointing from $(\mathbf{x}', \tau')$ to $(\mathbf{x}, \tau)$ represents the noninteracting Green's function $G_{0;\alpha,\alpha'}(\mathbf{x}, \tau; \mathbf{x}', \tau')$. In Figure 4 we have, for clarity sake, also explicitly indicated the various coordinates and spin degrees of freedom that we have to either integrate or sum over, respectively. It is, however, much more common in practice to suppress in Feynman diagrams those degrees of freedom that have to be integrated or summed over, and denote only the degrees of freedom on which the quantity of interest depends explicitly. For example, for the numerator of equation (2.80) we obtain

$$\begin{aligned} & - \int d[\phi^*] d[\phi] \phi_\alpha(\mathbf{x}, \tau) \phi_{\alpha'}^*(\mathbf{x}', \tau') e^{-S_0[\phi^*, \phi]/\hbar} \left(1 - \frac{S_{\text{int}}[\phi^*, \phi]}{\hbar} \right) \quad (2.83) \\ & = Z_0 \left(-\langle \phi_\alpha(\mathbf{x}, \tau) \phi_{\alpha'}^*(\mathbf{x}', \tau') \rangle_0 + \frac{1}{\hbar} \langle \phi_\alpha(\mathbf{x}, \tau) \phi_{\alpha'}^*(\mathbf{x}', \tau') S_{\text{int}}[\phi^*, \phi] \rangle_0 \right), \end{aligned}$$

whose diagrammatic equivalent is then given in Figure 5. Up to first order the interacting Green's function, which is represented by a thick arrowed line, obeys the equation shown in Figure 6. Note that the so-called disconnected diagrams have exactly cancelled. This is a general feature that

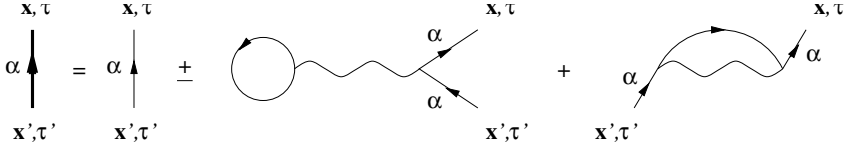


Fig. 6. Interacting Green's function up to first order in the interaction.

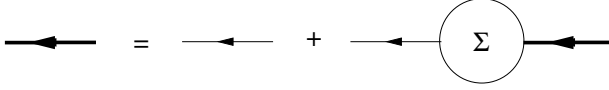


Fig. 7. Exact Dyson equation for the interacting Green's function.

happens for any expectation value, *i.e.*, the disconnected diagrams that occur in the numerator are always exactly cancelled by the denominator [18, 19].

One can also show that the general structure of the perturbation expansion of the Green's function is as in Figure 7, in which only one-particle irreducible diagrams contribute to the selfenergy $\hbar\Sigma$. These one-particle irreducible diagrams can be distinguished from the fact that they do not become disconnected if we cut a single thin arrowed line. This is Dyson's equation [20]. It is particularly insightful for a homogeneous gas or for a trapped gas in the weak-coupling limit, since then the one-particle states $\chi_{\mathbf{n}}(\mathbf{x})$ are not affected by the interactions and the exact one-particle propagator can be written as

$$G_{\alpha,\alpha'}(\mathbf{x}, \tau; \mathbf{x}', \tau') = \sum_{\mathbf{n}, n} G_{\alpha,\alpha'}(\mathbf{n}, i\omega_n) \chi_{\mathbf{n}}(\mathbf{x}) \chi_{\mathbf{n}}^*(\mathbf{x}') \frac{e^{-i\omega_n(\tau-\tau')}}{\hbar\beta}. \quad (2.84)$$

Note that for realistic trapped atomic gases this weak-coupling limit is essentially always realized in the normal phase of the gas. It is, therefore, also of some experimental interest to consider that limit in more detail first.

One then finds that the Dyson equation in first instance becomes

$$G_{\alpha,\alpha'}(\mathbf{n}, i\omega_n) = G_{0;\alpha,\alpha'}(\mathbf{n}, i\omega_n) + \sum_{\alpha'', \alpha'''} G_{0;\alpha,\alpha''}(\mathbf{n}, i\omega_n) \Sigma_{\alpha'', \alpha'''}(\mathbf{n}, i\omega_n) G_{\alpha''', \alpha'}(\mathbf{n}, i\omega_n). \quad (2.85)$$

Because $G_{0;\alpha,\alpha'}(\mathbf{n}, i\omega_n) = G_{0;\alpha}(\mathbf{n}, i\omega_n) \delta_{\alpha,\alpha'}$ and because we have assumed the interactions to be spin independent, we can easily convince ourselves that in perturbation theory it is always true that the selfenergy obeys $\Sigma_{\alpha'', \alpha'''}(\mathbf{n}, i\omega_n) = \Sigma_{\alpha''}(\mathbf{n}, i\omega_n) \delta_{\alpha'', \alpha'''}$ and as a result also that up to all orders in the interaction $G_{\alpha,\alpha'}(\mathbf{n}, i\omega_n) = G_{\alpha}(\mathbf{n}, i\omega_n) \delta_{\alpha,\alpha'}$. As we will see

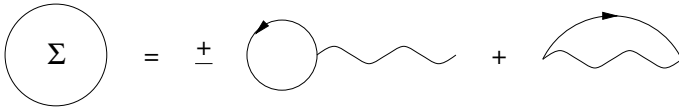


Fig. 8. Selfenergy up to first order in the interaction.

in Section 2.6, however, nonperturbative effect can change this result due to the phenomena of spontaneous broken symmetry. Ignoring the latter for the moment, we find for each spin state the uncoupled equation

$$G_{\alpha}(\mathbf{n}, i\omega_n) = G_{0;\alpha}(\mathbf{n}, i\omega_n) + G_{0;\alpha}(\mathbf{n}, i\omega_n) \Sigma_{\alpha}(\mathbf{n}, i\omega_n) G_{\alpha}(\mathbf{n}, i\omega_n), \quad (2.86)$$

or

$$\begin{aligned} \frac{1}{G_{\alpha}(\mathbf{n}, i\omega_n)} &= \frac{1}{G_{0;\alpha}(\mathbf{n}, i\omega_n)} - \Sigma_{\alpha}(\mathbf{n}, i\omega_n) \\ &= -\frac{1}{\hbar}(-i\hbar\omega_n + \epsilon_{\mathbf{n},\alpha} - \mu) - \Sigma_{\alpha}(\mathbf{n}, i\omega_n). \end{aligned} \quad (2.87)$$

Hence

$$G_{\alpha}(\mathbf{n}, i\omega_n) = \frac{-\hbar}{-i\hbar\omega_n + \epsilon_{\mathbf{n},\alpha} + \hbar\Sigma_{\alpha}(\mathbf{n}, i\omega_n) - \mu}, \quad (2.88)$$

which shows that the poles in the Green's function are indeed shifted by the interactions.

In our lowest order calculation we have found for the selfenergy the diagrammatic result shown in Figure 8. This is the most simple approximation we can think of. In the weak-coupling limit it is mathematically equal to

$$\begin{aligned} \hbar\Sigma_{\alpha}(\mathbf{n}, i\omega_n) &= \sum_{\mathbf{n}', \alpha'} V_{\mathbf{n}, \mathbf{n}'; \mathbf{n}, \mathbf{n}'} \frac{1}{e^{\beta(\epsilon_{\mathbf{n}', \alpha'} - \mu)} \mp 1} \\ &\mp \sum_{\mathbf{n}'} V_{\mathbf{n}', \mathbf{n}; \mathbf{n}, \mathbf{n}'} \frac{1}{e^{\beta(\epsilon_{\mathbf{n}', \alpha} - \mu)} \mp 1} \\ &= \sum_{\mathbf{n}', \alpha'} (V_{\mathbf{n}, \mathbf{n}'; \mathbf{n}, \mathbf{n}'} \pm V_{\mathbf{n}', \mathbf{n}; \mathbf{n}, \mathbf{n}'} \delta_{\alpha, \alpha'}) \frac{1}{e^{\beta(\epsilon_{\mathbf{n}', \alpha'} - \mu)} \mp 1}. \end{aligned} \quad (2.89)$$

The first term is known as the direct or Hartree, and the second term as the exchange or Fock contribution to the selfenergy. From equation (2.89) we conclude that the matrix elements of the interaction enter only in the combination $V_{\mathbf{n}, \mathbf{n}'; \mathbf{n}, \mathbf{n}'} \pm V_{\mathbf{n}', \mathbf{n}; \mathbf{n}, \mathbf{n}'} \delta_{\alpha, \alpha'}$. Clearly, this is a reflection of the Pauli principle, which forces the effective interaction between two fermionic atoms in the same state $|\mathbf{n}, \alpha\rangle$ to vanish.

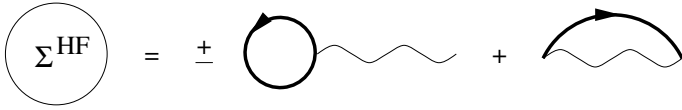


Fig. 9. Hartree–Fock approximation for the selfenergy.

To make the theory selfconsistent we should use in the expression for the selfenergy not the noninteracting propagators, but precisely those that follow from the Dyson equation. This is the Hartree–Fock approximation, which is diagrammatically given in Figure 9. It leads in the weak-coupling limit to the new dispersion relation $\hbar\omega_{\mathbf{n},\alpha} = \epsilon_{\mathbf{n},\alpha} + \hbar\Sigma_{\alpha}^{\text{HF}}(\mathbf{n}, 0) - \mu$ for the “dressed” particles or quasiparticles of the gas, where the selfenergy is essentially also found from equation (2.89). We only have to replace in the right-hand side $\epsilon_{\mathbf{n}',\alpha'} - \mu$ by $\epsilon_{\mathbf{n}',\alpha'} + \hbar\Sigma_{\alpha'}^{\text{HF}}(\mathbf{n}', 0) - \mu$. In this manner we have thus obtained an approximation to the interacting Green’s function that is nonperturbative in the interaction and effectively sums an infinite number of Feynman diagrams. Of course, the Hartree–Fock approximation can also be used in the strong-coupling limit. In that case it diagrammatically still corresponds to the solution of the Dyson equation of Figure 7, with a selfenergy as shown in Figure 9. However, we are then no longer allowed to assume that the exact Green’s function is diagonal in the eigenstates $\chi_{\mathbf{n}}(\mathbf{x})$ of the external trapping potential. To see more explicitly what this means physically, it is convenient to rederive the Hartree–Fock theory without making use of perturbation theory.

2.6 Hartree–Fock theory for an atomic Fermi gas

Because the Hartree–Fock theory is very useful in a large number of circumstances, and because we want to illustrate a very useful technique which is nowadays often used in the literature, we are now going to reproduce the above results without making use of a diagrammatic expansion. We consider for simplicity a fermionic mixture with an equal number of atoms in two hyperfine states and start by splitting our spin-independent interaction $V(\mathbf{x} - \mathbf{x}')$ into two spin-dependent parts such that one contributes only to the Hartree diagram and the other only to the Fock diagram. Denoting a spin-dependent interaction by $V_{\alpha',\beta';\alpha,\beta}(\mathbf{x} - \mathbf{x}')$ we thus want that

$$V(\mathbf{x} - \mathbf{x}')\delta_{\alpha,\alpha'}\delta_{\beta,\beta'} = V_{\alpha',\beta';\alpha,\beta}^{\text{H}}(\mathbf{x} - \mathbf{x}') + V_{\alpha',\beta';\alpha,\beta}^{\text{F}}(\mathbf{x} - \mathbf{x}') \quad (2.90)$$

with $\sum_{\beta} V_{\beta,\alpha;\alpha,\beta}^{\text{H}}(\mathbf{x} - \mathbf{x}') = \sum_{\beta} V_{\alpha,\beta;\alpha,\beta}^{\text{F}}(\mathbf{x} - \mathbf{x}') = 0$. Using operators in spin space, a possible solution to these equations is

$$\hat{V}^{\text{H}} = \frac{2}{3}(2 - \hat{P}_{12})V(\mathbf{x} - \mathbf{x}') \quad (2.91)$$

and

$$\hat{V}^F = \frac{1}{3}(2\hat{P}_{12} - 1)V(\mathbf{x} - \mathbf{x}'), \quad (2.92)$$

where $\hat{P}_{12} = (1 + \hat{\sigma}_1 \cdot \hat{\sigma}_2)/2$ is the exchange operator of the spins of atoms 1 and 2, and $\sigma_{\alpha,\alpha'}$ are the usual Pauli matrices. Clearly, we now have

$$\begin{aligned} S_{\text{int}}[\phi^*, \phi] = & \frac{1}{2} \sum_{\alpha, \alpha'; \beta, \beta'} \int_0^{\hbar\beta} d\tau \int d\mathbf{x} \int d\mathbf{x}' \\ & \times \left\{ \phi_{\alpha'}^*(\mathbf{x}, \tau) \phi_{\alpha}(\mathbf{x}, \tau) V_{\alpha', \beta'; \alpha, \beta}^H(\mathbf{x} - \mathbf{x}') \phi_{\beta'}^*(\mathbf{x}', \tau) \phi_{\beta}(\mathbf{x}', \tau) \right. \\ & \left. - \phi_{\alpha'}^*(\mathbf{x}, \tau) \phi_{\beta}(\mathbf{x}', \tau) V_{\alpha', \beta'; \alpha, \beta}^F(\mathbf{x} - \mathbf{x}') \phi_{\beta'}^*(\mathbf{x}', \tau) \phi_{\alpha}(\mathbf{x}, \tau) \right\}, \end{aligned} \quad (2.93)$$

which we write as

$$S_{\text{int}}[\phi^*, \phi] \equiv \frac{1}{2}(\phi^* \phi | V^H | \phi^* \phi) - \frac{1}{2}(\phi^* \phi | | V^F | | \phi^* \phi). \quad (2.94)$$

We next apply a so-called Hubbard-Stratonovich transformation [21, 22] to both the Hartree and the Fock parts of the interaction. First the Hartree part.

We note that $e^{-S_{\text{int}}^H[\phi^*, \phi]}$ can be written as a functional integral over the four real fields contained in $\kappa_{\alpha, \alpha'}(\mathbf{x}, \tau) \equiv \kappa_0(\mathbf{x}, \tau) \delta_{\alpha, \alpha'} + \boldsymbol{\kappa}(\mathbf{x}, \tau) \cdot \boldsymbol{\sigma}_{\alpha, \alpha'}$ as

$$\begin{aligned} \exp \left\{ -\frac{1}{2\hbar}(\phi^* \phi | V^H | \phi^* \phi) \right\} = \\ \int d[\kappa] \exp \left\{ \frac{1}{2\hbar}(\kappa | V^{H-1} | \kappa) - \frac{1}{2\hbar}(\kappa | \phi^* \phi) - \frac{1}{2\hbar}(\phi^* \phi | \kappa) \right\}. \end{aligned} \quad (2.95)$$

If we put $S_{\text{int}}^F[\phi^*, \phi] = 0$ for a moment, we can substitute this equality in the partition function to obtain $Z = \int d[\kappa] d[\phi^*] d[\phi] e^{-S[\kappa, \phi^*, \phi]/\hbar}$ with the action

$$\begin{aligned} S[\kappa, \phi^*, \phi] = & -\frac{1}{2}(\kappa | V^{H-1} | \kappa) + \sum_{\alpha, \alpha'} \int_0^{\hbar\beta} d\tau \int d\mathbf{x} \phi_{\alpha}^*(\mathbf{x}, \tau) \left\{ \left(\hbar \frac{\partial}{\partial \tau} \right. \right. \\ & \left. \left. - \frac{\hbar^2 \nabla^2}{2m} + V^{\text{ex}}(\mathbf{x}) + \epsilon_{\alpha} - \mu \right) \delta_{\alpha, \alpha'} + \kappa_{\alpha, \alpha'}(\mathbf{x}, \tau) \right\} \phi_{\alpha'}(\mathbf{x}, \tau). \end{aligned} \quad (2.96)$$

We see that in this manner the action for the fermions has become quadratic with a selfenergy $\hbar \Sigma_{\alpha, \alpha'}(\mathbf{x}, \tau; \mathbf{x}', \tau') = \kappa_{\alpha, \alpha'}(\mathbf{x}, \tau) \delta(\mathbf{x} - \mathbf{x}') \delta(\tau - \tau')$. Hence, we can now integrate out the fermion fields to obtain $Z = \int d[\kappa] e^{-S^{\text{eff}}[\kappa]/\hbar}$ and

$$S^{\text{eff}}[\kappa] = -\frac{1}{2}(\kappa | V^{H-1} | \kappa) - \hbar \text{Tr}[\ln(-G^{-1})], \quad (2.97)$$

with $G^{-1} = G_0^{-1} - \Sigma$ also a functional of $\kappa_{\alpha,\alpha'}(\mathbf{x}, \tau)$. Up to now we have not made any approximations and have only performed an exact rewriting of the partition function. However, the action $S^{\text{eff}}[\kappa]$ contains all powers of the fields $\kappa_{\alpha,\alpha'}(\mathbf{x}, \tau)$ and is thus quite complicated. It may therefore appear that we have not made any progress.

This is not the case, because the partition function will be largest for configurations that minimize the action $S^{\text{eff}}[\kappa]$. To make use of this observation, we expand the action around its minimum, *i.e.*, we put $\kappa_{\alpha,\alpha'}(\mathbf{x}, \tau) = \langle \kappa_{\alpha,\alpha'}(\mathbf{x}) \rangle + \delta \kappa_{\alpha,\alpha'}(\mathbf{x}, \tau)$ and require that $\delta S^{\text{eff}}[\kappa] / \delta \kappa_{\alpha,\alpha'}(\mathbf{x}, \tau)|_{\kappa=\langle \kappa \rangle} = 0$. If we neglect the fluctuations, we find that $Z \simeq e^{-S^{\text{eff}}[\langle \kappa \rangle] / \hbar}$. This will turn out to be the Hartree approximation, as we will show now. First of all we have

$$G^{-1} = G_0^{-1} - \langle \kappa \rangle / \hbar - \delta \kappa / \hbar \equiv G^{\text{H}^{-1}} - \delta \kappa / \hbar = G^{\text{H}^{-1}} (1 - G^{\text{H}} \delta \kappa / \hbar). \quad (2.98)$$

Substituting this in equation (2.97) gives us for the terms linear in the fluctuations

$$-\hbar \text{Tr}[-G^{\text{H}} \delta \kappa / \hbar] - (\delta \kappa | V^{\text{H}^{-1}} | \langle \kappa \rangle).$$

If $\langle \kappa_{\alpha,\alpha'}(\mathbf{x}) \rangle$ is indeed a minimum of the action $S^{\text{eff}}[\kappa]$, these linear terms have to vanish, which implies that

$$\langle \kappa_{\alpha',\alpha}(\mathbf{x}) \rangle = \sum_{\beta,\beta'} \int d\mathbf{x} V_{\alpha',\beta';\alpha,\beta}^{\text{H}}(\mathbf{x} - \mathbf{x}') G_{\beta,\beta'}^{\text{H}}(\mathbf{x}', \tau; \mathbf{x}', \tau^+). \quad (2.99)$$

As promised, this is precisely the most general mathematical expression for the Hartree contribution to the selfenergy in Figure 9. Taking again $\langle \kappa_{\alpha',\alpha}(\mathbf{x}) \rangle = \kappa(\mathbf{x}) \delta_{\alpha',\alpha}$, we also have that the Hartree approximation to the one-particle propagator obeys $G_{\beta,\beta'}^{\text{H}}(\mathbf{x}', \tau; \mathbf{x}', \tau^+) = n(\mathbf{x}') \delta_{\beta,\beta'} / 2$, with $n(\mathbf{x}')$ the average total atomic density, and we obtain the usual Hartree selfenergy

$$\kappa(\mathbf{x}) = \sum_{\beta} \int d\mathbf{x}' V_{\alpha,\beta;\alpha,\beta}^{\text{H}}(\mathbf{x} - \mathbf{x}') \frac{n(\mathbf{x}')}{2} = \int d\mathbf{x}' V(\mathbf{x} - \mathbf{x}') n(\mathbf{x}'). \quad (2.100)$$

Now we again want to include the Fock part of the interaction and treat this also by a Hubbard-Stratonovich transformation. This requires introducing four real fields that depend on two spatial coordinates. They are denoted by $\lambda_{\alpha,\alpha'}(\mathbf{x}, \mathbf{x}', \tau)$. Schematically we then use

$$\begin{aligned} & \exp \left\{ \frac{1}{2\hbar} (\phi^* \phi | | V^{\text{F}} | | \phi^* \phi) \right\} \\ &= \int d[\lambda] \exp \left\{ -\frac{1}{2\hbar} (\lambda | | V^{\text{F}^{-1}} | | \lambda) + \frac{1}{2\hbar} (\lambda | | \phi^* \phi) + \frac{1}{2\hbar} (\phi^* \phi | | \lambda) \right\}, \end{aligned} \quad (2.101)$$

which leads to the total selfenergy

$$\hbar \Sigma_{\alpha, \alpha'}(\mathbf{x}, \tau; \mathbf{x}', \tau') = [\kappa_{\alpha, \alpha'}(\mathbf{x}, \tau) \delta(\mathbf{x} - \mathbf{x}') - \lambda_{\alpha, \alpha'}(\mathbf{x}, \mathbf{x}', \tau)] \delta(\tau - \tau') \quad (2.102)$$

and after integration over the fermion fields to the effective action

$$S^{\text{eff}}[\kappa, \lambda] = -\frac{1}{2}(\kappa | V^{\text{H}^{-1}} | \kappa) + \frac{1}{2}(\lambda | | V^{\text{F}^{-1}} | | \lambda) - \hbar \text{Tr}[\ln(-G^{-1})]. \quad (2.103)$$

Requiring now that also $\delta S^{\text{eff}}[\kappa, \lambda] / \delta \lambda_{\alpha, \alpha'}(\mathbf{x}, \mathbf{x}', \tau) |_{\lambda=\langle \lambda \rangle} = 0$, then leads to the expected Fock selfenergy

$$\langle \lambda_{\alpha', \alpha}(\mathbf{x}', \mathbf{x}) \rangle = \sum_{\beta, \beta'} \int d\mathbf{x}' V_{\beta', \alpha'; \alpha, \beta}^{\text{F}}(\mathbf{x} - \mathbf{x}') G_{\beta', \beta}^{\text{HF}}(\mathbf{x}', \tau; \mathbf{x}, \tau^+). \quad (2.104)$$

In the symmetric case it simply becomes $\langle \lambda_{\alpha', \alpha}(\mathbf{x}', \mathbf{x}) \rangle = \lambda(\mathbf{x}', \mathbf{x}) \delta_{\alpha', \alpha}$ with

$$\lambda(\mathbf{x}', \mathbf{x}) = V(\mathbf{x} - \mathbf{x}') n(\mathbf{x}', \mathbf{x}) \quad (2.105)$$

and $n(\mathbf{x}', \mathbf{x}) = \sum_{\beta} G_{\beta, \beta}^{\text{HF}}(\mathbf{x}', \tau; \mathbf{x}, \tau^+) / 2 = \sum_{\beta} \langle \psi_{\beta}^{\dagger}(\mathbf{x}, \tau) \psi_{\beta}(\mathbf{x}', \tau) \rangle / 2$ exactly the Hartree–Fock approximation to the off-diagonal part of the one-particle density matrix.

Note that to actually perform the Hartree–Fock calculation in the latter case, we need to be able to determine the Green's function $G_{\alpha, \alpha'}^{\text{HF}}(\mathbf{x}, \tau; \mathbf{x}', \tau')$. The easiest way to do so, is by realizing that it is the Green's function of the operator in the fermionic piece of the action $S[\kappa, \lambda, \phi^*, \phi]$ obtained after the Hubbard–Stratonovich transformations. If we diagonalize this operator by solving the eigenvalue problem

$$\left\{ -\frac{\hbar^2 \nabla^2}{2m} + V^{\text{ex}}(\mathbf{x}) + \kappa(\mathbf{x}) - \epsilon'_{\mathbf{n}} \right\} \chi'_{\mathbf{n}}(\mathbf{x}) - \int d\mathbf{x}' \lambda(\mathbf{x}, \mathbf{x}') \chi'_{\mathbf{n}}(\mathbf{x}') = 0, \quad (2.106)$$

the desired one-particle propagator acquires the ideal gas form

$$G_{\alpha, \alpha'}^{\text{HF}}(\mathbf{x}, \tau; \mathbf{x}', \tau') = \delta_{\alpha, \alpha'} \sum_{\mathbf{n}, n} \frac{-\hbar}{-i\hbar\omega_n + \epsilon'_{\mathbf{n}, \alpha} - \mu} \chi'_{\mathbf{n}}(\mathbf{x}) \chi_{\mathbf{n}}'^*(\mathbf{x}') \frac{e^{-i\omega_n(\tau - \tau')}}{\hbar\beta}, \quad (2.107)$$

with new one-particle energies $\epsilon'_{\mathbf{n}, \alpha} = \epsilon'_{\mathbf{n}} + \epsilon_{\alpha}$ and eigenstates $\chi'_{\mathbf{n}}(\mathbf{x})$ that incorporate the average effect of the interactions of an atom with all the other atoms in the gas. Clearly, in the cases that the eigenstates are not affected by these so-called mean-field effects, we recover the weak-coupling results of the previous section.

Although we have thus precisely reproduced our diagrammatic result, there are two important advantages in using the Hubbard-Stratonovich transformation. First, it is in principle exact, and allows us to also calculate corrections to the Hartree-Fock approximation. For example, if we expand $S^{\text{eff}}[\kappa, \lambda]$ up to quadratic order in $\delta\kappa$ and $\delta\lambda$, and neglect all higher orders, we find the so-called Generalized Random Phase Approximation. The latter approach actually gives us also the opportunity to study the density fluctuations and therefore the collective excitations of the gas. We return to this important topic in Section 3.5. Second, it allows for a beautiful way to describe phase transitions. As mentioned previously, in perturbation theory we always find for a homogeneous gas that $G_{\alpha, \alpha'}(\mathbf{x}, \tau; \mathbf{x}, \tau^+) = n\delta_{\alpha, \alpha'}/2$ due to the same feature of $G_{0; \alpha, \alpha'}(\mathbf{x}, \tau; \mathbf{x}, \tau^+)$. From a fundamental point of view this is a result of the translational invariance of the gas and of the rotational symmetry in spin space. However, we can imagine that in principle we can also find selfconsistent solutions that do not have this property. We then have a spontaneous breaking of symmetry and therefore a phase transition in our system. For example, if below a certain temperature $G_{\alpha, \alpha'}(\mathbf{x}, \tau; \mathbf{x}, \tau^+) = n(\mathbf{x})\delta_{\alpha, \alpha'}/2$, we are dealing with a transition to a charge density wave or (Wigner) crystal. If on the other hand $G_{\alpha, \alpha'}(\mathbf{x}, \tau; \mathbf{x}, \tau^+) = n\delta_{\alpha, \alpha'}/2 + \mathbf{m} \cdot \boldsymbol{\sigma}_{\alpha, \alpha'}$ the gas is in a ferromagnetic phase. For a spin-density wave we even have that $G_{\alpha, \alpha'}(\mathbf{x}, \tau; \mathbf{x}, \tau^+) = n\delta_{\alpha, \alpha'}/2 + \mathbf{m}(\mathbf{x}) \cdot \boldsymbol{\sigma}_{\alpha, \alpha'}$. In all these cases the Hubbard-Stratonovich approach used above leads in a natural way to the appropriate Landau theory of the phase transition. Since the Landau theory is also very useful for the understanding of superfluidity in atomic gases, which is clearly the primary goal of the present course, we use the next section to give a short introduction into this subject.

2.7 Landau theory of phase transitions

In this summary of the Landau theory of phase transitions, we restrict ourselves in first instance to the homogeneous case because this makes the discussion more transparent. However, at the end of the section we also briefly mention how the inhomogeneity enters the theory. We have seen, for example in the Hartree-Fock theory discussed above, that the Green's function $G_{\alpha, \alpha'}(\mathbf{x}, \tau; \mathbf{x}, \tau^+) = n\delta_{\alpha, \alpha'}/2 + \langle \mathbf{s} \rangle \cdot \boldsymbol{\sigma}_{\alpha, \alpha'}$ can have a nonzero value of the average spin density $\langle \mathbf{s} \rangle = \langle \hat{\psi}_{\alpha}^{\dagger}(\mathbf{x}, \tau) \boldsymbol{\sigma}_{\alpha, \alpha'} \hat{\psi}_{\alpha'}(\mathbf{x}, \tau) \rangle / 2$, which is usually called the magnetization $\mathbf{m}$ in this context. This signals a phase transition to a ferromagnetic phase and the magnetization is called the order parameter of this transition. In the previous section we have also seen how we can, in principle exactly, obtain an expression for the partition function as

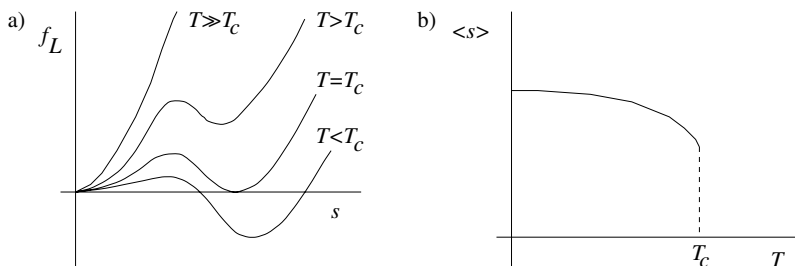


Fig. 10. Qualitative behaviour of a) the Landau free energy and b) the order parameter for a discontinuous phase transition.

a functional integral over the field $\mathbf{s}(\mathbf{x}, \tau)$, *i.e.*,

$$Z = \int d[\mathbf{s}] e^{-S^{\text{eff}}[\mathbf{s}]/\hbar}. \quad (2.108)$$

We just have to integrate out the fields κ_0 and $\lambda_{\alpha, \alpha'}$. For space and time independent values of the magnetization $\mathbf{s}$ the action $S^{\text{eff}}[\mathbf{s}]$ is $\hbar\beta V f_L(\mathbf{s})$, where $f_L(\mathbf{s})$ is the Landau free-energy density and V is the total volume of system. Because of the symmetry of $S[\phi^*, \phi]$ under rotations of the spin, this free-energy density must also be rotationally invariant and can therefore only depend on the magnitude of $\mathbf{s}$, which we denote by s . If a phase transition occurs the behaviour of $f_L(s)$ can essentially fall only into two categories.

At temperatures very high compared to the critical temperature T_c , the system is fully disordered and the free energy $f_L(s)$ must have a single minimum at $s = 0$ to make sure that the order parameter $\langle s \rangle$ is zero. Bringing the temperature closer to T_c , however, the free energy can develop a second local minimum. As long as the free energy in this second local minimum is higher than the minimum at $s = 0$, the equilibrium value of $\langle s \rangle$ will still be zero and no phase transition has occurred. Lowering the temperature further, the value of the free energy in the second minimum decrease until, precisely at the critical temperature T_c , it is equal to the free energy at $s = 0$. For temperatures below this critical one the second minimum has actually become the global minimum of the free energy, which implies that $\langle s \rangle \neq 0$ and we are in the ordered phase. In this scenario the order parameter has always a discontinuity at the critical temperature. As a result, this corresponds to a discontinuous, or first-order, phase transition. The behaviour of the free energy and the order parameter is illustrated in Figure 10. This should be compared with the behaviour of the free energy and the order parameter for a continuous, *i.e.*, second or higher order, phase transition, which is quite different and depicted in Figure 11. Now the Landau free energy $f_L(s)$ has always a single minimum, which for temperatures above T_c is at $s = 0$ but

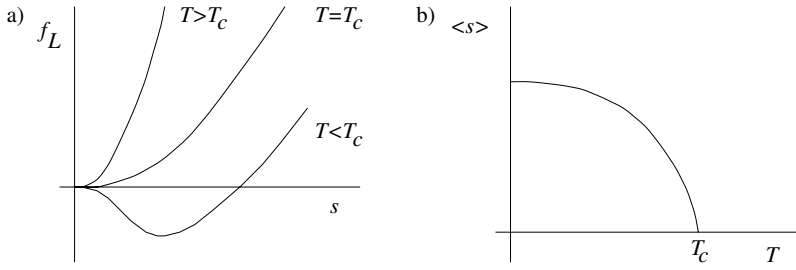


Fig. 11. Qualitative behaviour of a) the Landau free energy and b) the order parameter for a continuous phase transition.

at temperatures below the critical temperature shifts to a nonzero value of s . In particular, the order parameter thus shows no discontinuity at T_c .

In the case of a second-order phase transition, we conclude that near the critical temperature $\langle s \rangle$ is very small. As a result we can then expand the Landau free-energy density in powers of s . Because the free energy must also be symmetric under $s \rightarrow -s$, we have

$$f_L(s) = \alpha(T)|s|^2 + \frac{\beta}{2}|s|^4, \quad (2.109)$$

with $\beta > 0$ and $\alpha(T) = \alpha_0(T/T_c - 1)$. Thus if $T > T_c$ we have $\alpha(T) > 0$ and $\langle s \rangle = 0$. But for $T < T_c$, $\alpha(T)$ becomes negative and we have

$$\langle s \rangle = \sqrt{\frac{\alpha_0}{\beta} \left(1 - \frac{T}{T_c} \right)}. \quad (2.110)$$

Note that the free-energy density in this minimum is $-\alpha_0^2(1-T/T_c)^2/2\beta < 0$ and has a discontinuity in its second derivative with respect to the temperature. Historically, this is the reason why the corresponding phase transition was named to be of second order.

In fact, the Landau theory of second order phase transitions is slightly more involved, because it also considers slow spatial fluctuations in $\mathbf{s}$. Since a uniform rotation of $\mathbf{s}$ costs no energy, we must have that the free energy is

$$F_L[\mathbf{s}] = \int d\mathbf{x} \left(\gamma(\nabla \mathbf{s}(\mathbf{x}))^2 + \alpha(T)|\mathbf{s}(\mathbf{x})|^2 + \frac{\beta}{2}|\mathbf{s}(\mathbf{x})|^4 \right) \quad (2.111)$$

and $Z \simeq \int d[\mathbf{s}] e^{-\beta F_L[\mathbf{s}]}$. Landau theory now essentially corresponds to minimizing $F_L[\mathbf{s}]$ and taking only quadratic fluctuations into account. Taking also higher order fluctuations into account turns out to be very difficult. It requires Renormalization Group methods, which we are not going to

treat here and that can be found in the literature [18]. The effects of these fluctuation corrections to Landau theory are generally known as critical phenomena. Interestingly, they do not occur in first-order phase transitions. More importantly for our purposes is, however, that for atomic gases the fluctuations are only important in a small temperature interval around the critical temperature. For many applications it is, therefore, possible to neglect them. What usually cannot be neglected is the effect of the inhomogeneity of the gas. In the context of Landau theory that implies that the coefficients $\alpha(T)$, β and γ in equation (2.111) become also dependent on the spatial position in the trapping potential. We will see several examples of this feature in the following.

2.8 Superfluidity and superconductivity

We finally want to consider two important second-order phase transitions, that are purely due to quantum effects and can be conveniently treated with the methods that we have developed so far. Moreover, they occur very often in nature, for example in metals, in liquid helium and recently of course also in atomic gases of rubidium [10], lithium [11], sodium [12] and hydrogen [23].

2.8.1 Superfluidity

Let us first consider the last case, which is associated with a gas of spin-less bosons. For the low temperatures of interest the action is

$$S[\phi^*, \phi] = \int_0^{\hbar\beta} d\tau \int d\mathbf{x} \phi^*(\mathbf{x}, \tau) \left\{ \hbar \frac{\partial}{\partial \tau} - \frac{\hbar^2 \nabla^2}{2m} + V^{\text{ex}}(\mathbf{x}) - \mu \right\} \phi(\mathbf{x}, \tau) \\ + \frac{1}{2} \int_0^{\hbar\beta} d\tau \int d\mathbf{x} V_0 \phi^*(\mathbf{x}, \tau) \phi^*(\mathbf{x}, \tau) \phi(\mathbf{x}, \tau) \phi(\mathbf{x}, \tau), \quad (2.112)$$

where $V(\mathbf{x} - \mathbf{x}')$ is taken to be equal to $V_0 \delta(\mathbf{x} - \mathbf{x}')$. The justification for this simplification is, roughly speaking, that the thermal de Broglie wavelength $\Lambda_{\text{th}} = (2\pi\hbar^2/mk_B T)^{1/2}$ of the atoms is much larger than the range of the interatomic interaction. In this system the phase transition of interest is Bose-Einstein condensation. The associated order parameter is $\langle \phi(\mathbf{x}, \tau) \rangle$, since for time independent $\phi(\mathbf{x}, \tau)$ the above action has precisely the form of a Landau theory with a “free-energy” of

$$F_L[\phi^*, \phi] \\ = \int d\mathbf{x} \left(\frac{\hbar^2}{2m} |\nabla \phi(\mathbf{x})|^2 + (V^{\text{ex}}(\mathbf{x}) - \mu) |\phi(\mathbf{x})|^2 + \frac{V_0}{2} |\phi(\mathbf{x})|^4 \right). \quad (2.113)$$

We conclude that in lowest order the critical temperature is determined by $\mu(T_c) = \epsilon_0$, because then the configurations $\phi(\mathbf{x}) \propto \chi_0(\mathbf{x})$ precisely make

a vanishing contribution to the quadratic part of the “free energy”. This condition makes sense, because it is exactly the condition that we have a Bose-Einstein condensation in the ideal case: In the ideal Bose gas the number of particles in the one-particle ground state is $N_0 = 1/(e^{\beta(\epsilon_0 - \mu)} - 1)$, which indeed diverges for $\mu = \epsilon_0$.

To determine the corrections to this result we now explicitly substitute $\phi(\mathbf{x}, \tau) = \phi_0(\mathbf{x}) + \phi'(\mathbf{x}, \tau)$ into our functional integral. It is for lateron important to realize that to consistently define the fluctuations $\phi'(\mathbf{x}, \tau)$ in this manner, we also have to require that

$$\int d\mathbf{x} \phi_0^*(\mathbf{x})\phi'(\mathbf{x}, \tau) + \int d\mathbf{x} \phi_0(\mathbf{x})\phi'^*(\mathbf{x}, \tau) = 0. \quad (2.114)$$

The physical reason behind this condition is that $\phi'(\mathbf{x}, \tau)$ should contain all the configurations that are orthogonal to $\phi_0(\mathbf{x})$. In principle, therefore, it should also contain configurations that in effect only multiply $\phi_0(\mathbf{x})$ by a global phase. Such fluctuations lead to the phenomena of phase “diffusion” and are discussed in Section 3.2. In full detail we find after the above substitution that

$$S[\phi'^*, \phi'] = \hbar\beta F_L[\phi_0^*, \phi_0] + S_0[\phi'^*, \phi'] + S_{\text{int}}[\phi'^*, \phi'], \quad (2.115)$$

where the linear and quadratic terms are given by

$$\begin{aligned} S_0[\phi'^*, \phi'] &= \int_0^{\hbar\beta} d\tau \int d\mathbf{x} \phi'^*(\mathbf{x}, \tau) \left\{ -\frac{\hbar^2 \nabla^2}{2m} + V^{\text{ex}}(\mathbf{x}) - \mu + V_0 |\phi_0(\mathbf{x})|^2 \right\} \phi_0(\mathbf{x}) \\ &+ \int_0^{\hbar\beta} d\tau \int d\mathbf{x} \phi'(\mathbf{x}, \tau) \left\{ -\frac{\hbar^2 \nabla^2}{2m} + V^{\text{ex}}(\mathbf{x}) - \mu + V_0 |\phi_0(\mathbf{x})|^2 \right\} \phi_0^*(\mathbf{x}) \\ &+ \int_0^{\hbar\beta} d\tau \int d\mathbf{x} \phi'^*(\mathbf{x}, \tau) \\ &\times \left\{ \hbar \frac{\partial}{\partial \tau} - \frac{\hbar^2 \nabla^2}{2m} + V^{\text{ex}}(\mathbf{x}) - \mu + 2V_0 |\phi_0(\mathbf{x})|^2 \right\} \phi'(\mathbf{x}, \tau) \\ &+ \frac{1}{2} \int_0^{\hbar\beta} d\tau \int d\mathbf{x} V_0 (\phi_0(\mathbf{x}))^2 \phi'^*(\mathbf{x}, \tau) \phi'^*(\mathbf{x}, \tau) \\ &+ \frac{1}{2} \int_0^{\hbar\beta} d\tau \int d\mathbf{x} V_0 (\phi_0^*(\mathbf{x}))^2 \phi'(\mathbf{x}, \tau) \phi'(\mathbf{x}, \tau), \end{aligned} \quad (2.116)$$

and the cubic and quartic terms by

$$\begin{aligned}
 S_{\text{int}}[\phi'^*, \phi'] = & \int_0^{\hbar\beta} d\tau \int d\mathbf{x} V_0 \phi_0(\mathbf{x}) \phi'^*(\mathbf{x}, \tau) \phi'^*(\mathbf{x}, \tau) \phi'(\mathbf{x}, \tau) \\
 & + \int_0^{\hbar\beta} d\tau \int d\mathbf{x} V_0 \phi_0^*(\mathbf{x}) \phi'^*(\mathbf{x}, \tau) \phi'(\mathbf{x}, \tau) \phi'(\mathbf{x}, \tau) \\
 & + \frac{1}{2} \int_0^{\hbar\beta} d\tau \int d\mathbf{x} V_0 \phi'^*(\mathbf{x}, \tau) \phi'^*(\mathbf{x}, \tau) \phi'(\mathbf{x}, \tau) \phi'(\mathbf{x}, \tau),
 \end{aligned} \quad (2.117)$$

respectively.

In the Bogoliubov approximation we neglect the last three interaction terms [24]. Furthermore, to make sure that $\langle \phi(\mathbf{x}, \tau) \rangle = \phi_0(\mathbf{x})$ or $\langle \phi'(\mathbf{x}, \tau) \rangle = 0$, we need to require that the terms linear in ϕ' and ϕ'^* drop out of the action $S_0[\phi'^*, \phi']$. Clearly, this implies that

$$\left(-\frac{\hbar^2 \nabla^2}{2m} + V^{\text{ex}}(\mathbf{x}) + V_0 |\phi_0(\mathbf{x})|^2 \right) \phi_0(\mathbf{x}) = \mu \phi_0(\mathbf{x}), \quad (2.118)$$

which is the same result as obtained from minimizing the Landau “free-energy” $F_L[\phi^*, \phi]$. In the context of trapped atomic gases, this equation is known as the Gross-Pitaevskii equation [25]. It determines the macroscopic wave function of the condensate. The reason for calling $\phi_0(\mathbf{x})$ the macroscopic wave function follows from the fact that the total density of the gas now obeys

$$n(\mathbf{x}) = \langle \phi(\mathbf{x}, \tau) \phi^*(\mathbf{x}, \tau^+) \rangle = |\phi_0(\mathbf{x})|^2 + \langle \phi'(\mathbf{x}, \tau) \phi'^*(\mathbf{x}, \tau^+) \rangle. \quad (2.119)$$

The total number of condensate atoms thus equals $N_0 = \int d\mathbf{x} |\phi_0(\mathbf{x})|^2$. As equation (2.119) shows, it is in general always smaller than the total number of atoms in the gas due to the effect of the fluctuations. Note that in our present formulation the average $\langle \phi'(\mathbf{x}, \tau) \phi'^*(\mathbf{x}, \tau^+) \rangle$ physically describes not only the depletion of the condensate due to the usual thermal fluctuations known from the ideal Bose gas, but also due to the interactions, *i.e.*, purely due to quantum fluctuations.

Assuming that we have solved for the Gross-Pitaevskii equation, the fluctuation corrections are in the Bogoliubov theory determined by a quadratic action of the form

$$\begin{aligned}
 S_B[\phi'^*, \phi'] = & -\frac{\hbar}{2} \int_0^{\hbar\beta} d\tau \int d\mathbf{x} [\phi'^*(\mathbf{x}, \tau), \phi'(\mathbf{x}, \tau)] \cdot \mathbf{G}^{-1} \cdot \begin{bmatrix} \phi'(\mathbf{x}, \tau) \\ \phi'^*(\mathbf{x}, \tau) \end{bmatrix}, \quad (2.120)
 \end{aligned}$$

where the associated Green’s function $\mathbf{G}$ has now a matrix structure because not only the normal average $\langle \phi'(\mathbf{x}, \tau) \phi'^*(\mathbf{x}', \tau') \rangle$ but also the anomalous

average $\langle \phi'(\mathbf{x}, \tau) \phi'(\mathbf{x}', \tau') \rangle$ is now unequal to zero. We thus have that

$$-\mathbf{G}(\mathbf{x}, \tau; \mathbf{x}', \tau') = \left\langle \left[\begin{array}{c} \phi'(\mathbf{x}, \tau) \\ \phi'^*(\mathbf{x}, \tau) \end{array} \right] \cdot [\phi'^*(\mathbf{x}', \tau'), \phi'(\mathbf{x}', \tau')] \right\rangle. \quad (2.121)$$

From equation (2.116) we in fact find that in the Bogoliubov approximation

$$\mathbf{G}^{-1}(\mathbf{x}, \tau; \mathbf{x}', \tau') = \mathbf{G}_0^{-1}(\mathbf{x}, \tau; \mathbf{x}', \tau') \quad (2.122)$$

$$- \frac{1}{\hbar} \left[\begin{array}{cc} 2V_0|\phi_0(\mathbf{x})|^2 & V_0(\phi_0(\mathbf{x}))^2 \\ V_0(\phi_0^*(\mathbf{x}))^2 & 2V_0|\phi_0(\mathbf{x})|^2 \end{array} \right] \delta(\mathbf{x} - \mathbf{x}') \delta(\tau - \tau').$$

with the noninteracting Green's function $\mathbf{G}_0$ defined by

$$\mathbf{G}_0^{-1}(\mathbf{x}, \tau; \mathbf{x}', \tau') = \left[\begin{array}{cc} G_0^{-1}(\mathbf{x}, \tau; \mathbf{x}', \tau') & 0 \\ 0 & G_0^{-1}(\mathbf{x}', \tau'; \mathbf{x}, \tau) \end{array} \right] \quad (2.123)$$

and, of course,

$$G_0^{-1}(\mathbf{x}, \tau; \mathbf{x}', \tau') = -\frac{1}{\hbar} \left\{ \hbar \frac{\partial}{\partial \tau} - \frac{\hbar^2 \nabla^2}{2m} + V^{\text{ex}}(\mathbf{x}) - \mu \right\} \delta(\mathbf{x} - \mathbf{x}') \delta(\tau - \tau'). \quad (2.124)$$

This is clearly only the lowest order result for the Green's function, because a perturbative treatment of $S_{\text{int}}[\phi'^*, \phi']$ leads, in the same way as in Section 2.5, to higher order corrections. In general, the Dyson equation is, however, always of the form

$$\left[\begin{array}{cc} G_{11} & G_{12} \\ G_{21} & G_{22} \end{array} \right]^{-1} = \left[\begin{array}{cc} G_0^{-1} & 0 \\ 0 & G_0^{-1} \end{array} \right] - \left[\begin{array}{cc} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{array} \right]. \quad (2.125)$$

The off-diagonal elements are again called anomalous, since they vanish in the normal phase of the gas. Diagrammatically the Dyson equations for G_{11} and G_{21} are shown in Figure 12.

The selfenergy in the Bogoliubov approximation is

$$\hbar \Sigma(\mathbf{x}, \tau; \mathbf{x}', \tau') \quad (2.126)$$

$$= \left[\begin{array}{cc} 2V_0|\phi_0(\mathbf{x})|^2 & V_0(\phi_0(\mathbf{x}))^2 \\ V_0(\phi_0^*(\mathbf{x}))^2 & 2V_0|\phi_0(\mathbf{x})|^2 \end{array} \right] \delta(\mathbf{x} - \mathbf{x}') \delta(\tau - \tau'). \quad (2.127)$$

Because we have completely neglected the cubic and quartic terms in the action to obtain this selfenergy, the Bogoliubov approach is only valid if the fluctuations are sufficiently small. Physically, this implies that the depletion of the condensate must be small. It can, therefore, not be applied to liquid helium, but is expected to be valid for a weakly-interacting atomic

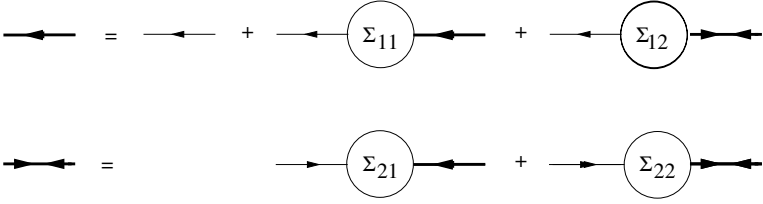


Fig. 12. Exact Dyson equation for the interacting normal and anomalous Green's functions.

gas at such low temperature that it essentially only consists of a condensate. Under these conditions the Bogoliubov theory not only predicts the condensate density profile $n_0(\mathbf{x}) = |\phi_0(\mathbf{x})|^2$ but also the collective modes of the condensate. Both these predictions have been accurately verified in recent experiments [26–28]. Theoretically, the eigenfrequencies of the collective modes are again determined by the poles in the one-particle Green's function. To understand more clearly how these can be determined, we first consider a homogeneous Bose gas.

In a box with volume $V = L^3$ the one-particle states are most easily characterized by the wavevector $\mathbf{k} = (2\pi/L)\mathbf{n}$ and equal to $e^{i\mathbf{k}\cdot\mathbf{x}}/\sqrt{V}$. The one-particle energies are thus $\epsilon_{\mathbf{k}} = \hbar^2\mathbf{k}^2/2m$. Moreover, the Gross-Pitaevskii equation reduces to $\mu = V_0|\phi_0|^2$ in that case, because the Landau “free-energy” is minimized for a macroscopic wave function that is independent of the position in the box. Making use of this fact, equation (2.122) can immediately be solved by a Fourier transformation. The result is

$$-\hbar\mathbf{G}^{-1}(\mathbf{k}, i\omega_n) = \begin{bmatrix} -i\hbar\omega_n + \epsilon_{\mathbf{k}} + V_0|\phi_0|^2 & V_0\phi_0^2 \\ V_0\phi_0^{*2} & i\hbar\omega_n + \epsilon_{\mathbf{k}} + V_0|\phi_0|^2 \end{bmatrix}. \quad (2.128)$$

Clearly there are poles in $G(\mathbf{k}, \omega)$ if the determinant of the right-hand side is zero or if

$$\hbar\omega = \hbar\omega_{\mathbf{k}} \equiv \sqrt{\epsilon_{\mathbf{k}}^2 + 2V_0|\phi_0|^2\epsilon_{\mathbf{k}}} = \sqrt{\epsilon_{\mathbf{k}}^2 + 2V_0n_0\epsilon_{\mathbf{k}}}. \quad (2.129)$$

This is the famous Bogoliubov dispersion of the collective excitations. Note that to finish the calculation we still have to obtain the condensate density $n_0 = |\phi_0|^2$. This is determined by the total density of the gas, which obeys

$$n = |\phi_0|^2 - G_{11}(\mathbf{x}, \tau; \mathbf{x}, \tau^+) = n_0 + n', \quad (2.130)$$

with n' the density of the “above” condensate particles. By inverting the right-hand side of equation (2.128), we find that the noncondensate density

is equal to

$$\begin{aligned}
 n' &= \lim_{\eta \downarrow 0} \frac{\hbar}{V \hbar \beta} \sum_{\mathbf{k} \neq \mathbf{0}, n} e^{i\omega_n \eta} \frac{i\hbar\omega_n + \epsilon_{\mathbf{k}} + V_0 n_0}{(\hbar\omega_n)^2 + (\hbar\omega_{\mathbf{k}})^2} \\
 &= \frac{1}{V} \sum_{\mathbf{k} \neq \mathbf{0}} \left(\frac{\epsilon_{\mathbf{k}} + V_0 n_0}{\hbar\omega_{\mathbf{k}}} \frac{1}{e^{\beta \hbar\omega_{\mathbf{k}}} - 1} + \frac{\epsilon_{\mathbf{k}} + V_0 n_0 - \hbar\omega_{\mathbf{k}}}{2\hbar\omega_{\mathbf{k}}} \right). \quad (2.131)
 \end{aligned}$$

For a given density and temperature, the last two equations thus fully determine the condensate density. Note that equation (2.131) explicitly shows that the condensate is indeed depleted both by thermal as well as quantum effects.

The generalization to the inhomogeneous case is straightforward. First we again have to solve the Gross-Pitaevskii equation at a fixed chemical potential. Given the condensate wave function, we can then calculate the collective mode frequencies by finding the poles of $\mathbf{G}$, or equivalently but more conveniently, the zero's of $\mathbf{G}^{-1}$. Clearly, the latter are located at $\hbar\omega = \hbar\omega_{\mathbf{n}}$, where $\hbar\omega_{\mathbf{n}}$ is found from the eigenvalue problem

$$\begin{aligned}
 \begin{bmatrix} \hat{K} + 2V_0|\phi_0(\mathbf{x})|^2 & V_0(\phi_0(\mathbf{x}))^2 \\ V_0(\phi_0^*(\mathbf{x}))^2 & \hat{K} + 2V_0|\phi_0(\mathbf{x})|^2 \end{bmatrix} \cdot \begin{bmatrix} u_{\mathbf{n}}(\mathbf{x}) \\ v_{\mathbf{n}}(\mathbf{x}) \end{bmatrix} \\
 = \hbar\omega_{\mathbf{n}} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \cdot \begin{bmatrix} u_{\mathbf{n}}(\mathbf{x}) \\ v_{\mathbf{n}}(\mathbf{x}) \end{bmatrix} \quad (2.132)
 \end{aligned}$$

and we introduced the operator $\hat{K} = -\hbar^2 \nabla^2 / 2m + V^{\text{ex}}(\mathbf{x}) - \mu$. This is de Bogoliubov-de Gennes equation that has recently been applied with great succes to the collective modes of a Bose condensed rubidium and sodium gas [29, 30]. Note that a special solution with $\hbar\omega_{\mathbf{0}} = 0$ is given by $[u_{\mathbf{0}}(\mathbf{x}), v_{\mathbf{0}}(\mathbf{x})] = [\phi_0(\mathbf{x}), -\phi_0^*(\mathbf{x})]$. As a result we can, by making use of the fact that the left-hand side of the Bogoliubov-de Gennes equation involves a hermitian operator, easily proof that all the solutions obey

$$\int d\mathbf{x} \phi_0^*(\mathbf{x}) u_{\mathbf{n}}(\mathbf{x}) + \int d\mathbf{x} \phi_0(\mathbf{x}) v_{\mathbf{n}}(\mathbf{x}) = 0, \quad (2.133)$$

as required by the condition in equation (2.114). Moreover, we can similary show that the solutions with $\hbar\omega_{\mathbf{n}} > 0$ can always be normalized as [31]

$$\int d\mathbf{x} (|u_{\mathbf{n}}(\mathbf{x})|^2 - |v_{\mathbf{n}}(\mathbf{x})|^2) = 1. \quad (2.134)$$

Physically, the zero frequency solution $\mathbf{n} = \mathbf{0}$ describes the dynamics of the global phase of the condensate [32]. Because of the so-called $U(1)$ symmetry of the action, *i.e.*, its invariance under the simultaneous phase changes $\phi(\mathbf{x}, \tau) \rightarrow e^{i\vartheta} \phi(\mathbf{x}, \tau)$ and $\phi^*(\mathbf{x}, \tau) \rightarrow e^{-i\vartheta} \phi^*(\mathbf{x}, \tau)$, this solution is essentially of no importance to the thermodynamic properties of a macroscopic

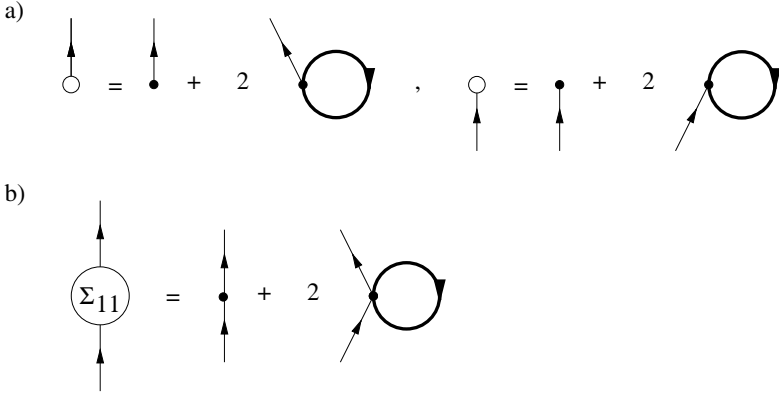


Fig. 13. Hartree–Fock corrections to a) the linear and b) the quadratic interaction terms of the Bogoliubov theory. This represents the Popov theory.

gas sample and is therefore usually neglected. Nevertheless, it has from a fundamental point of view some interesting consequences, as we will see in Section 3.2. Knowing all the eigenstates of $\mathbf{G}^{-1}$ we can then easily perform the inversion and finally again determine the density profile of the noncondensed atoms. Keeping the physical significance of the zero frequency mode in mind, we ultimately find,

$$n'(\mathbf{x}) = \sum_{\mathbf{n} \neq \mathbf{0}} \left((|u_{\mathbf{n}}(\mathbf{x})|^2 + |v_{\mathbf{n}}(\mathbf{x})|^2) \frac{1}{e^{\beta \hbar \omega_{\mathbf{n}}} - 1} + |v_{\mathbf{n}}(\mathbf{x})|^2 \right), \quad (2.135)$$

which may be compared with equation (2.131).

At temperatures near absolute zero, we have as a good approximation that $n'(\mathbf{x}) = 0$ and the Bogoliubov theory applies. However at nonzero temperatures we thermally excite particles and $n'(\mathbf{x})$ becomes nonzero. If we treat the effect of the noncondensate part of the gas in the Hartree–Fock approximation, we find that $S_{\text{int}}[\phi'^*, \phi']$ on average adds

$$\begin{aligned} S_{\text{int}}^{\text{HF}}[\phi'^*, \phi'] &= 2 \int_0^{\hbar\beta} d\tau \int d\mathbf{x} V_0 n'(\mathbf{x}) \phi'^*(\mathbf{x}, \tau) \phi_0(\mathbf{x}) \\ &\quad + 2 \int_0^{\hbar\beta} d\tau \int d\mathbf{x} V_0 n'(\mathbf{x}) \phi'(\mathbf{x}, \tau) \phi_0^*(\mathbf{x}) \\ &\quad + 2 \int_0^{\hbar\beta} d\tau \int d\mathbf{x} V_0 n'(\mathbf{x}) \phi'^*(\mathbf{x}, \tau) \phi'(\mathbf{x}, \tau), \end{aligned} \quad (2.136)$$

to the action $S_0[\phi'^*, \phi']$. In Figure 13 we indicate how this can be understood diagrammatically. Performing the same analysis as before, we conclude that

the Gross-Pitaevskii equation is modified to

$$\left(-\frac{\hbar^2 \nabla^2}{2m} + V^{\text{ex}}(\mathbf{x}) + 2V_0 n'(\mathbf{x}) + V_0 |\phi_0(\mathbf{x})|^2 \right) \phi_0(\mathbf{x}) = \mu \phi_0(\mathbf{x}), \quad (2.137)$$

and the normal selfenergies are changed into $2V_0 |\phi_0(\mathbf{x})|^2 + 2V_0 n'(\mathbf{x}) = 2V_0 n(\mathbf{x})$. The Bogoliubov-de Gennes equation for the elementary excitations is, therefore, now given by

$$\begin{aligned} \begin{bmatrix} \hat{K} + 2V_0 n(\mathbf{x}) & V_0 (\phi_0(\mathbf{x}))^2 \\ V_0 (\phi_0^*(\mathbf{x}))^2 & \hat{K} + 2V_0 n(\mathbf{x}) \end{bmatrix} \cdot \begin{bmatrix} u_{\mathbf{n}}(\mathbf{x}) \\ v_{\mathbf{n}}(\mathbf{x}) \end{bmatrix} \\ = \hbar \omega_{\mathbf{n}} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \cdot \begin{bmatrix} u_{\mathbf{n}}(\mathbf{x}) \\ v_{\mathbf{n}}(\mathbf{x}) \end{bmatrix}. \end{aligned} \quad (2.138)$$

These last two equations in combination with equation (2.135) are known as the Popov theory in the recent literature [33]. It is much studied at present in the context of Bose-Einstein condensation in atomic gases, and has been applied with succes to the equilibrium density profile of the gas below the critical temperature [34]. It has also been used to determine the collective mode frequencies of the gas at nonzero temperatures, however, with much less success [35, 36]. The reason for the failure of the Popov theory in this case is that the Bogoliubov-de Gennes equation in equation (2.138) describes physically only the motion of the condensate in the presence of a static noncondensed cloud and not the dynamics of the noncondensed cloud itself. How that can be achieved is discussed later on in Section 3.5, when we have obtained a better understanding of the nonequilibrium theory. Now we briefly want to make a connection to the interaction parameter V_0 used in the Bogoliubov and Popov theories and the specific two-body scattering properties of the atomic gas of interest in a particular experiment.

2.8.2 Some atomic physics

In the previous section we mentioned that the Bogoliubov theory, and to a certain extent also the Popov theory, agree very well with experiment. It is clear, however, that to apply these theories to an actual experiment we need to know the interaction parameter V_0 . In the case of atomic gases it is indeed possible to perform an *ab initio* calculation of this quantity, something which for instance cannot be done for liquid helium. The reason why V_0 can be determined for atomic gases, is that under the experimental conditions of interest the densities are always so low that we only need to consider all two-body processes taking place in the gas and we can neglect three-body and higher-body processes. This implies physically that we only have to calculate and add the quantum mechanical amplitudes for two atoms to scatter of each other an arbitrary number of times. Diagrammatically

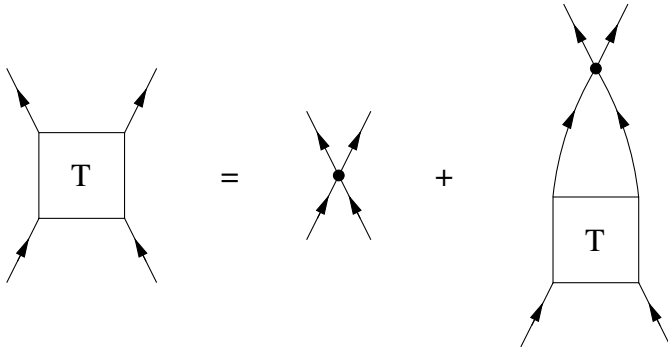


Fig. 14. T-matrix equation for the effective interatomic interaction.

the procedure can essentially be summarized by the T-matrix equation in Figure 14, because by iteration of this equation we easily see that we are indeed summing all two-body interaction processes.

Denoting the total momentum of the two incoming particles by $\hbar\mathbf{K}$ and the sum of the two Matsubara frequencies by Ω_n , the T-matrix equation in Figure 14 can, with our knowledge of how to perform the Matsubara sum in the right-hand side, easily be shown to be mathematically equivalent to

$$T(\mathbf{K}, i\Omega_n) = V_0 + \frac{V_0}{V} \sum_{\mathbf{k}} \frac{1}{i\hbar\Omega_n - \epsilon_{\mathbf{K}/2+\mathbf{k}} - \epsilon_{\mathbf{K}/2-\mathbf{k}} + 2\mu} \quad (2.139)$$

$$\times \left(1 + \frac{1}{e^{\beta(\epsilon_{\mathbf{K}/2+\mathbf{k}}-\mu)} - 1} + \frac{1}{e^{\beta(\epsilon_{\mathbf{K}/2-\mathbf{k}}-\mu)} - 1} \right) T(\mathbf{K}, i\Omega_n).$$

It is immediately solved by

$$\frac{1}{T(\mathbf{K}, i\Omega_n)} = \frac{1}{V_0} - \frac{1}{V} \sum_{\mathbf{k}} \frac{1}{i\hbar\Omega_n - \epsilon_{\mathbf{K}/2+\mathbf{k}} - \epsilon_{\mathbf{K}/2-\mathbf{k}} + 2\mu}$$

$$\times \left(1 + \frac{1}{e^{\beta(\epsilon_{\mathbf{K}/2+\mathbf{k}}-\mu)} - 1} + \frac{1}{e^{\beta(\epsilon_{\mathbf{K}/2-\mathbf{k}}-\mu)} - 1} \right). \quad (2.140)$$

Note that this is a somewhat formal result, because the momentum sum in the right-hand side has an ultra-violet divergence, which from a field-theoretical point of view requires a renormalization procedure.

The physical reason for the divergence is that we have used the approximate potential $V_0\delta(\mathbf{x} - \mathbf{x}')$ instead of the actual interatomic potential $V(\mathbf{x} - \mathbf{x}')$. The argument for using the δ -function approximation was that the thermal de Broglie wavelength of the atoms is for the ultra-low temperatures of interest always much larger than the typical range of the interaction. We now see that this argument is not fully correct, because if we calculate

corrections in perturbation theory, we have to deal with momentum sums which are not always restricted to momenta of order $\hbar/\Lambda_{\text{th}}$ and are therefore sensitive to the precise details of the interaction potential.

To cure this disease we note that if we put in equation (2.139) the Bose occupation numbers equal to zero, we precisely get the T-matrix or Lippmann-Schwinger equation [37] for two atoms interacting with the potential $V_0\delta(\mathbf{x} - \mathbf{x}')$. Furthermore, if the atoms interact with the potential $V(\mathbf{x} - \mathbf{x}')$ the solution of the corresponding Lippmann-Schwinger equation is known from elementary scattering theory to be equal to $4\pi a\hbar^2/m$ for small incoming momenta and energies, where a is the s -wave scattering length. We thus conclude that we must interpret

$$\frac{1}{V_0} - \frac{1}{V} \sum_{\mathbf{k}} \frac{1}{i\hbar\Omega_n - \epsilon_{\mathbf{K}/2+\mathbf{k}} - \epsilon_{\mathbf{K}/2-\mathbf{k}} + 2\mu}$$

as being equal to $m/4\pi a\hbar^2$ and, therefore, that the desired T-matrix in principle obeys

$$\begin{aligned} \frac{1}{T(\mathbf{K}, i\Omega_n)} &= \frac{m}{4\pi a\hbar^2} - \frac{1}{V} \sum_{\mathbf{k}} \frac{1}{i\hbar\Omega_n - \epsilon_{\mathbf{K}/2+\mathbf{k}} - \epsilon_{\mathbf{K}/2-\mathbf{k}} + 2\mu} \\ &\times \left(\frac{1}{e^{\beta(\epsilon_{\mathbf{K}/2+\mathbf{k}}-\mu)} - 1} + \frac{1}{e^{\beta(\epsilon_{\mathbf{K}/2-\mathbf{k}}-\mu)} - 1} \right). \end{aligned} \quad (2.141)$$

To obtain an accurate theory for a trapped atomic Bose gas that includes the effect of all two-body processes, we should now use instead of V_0 the above T-matrix in the Bogoliubov or Popov theories. Of course, in the normal phase the same is true for the Hartree-Fock theory. If the temperature is not too close to the critical temperature for Bose-Einstein condensation, it turns out that $T(\mathbf{K}, i\Omega_n) \simeq 4\pi a\hbar^2/m$ and we arrive at the conclusion that for an application to realistic atomic gases we must replace everywhere in Section 2.8.1 the interaction parameter V_0 by $4\pi a\hbar^2/m$. For temperatures close to the critical temperature, this is however no longer true and the Bose distribution functions have a nonnegligible effect on the T-matrix [38, 39]. The theory that, by using “dressed” one-particle propagators in Figure 14, selfconsistently includes these effects of the medium on the scattering properties of the atoms is known as the many-body T-matrix theory. It results in an effective interaction that, to avoid confusion, is denoted by $T^{(+)}(\mathbf{K}, \Omega)$ in Section 3.4. As we will see then, it plays a crucial role if we want to arrive at a consistent description of condensate formation in an atomic Bose gas.

2.8.3 Superconductivity

Finally, we want to briefly discuss the Bardeen-Cooper-Schrieffer or BCS theory of superconductivity [40], which has received considerable attention

recently in connection with ongoing experiments with the fermionic isotope of lithium. The reasons for this will become clear shortly. We are in that case dealing with effective spin 1/2 fermions and the action is taken to be

$$S[\phi^*, \phi] = \sum_{\alpha=\uparrow, \downarrow} \int_0^{\hbar\beta} d\tau \int d\mathbf{x} \, \phi_\alpha^*(\mathbf{x}, \tau) \left\{ \hbar \frac{\partial}{\partial \tau} - \frac{\hbar^2 \nabla^2}{2m} - \mu \right\} \phi_\alpha(\mathbf{x}, \tau) \\ + \int_0^{\hbar\beta} d\tau \int d\mathbf{x} \, V_0 \phi_\uparrow^*(\mathbf{x}, \tau) \phi_\downarrow^*(\mathbf{x}, \tau) \phi_\downarrow(\mathbf{x}, \tau) \phi_\uparrow(\mathbf{x}, \tau). \quad (2.142)$$

Note that the use of a single chemical potential implies that we only consider the optimal case of an equal density in each hyperfine state. This situation is optimal in the sense that, for unequal densities in each hyperfine state, it is no longer possible to pair up all the atoms in the gas. As a result the critical temperature of the gas drops dramatically, and in general becomes experimentally inaccessible. The effect is to a large extent analogous to putting superfluid ^3He in an homogeneous magnetic field. Furthermore, we in first instance consider the homogeneous case, because we want to illustrate in this section the local-density approximation to include the effect of the external trapping potential. Physically, this approximation treats the gas as consisting of a large number of independent gases that are in diffusive equilibrium with each other. Such an approach only works if the correlation length of the gas is much smaller than the typical length scale associated with changes of the external potential. Fortunately, this is almost always the case for realistic trapped atomic gases and for that reason the local-density approximation is often used in practice.

The BCS theory is the theory of Bose-Einstein condensation of so-called Cooper pairs. This means that the order parameter is $\langle \phi_\downarrow(\mathbf{x}, \tau) \phi_\uparrow(\mathbf{x}, \tau) \rangle$, in analogy with the order parameter $\langle \phi(\mathbf{x}, \tau) \rangle$ for the Bose case just discussed. Furthermore, it requires that the interaction parameter V_0 is negative, since otherwise the formation of pairs would not be energetically favorable. From now on we assume, therefore, that this is the case. The condensate of Cooper pairs can also be nicely treated with a Hubbard-Stratonovich transformation. We now introduce a complex field $\Delta(\mathbf{x}, \tau)$ and use

$$\exp \left\{ -\frac{1}{\hbar} \int_0^{\hbar\beta} d\tau \int d\mathbf{x} \, V_0 \phi_\uparrow^*(\mathbf{x}, \tau) \phi_\downarrow^*(\mathbf{x}, \tau) \phi_\downarrow(\mathbf{x}, \tau) \phi_\uparrow(\mathbf{x}, \tau) \right\} \quad (2.143) \\ = \int d[\Delta^*] d[\Delta] \exp \left\{ \frac{1}{\hbar} \int_0^{\hbar\beta} d\tau \int d\mathbf{x} \, \left(\frac{|\Delta(\mathbf{x}, \tau)|^2}{V_0} \right. \right. \\ \left. \left. + \Delta^*(\mathbf{x}, \tau) \phi_\downarrow(\mathbf{x}, \tau) \phi_\uparrow(\mathbf{x}, \tau) + \phi_\uparrow^*(\mathbf{x}, \tau) \phi_\downarrow^*(\mathbf{x}, \tau) \Delta(\mathbf{x}, \tau) \right) \right\}.$$

This leads to a partition function with the action

$$S[\Delta^*, \Delta, \phi^*, \phi] = - \int_0^{\hbar\beta} d\tau \int d\mathbf{x} \frac{|\Delta(\mathbf{x}, \tau)|^2}{V_0} - \frac{\hbar}{2} \int_0^{\hbar\beta} d\tau \int d\mathbf{x} [\phi_\downarrow^*(\mathbf{x}, \tau), \phi_\uparrow(\mathbf{x}, \tau)] \cdot \mathbf{G}^{-1} \cdot \begin{bmatrix} \phi_\downarrow(\mathbf{x}, \tau) \\ \phi_\uparrow^*(\mathbf{x}, \tau) \end{bmatrix}, \quad (2.144)$$

where

$$\mathbf{G}^{-1}(\mathbf{x}, \tau; \mathbf{x}', \tau') = \mathbf{G}_0^{-1}(\mathbf{x}, \tau; \mathbf{x}', \tau') - \frac{1}{\hbar} \begin{bmatrix} 0 & \Delta(\mathbf{x}, \tau) \\ \Delta^*(\mathbf{x}, \tau) & 0 \end{bmatrix} \delta(\mathbf{x} - \mathbf{x}') \delta(\tau - \tau'), \quad (2.145)$$

and the noninteracting Green's function $\mathbf{G}_0$ is defined by

$$\mathbf{G}_0^{-1}(\mathbf{x}, \tau; \mathbf{x}', \tau') = \begin{bmatrix} G_0^{-1}(\mathbf{x}, \tau; \mathbf{x}', \tau') & 0 \\ 0 & -G_0^{-1}(\mathbf{x}', \tau'; \mathbf{x}, \tau) \end{bmatrix} \quad (2.146)$$

and

$$G_0^{-1}(\mathbf{x}, \tau; \mathbf{x}', \tau') = -\frac{1}{\hbar} \left\{ \hbar \frac{\partial}{\partial \tau} - \frac{\hbar^2 \nabla^2}{2m} - \mu \right\} \delta(\mathbf{x} - \mathbf{x}') \delta(\tau - \tau'). \quad (2.147)$$

We thus see that the fermionic part has exactly the same matrix structure as in the case of a condensed Bose gas, only the selfenergy is now

$$\begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{21} & \Sigma_{22} \end{bmatrix} = \frac{1}{\hbar} \begin{bmatrix} 0 & \Delta(\mathbf{x}, \tau) \\ \Delta^*(\mathbf{x}, \tau) & 0 \end{bmatrix} \delta(\mathbf{x} - \mathbf{x}') \delta(\tau - \tau'). \quad (2.148)$$

If we again integrate out the fermion fields, we get the effective action

$$S^{\text{eff}}[\Delta^*, \Delta] = - \int_0^{\hbar\beta} d\tau \int d\mathbf{x} \frac{|\Delta(\mathbf{x}, \tau)|^2}{V_0} - \hbar \text{Tr}[\ln(-\mathbf{G}^{-1})], \quad (2.149)$$

which we can expand in powers of Δ by using $\mathbf{G}^{-1} = \mathbf{G}_0^{-1} - \Sigma = \mathbf{G}_0^{-1}(1 - \mathbf{G}_0 \Sigma)$ and therefore

$$-\hbar \text{Tr}[\ln(-\mathbf{G}^{-1})] = -\hbar \text{Tr}[\ln(-\mathbf{G}_0^{-1})] + \hbar \sum_{m=1}^{\infty} \frac{1}{m} \text{Tr}[(\mathbf{G}_0 \Sigma)^m]. \quad (2.150)$$

Explicite calculation [41] shows that for space and time independent Δ we obtain a “free-energy” density of the form of the Landau-theory of second-order phase transitions, *i.e.*,

$$f_L(|\Delta|) = \alpha(T) |\Delta|^2 + N(0) \frac{7\zeta(3)}{16(\pi T_c)^2} |\Delta|^4, \quad (2.151)$$

with as expected

$$\alpha(T) = -\frac{1}{V_0} + \frac{1}{V} \sum_{\mathbf{k}} \frac{1}{2(\epsilon_{\mathbf{k}} - \mu)} \left(1 - \frac{2}{e^{\beta(\epsilon_{\mathbf{k}} - \mu)} + 1} \right) \quad (2.152)$$

$$\equiv N(0) \ln \left(\frac{T}{T_c} \right) \simeq N(0) \left(\frac{T}{T_c} - 1 \right). \quad (2.153)$$

Here $N(0)$ is the density of states of a single spin state at the Fermi energy $\epsilon_F \equiv \hbar^2 k_F^2 / 2m$ and the critical temperature is given by

$$T_c = \frac{8e^{\gamma-2}}{\pi} \frac{\epsilon_F}{k_B} \exp \left\{ -\frac{\pi}{2k_F|a|} \right\}, \quad (2.154)$$

if we use the same renormalization procedure as in Section 2.8.2 to eliminate the interaction parameter V_0 in favor of the negative s -wave scattering length a .

Below T_c we thus have a nonzero average $\langle \Delta(\mathbf{x}, \tau) \rangle \equiv \Delta_0$. Using this in the Green's function for the fermions and neglecting fluctuations, we find in momentum space that

$$-\hbar \mathbf{G}^{-1}(\mathbf{k}, i\omega_n) = \begin{bmatrix} -i\hbar\omega_n + \epsilon_{\mathbf{k}} - \mu & \Delta_0 \\ \Delta_0^* & -(i\hbar\omega_n + \epsilon_{\mathbf{k}} - \mu) \end{bmatrix} \quad (2.155)$$

and therefore poles in $\mathbf{G}(\mathbf{k}, \omega)$ if

$$\hbar\omega = \hbar\omega_{\mathbf{k}} = \sqrt{(\epsilon_{\mathbf{k}} - \mu)^2 + |\Delta_0|^2}. \quad (2.156)$$

This dispersion relation has clearly a gap of magnitude $|\Delta_0|$ at the Fermi surface. As a consequence $|\Delta_0|$ is known as the BCS gap parameter. Note that the critical temperature below which the gap becomes nonzero depends exponentially on the parameter $\pi/2k_F|a|$. For typical atomic gases this is a quantity which is much larger than one, and the BCS transition is experimentally inaccessible. The only exception at the moment appears to be ${}^6\text{Li}$, with its anomalously large and negative triplet scattering length of $-2160 a_0$ [42]. This explains the present interest in spin-polarized atomic lithium.

In view of this exciting possibility, we have recently studied the equilibrium properties of atomic lithium in a harmonic oscillator potential $V^{\text{ex}}(\mathbf{x}) = m\omega^2 \mathbf{x}^2 / 2$, with a trapping frequency of $\omega/2\pi = 144 \text{ Hz}$ [43]. To incorporate the effect of the external potential we have, as mentioned above, applied the local-density approximation. The result is shown in Figure 15. Note that the use of the local-density approximation implies that we perform the above outlined homogeneous calculation for each point in space with a chemical potential that is equal to

$$\mu(\mathbf{x}) = \mu - \frac{1}{2}m\omega^2 \mathbf{x}^2 - \frac{4\pi a \hbar^2}{m} \frac{n(\mathbf{x})}{2}. \quad (2.157)$$

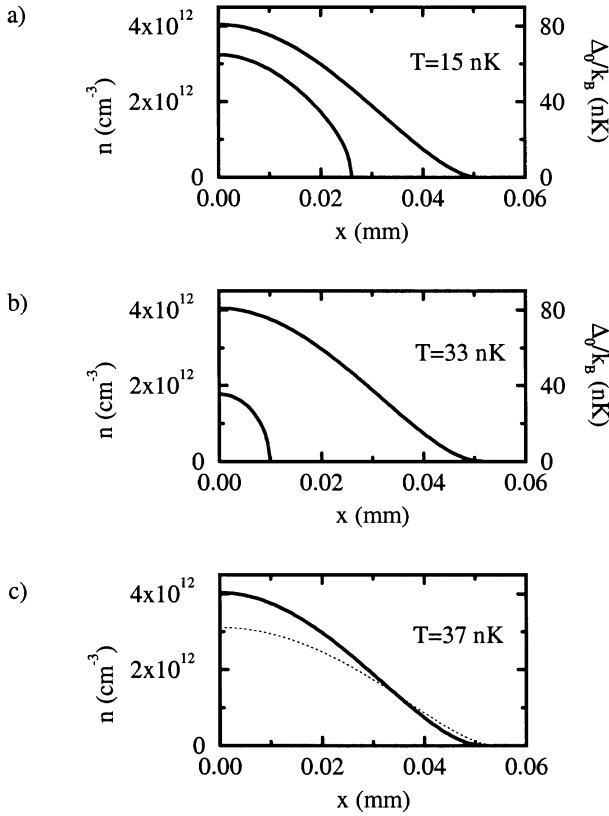


Fig. 15. Density distribution $n(x)$ and energy gap $\Delta_0(x)$ for a ${}^6\text{Li}$ atomic gas consisting of 2.865×10^5 atoms in each spin state a) at $T = 15 \text{ nK}$, b) at $T = 33 \text{ nK}$, slightly below T_c , and c) at $T = T_c = 37 \text{ nK}$. The left scale of each plot refers to the density and the right scale to the energy gap. The dotted line in c) shows the density distribution for an ideal Fermi gas with the same number of particles and at the same temperature.

The third term in the right-hand side represents the mean-field effect of the Hartree contribution to the selfenergy of the fermions. Since our Hubbard-Stratonovich procedure is in principle exact, it is not immediately clear why such a term must be included in the theory. It can, however, be shown that it arises from the fluctuations of the BCS gap parameter. With this remark, we end our development of the equilibrium field theory of trapped atomic gases. We now turn our attention to the nonequilibrium field theory.

3 Nonequilibrium field theory

As we have already seen several times, the equilibrium field theory gives us also information on dynamical properties of the gas by means of the substitution $\omega_n \rightarrow -i\omega$ or equivalently $\tau \rightarrow it$. However, the Popov theory of Bose-Einstein condensation has shown us that we have to be very careful with this procedure, because we may not always end up with the correct physics needed for a discription of a particular experiment. It is for these cases that a truly nonequilibrium field theory is required and the development of such a theory is the topic of Section 3.3. Before embarking on that, however, we first consider two important dynamical problems where the equilibrium theory does give us all the answers.

3.1 Macroscopic quantum tunneling of a condensate

In a Bose gas with effectively attractive interactions, *i.e.*, with a negative scattering length a , a condensate will always have the tendency to collapse to a high density state due to the gain in energy that can be obtained in this way [44]. The most important question in this context is, therefore, if a condensate can exist sufficiently long to be experimentally observed. Neglecting the variation of the noncondensate density on the size of the condensate [45, 46], we know from the Popov theory that the dynamics of the collapse is, apart from an unimportant shift in the chemical potential, determined by the Gross-Pitaevskii equation [25]

$$i\hbar \frac{\partial}{\partial t} \langle \phi(\mathbf{x}, t) \rangle = \left\{ -\frac{\hbar^2 \nabla^2}{2m} + V^{\text{ex}}(\mathbf{x}) - \mu + \frac{4\pi a \hbar^2}{m} |\langle \phi(\mathbf{x}, t) \rangle|^2 \right\} \langle \phi(\mathbf{x}, t) \rangle. \quad (3.1)$$

More precisely, this determines only the semiclassical dynamics. If we also want to study the quantum fluctuations, which is necessary if we are also interested in how the condensate tunnels through the macroscopic energy barrier, it is most convenient to calculate the grand canonical partition function of the condensate [47]. Quantizing the Gross-Pitaevskii equation we obtain for this partition function the functional integral

$$Z(\mu) = \int d[\phi^*] d[\phi] \exp \left\{ -\frac{1}{\hbar} S[\phi^*, \phi] \right\}, \quad (3.2)$$

over the complex field $\phi(\mathbf{x}, \tau)$ and with the Euclidian action

$$S[\phi^*, \phi] = \int_0^{\hbar\beta} d\tau \int d\mathbf{x} \phi^*(\mathbf{x}, \tau) \left(\hbar \frac{\partial}{\partial \tau} + \frac{\hbar^2 \nabla^2}{2m} + V^{\text{ex}}(\mathbf{x}) - \mu + \frac{2\pi a \hbar^2}{m} |\phi(\mathbf{x}, \tau)|^2 \right) \phi(\mathbf{x}, \tau). \quad (3.3)$$

As always for Bose systems, the integration is only over fields that are periodic on the imaginary time axis.

Although it has recently been shown by Freire and Arovas that the tunneling process can also be studied in terms of the complex field $\phi(\mathbf{x}, \tau)$ [48], we believe that it leads to somewhat more physical insight if we use instead the fields $\rho(\mathbf{x}, \tau)$ and $\theta(\mathbf{x}, \tau)$ that correspond to the density and phase fluctuations of the condensate, respectively. They are introduced by performing the canonical variable transformation [33]

$$\phi(\mathbf{x}, \tau) = \sqrt{\rho(\mathbf{x}, \tau)} e^{i\theta(\mathbf{x}, \tau)}$$

in the functional integral for the partition function. As a result we find

$$Z(\mu) = \int d[\rho] d[\theta] \exp \left\{ -\frac{1}{\hbar} S[\rho, \theta; \mu] \right\}, \quad (3.4)$$

with

$$\begin{aligned} S[\rho, \theta; \mu] = & \int_0^{\hbar\beta} d\tau \int d\mathbf{x} \left(i\hbar \rho(\mathbf{x}, \tau) \frac{\partial \theta(\mathbf{x}, \tau)}{\partial \tau} \right. \\ & + \frac{\hbar^2 \rho(\mathbf{x}, \tau)}{2m} (\nabla \theta(\mathbf{x}, \tau))^2 + \frac{\hbar^2}{8m\rho(\mathbf{x}, \tau)} (\nabla \rho(\mathbf{x}, \tau))^2 \\ & \left. + V^{\text{ex}}(\mathbf{x}) \rho(\mathbf{x}, \tau) - \mu \rho(\mathbf{x}, \tau) + \frac{2\pi a \hbar^2}{m} \rho^2(\mathbf{x}, \tau) \right). \end{aligned} \quad (3.5)$$

Next, we notice that this action is only quadratic in the phase fluctuations. The field $\theta(\mathbf{x}, \tau)$ can therefore be integrated over exactly, because it only involves the evaluation of a Gaussian integral.

Compared to ordinary Gaussian integrals there is, however, one slight complication which is associated with the fact that $\theta(\mathbf{x}, \tau)$ are phase variables. This implies that the periodicity of the original field $\phi(\mathbf{x}, \tau)$ only constraints the phase field $\theta(\mathbf{x}, \tau)$ to be periodic up to a multiple of 2π . To evaluate the grand canonical partition function in equation (3.4) we must therefore first integrate over all fields $\theta(\mathbf{x}, \tau)$ that obey the boundary condition $\theta(\mathbf{x}, \hbar\beta) = \theta(\mathbf{x}, 0) + 2\pi j$ and subsequently sum over all possible integers j . Because these different boundary conditions only affect the zero-momentum part of $\theta(\mathbf{x}, \tau)$ we first have to evaluate the sum

$$\sum_j \int^{\theta_{\mathbf{0}}(\hbar\beta) = \theta_{\mathbf{0}}(0) + 2\pi j} d[\theta_{\mathbf{0}}] \exp \left\{ -i \int_0^{\hbar\beta} d\tau N_{\mathbf{0}}(\tau) \frac{\partial \theta_{\mathbf{0}}(\tau)}{\partial \tau} \right\},$$

with $N_{\mathbf{0}}(\tau) = \int d\mathbf{x} \rho(\mathbf{x}, \tau)$ the number of condensate particles. After performing a partial integration on the integral in the exponent, we can carry

out the path integration over $\theta_0(\tau)$ to obtain

$$\sum_j e^{2\pi i N_0 j} \delta \left[\frac{\partial N_0(\tau)}{\partial \tau} \right].$$

As expected, the integration over the global phase of the condensate leads to the constraint of a constant number of condensate particles, *i.e.*, $N_0(\tau) = N_0$. Moreover, we have $\sum_j e^{2\pi i N_0 j} = \sum_j \delta(N_0 - j)$, which restricts the number of condensate particles to an integer. Putting all these results together, we see that the integration over the zero-momentum part of $\rho(\mathbf{x}, \tau)$ is only a sum over the number of condensate particles and we have that

$$Z(\mu) = \sum_{N_0} e^{\beta \mu N_0} Z_{N_0}. \quad (3.6)$$

Here we introduced the canonical partition function of the condensate, which is apparently equal to the functional integral

$$Z_{N_0} = \int d[\rho] d[\theta] \exp \left\{ -\frac{1}{\hbar} S[\rho, \theta; 0] \right\} \quad (3.7)$$

over all the nonzero momentum components of the density and phase fields.

The integration over the nonzero momentum components of the phase field $\theta(\mathbf{x}, \tau)$ is easily performed, because it now involves an ordinary Gaussian integral. Introducing the Green's function for the phase fluctuations $G(\mathbf{x}, \mathbf{x}'; \rho)$ by

$$\frac{\hbar}{m} ((\nabla \rho) \cdot \nabla + \rho \nabla^2) G(\mathbf{x}, \mathbf{x}'; \rho) = \delta(\mathbf{x} - \mathbf{x}'), \quad (3.8)$$

we immediately obtain the desired effective action for the density field

$$\begin{aligned} S^{\text{eff}}[\rho] = & \int_0^{\hbar\beta} d\tau \int d\mathbf{x} \int d\mathbf{x}' \left(-\frac{\hbar}{2} \frac{\partial \rho(\mathbf{x}, \tau)}{\partial \tau} G(\mathbf{x}, \mathbf{x}'; \rho) \frac{\partial \rho(\mathbf{x}', \tau)}{\partial \tau} \right) \\ & + \int_0^{\hbar\beta} d\tau \int d\mathbf{x} \left(\frac{\hbar^2}{8m\rho(\mathbf{x}, \tau)} (\nabla \rho(\mathbf{x}, \tau))^2 \right. \\ & \left. + V^{\text{ex}}(\mathbf{x}) \rho(\mathbf{x}, \tau) + \frac{2\pi a \hbar^2}{m} \rho^2(\mathbf{x}, \tau) \right). \end{aligned} \quad (3.9)$$

Being an action for the density fluctuations of the condensate, $S^{\text{eff}}[\rho]$ also describes all the collisionless modes of the condensate. This is important for our purposes, because the mode which becomes unstable first, determines precisely how the condensate collapses. Moreover, it determines the probability with which the collapse is going to take place, both for quantum and thermal fluctuations, since the energy barrier is smallest in that direction of

the configuration space. It should be noted that as long as we can neglect the interaction between the condensate and the thermal cloud, the action $S^{\text{eff}}[\rho]$ describes also the collective modes of a gas with positive scattering length. For various other theoretical approaches that have been applied under these conditions see, for example, references [29, 30, 49–55]. The actual measurements of the collective mode frequencies have been performed by Jin *et al.* [26] and Mewes *et al.* [27] and are at sufficiently low temperatures indeed in good agreement with the theoretical predictions [35, 36]. We expect the same to be true for a gas with effectively attractive interactions and, therefore, the action $S^{\text{eff}}[\rho]$ to be a good starting point for the following discussion.

To obtain the collisionless modes explicitly we consider first the case of an ideal Bose gas by putting $a = 0$. For the ideal Bose gas we expect the gaussian profile

$$\rho(\mathbf{x}; q(\tau)) = N_0 \left(\frac{1}{\pi q^2(\tau)} \right)^{3/2} \exp \left(-\frac{\mathbf{x}^2}{q^2(\tau)} \right) \quad (3.10)$$

to describe an exact mode of the condensate. The reason is that in the noninteracting case we can make a density fluctuation by taking one particle from the condensate and putting that in one of the excited states of the external potential. The corresponding density fluctuation obeys

$$\delta\rho(\mathbf{x}, t) \propto e^{-i(\epsilon_{\mathbf{n}} - \epsilon_0)t/\hbar} \chi_{\mathbf{n}}^*(\mathbf{x}) \chi_0(\mathbf{x}).$$

For the experimentally relevant case of an isotropic harmonic oscillator [11] it is more convenient to use instead of the cartesian quantum numbers $\mathbf{n}$, the two angular momentum quantum numbers ℓ and m and the quantum number n that counts the number of nodes in the radial wave function $\chi_{n\ell}(x)$. The density fluctuation then becomes

$$\delta\rho(\mathbf{x}, t) \propto e^{-i(2n+\ell)\omega t} \chi_{n\ell}(x) Y_{\ell m}^*(\hat{\mathbf{x}}) \frac{e^{-x^2/2l^2}}{(\pi l^2)^{3/4}},$$

with $\epsilon_{n\ell m} - \epsilon_{000} = (2n + \ell)\hbar\omega$ the excitation energy and $l = (\hbar/m\omega)^{1/2}$ the size of the condensate wave function. Comparing this now with the expansion of the gaussian profile in equation (3.10) around the groundstate density profile, which is obtained by substituting $q(\tau) = l + \delta q(\tau)$, we find that

$$\delta\rho(\mathbf{x}, \tau) = -\sqrt{6}N_0 \frac{\delta q(\tau)}{l} \chi_{10}(x) Y_{00}^*(\hat{\mathbf{x}}) \frac{e^{-x^2/2l^2}}{(\pi l^2)^{3/4}} \quad (3.11)$$

has precisely the same form as a density fluctuation in which one particle is taken from the condensate and put into the harmonic oscillator state

with quantum numbers $(n\ell m) = (100)$. The frequency of this so-called “breathing” mode described by the gaussian density profile must therefore be equal to 2ω .

To proof that this is indeed correct, we need to evaluate the effective action $S^{\text{eff}}[\rho]$, and hence the Green’s function $G(\mathbf{x}, \mathbf{x}'; \rho)$, for a gaussian density profile. Substituting such a profile in equation (3.8) immediately leads to $G(\mathbf{x}, \mathbf{x}'; \rho) = G(\mathbf{x}, \mathbf{x}'; q)/\rho(\mathbf{x}'; q)$, with

$$\frac{\hbar}{m} \left(-\frac{2}{q^2} \mathbf{x} \cdot \nabla + \nabla^2 \right) G(\mathbf{x}, \mathbf{x}'; q) = \delta(\mathbf{x} - \mathbf{x}'). \quad (3.12)$$

The latter equation can be solved, if we can solve the eigenvalue problem

$$\left(\nabla^2 - \frac{2x}{q^2} \frac{\partial}{\partial x} \right) \xi(\mathbf{x}) = \lambda \xi(\mathbf{x}). \quad (3.13)$$

This turns out to be an easy task, because substituting

$$\xi_{n\ell m}(\mathbf{x}) = \xi_{n\ell}(x) \frac{e^{x^2/2q^2}}{x} Y_{\ell m}(\hat{\mathbf{x}}) \quad (3.14)$$

gives essentially the radial Schrödinger equation for an isotropic harmonic oscillator with frequency $\omega_q = \hbar/mq^2$, i.e.,

$$-\frac{2m}{\hbar^2} \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{1}{2} m \omega_q^2 x^2 + \frac{\hbar^2 \ell(\ell+1)}{2m x^2} - \frac{3}{2} \hbar \omega_q \right) \xi_{n\ell}(x) = \lambda_{n\ell} \xi_{n\ell}(x). \quad (3.15)$$

The desired eigenfunctions are therefore $\xi_{n\ell m}(\mathbf{x}; q) = \varphi_{n\ell m}(\mathbf{x}) e^{x^2/2q^2}$, with $\varphi_{n\ell m}(\mathbf{x})$ the properly normalized harmonic oscillator states with the energies $(2n + \ell + 3/2)\hbar\omega_q$, and the corresponding eigenvalues are $\lambda_{n\ell}(q) = -2(2n + \ell)/q^2$. Introducing finally the “dual” eigenfunctions $\bar{\xi}_{n\ell m}(\mathbf{x}; q) \equiv \varphi_{n\ell m}^*(\mathbf{x}) e^{-x^2/2q^2}$, the Green’s function $G(\mathbf{x}, \mathbf{x}'; q)$ is given by

$$G(\mathbf{x}, \mathbf{x}'; q) = \sum'_{n\ell m} \xi_{n\ell m}(\mathbf{x}; q) \frac{m}{\hbar \lambda_{n\ell}(q)} \bar{\xi}_{n\ell m}(\mathbf{x}'; q). \quad (3.16)$$

Note that the prime on the summation sign indicates that the sum is over all quantum numbers except $(n\ell m) = (000)$. The latter is excluded because the associated eigenfunction $\xi_{000}(\mathbf{x}; q)$ is just a constant and thus does not contribute to $G(\mathbf{x}, \mathbf{x}'; \rho)$, which is defined as the Green’s function for all phase fluctuations with nonvanishing momenta.

Putting all these results together, we see that the dynamics of the collective variable $q(\tau)$ is determined by the action

$$\begin{aligned} S^{\text{eff}}[q] &= \int_0^{\hbar\beta} d\tau \left\{ \frac{3mN_0}{4} \left(\frac{dq}{d\tau} \right)^2 + N_0 \left(\frac{3\hbar^2}{4mq^2} + \frac{3}{4}m\omega^2 q^2 \right) \right\} \\ &\equiv \int_0^{\hbar\beta} d\tau \left\{ \frac{1}{2}m^* \left(\frac{dq}{d\tau} \right)^2 + V(q) \right\}, \end{aligned} \quad (3.17)$$

that is equivalent to the action of a particle with effective mass $m^* = 3mN_0/2$ in a potential $V(q) = N_0(3\hbar^2/4mq^2 + 3m\omega^2 q^2/4)$. As expected from our previous remarks, this potential has a minimum for $q = l$ and can be expanded near its minimum as

$$V(q) \simeq \frac{3}{2}N_0\hbar\omega + \frac{1}{2}m^*(2\omega)^2(\delta q)^2. \quad (3.18)$$

It thus confirms that the gaussian profile describes a breathing mode with frequency 2ω around an equilibrium density profile that is given by $\rho(\mathbf{x}; l) = N_0|\chi_{000}(\mathbf{x})|^2$.

Our next task is to investigate how interactions affect this result. Considering again only Gaussian density profiles, the action $S^{\text{eff}}[q]$ is again that of a particle with effective mass $m^* = 3mN_0/2$ but now in the potential [56]

$$V(q) = N_0 \left(\frac{3\hbar^2}{4mq^2} + \frac{3}{4}m\omega^2 q^2 - \frac{N_0}{\sqrt{2\pi}} \frac{\hbar^2 |a|}{mq^3} \right). \quad (3.19)$$

The physically most important feature of this potential is that it is unbounded from below, since $V(q) \rightarrow -\infty$ if $q \downarrow 0$. Hence, the condensate indeed always has the tendency to collapse to the high-density state $\lim_{q \downarrow 0} \rho(\mathbf{x}; q) = N_0\delta(\mathbf{x})$. However, if the number of condensate particles is sufficiently small, or more precisely if [57]

$$N_0 < \frac{2\sqrt{2\pi}}{5^{5/4}} \frac{l}{|a|} \simeq 0.68 \frac{l}{|a|}, \quad (3.20)$$

the condensate has to overcome a macroscopic energy barrier before it can collapse. Under these conditions the condensate is therefore really metastable and can in principle be observed experimentally. The most important question in this respect is of course: How metastable is the condensate? Within the gaussian approximation this question is easily answered, because then the dynamics of the condensate is equivalent to the dynamics of a particle in an unstable potential, as we have just seen. We therefore only need to evaluate the WKB-expression for the tunneling rate [58] and compare this to the rate of decay due to thermal fluctuations by calculating

also the height of the energy barrier. The outcome of this comparison for the conditions of the experiment with atomic ^7Li is presented in reference [59] and shows that, for the relatively high temperatures $T \gg \hbar\omega/k_B$ that have been obtained thusfar [11], the decay by means of thermal fluctuations over the energy barrier is the dominant decay mechanism of the condensate.

More important for our purposes, however, is that sufficiently close to the maximum number of condensate particles N_{max} the collective decay of the condensate discussed above is always much more probable than the decay due to two and three-body collisions that lead to a spin-flip or the formation of ^7Li molecules, respectively. As a result the collapse of the condensate should be observable within the finite lifetime of the gas. In fact, on the basis of this separation of time scales we expect the condensate to go through a number of growth and collapse cycles [59, 60]. Physically this picture arises as follows. Starting from a gas with a number of atoms $N \gg N_{\text{max}}$, the condensate will initially grow as a response to evaporative cooling. However, if the number of condensate atoms starts to come close to N_{max} , the condensate fluctuates over the energy barrier and collapses in a very short time of $\mathcal{O}(1/\omega)$ [61]. During the collapse the condensate density increases rapidly and two and three-body inelastic processes quickly remove almost all the atoms from the condensate. After this has occurred the condensate grows again from the noncondensed part of the gas and a new growth and collapse cycle begins. It is only after many of these cycles that enough atoms are removed for the gas to relax to an equilibrium with a number of condensate particles that is less than N_{max} . This is shown quantitatively in Figure 16 for the experimental conditions of interest.

A final issue which needs to be addressed at this point is the actual dynamics of the collapse and, in particular, how we must include the effect of the inelastic growth and decay processes on this dynamics. Unfortunately, the inclusion of these effects is rather complicated and we need the results of Section 3.4 to be able to correctly address this problem. It is, however, of some interest because Sackett *et al.* have recently observed that after a single collapse there remains a remnant of the condensate with about 10% of the initial number of atoms [62]. At present, it is an important open problem to theoretically understand the magnitude of this remnant.

3.2 Phase diffusion

As we have just seen explicitly, a particularly interesting consequence of the finite size of the gas is that quantum fluctuations play a much more important role. Although this is especially true for the case of attractive interactions that we considered in Section 3.1, it is also true for a Bose gas with repulsive interactions. A striking example in this respect is the phenomenon of phase “diffusion”, which was recently discussed by Lewenstein and You [32]. We rederive their results for a trapped Bose gas in a

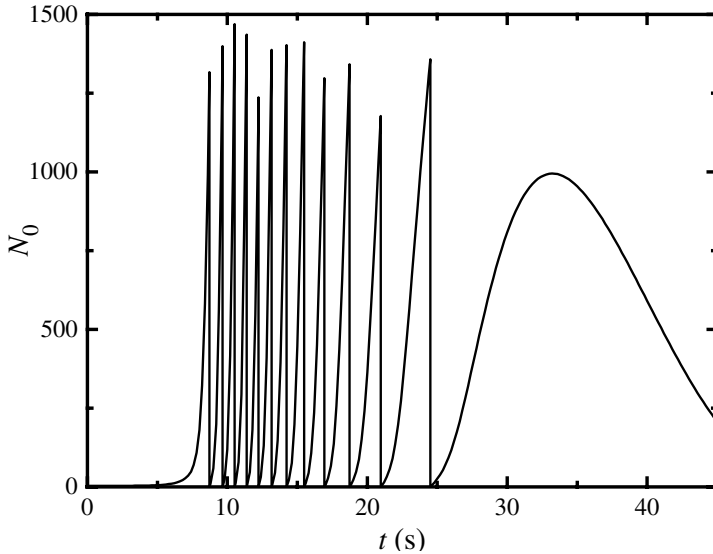


Fig. 16. Typical evolution of condensate number N_0 in response to evaporative cooling. The long-time decay of the condensate is due to two and three-body inelastic collisions.

moment, but first consider also the same phenomenon for a neutral and homogeneous superconductor. In this manner it is possible to bring out the physics involved more clearly.

Using the approach of Section 2.8.3, it can be shown that at zero temperature the dynamics of the superconducting order parameter, *i.e.*, the BCS gap parameter $\Delta(\mathbf{x}, t)$ that is proportional to the wave function of the condensate of Cooper pairs, is in a good approximation determined by a time-dependent Ginzburg-Landau theory [41, 63, 64] with the action

$$S^{\text{eff}}[\Delta^*, \Delta] = \frac{N(0)}{4} \int dt \int d\mathbf{x} \left\{ \frac{\hbar^2}{|\Delta_0|^2} \left| \frac{\partial \Delta}{\partial t} \right|^2 - \frac{\hbar^2 v_F^2}{3|\Delta_0|^2} |\nabla \Delta|^2 + 2|\Delta|^2 \left(1 - \frac{|\Delta|^2}{2|\Delta_0|^2} \right) \right\}, \quad (3.21)$$

where $N(0)$ is the density of states for one spin projection at the Fermi energy $\epsilon_F = mv_F^2/2$ and Δ_0 is the equilibrium value of the order parameter [65]. Writing the complex order parameter in terms of an amplitude and a phase, we immediately observe that the amplitude fluctuations are gapped [66] and can, therefore, be safely neglected at large length scales. The long-wavelength dynamics of the superconductor is thus dominated by

the phase fluctuations, according to the action

$$S^{\text{eff}}[\theta] = \frac{N(0)\hbar^2}{4} \int dt \int d\mathbf{x} \left\{ \left(\frac{\partial \theta}{\partial t} \right)^2 - \frac{v_F^2}{3} (\nabla \theta)^2 \right\}. \quad (3.22)$$

This also implies that the global phase $\theta_0(t) = \int d\mathbf{x} \theta(\mathbf{x}, t)/V$ of the superconductor has a dynamics that is governed by

$$S^{\text{eff}}[\theta_0] = \frac{N(0)N\hbar^2}{4n} \int dt \left(\frac{d\theta_0}{dt} \right)^2, \quad (3.23)$$

using the fact that the total volume V of the system is given by N/n .

Up to now our discussion has again been semiclassical. To consider also the quantum fluctuations, we have to quantize this theory by applying the usual rules of quantum mechanics. Doing so, we find that the wave function of the overall phase obeys a Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \Psi(\theta_0; t) = -\frac{n}{N(0)N} \frac{\partial^2}{\partial \theta_0^2} \Psi(\theta_0; t), \quad (3.24)$$

with a “diffusion” constant that can easily be shown to be equal to the quantity $(2/\hbar)\partial\epsilon_F/\partial N$ [67] and is, most importantly for our purposes, proportional to $1/N$. In the thermodynamic limit $N \rightarrow \infty$ a state with a well defined stationary phase is clearly a solution and we are then dealing with a system having a spontaneously broken $U(1)$ symmetry. However, for a finite (and fixed) number of particles the global phase cannot be well defined at all times and always has to “diffuse” in accordance with the above Schrödinger equation. Note also that in the groundstate the phase is fully undetermined and $|\Psi(\theta_0; t)|^2 = 1/2\pi$. Maybe surprisingly, the same calculation is somewhat more complicated for a Bose gas because the amplitude fluctuations of the order parameter cannot be neglected even at the largest length scales. However, taking these amplitude fluctuations into account properly, we nevertheless arrive at an action that is equivalent to equation (3.23) and hence again leads to the phenomenon of phase “diffusion”.

We start again from the action $S[\rho, \theta; \mu]$ for the condensate. The difference with the previous subsection is, however, that now we are not so much interested in the dynamics of the density but in the phase dynamics instead. Therefore we now want to integrate over the density field $\rho(\mathbf{x}, \tau)$. This cannot be done exactly and we therefore here consider only the strong-coupling limit, which was also treated by Lewenstein and You [32]. In that limit we are allowed to neglect the gradient of the average density profile [68] and

the action $S[\rho, \theta; \mu]$ is for the longest wavelengths well approximated by

$$S[\rho, \theta; \mu] = \int_0^{\hbar\beta} d\tau \int d\mathbf{x} \left(i\hbar\rho(\mathbf{x}, \tau) \frac{\partial\theta(\mathbf{x}, \tau)}{\partial\tau} + V^{\text{ex}}(\mathbf{x})\rho(\mathbf{x}, \tau) - \mu\rho(\mathbf{x}, \tau) + \frac{2\pi a\hbar^2}{m}\rho^2(\mathbf{x}, \tau) \right). \quad (3.25)$$

In equilibrium the average density profile of the condensate thus obeys

$$\langle\rho(\mathbf{x})\rangle = \frac{m}{4\pi a\hbar^2} (\mu - V^{\text{ex}}(\mathbf{x})) \Theta(\mu - V^{\text{ex}}(\mathbf{x})). \quad (3.26)$$

Performing now the shift $\rho(\mathbf{x}, \tau) = \langle\rho(\mathbf{x})\rangle + \delta\rho(\mathbf{x}, \tau)$, we find for the zero-momentum part of the action [69]

$$S[\delta N_0, \theta_0; \mu] = \hbar\beta E_0(\mu) + \int_0^{\hbar\beta} d\tau \left(i\hbar\delta N_0 \frac{d\theta_0}{d\tau} + \frac{2\pi a\hbar^2}{mV_0(\mu)} (\delta N_0)^2 \right), \quad (3.27)$$

where $E_0(\mu)$ and $V_0(\mu)$ correspond, respectively, to the energy and the volume of the condensate in the so-called Thomas-Fermi approximation [70]. Moreover, $\delta N_0(\tau) = \int d\mathbf{x} \delta\rho(\mathbf{x}, \tau)$ represents the fluctuations in the total number of condensate particles in that same approximation, implying that the density fluctuations $\delta\rho(\mathbf{x}, \tau)$ are only nonzero in that region of space where the condensate density does not vanish.

Performing now the integration over the number fluctuations $\delta N_0(\tau)$ and the usual Wick rotation to real times $\tau \rightarrow it$, we immediately see that the effective action for the global phase of the condensate has precisely the same form as in equation (3.23), *i.e.*,

$$S^{\text{eff}}[\theta_0; \mu] = \frac{mV_0(\mu)}{8\pi a} \int dt \left(\frac{d\theta_0}{dt} \right)^2. \quad (3.28)$$

The appropriate “diffusion” constant is therefore equal to $2\pi a\hbar/mV_0(\mu)$, which can easily be shown to be equal to $(1/2\hbar)\partial\mu/\partial N_0$ if we make use of the fact that in the Thomas-Fermi approximation the chemical potential obeys $\mu = m\omega^2 R_{\text{TF}}^2/2$ and the radius of the condensate is given by $R_{\text{TF}} = (15a\hbar^2 N_0/m^2\omega^2)^{1/5}$ [56]. Hence, the “diffusion” constant is proportional to $1/N_0^{3/5}$. Note that if the condensate were contained in a box the “diffusion” constant would be proportional to $1/N_0$ instead. It is important to note also that, in contrast to the case of a fermionic superfluid, we have to integrate over the amplitude fluctuations of the order parameter to arrive at a quadratic action for the phase fluctuations. This leads to the important conclusion that for a bosonic superfluid it is impossible to be in a state with only phase fluctuations and no density fluctuations, even at the largest length scales.

3.3 Quantum kinetic theory

For simplicity we restrict ourselves for the rest of this course to the case of a doubly-polarized atomic Bose gas, which for most practical purposes can be seen as a gas of spin-less bosons [71]. Once we have understood the quantum kinetic theory for this particular case, however, we can easily generalize to multi-component Bose gases that are receiving considerable attention at present [72]. Furthermore, the same methods can also be used for fermionic gases and have recently already been applied to the problem of Cooper-pair formation in a two-component fermion gas [73].

3.3.1 Ideal Bose gas

In textbooks an ideal Bose gas is generally discussed in terms of the average occupation numbers of the one-particle states $\chi_{\mathbf{n}}(\mathbf{x})$ [74]. Given the density matrix $\hat{\rho}(t_0)$ of the gas at an initial time t_0 , these occupation numbers obey

$$N_{\mathbf{n}}(t) = \text{Tr} \left[\hat{\rho}(t_0) \hat{\psi}_{\mathbf{n}}^{\dagger}(t) \hat{\psi}_{\mathbf{n}}(t) \right], \quad (3.29)$$

with $\hat{\psi}_{\mathbf{n}}^{\dagger}(t)$ and $\hat{\psi}_{\mathbf{n}}(t)$ the usual (Heisenberg picture) creation and annihilation operators of second quantization, respectively. Because the Hamiltonian of the gas

$$\hat{H} = \sum_{\mathbf{n}} \epsilon_{\mathbf{n}} \hat{\psi}_{\mathbf{n}}^{\dagger}(t) \hat{\psi}_{\mathbf{n}}(t) \quad (3.30)$$

commutes with the number operators $\hat{N}_{\mathbf{n}}(t) = \hat{\psi}_{\mathbf{n}}^{\dagger}(t) \hat{\psi}_{\mathbf{n}}(t)$, the nonequilibrium dynamics of the system is trivial and the average occupation numbers are at all times equal to their value at the initial time t_0 . If we are also interested in fluctuations, it is convenient to introduce the eigenstates of the number operators, *i.e.*,

$$|\{N_{\mathbf{n}}\}; t\rangle = \prod_{\mathbf{n}} \frac{\left(\hat{\psi}_{\mathbf{n}}^{\dagger}(t)\right)^{N_{\mathbf{n}}}}{\sqrt{N_{\mathbf{n}}!}} |0\rangle, \quad (3.31)$$

and to consider the full probability distribution

$$P(\{N_{\mathbf{n}}\}; t) = \text{Tr} [\hat{\rho}(t_0) |\{N_{\mathbf{n}}\}; t\rangle \langle \{N_{\mathbf{n}}\}; t|], \quad (3.32)$$

which is again independent of time for an ideal Bose gas. The average occupation numbers are then determined by

$$N_{\mathbf{n}}(t) = \sum_{\{N_{\mathbf{n}}\}} N_{\mathbf{n}} P(\{N_{\mathbf{n}}\}; t) \quad (3.33)$$

and the fluctuations can be obtained from similar expressions.

As indicated in Section 3.2, we are also interested in the phase dynamics of the gas. In analogy with the occupation number representation in equation (3.32), we can now obtain a completely different description of the Bose gas by making use of coherent states and considering the probability distribution $P[\phi^*, \phi; t]$. Although we expect that this probability distribution is again independent of time, let us nevertheless proceed to derive its equation of motion in a way that can be generalized later on when we consider an interacting Bose gas. First, we use that

$$P[\phi^*, \phi; t] = \int d[\phi_0^*] d[\phi_0] P[\phi_0^*, \phi_0; t_0] \frac{|\langle \phi; t | \phi_0; t_0 \rangle|^2}{\langle \phi; t | \phi; t \rangle \langle \phi_0; t_0 | \phi_0; t_0 \rangle} . \quad (3.34)$$

This is a particularly useful result, because the time dependence is now completely determined by the matrix element $\langle \phi; t | \phi_0; t_0 \rangle$ for which the functional integral representation is well known from our discussion in Section 2.3. It is given by a “path” integral over all complex field evolutions $\psi(\mathbf{x}, t_+) = \sum_{\mathbf{n}} \psi_{\mathbf{n}}(t_+) \chi_{\mathbf{n}}(\mathbf{x})$ from t_0 to t . More precisely we have

$$\langle \phi; t | \phi_0; t_0 \rangle = \int_{\psi(\mathbf{x}, t_0) = \phi_0(\mathbf{x})}^{\psi^*(\mathbf{x}, t) = \phi^*(\mathbf{x})} d[\psi^*] d[\psi] \exp \left\{ \frac{i}{\hbar} S_+[\psi^*, \psi] \right\} , \quad (3.35)$$

with the forward action $S_+[\psi^*, \psi]$ given by

$$\begin{aligned} S_+[\psi^*, \psi] &= \sum_{\mathbf{n}} \left\{ -i\hbar \psi_{\mathbf{n}}^*(t) \psi_{\mathbf{n}}(t) \right. \\ &\quad \left. + \int_{t_0}^t dt_+ \psi_{\mathbf{n}}^*(t_+) \left(i\hbar \frac{\partial}{\partial t_+} - \epsilon_{\mathbf{n}} \right) \psi_{\mathbf{n}}(t_+) \right\} . \end{aligned} \quad (3.36)$$

In the same manner the matrix element $\langle \phi; t | \phi_0; t_0 \rangle^* = \langle \phi_0; t_0 | \phi; t \rangle$ can be written as a “path” integral over all possible field configurations $\psi(\mathbf{x}, t_-) = \sum_{\mathbf{n}} \psi_{\mathbf{n}}(t_-) \chi_{\mathbf{n}}(\mathbf{x})$ evolving backward in time from t to t_0 , i.e.,

$$\langle \phi; t | \phi_0; t_0 \rangle^* = \int_{\psi(\mathbf{x}, t) = \phi(\mathbf{x})}^{\psi^*(\mathbf{x}, t_0) = \phi_0^*(\mathbf{x})} d[\psi^*] d[\psi] \exp \left\{ \frac{i}{\hbar} S_-[\psi^*, \psi] \right\} , \quad (3.37)$$

with a backward action

$$\begin{aligned} S_-[\psi^*, \psi] &= \sum_{\mathbf{n}} \left\{ -i\hbar \psi_{\mathbf{n}}^*(t_0) \psi_{\mathbf{n}}(t_0) \right. \\ &\quad \left. + \int_t^{t_0} dt_- \psi_{\mathbf{n}}^*(t_-) \left(i\hbar \frac{\partial}{\partial t_-} - \epsilon_{\mathbf{n}} \right) \psi_{\mathbf{n}}(t_-) \right\} \\ &= \sum_{\mathbf{n}} \left\{ -i\hbar \psi_{\mathbf{n}}^*(t) \psi_{\mathbf{n}}(t) \right. \\ &\quad \left. + \int_t^{t_0} dt_- \psi_{\mathbf{n}}(t_-) \left(-i\hbar \frac{\partial}{\partial t_-} - \epsilon_{\mathbf{n}} \right) \psi_{\mathbf{n}}^*(t_-) \right\} . \end{aligned} \quad (3.38)$$

Putting all these results together, we see that the probability distribution $P[\phi^*, \phi; t]$ can in fact be represented by a functional integral over all fields $\psi(\mathbf{x}, t)$ that evolve backwards from t to t_0 and then forward in time from t_0 to t . Absorbing the factor $P[\phi_0^*, \phi_0; t_0]$ into the measure of the functional integral, we thus arrive at the desired result that

$$P[\phi^*, \phi; t] = \int_{\psi(\mathbf{x}, t) = \phi(\mathbf{x})}^{\psi^*(\mathbf{x}, t) = \phi^*(\mathbf{x})} d[\psi^*] d[\psi] \exp \left\{ \frac{i}{\hbar} S[\psi^*, \psi] \right\}, \quad (3.39)$$

where the total (backward-forward) action in first instance obeys

$$\begin{aligned} S[\psi^*, \psi] &= S_-[\psi^*, \psi] + S_+[\psi^*, \psi] = -i\hbar \sum_{\mathbf{n}} (\psi_{\mathbf{n}}^*(t) \psi_{\mathbf{n}}(t) - |\phi_{\mathbf{n}}|^2) \\ &+ \sum_{\mathbf{n}} \int_{\mathcal{C}^t} dt' \left\{ \frac{1}{2} \left(\psi_{\mathbf{n}}^*(t') i\hbar \frac{\partial}{\partial t'} \psi_{\mathbf{n}}(t') \right. \right. \\ &\quad \left. \left. - \psi_{\mathbf{n}}(t') i\hbar \frac{\partial}{\partial t'} \psi_{\mathbf{n}}^*(t') \right) - \epsilon_{\mathbf{n}} \psi_{\mathbf{n}}^*(t') \psi_{\mathbf{n}}(t') \right\}, \end{aligned} \quad (3.40)$$

and the integration along the Schwinger-Keldysh contour $\mathcal{C}^t$ is defined by $\int_{\mathcal{C}^t} dt' = \int_t^{t_0} dt_- + \int_{t_0}^t dt_+$ [75–77]. Note also that in equation (3.39) we have explicitly specified the boundary conditions on the functional integral. It is interesting to mention that these boundary conditions are essentially dictated by the topological terms in the action $S[\psi^*, \psi]$, which is a general feature of the path-integral formulation of quantum mechanics due to the fact that the quantum theory should have the correct (semi)classical limit [78]. Making use of the periodicity of the field $\psi(\mathbf{x}, t)$ on the Schwinger-Keldysh contour, the variational principle $\delta S[\psi^*, \psi] / \delta \psi_{\mathbf{n}}^*(t_{\pm}) = 0$ indeed leads not only to the Euler-Lagrange equation

$$i\hbar \frac{\partial}{\partial t_{\pm}} \psi_{\mathbf{n}}(t_{\pm}) = \epsilon_{\mathbf{n}} \psi_{\mathbf{n}}(t_{\pm}), \quad (3.41)$$

which agrees with the Heisenberg equation of motion $i\hbar \partial \hat{\psi}_{\mathbf{n}}(t_{\pm}) / \partial t_{\pm} = [\hat{\psi}_{\mathbf{n}}(t_{\pm}), H]$ for the annihilation operators, but also with the appropriate boundary condition $\delta \psi_{\mathbf{n}}^*(t) = 0$. In the same way we find the complex conjugate results if we require that $\delta S[\psi^*, \psi] / \delta \psi_{\mathbf{n}}(t_{\pm}) = 0$. Substituting the boundary conditions in equation (3.40) and performing a partial integration, we then finally obtain for the action

$$S[\psi^*, \psi] = \sum_{\mathbf{n}} \int_{\mathcal{C}^t} dt' \psi_{\mathbf{n}}^*(t') \left(i\hbar \frac{\partial}{\partial t'} - \epsilon_{\mathbf{n}} \right) \psi_{\mathbf{n}}(t'), \quad (3.42)$$

which we for completeness sake also rewrite as

$$S[\psi^*, \psi] = \int_{\mathcal{C}^t} dt' \int d\mathbf{x} \psi^*(\mathbf{x}, t') \left(i\hbar \frac{\partial}{\partial t'} + \frac{\hbar^2 \nabla^2}{2m} - V^{\text{ex}}(\mathbf{x}) \right) \psi(\mathbf{x}, t'). \quad (3.43)$$

We are now in a position to derive the equation of motion, *i.e.*, the Fokker-Planck equation, for the probability distribution $P[\phi^*, \phi; t]$. This is most easily achieved by performing the variable transformation $\psi(\mathbf{x}, t_{\pm}) = \phi(\mathbf{x}, t') \pm \xi(\mathbf{x}, t')/2$ in equation (3.39). In this manner the fields $\psi(\mathbf{x}, t_-)$ and $\psi(\mathbf{x}, t_+)$ that live on the backward and forward branch of the Schwinger-Keldysh contour, respectively, are “projected” onto the real time axis. Moreover, at the same time we effect a separation between the (semi)classical dynamics described by $\phi(\mathbf{x}, t')$ and the quantum fluctuations determined by $\xi(\mathbf{x}, t')$. After the transformation we have

$$P[\phi^*, \phi; t] = \int_{\phi(\mathbf{x}, t) = \phi(\mathbf{x})}^{\phi^*(\mathbf{x}, t) = \phi^*(\mathbf{x})} d[\phi^*] d[\phi] \int d[\xi^*] d[\xi] \exp \left\{ \frac{i}{\hbar} S[\phi^*, \phi; \xi^*, \xi] \right\}, \quad (3.44)$$

with

$$S[\phi^*, \phi; \xi^*, \xi] = \sum_{\mathbf{n}} \int_{t_0}^t dt' \left\{ \phi_{\mathbf{n}}^*(t') \left(i\hbar \frac{\partial}{\partial t'} - \epsilon_{\mathbf{n}} \right) \xi_{\mathbf{n}}(t') + \xi_{\mathbf{n}}^*(t') \left(i\hbar \frac{\partial}{\partial t'} - \epsilon_{\mathbf{n}} \right) \phi_{\mathbf{n}}(t') \right\}. \quad (3.45)$$

Because this action is linear in $\xi_{\mathbf{n}}(t')$ and $\xi_{\mathbf{n}}^*(t')$, the integration over the quantum fluctuations leads just to a constraint and we find that

$$P[\phi^*, \phi; t] = \int_{\phi(\mathbf{x}, t) = \phi(\mathbf{x})}^{\phi^*(\mathbf{x}, t) = \phi^*(\mathbf{x})} d[\phi^*] d[\phi] \times \prod_{\mathbf{n}} \delta \left[\left(-i \frac{\partial}{\partial t'} - \frac{\epsilon_{\mathbf{n}}}{\hbar} \right) \phi_{\mathbf{n}}^*(t') \cdot \left(i \frac{\partial}{\partial t'} - \frac{\epsilon_{\mathbf{n}}}{\hbar} \right) \phi_{\mathbf{n}}(t') \right] \quad (3.46)$$

or equivalently that

$$P[\phi^*, \phi; t] = \int d[\phi_0^*] d[\phi_0] P[\phi_0^*, \phi_0; t_0] \prod_{\mathbf{n}} \delta (|\phi_{\mathbf{n}} - \phi_{\mathbf{n}}^{\text{cl}}(t)|^2), \quad (3.47)$$

where we introduced the quantity $\phi_{\mathbf{n}}^{\text{cl}}(t)$ obeying the semiclassical equation of motion

$$i\hbar \frac{\partial}{\partial t} \phi_{\mathbf{n}}^{\text{cl}}(t) = \epsilon_{\mathbf{n}} \phi_{\mathbf{n}}^{\text{cl}}(t) \quad (3.48)$$

and the initial condition $\phi_{\mathbf{n}}^{\text{cl}}(t_0) = \phi_{0; \mathbf{n}}$.

The latter equation is thus solved by $\phi_{\mathbf{n}}^{\text{cl}}(t) = \phi_{0; \mathbf{n}} e^{-i\epsilon_{\mathbf{n}}(t-t_0)/\hbar}$ and we conclude from a simple change of variables in equation (3.47) that for an

ideal Bose gas $P[\phi^*, \phi; t] = P[\phi^*, \phi; t_0]$, as expected. We also see from equation (3.47) that the desired equation of motion for $P[\phi^*, \phi; t]$ reads

$$i\hbar \frac{\partial}{\partial t} P[\phi^*, \phi; t] = - \left(\sum_{\mathbf{n}} \frac{\partial}{\partial \phi_{\mathbf{n}}} \epsilon_{\mathbf{n}} \phi_{\mathbf{n}} \right) P[\phi^*, \phi; t] + \left(\sum_{\mathbf{n}} \frac{\partial}{\partial \phi_{\mathbf{n}}^*} \epsilon_{\mathbf{n}} \phi_{\mathbf{n}}^* \right) P[\phi^*, \phi; t]. \quad (3.49)$$

This is indeed the correct Fokker-Planck equation for an ideal Bose gas [79]. To see that we first consider $\langle \phi_{\mathbf{n}} \rangle(t) = \int d[\phi^*] d[\phi] \phi_{\mathbf{n}} P[\phi^*, \phi; t]$. Multiplying equation (3.49) with $\phi_{\mathbf{n}}$ and integrating over $\phi(\mathbf{x})$, we easily find after a partial integration that

$$i\hbar \frac{\partial}{\partial t} \langle \phi_{\mathbf{n}} \rangle(t) = \epsilon_{\mathbf{n}} \langle \phi_{\mathbf{n}} \rangle(t), \quad (3.50)$$

which precisely corresponds to the equation of motion of the expectation value $\langle \hat{\psi}_{\mathbf{n}}(t) \rangle = \text{Tr}[\hat{\rho}(t_0) \hat{\psi}_{\mathbf{n}}(t)]$ in the operator formalism. Similarly, we find that

$$i\hbar \frac{\partial}{\partial t} \langle \phi_{\mathbf{n}}^* \rangle(t) = -\epsilon_{\mathbf{n}} \langle \phi_{\mathbf{n}}^* \rangle(t), \quad (3.51)$$

in agreement with the result for $\langle \hat{\psi}_{\mathbf{n}}^\dagger(t) \rangle = \text{Tr}[\hat{\rho}(t_0) \hat{\psi}_{\mathbf{n}}^\dagger(t)]$.

Next we consider the average of $|\phi_{\mathbf{n}}|^2$, for which we immediately obtain

$$i\hbar \frac{\partial}{\partial t} \langle |\phi_{\mathbf{n}}|^2 \rangle(t) = 0. \quad (3.52)$$

We expect this result to be related to the fact that in the operator formalism the occupation numbers $N_{\mathbf{n}}(t)$ are independent of time. Although this turns out to be true, to give the precise relation between $\langle |\phi_{\mathbf{n}}|^2 \rangle(t)$ and $N_{\mathbf{n}}(t)$ is complicated by the fact that at equal times the operators $\hat{\psi}_{\mathbf{n}}(t)$ and $\hat{\psi}_{\mathbf{n}}^\dagger(t)$ do not commute. However, the path-integral formulation of quantum mechanics is only capable of calculating time-ordered operator products [80]. In our case this implies that $\langle |\phi_{\mathbf{n}}|^2 \rangle(t)$ is the value at $t' = t$ of

$$\text{Tr} \left[\hat{\rho}(t_0) T_{C^t} \left(\hat{\psi}_{\mathbf{n}}(t) \hat{\psi}_{\mathbf{n}}^\dagger(t') \right) \right] = \Theta(t, t') \text{Tr} \left[\hat{\rho}(t_0) \hat{\psi}_{\mathbf{n}}(t) \hat{\psi}_{\mathbf{n}}^\dagger(t') \right] + \Theta(t', t) \text{Tr} \left[\hat{\rho}(t_0) \hat{\psi}_{\mathbf{n}}^\dagger(t') \hat{\psi}_{\mathbf{n}}(t) \right], \quad (3.53)$$

with T_{C^t} the time-ordering operator on the Schwinger-Keldysh contour and $\Theta(t, t')$ the corresponding Heaviside function. Since the Heaviside function is equal to 1/2 at equal times [81], we conclude that

$$\langle |\phi_{\mathbf{n}}|^2 \rangle(t) = N_{\mathbf{n}}(t) + \frac{1}{2} \quad (3.54)$$

and that equation (3.52) is thus fully consistent with the operator formalism. An intuitive understanding of the relation between $\langle |\phi_{\mathbf{n}}|^2 \rangle(t)$ and the occupation numbers can be obtained by noting that, since all our manipulations up to now have been exact, we expect $\langle |\phi_{\mathbf{n}}|^2 \rangle(t)$ to contain both classical and quantum fluctuations. These correspond precisely to the contributions $N_{\mathbf{n}}(t)$ and $1/2$, respectively.

Finally we need to discuss the stationary solutions of the Fokker-Planck equation. It is not difficult to show that any functional that only depends on the amplitudes $|\phi_{\mathbf{n}}|^2$ is a solution. As it stands the Fokker-Planck equation, therefore, does not lead to a unique equilibrium distribution. This is not surprising, because for an isolated, ideal Bose gas there is no mechanism for redistributing the particles over the various energy levels and thus for relaxation towards equilibrium. However, the situation changes when we allow the bosons in the trap to tunnel back and forth to a reservoir at a temperature T . The corrections to the Fokker-Planck equation that are required to describe the physics in this case are considered next. However, to determine these corrections in the most convenient way, we have to slightly generalize the above theory because with the probability distribution $P[\phi^*, \phi; t]$ we are only able to study spatial, but not temporal correlations in the Bose gas.

To study also those we follow the by now well-known procedure in quantum field theory and construct a generating functional $Z[J, J^*]$ for all (time-ordered) correlation functions. It is obtained by performing two steps. First, we introduce the probability distribution $P_J[\phi^*, \phi; t]$ for a Bose gas in the presence of the external currents $J(\mathbf{x}, t)$ and $J^*(\mathbf{x}, t)$ by adding to the Hamiltonian the terms

$$-\hbar \int d\mathbf{x} \left(\hat{\psi}(\mathbf{x}, t) J^*(\mathbf{x}, t) + J(\mathbf{x}, t) \hat{\psi}^\dagger(\mathbf{x}, t) \right) = \\ -\hbar \sum_{\mathbf{n}} \left(\hat{\psi}_{\mathbf{n}}(t) J_{\mathbf{n}}^*(t) + J_{\mathbf{n}}(t) \hat{\psi}_{\mathbf{n}}^\dagger(t) \right).$$

As a result we have

$$P_J[\phi^*, \phi; t] = \int_{\psi(\mathbf{x}, t) = \phi(\mathbf{x})}^{\psi^*(\mathbf{x}, t) = \phi^*(\mathbf{x})} d[\psi^*] d[\psi] \exp \left\{ \frac{i}{\hbar} S[\psi^*, \psi] \right\} \\ \times \exp \left\{ i \int_{\mathcal{C}^t} dt' \int d\mathbf{x} \left(\psi(\mathbf{x}, t') J^*(\mathbf{x}, t') + J(\mathbf{x}, t') \psi^*(\mathbf{x}, t') \right) \right\}. \quad (3.55)$$

Second, we integrate this expression over $\phi(\mathbf{x})$ to obtain the desired generating functional. Hence

$$\begin{aligned} Z[J, J^*] &= \int d[\phi^*] d[\phi] P_J[\phi^*, \phi; t] = \int d[\psi^*] d[\psi] \exp \left\{ \frac{i}{\hbar} S[\psi^*, \psi] \right\} \\ &\times \exp \left\{ i \int_{\mathcal{C}^\infty} dt \int d\mathbf{x} (\psi(\mathbf{x}, t) J^*(\mathbf{x}, t) + J(\mathbf{x}, t) \psi^*(\mathbf{x}, t)) \right\}. \end{aligned} \quad (3.56)$$

It is important to realize that $Z[J, J^*]$ is indeed independent of the time t because of the fact that $P_J[\phi^*, \phi; t]$ is a probability distribution and thus properly normalized. We are therefore allowed to deform the contour $\mathcal{C}^t$ to any closed contour that runs through t_0 . Since we are in principle interested in all times $t \geq t_0$, the most convenient choice is the countour that runs backward from infinity to t_0 and then forwards from t_0 to infinity. This contour is denoted by $\mathcal{C}^\infty$ and also called the Schwinger-Keldysh contour in the following because there is in practice never confusion with the more restricted contour $\mathcal{C}^t$ that is required when we consider a probability distribution. With this choice it is also clear that $Z[J, J^*]$ is a generating functional. Indeed, equation (3.56) shows explicitly that all time-ordered correlation functions can be obtained by functional differentiation with respect to the currents $J(\mathbf{x}, t)$ and $J^*(\mathbf{x}, t)$. We have, for instance, that

$$\text{Tr}[\hat{\rho}(t_0) \hat{\psi}(\mathbf{x}, t)] = \frac{1}{i} \frac{\delta}{\delta J^*(\mathbf{x}, t)} Z[J, J^*] \Big|_{J, J^*=0} \quad (3.57)$$

and similarly that

$$\begin{aligned} &\text{Tr} \left[\hat{\rho}(t_0) T_{\mathcal{C}^\infty} \left(\hat{\psi}(\mathbf{x}, t) \hat{\psi}^\dagger(\mathbf{x}', t') \right) \right] \\ &= \frac{1}{i^2} \frac{\delta^2}{\delta J^*(\mathbf{x}, t) \delta J(\mathbf{x}', t')} Z[J, J^*] \Big|_{J, J^*=0}. \end{aligned} \quad (3.58)$$

Note that the times t and t' always have to be larger or equal to t_0 for these identities to be valid.

3.3.2 Ideal Bose gas in contact with a reservoir

Inspired by the Caldeira-Leggett model for a particle experiencing friction [82], we take for the reservoir an ideal gas of N bosons in a box with volume V . The states in this box are labeled by the momentum $\hbar \mathbf{k}$ and equal to $\chi_{\mathbf{k}}(\mathbf{x}) = e^{i\mathbf{k} \cdot \mathbf{x}} / \sqrt{V}$. They have an energy $\epsilon(\mathbf{k}) = \hbar^2 \mathbf{k}^2 / 2m + \Delta V^{\text{ex}}$, where ΔV^{ex} accounts for a possible bias between the potential energies of a particle in the center of the trap and a particle in the reservoir. The reservoir

is also taken to be sufficiently large that it can be treated in the thermodynamic limit and is in an equilibrium with temperature T and chemical potential μ for times $t < t_0$. At t_0 it is brought into contact with the trap by means of a tunnel Hamiltonian

$$\hat{H}^{\text{int}} = \frac{1}{\sqrt{V}} \sum_{\mathbf{n}} \sum_{\mathbf{k}} \left(t_{\mathbf{n}}(\mathbf{k}) \hat{\psi}_{\mathbf{n}}(t) \hat{\psi}_{\mathbf{k}}^{\dagger}(t) + t_{\mathbf{n}}^*(\mathbf{k}) \hat{\psi}_{\mathbf{k}}(t) \hat{\psi}_{\mathbf{n}}^{\dagger}(t) \right), \quad (3.59)$$

with complex tunneling matrix elements $t_{\mathbf{n}}(\mathbf{k})$ that for simplicity are assumed to be almost constant for momenta $\hbar k$ smaller than a cutoff $\hbar k_c$ but to vanish rapidly for momenta larger than this ultraviolet cutoff. Moreover, we consider here only the low-temperature regime in which the thermal de Broglie wavelength $\Lambda_{\text{th}} = (2\pi\hbar^2/mk_B T)^{1/2}$ of the particles obeys $\Lambda_{\text{th}} \gg 1/k_c$, since this is the most appropriate limit for realistic atomic gases.

To study the evolution of the combined system for times $t \geq t_0$ we thus have to deal with the action

$$\begin{aligned} S[\psi^*, \psi; \psi_{\text{R}}^*, \psi_{\text{R}}] = & \sum_{\mathbf{n}} \int_{\mathcal{C}^\infty} dt \, \psi_{\mathbf{n}}^*(t) \left(i\hbar \frac{\partial}{\partial t} - \epsilon_{\mathbf{n}} + \mu \right) \psi_{\mathbf{n}}(t) \\ & + \sum_{\mathbf{k}} \int_{\mathcal{C}^\infty} dt \, \psi_{\mathbf{k}}^*(t) \left(i\hbar \frac{\partial}{\partial t} - \epsilon(\mathbf{k}) + \mu \right) \psi_{\mathbf{k}}(t) \\ & - \frac{1}{\sqrt{V}} \sum_{\mathbf{n}} \sum_{\mathbf{k}} \int_{\mathcal{C}^\infty} dt \, (t_{\mathbf{n}}(\mathbf{k}) \psi_{\mathbf{n}}(t) \psi_{\mathbf{k}}^*(t) \\ & + t_{\mathbf{n}}^*(\mathbf{k}) \psi_{\mathbf{k}}(t) \psi_{\mathbf{n}}^*(t)) \end{aligned} \quad (3.60)$$

if we measure all energies relative to the chemical potential and also introduce the complex field $\psi_{\text{R}}(\mathbf{x}, t) = \sum_{\mathbf{k}} \psi_{\mathbf{k}}(t) \chi_{\mathbf{k}}(\mathbf{x})$ for the degrees of freedom of the reservoir. However, we are only interested in the evolution of the Bose gas in the trap and therefore only in the time-ordered correlation functions of this part of the system. The corresponding generating functional

$$\begin{aligned} Z[J, J^*] = & \int d[\psi^*] d[\psi] \int d[\psi_{\text{R}}^*] d[\psi_{\text{R}}] \exp \left\{ \frac{i}{\hbar} S[\psi^*, \psi; \psi_{\text{R}}^*, \psi_{\text{R}}] \right\} \\ & \times \exp \left\{ i \int_{\mathcal{C}^\infty} dt \int d\mathbf{x} \, (\psi(\mathbf{x}, t) J^*(\mathbf{x}, t) + J(\mathbf{x}, t) \psi^*(\mathbf{x}, t)) \right\} \end{aligned} \quad (3.61)$$

is of the same form as the functional integral in equation (3.56), but now with an effective action that is defined by

$$\exp \left\{ \frac{i}{\hbar} S^{\text{eff}}[\psi^*, \psi] \right\} \equiv \int d[\psi_{\text{R}}^*] d[\psi_{\text{R}}] \exp \left\{ \frac{i}{\hbar} S[\psi^*, \psi; \psi_{\text{R}}^*, \psi_{\text{R}}] \right\}. \quad (3.62)$$

Hence, our next task is to integrate out the field $\psi_R(\mathbf{x}, t)$, which can be done exactly because it only requires the integration of a gaussian.

To familiarize ourselves with the Schwinger-Keldysh formalism, we perform the gaussian integration here in some detail. In principle, this can of course be done explicitly by making use of the fact that the initial density matrix $\hat{\rho}_R(t_0)$ of the reservoir can be expanded in the projection operators on the coherent states by using the coefficients

$$\rho_R[|\phi_R|^2; t_0] = \prod_{\mathbf{k}} \frac{1}{N(\mathbf{k})} e^{-|\phi_{\mathbf{k}}|^2/N(\mathbf{k})}, \quad (3.63)$$

with $N(\mathbf{k}) = 1/(e^{\beta(\epsilon(\mathbf{k})-\mu)} - 1)$ the appropriate Bose distribution function and $\beta = 1/k_B T$. However, in practice it is much more easy to use a different procedure. It is based on the observation that if we introduce the δ function on the Schwinger-Keldysh contour defined by $\int_{\mathcal{C}^\infty} dt' \delta(t, t') = 1$ and the Green's function $G(\mathbf{k}; t, t')$ obeying

$$\left(i\hbar \frac{\partial}{\partial t} - \epsilon(\mathbf{k}) + \mu \right) G(\mathbf{k}; t, t') = \hbar \delta(t, t'), \quad (3.64)$$

the action $S[\psi^*, \psi; \psi_R^*, \psi_R]$ can be written as a complete square, or more precisely as the sum of two squares $S_1[\psi^*, \psi]$ and $S_2[\psi^*, \psi; \psi_R^*, \psi_R]$ that are given by

$$\begin{aligned} S_1[\psi^*, \psi] &= \sum_{\mathbf{n}} \int_{\mathcal{C}^\infty} dt \psi_{\mathbf{n}}^*(t) \left(i\hbar \frac{\partial}{\partial t} - \epsilon_{\mathbf{n}} + \mu \right) \psi_{\mathbf{n}}(t) \\ &\quad - \frac{1}{\hbar V} \sum_{\mathbf{n}, \mathbf{n}'} \sum_{\mathbf{k}} \int_{\mathcal{C}^\infty} dt \int_{\mathcal{C}^\infty} dt' \psi_{\mathbf{n}}^*(t) t_{\mathbf{n}}^*(\mathbf{k}) G(\mathbf{k}; t, t') t_{\mathbf{n}'}(\mathbf{k}) \psi_{\mathbf{n}'}(t') \end{aligned} \quad (3.65)$$

and

$$\begin{aligned} S_2[\psi^*, \psi; \psi_R^*, \psi_R] &= \sum_{\mathbf{k}} \int_{\mathcal{C}^\infty} dt \left(\psi_{\mathbf{k}}^*(t) \right. \\ &\quad \left. - \frac{1}{\hbar \sqrt{V}} \sum_{\mathbf{n}} \int_{\mathcal{C}^\infty} dt' t_{\mathbf{n}}^*(\mathbf{k}) \psi_{\mathbf{n}}^*(t') G(\mathbf{k}; t', t) \right) \\ &\quad \times \left(i\hbar \frac{\partial}{\partial t} - \epsilon(\mathbf{k}) + \mu \right) \\ &\quad \times \left(\psi_{\mathbf{k}}(t) - \frac{1}{\hbar \sqrt{V}} \sum_{\mathbf{n}} \int_{\mathcal{C}^\infty} dt' G(\mathbf{k}; t, t') \psi_{\mathbf{n}}(t') t_{\mathbf{n}}(\mathbf{k}) \right), \end{aligned} \quad (3.66)$$

respectively. Since the first term is independent of the field $\psi_R(\mathbf{x}, t)$, we only need to evaluate $\int d[\psi_R^*] d[\psi_R] \exp(iS_2[\psi^*, \psi; \psi_R^*, \psi_R]/\hbar)$. Performing

a shift in the integration variables, we however see that this functional integral is equal to

$$\int d[\psi_R^*]d[\psi_R] \exp \left\{ \frac{i}{\hbar} \sum_{\mathbf{k}} \int_{C^\infty} dt \psi_{\mathbf{k}}^*(t) \left(i\hbar \frac{\partial}{\partial t} - \epsilon(\mathbf{k}) + \mu \right) \psi_{\mathbf{k}}(t) \right\} \\ = \text{Tr}[\rho_R(t_0)] = 1. \quad (3.67)$$

As a result the effective action $S^{\text{eff}}[\psi^*, \psi]$ is just equal to $S_1[\psi^*, \psi]$, which can be slightly rewritten to read

$$S^{\text{eff}}[\psi^*, \psi] = \sum_{\mathbf{n}, \mathbf{n}'} \int_{C^\infty} dt \int_{C^\infty} dt' \\ \times \psi_{\mathbf{n}}^*(t) \left\{ \left(i\hbar \frac{\partial}{\partial t} - \epsilon_{\mathbf{n}} + \mu \right) \delta_{\mathbf{n}, \mathbf{n}'} \delta(t, t') - \hbar \Sigma_{\mathbf{n}, \mathbf{n}'}(t, t') \right\} \psi_{\mathbf{n}'}(t'), \quad (3.68)$$

with a selfenergy $\Sigma_{\mathbf{n}, \mathbf{n}'}(t, t')$ obeying

$$\hbar \Sigma_{\mathbf{n}, \mathbf{n}'}(t, t') = \frac{1}{\hbar V} \sum_{\mathbf{k}} t_{\mathbf{n}}^*(\mathbf{k}) G(\mathbf{k}; t, t') t_{\mathbf{n}'}(\mathbf{k}). \quad (3.69)$$

This is our first example of an effective action describing the nonequilibrium dynamics of a Bose gas. Before we can study its consequences we clearly first need to determine the Green's function $G(\mathbf{k}; t, t')$ in terms of which the selfenergy is expressed. Although we know that this Green's function fulfills equation (3.64), we cannot directly solve this equation because we do not know the appropriate boundary condition at $t = t'$. To calculate $G(\mathbf{k}; t, t')$ we therefore have to proceed differently. It is however clear from equation (3.64) that $G(\mathbf{k}; t, t')$ is a property of the reservoir and we thus expect that it can somehow be related to a time-ordered correlation function of this reservoir. To see that explicitly we consider again the generating functional of these correlation functions, *i.e.*,

$$Z_R[J, J^*] = \int d[\psi_R^*]d[\psi_R] \\ \times \exp \left\{ \frac{i}{\hbar} \sum_{\mathbf{k}} \int_{C^\infty} dt \psi_{\mathbf{k}}^*(t) \left(i\hbar \frac{\partial}{\partial t} - \epsilon(\mathbf{k}) + \mu \right) \psi_{\mathbf{k}}(t) \right\} \\ \times \exp \left\{ i \sum_{\mathbf{k}} \int_{C^\infty} dt (\psi_{\mathbf{k}}(t) J_{\mathbf{k}}^*(t) + J_{\mathbf{k}}(t) \psi_{\mathbf{k}}^*(t)) \right\}. \quad (3.70)$$

It is again a gaussian integral and can thus be evaluated in the same manner as before. The result is now

$$Z_R[J, J^*] = \exp \left\{ -i \sum_{\mathbf{k}} \int_{C^\infty} dt \int_{C^\infty} dt' J_{\mathbf{k}}^*(t) G(\mathbf{k}; t, t') J_{\mathbf{k}}(t') \right\}, \quad (3.71)$$

which shows by means of equation (3.58) that

$$iG(\mathbf{k}; t, t') = \text{Tr} \left[\hat{\rho}_R(t_0) T_{C^\infty} \left(\hat{\psi}_{\mathbf{k}}(t) \hat{\psi}_{\mathbf{k}}^\dagger(t') \right) \right]. \quad (3.72)$$

Note first of all that this is indeed consistent with equation (3.64), because the right-hand side obeys

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} \text{Tr} \left[\hat{\rho}_R(t_0) T_{C^\infty} \left(\hat{\psi}_{\mathbf{k}}(t) \hat{\psi}_{\mathbf{k}}^\dagger(t') \right) \right] &= i\hbar \delta(t, t') \text{Tr} \left[\hat{\rho}_R(t_0) [\hat{\psi}_{\mathbf{k}}(t), \hat{\psi}_{\mathbf{k}}^\dagger(t)] \right] \\ &+ \text{Tr} \left[\hat{\rho}_R(t_0) T_{C^\infty} \left(i\hbar \frac{\partial}{\partial t} \hat{\psi}_{\mathbf{k}}(t) \hat{\psi}_{\mathbf{k}}^\dagger(t') \right) \right] \\ &= i\hbar \delta(t, t') + (\epsilon(\mathbf{k}) - \mu) \text{Tr} \left[\hat{\rho}_R(t_0) T_{C^\infty} \left(\hat{\psi}_{\mathbf{k}}(t) \hat{\psi}_{\mathbf{k}}^\dagger(t') \right) \right] \end{aligned} \quad (3.73)$$

in the operator formalism. Moreover, from this identification we see that the desired solution fulfilling the appropriate boundary conditions is apparently

$$G(\mathbf{k}; t, t') = -ie^{-i(\epsilon(\mathbf{k}) - \mu)(t - t')/\hbar} \{ \Theta(t, t') (1 + N(\mathbf{k})) + \Theta(t', t) N(\mathbf{k}) \}. \quad (3.74)$$

The specific dependence on the backward and forward branches of the Schwinger-Keldysh contour is thus solely determined by the Heaviside function $\Theta(t, t')$. As a result it is convenient to decompose the Green's function into its analytic pieces $G^>(\mathbf{k}; t - t')$ and $G^<(\mathbf{k}; t - t')$ [83] by means of

$$G(\mathbf{k}; t, t') = \Theta(t, t') G^>(\mathbf{k}; t - t') + \Theta(t', t) G^<(\mathbf{k}; t - t'). \quad (3.75)$$

Due to the fact that we are always dealing with time-ordered correlation functions, such a decomposition turns out to be a generic feature of all the functions on the Schwinger-Keldysh contour that we will encounter in the following [84]. For a general function $F(t, t')$, it is however also possible to have δ -function singularities. If that happens the correct decomposition is

$$F(t, t') = F^\delta(t) \delta(t, t') + \Theta(t, t') F^>(t, t') + \Theta(t', t) F^<(t, t'). \quad (3.76)$$

This more general decomposition is not required here, but will be needed in Section 3.4 when we determine the effective interaction between two atoms in a gas.

Having obtained the Green's function of the reservoir, we can now return to our discussion of the effective action $S^{\text{eff}}[\psi^*, \psi]$ for the Bose gas in the trap. Although we have chosen to derive in equation (3.68) the effective action for the generating functional $Z[J, J^*]$, it is straightforward to show that the effective action for the probability distribution $P[\phi^*, \phi; t]$ is obtained by only replacing the contour C^∞ by C^t . In the following we therefore no longer always specify all the boundary conditions on the time

integration, if the precise details of this integration are not important and the discussion applies equally well to both cases. Keeping this in mind, we now again perform the transformation $\psi_{\mathbf{n}}(t_{\pm}) = \phi_{\mathbf{n}}(t) \pm \xi_{\mathbf{n}}(t)/2$ to explicitly separate the (semi)classical dynamics from the effect of fluctuations. It leads in first instance to [85]

$$\begin{aligned}
S^{\text{eff}}[\phi^*, \phi; \xi^*, \xi] = & \sum_{\mathbf{n}} \int_{t_0} dt \phi_{\mathbf{n}}^*(t) \left(i\hbar \frac{\partial}{\partial t} - \epsilon_{\mathbf{n}} + \mu \right) \xi_{\mathbf{n}}(t) \\
& + \sum_{\mathbf{n}} \int_{t_0} dt \xi_{\mathbf{n}}^*(t) \left(i\hbar \frac{\partial}{\partial t} - \epsilon_{\mathbf{n}} + \mu \right) \phi_{\mathbf{n}}(t) \\
& - \sum_{\mathbf{n}, \mathbf{n}'} \int_{t_0} dt \int_{t_0} dt' \phi_{\mathbf{n}}^*(t) \hbar \Sigma_{\mathbf{n}, \mathbf{n}'}^{(-)}(t - t') \xi_{\mathbf{n}'}(t') \\
& - \sum_{\mathbf{n}, \mathbf{n}'} \int_{t_0} dt \int_{t_0} dt' \xi_{\mathbf{n}}^*(t) \hbar \Sigma_{\mathbf{n}, \mathbf{n}'}^{(+)}(t - t') \phi_{\mathbf{n}'}(t') \\
& - \frac{1}{2} \sum_{\mathbf{n}, \mathbf{n}'} \int_{t_0} dt \int_{t_0} dt' \xi_{\mathbf{n}}^*(t) \hbar \Sigma_{\mathbf{n}, \mathbf{n}'}^K(t - t') \xi_{\mathbf{n}'}(t'), \quad (3.77)
\end{aligned}$$

where we introduced the retarded and advanced components of the self-energy

$$\Sigma_{\mathbf{n}, \mathbf{n}'}^{(\pm)}(t - t') = \pm \Theta(\pm(t - t')) (\Sigma_{\mathbf{n}, \mathbf{n}'}^{>}(t - t') - \Sigma_{\mathbf{n}, \mathbf{n}'}^{<}(t - t')) \quad (3.78)$$

that affect the terms in the action that are linear in $\xi_{\mathbf{n}}^*(t)$ and $\xi_{\mathbf{n}}(t)$, respectively, and also the Keldysh component

$$\Sigma_{\mathbf{n}, \mathbf{n}'}^K(t - t') = (\Sigma_{\mathbf{n}, \mathbf{n}'}^{>}(t - t') + \Sigma_{\mathbf{n}, \mathbf{n}'}^{<}(t - t')) \quad (3.79)$$

that is associated with the part quadratic in the fluctuations.

The physical content of these various components of the selfenergy is understood most clearly if we now apply again the beautiful functional-integral procedure that is due to Hubbard and Stratonovich. The basic idea is to write the factor

$$\exp \left\{ -\frac{i}{2} \sum_{\mathbf{n}, \mathbf{n}'} \int_{t_0} dt \int_{t_0} dt' \xi_{\mathbf{n}}^*(t) \Sigma_{\mathbf{n}, \mathbf{n}'}^K(t - t') \xi_{\mathbf{n}'}(t') \right\}$$

in the integrant of $\int d[\phi^*] d[\phi] \int d[\xi^*] d[\xi] \exp(iS^{\text{eff}}[\phi^*, \phi; \xi^*, \xi]/\hbar)$ as a gaussian integral over a complex field $\eta(\mathbf{x}, t)$. It is equivalent, but in practice more convenient, to just multiply the integrant by a factor 1 that is

written as a gaussian integral $\int d[\eta^*]d[\eta] \exp(iS^{\text{eff}}[\eta^*, \eta]/\hbar)$ with

$$\begin{aligned}
 S^{\text{eff}}[\eta^*, \eta] = & \frac{1}{2} \sum_{\mathbf{n}, \mathbf{n}'} \int_{t_0} dt \int_{t_0} dt' \left(2\eta_{\mathbf{n}}^*(t) \right. \\
 & - \sum_{\mathbf{n}''} \int_{t_0} dt'' \xi_{\mathbf{n}''}^*(t'') \hbar \Sigma_{\mathbf{n}'', \mathbf{n}}^K(t'' - t) \Big) \\
 & \times (\hbar \Sigma_{\mathbf{n}, \mathbf{n}'}^K)^{-1}(t - t') \left(2\eta_{\mathbf{n}'}(t') \right. \\
 & - \sum_{\mathbf{n}''} \int_{t_0} dt'' \hbar \Sigma_{\mathbf{n}', \mathbf{n}''}^K(t' - t'') \xi_{\mathbf{n}''}(t'') \Big) \quad (3.80)
 \end{aligned}$$

a complete square. Adding this to $S^{\text{eff}}[\phi^*, \phi; \xi^*, \xi]$ the total effective action becomes

$$\begin{aligned}
 S^{\text{eff}}[\phi^*, \phi; \xi^*, \xi; \eta^*, \eta] = & \sum_{\mathbf{n}, \mathbf{n}'} \int_{t_0} dt \int_{t_0} dt' \phi_{\mathbf{n}}^*(t) \left\{ \left(i\hbar \frac{\partial}{\partial t} - \epsilon_{\mathbf{n}} \right. \right. \quad (3.81) \\
 & + \mu \Big) \delta_{\mathbf{n}, \mathbf{n}'} \delta(t - t') - \hbar \Sigma_{\mathbf{n}, \mathbf{n}'}^{(-)}(t - t') \Big\} \xi_{\mathbf{n}'}(t') \\
 & + \sum_{\mathbf{n}, \mathbf{n}'} \int_{t_0} dt \int_{t_0} dt' \xi_{\mathbf{n}}^*(t) \left\{ \left(i\hbar \frac{\partial}{\partial t} - \epsilon_{\mathbf{n}} \right. \right. \\
 & + \mu \Big) \delta_{\mathbf{n}, \mathbf{n}'} \delta(t - t') - \hbar \Sigma_{\mathbf{n}, \mathbf{n}'}^{(+)}(t - t') \Big\} \phi_{\mathbf{n}'}(t') \\
 & - \sum_n \int_{t_0} dt (\eta_n^*(t) \xi_n(t) + \xi_n^*(t) \eta_n(t)) \\
 & + 2 \sum_{\mathbf{n}, \mathbf{n}'} \int_{t_0} dt \int_{t_0} dt' \eta_{\mathbf{n}}^*(t) (\hbar \Sigma_{\mathbf{n}, \mathbf{n}'}^K)^{-1}(t - t') \eta_{\mathbf{n}'}(t')
 \end{aligned}$$

and is thus linear in $\xi_{\mathbf{n}}(t)$ and $\xi_{\mathbf{n}}^*(t)$. Integrating over these fluctuations we conclude from this action that the field $\phi(\mathbf{x}, t)$ is constraint to obey the Langevin equations [86]

$$i\hbar \frac{\partial}{\partial t} \phi_{\mathbf{n}}(t) = (\epsilon_{\mathbf{n}} - \mu) \phi_{\mathbf{n}}(t) + \sum_{\mathbf{n}'} \int_{t_0}^{\infty} dt' \hbar \Sigma_{\mathbf{n}, \mathbf{n}'}^{(+)}(t - t') \phi_{\mathbf{n}'}(t') + \eta_{\mathbf{n}}(t) \quad (3.82)$$

and

$$-i\hbar \frac{\partial}{\partial t} \phi_{\mathbf{n}}^*(t) = (\epsilon_{\mathbf{n}} - \mu) \phi_{\mathbf{n}}^*(t) + \sum_{\mathbf{n}'} \int_{t_0}^{\infty} dt' \phi_{\mathbf{n}'}^*(t') \hbar \Sigma_{\mathbf{n}', \mathbf{n}}^{(-)}(t' - t) + \eta_{\mathbf{n}}^*(t) \quad (3.83)$$

with gaussian noise terms $\eta_{\mathbf{n}}(t)$ and $\eta_{\mathbf{n}}^*(t)$ that from the last term in the right-hand side of equation (3.81) are seen to have the time correlations

$$\begin{aligned} \langle \eta_{\mathbf{n}}^*(t) \eta_{\mathbf{n}'}(t') \rangle &= \frac{i\hbar^2}{2} \Sigma_{\mathbf{n},\mathbf{n}'}^{\mathbf{K}}(t-t') \\ &= \frac{1}{2} \int \frac{d\mathbf{k}}{(2\pi)^3} (1 + 2N(\mathbf{k})) t_{\mathbf{n}}^*(\mathbf{k}) e^{-i(\epsilon(\mathbf{k})-\mu)(t-t')/\hbar} t_{\mathbf{n}'}(\mathbf{k}) \end{aligned} \quad (3.84)$$

in the thermodynamic limit. Moreover, in that limit the retarded selfenergy is equal to

$$\hbar \Sigma_{\mathbf{n},\mathbf{n}'}^{(+)}(t-t') = -\Theta(t-t') \frac{i}{\hbar} \int \frac{d\mathbf{k}}{(2\pi)^3} t_{\mathbf{n}}^*(\mathbf{k}) e^{-i(\epsilon(\mathbf{k})-\mu)(t-t')/\hbar} t_{\mathbf{n}'}(\mathbf{k}) \quad (3.85)$$

and the advanced selfenergy can be found from the relation $\Sigma_{\mathbf{n}',\mathbf{n}}^{(-)}(t'-t) = (\Sigma_{\mathbf{n},\mathbf{n}'}^{(+)}(t-t'))^*$. Note that the Heaviside functions in these retarded and advanced selfenergies are precisely such that equations (3.82) and (3.83) are causal, *i.e.*, the evolution of $\phi(\mathbf{x}, t)$ and $\phi^*(\mathbf{x}, t)$ depends only on their value at previous times. This is clearly a sensible result and explains why these components of the full selfenergy enter into the terms in the action that are linear in the fluctuations.

To understand why the Keldysh component enters into the terms that are quadratic in the fluctuations is more complicated and is related to the famous fluctuation-dissipation theorem [83,86,87]. Physically, the fluctuation-dissipation theorem ensures in our case that, due to the interactions with the reservoir, the gas in the trap now relaxes towards thermal equilibrium in the limit $t \rightarrow \infty$. Let us therefore study this limit in somewhat more detail. However, before we do so we would like to mention for completeness that if we apply the above Hubbard-Stratonovich transformation to the functional integral for the probability distribution $P[\phi^*, \phi; t]$, we immediately find that analogous to equation (3.47)

$$\begin{aligned} P[\phi^*, \phi; t] &= \int d[\eta^*] d[\eta] P[\eta^*, \eta] \int d[\phi_0^*] d[\phi_0] P[|\phi_0|^2; t_0] \\ &\quad \times \prod_{\mathbf{n}} \delta(|\phi_{\mathbf{n}} - \phi_{\mathbf{n}}^{\text{cl}}(t)|^2), \end{aligned} \quad (3.86)$$

where $\phi_{\mathbf{n}}^{\text{cl}}(t)$ now obeys the Langevin equation in equation (3.82) for a particular realization of the noise $\eta_{\mathbf{n}}(t)$ and with the initial condition $\phi_{\mathbf{n}}^{\text{cl}}(t_0) = \phi_{0,\mathbf{n}}$. Furthermore, the probability distribution for each realization of the

noise is given by

$$P[\eta^*, \eta] = \exp \left\{ \frac{2i}{\hbar} \sum_{\mathbf{n}, \mathbf{n}'} \int_{t_0}^t dt' \int_{t_0}^t dt'' \eta_{\mathbf{n}}^*(t') (\hbar \Sigma_{\mathbf{n}, \mathbf{n}'}^K)^{-1} (t' - t'') \eta_{\mathbf{n}'}(t'') \right\}. \quad (3.87)$$

This result shows explicitly that, as expected, the Fokker-Planck equation associated with the Langevin equations in equations (3.82) and (3.83) is in fact the desired Fokker-Planck equation for the probability distribution $P[\phi^*, \phi; t]$.

After this slight digression, we now return to the long-time behaviour of the gas. In the long-time limit two important simplifications occur. Looking at the expressions for the selfenergies, we see that their width as a function of the time difference $t - t'$ is at most of order $\mathcal{O}(\hbar/k_B T)$ in the low-temperature regime of interest where the thermal de Broglie wavelength of the particles obeys $\Lambda_{\text{th}} \gg 1/k_c$. If therefore $t \gg t_0 + \mathcal{O}(\hbar/k_B T)$ we are allowed to take the limit $t_0 \rightarrow -\infty$. Taking this limit means physically that we neglect the initial transients that are due to the precise way in which the contact between the trap and the reservoir is made, and focus on the “universal” dynamics that is independent of these details. In addition, at long times the dynamics of the gas is expected to be sufficiently slow that we can neglect the memory effects altogether. Finally, we consider here first the case of a reservoir that is so weakly coupled to the gas in the trap that we can treat the coupling with second order perturbation theory. As a result we can also neglect the nondiagonal elements of the selfenergies. In total we are then allowed to put (but see below)

$$\Sigma_{\mathbf{n}, \mathbf{n}'}^{(\pm), K}(t - t') \simeq \Sigma_{\mathbf{n}, \mathbf{n}}^{(\pm), K}(\epsilon_{\mathbf{n}} - \mu) \delta_{\mathbf{n}, \mathbf{n}'} \delta(t - t') \equiv \Sigma_{\mathbf{n}}^{(\pm), K} \delta_{\mathbf{n}, \mathbf{n}'} \delta(t - t'), \quad (3.88)$$

where the Fourier transform of the selfenergies is defined by

$$\Sigma_{\mathbf{n}, \mathbf{n}'}^{(\pm), K}(t - t') = \int d\epsilon \Sigma_{\mathbf{n}, \mathbf{n}'}^{(\pm), K}(\epsilon) \frac{e^{-i\epsilon(t-t')/\hbar}}{2\pi\hbar}. \quad (3.89)$$

Note that this implies in general that $\Sigma_{\mathbf{n}', \mathbf{n}}^{(-)}(\epsilon) = \left(\Sigma_{\mathbf{n}, \mathbf{n}'}^{(+)}(\epsilon) \right)^*$, and in particular therefore that $\Sigma_{\mathbf{n}}^{(-)} = \left(\Sigma_{\mathbf{n}}^{(+)} \right)^*$.

With these simplifications our Langevin equations become

$$i\hbar \frac{\partial}{\partial t} \phi_{\mathbf{n}}(t) = (\epsilon_{\mathbf{n}} + \hbar \Sigma_{\mathbf{n}}^{(+)} - \mu) \phi_{\mathbf{n}}(t) + \eta_{\mathbf{n}}(t) \quad (3.90)$$

and just the complex conjugate equation for $\phi_{\mathbf{n}}^*(t)$. The retarded selfenergy in this equation is given by

$$\hbar\Sigma_{\mathbf{n}}^{(+)} = \int \frac{d\mathbf{k}}{(2\pi)^3} t_{\mathbf{n}}^*(\mathbf{k}) \frac{1}{\epsilon_{\mathbf{n}}^+ - \epsilon(\mathbf{k})} t_{\mathbf{n}}(\mathbf{k}), \quad (3.91)$$

with $\epsilon_{\mathbf{n}}^+$ the usual notation for the limiting procedure $\epsilon_{\mathbf{n}} + i0$. It clearly has real and imaginary parts that we denote by $S_{\mathbf{n}}$ and $-R_{\mathbf{n}}$, respectively. Denoting the Cauchy principle value part of an integral by $\mathcal{P}$, they obey

$$S_{\mathbf{n}} = \int \frac{d\mathbf{k}}{(2\pi)^3} t_{\mathbf{n}}^*(\mathbf{k}) \frac{\mathcal{P}}{\epsilon_{\mathbf{n}} - \epsilon(\mathbf{k})} t_{\mathbf{n}}(\mathbf{k}) \quad (3.92)$$

and

$$R_{\mathbf{n}} = \pi \int \frac{d\mathbf{k}}{(2\pi)^3} \delta(\epsilon_{\mathbf{n}} - \epsilon(\mathbf{k})) |t_{\mathbf{n}}(\mathbf{k})|^2. \quad (3.93)$$

The interpretation of these results is quite obvious if we consider the average of the Langevin equation, *i.e.*,

$$i\hbar \frac{\partial}{\partial t} \langle \phi_{\mathbf{n}} \rangle(t) = (\epsilon_{\mathbf{n}} + S_{\mathbf{n}} - iR_{\mathbf{n}} - \mu) \langle \phi_{\mathbf{n}} \rangle(t), \quad (3.94)$$

which is solved by

$$\langle \phi_{\mathbf{n}} \rangle(t) = \langle \phi_{\mathbf{n}} \rangle(0) e^{-i(\epsilon_{\mathbf{n}} + S_{\mathbf{n}} - \mu)t/\hbar} e^{-R_{\mathbf{n}}t/\hbar}. \quad (3.95)$$

Hence the real part of the retarded selfenergy $S_{\mathbf{n}}$ represents the shift in the energy of state $\chi_{\mathbf{n}}(\mathbf{x})$ due to the coupling with the reservoir. Indeed, equation (3.92) agrees precisely with the value of this shift in second order perturbation theory. Moreover, the fact that $|\langle \phi_{\mathbf{n}} \rangle(t)|^2 = |\langle \phi_{\mathbf{n}} \rangle(0)|^2 e^{-2R_{\mathbf{n}}t/\hbar}$ shows that the average rate of decay $\Gamma_{\mathbf{n}}$ of the state $\chi_{\mathbf{n}}(\mathbf{x})$ is equal to $2R_{\mathbf{n}}/\hbar$, which, together with equation (3.93), exactly reproduces Fermi's Golden Rule.

From the equation of motion for the average $\langle \phi_{\mathbf{n}} \rangle(t)$ we can also conclude that the right-hand side of the Fokker-Planck equation contains the “streaming” terms

$$\begin{aligned} - \left(\sum_{\mathbf{n}} \frac{\partial}{\partial \phi_{\mathbf{n}}} (\epsilon_{\mathbf{n}} + \hbar\Sigma_{\mathbf{n}}^{(+)} - \mu) \phi_{\mathbf{n}} \right) P[\phi^*, \phi; t] \\ + \left(\sum_{\mathbf{n}} \frac{\partial}{\partial \phi_{\mathbf{n}}^*} (\epsilon_{\mathbf{n}} + \hbar\Sigma_{\mathbf{n}}^{(-)} - \mu) \phi_{\mathbf{n}}^* \right) P[\phi^*, \phi; t]. \end{aligned}$$

However, there must now also be a “diffusion” term due to the fact that the average $\langle |\phi_{\mathbf{n}}|^2 \rangle(t)$ is no longer independent of time since the interactions

with the reservoir can lead to changes in the occupation numbers $N_{\mathbf{n}}(t)$. To obtain the “diffusion” term we thus need to determine $i\hbar\partial\langle|\phi_{\mathbf{n}}|^2\rangle(t)/\partial t$. To do so we first formally solve the Langevin equation by

$$\phi_{\mathbf{n}}(t) = e^{-i(\epsilon_{\mathbf{n}} + \hbar\Sigma_{\mathbf{n}}^{(+)} - \mu)t/\hbar} \left\{ \phi_{\mathbf{n}}(0) - \frac{i}{\hbar} \int_0^t dt' \eta(t') e^{i(\epsilon_{\mathbf{n}} + \hbar\Sigma_{\mathbf{n}}^{(+)} - \mu)t'/\hbar} \right\}. \quad (3.96)$$

Multiplying this with the complex conjugate expression and taking the average, we obtain first of all

$$\langle|\phi_{\mathbf{n}}|^2\rangle(t) = e^{-2R_{\mathbf{n}}t/\hbar} \left\{ \langle|\phi_{\mathbf{n}}|^2\rangle(0) + \frac{i}{2}\Sigma_{\mathbf{n}}^K \int_0^t dt' e^{2R_{\mathbf{n}}t'/\hbar} \right\}, \quad (3.97)$$

which shows that

$$i\hbar \frac{\partial}{\partial t} \langle|\phi_{\mathbf{n}}|^2\rangle(t) = -2iR_{\mathbf{n}} \langle|\phi_{\mathbf{n}}|^2\rangle(t) - \frac{1}{2}\hbar\Sigma_{\mathbf{n}}^K. \quad (3.98)$$

Moreover, the Keldysh component of the selfenergy is given by

$$\hbar\Sigma_{\mathbf{n}}^K = -2\pi i \int \frac{d\mathbf{k}}{(2\pi)^3} (1 + 2N(\mathbf{k})) \delta(\epsilon_{\mathbf{n}} - \epsilon(\mathbf{k})) |t_{\mathbf{n}}(\mathbf{k})|^2 \quad (3.99)$$

and therefore obeys

$$\hbar\Sigma_{\mathbf{n}}^K = -2i(1 + 2N_{\mathbf{n}})R_{\mathbf{n}} \quad (3.100)$$

with $N_{\mathbf{n}} = (e^{\beta(\epsilon_{\mathbf{n}} - \mu)} - 1)^{-1}$ the Bose distribution function. This is in fact the fluctuation-dissipation theorem, because it relates the strength of the fluctuations determined by $\hbar\Sigma_{\mathbf{n}}^K$, to the amount of dissipation that is given by $R_{\mathbf{n}}$. As mentioned previously, the fluctuation-dissipation theorem ensures that the gas relaxes to thermal equilibrium. This we can already see from equation (3.98), because substitution of the fluctuation-dissipation theorem leads to

$$i\hbar \frac{\partial}{\partial t} \langle|\phi_{\mathbf{n}}|^2\rangle(t) = -2iR_{\mathbf{n}} \langle|\phi_{\mathbf{n}}|^2\rangle(t) + iR_{\mathbf{n}}(1 + 2N_{\mathbf{n}}), \quad (3.101)$$

which tells us that in equilibrium $\langle|\phi_{\mathbf{n}}|^2\rangle = N_{\mathbf{n}} + 1/2$. In fact, we have argued that in general $\langle|\phi_{\mathbf{n}}|^2\rangle(t) = N_{\mathbf{n}}(t) + 1/2$. Substituting this identity in equation (3.101) and realizing that $\Gamma_{\mathbf{n}}N_{\mathbf{n}} = \Gamma_{\mathbf{n}}N(\mathbf{k})$ due to the energy-conserving δ function in $\Gamma_{\mathbf{n}}$, we indeed obtain the correct rate equation for the average occupation numbers

$$\begin{aligned} \frac{\partial}{\partial t} N_{\mathbf{n}}(t) &= -\Gamma_{\mathbf{n}}N_{\mathbf{n}}(t) + \Gamma_{\mathbf{n}}N_{\mathbf{n}} \\ &= -\Gamma_{\mathbf{n}}N_{\mathbf{n}}(t)(1 + N(\mathbf{k})) + \Gamma_{\mathbf{n}}(1 + N_{\mathbf{n}}(t))N(\mathbf{k}), \end{aligned} \quad (3.102)$$

that might justly be called the quantum Boltzmann equation for the gas, because the right-hand side contains precisely the rates for scattering into and out of the reservoir.

Furthermore, equation (3.98) shows that the “diffusion” term in the Fokker-Planck equation is

$$-\left(\frac{1}{2}\sum_{\mathbf{n}}\frac{\partial^2}{\partial\phi_{\mathbf{n}}^*\partial\phi_{\mathbf{n}}}\hbar\Sigma_{\mathbf{n}}^K\right)P[\phi^*,\phi;t],$$

because the first term in the right-hand side of equation (3.98) is also present without the noise and is therefore already accounted for in the “streaming” terms. In total we have thus arrived at

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}P[\phi^*,\phi;t] = & -\left(\sum_{\mathbf{n}}\frac{\partial}{\partial\phi_{\mathbf{n}}}(\epsilon_{\mathbf{n}}+\hbar\Sigma_{\mathbf{n}}^{(+)}-\mu)\phi_{\mathbf{n}}\right)P[\phi^*,\phi;t] \\ & +\left(\sum_{\mathbf{n}}\frac{\partial}{\partial\phi_{\mathbf{n}}^*}(\epsilon_{\mathbf{n}}+\hbar\Sigma_{\mathbf{n}}^{(-)}-\mu)\phi_{\mathbf{n}}^*\right)P[\phi^*,\phi;t] \\ & -\left(\frac{1}{2}\sum_{\mathbf{n}}\frac{\partial^2}{\partial\phi_{\mathbf{n}}^*\partial\phi_{\mathbf{n}}}\hbar\Sigma_{\mathbf{n}}^K\right)P[\phi^*,\phi;t]. \end{aligned} \quad (3.103)$$

Using again the fluctuation-dissipation theorem, it is not difficult to show that the stationary solution of this Fokker-Planck equation is

$$P[\phi^*,\phi;\infty] = \prod_{\mathbf{n}} \frac{1}{N_{\mathbf{n}}+1/2} \exp\left\{-\frac{1}{N_{\mathbf{n}}+1/2}|\phi_{\mathbf{n}}|^2\right\}. \quad (3.104)$$

Although this appears to be quite reasonable, it is important to note that this result is not fully consistent because the “streaming” terms in equation (3.103) show that the energies of the states $\chi_{\mathbf{n}}(\mathbf{x})$ are shifted and equal to $\epsilon_{\mathbf{n}} + S_{\mathbf{n}}$. We therefore expect that the equilibrium occupation numbers are equal to the Bose distribution evaluated at those energies and not at the unshifted values $\epsilon_{\mathbf{n}}$. The reason for this inconsistency is, of course, that we have taken $\Sigma_{\mathbf{n}}^{(\pm),K}$ equal to $\Sigma_{\mathbf{n},\mathbf{n}}^{(\pm),K}(\epsilon_{\mathbf{n}} - \mu)$, which was only justified on the basis of second-order perturbation theory. We now, however, see that to obtain a fully consistent theory we must take instead $\Sigma_{\mathbf{n}}^{(\pm),K} \equiv \Sigma_{\mathbf{n},\mathbf{n}}^{(\pm),K}(\epsilon_{\mathbf{n}} + S_{\mathbf{n}} - \mu)$. This implies that to obtain the retarded selfenergy, we first have to solve for the real part

$$S_{\mathbf{n}} = \int \frac{d\mathbf{k}}{(2\pi)^3} t_{\mathbf{n}}^*(\mathbf{k}) \frac{\mathcal{P}}{\epsilon_{\mathbf{n}} + S_{\mathbf{n}} - \epsilon(\mathbf{k})} t_{\mathbf{n}}(\mathbf{k}) \quad (3.105)$$

and then substitute this into

$$R_{\mathbf{n}} = \pi \int \frac{d\mathbf{k}}{(2\pi)^3} \delta(\epsilon_{\mathbf{n}} + S_{\mathbf{n}} - \epsilon(\mathbf{k})) |t_{\mathbf{n}}(\mathbf{k})|^2 \quad (3.106)$$

to obtain the imaginary part. The fluctuation-dissipation theorem then again reads $\hbar \Sigma_{\mathbf{n}}^K = -2i(1 + 2N_{\mathbf{n}})R_{\mathbf{n}}$ but now with the equilibrium distribution $N_{\mathbf{n}} = (e^{\beta(\epsilon_{\mathbf{n}} + S_{\mathbf{n}} - \mu)} - 1)^{-1}$. As a consequence the quantum Boltzmann equation and the stationary state of the Fokker-Planck equation will now also contain these correct equilibrium occupation numbers [88].

Having arrived at the Fokker-Planck equation of our Caldeira-Leggett-like toy model, we have now demonstrated the use of essentially all the theoretical tools that are required for a discussion of a weakly interacting Bose gas. Before we start with this discussion, however, we want to make a final remark about the effect of the nondiagonal elements of the selfenergies. Physically, including these nondiagonal elements accounts for the change in the wave functions $\chi_{\mathbf{n}}(\mathbf{x})$ due to the interaction with the reservoir. It can clearly be neglected if the coupling with the reservoir is sufficiently weak, or more precisely if $|\hbar \Sigma_{\mathbf{n}', \mathbf{n}}^{(+)}(\epsilon_{\mathbf{n}} + S_{\mathbf{n}} - \mu)|$ is much smaller than the energy splitting $|\epsilon_{\mathbf{n}'} - \epsilon_{\mathbf{n}}|$ between the states in the trap. For a quantum dot in solid-state physics [89] this is often the case and for that reason we might call our toy model a bosonic quantum dot. However, in magnetically trapped atomic gases the average interaction energy between the atoms is already slightly below the Bose-Einstein condensation critical temperature larger than the typical energy splitting and the nondiagonal elements of the selfenergies are very important. Such a strong-coupling situation can, of course, also be treated in our Caldeira-Leggett like model. The main difference is that we need to expand our various fields not in the eigenstates of the trapping potential $\chi_{\mathbf{n}}(\mathbf{x})$ but in the eigenstates $\chi'_{\mathbf{n}}(\mathbf{x})$ of the nonlocal Schrödinger equation

$$\begin{aligned} \epsilon'_{\mathbf{n}} \chi'_{\mathbf{n}}(\mathbf{x}) = & \left(-\frac{\hbar^2 \nabla^2}{2m} + V^{\text{ex}}(\mathbf{x}) \right) \chi'_{\mathbf{n}}(\mathbf{x}) \\ & + \int d\mathbf{x}' \operatorname{Re} \left[\hbar \Sigma^{(+)}(\mathbf{x}, \mathbf{x}'; \epsilon'_{\mathbf{n}} - \mu) \right] \chi'_{\mathbf{n}}(\mathbf{x}') \end{aligned} \quad (3.107)$$

where $\epsilon'_{\mathbf{n}}$ are the new eigenvalues and the retarded selfenergie in coordinate space is $\hbar \Sigma^{(+)}(\mathbf{x}, \mathbf{x}'; \epsilon) = \sum_{\mathbf{n}, \mathbf{n}'} \chi_{\mathbf{n}}(\mathbf{x}) \hbar \Sigma_{\mathbf{n}, \mathbf{n}'}^{(+)}(\epsilon) \chi_{\mathbf{n}'}^*(\mathbf{x}')$. In this new basis the nondiagonal elements of the selfenergies can now be neglected and we find essentially the same results as before. We only need to replace $\epsilon_{\mathbf{n}} + S_{\mathbf{n}}$ by $\epsilon'_{\mathbf{n}}$ and $t_{\mathbf{n}}(\mathbf{k})$ by $\sum_{\mathbf{n}'} (\int d\mathbf{x} \chi'_{\mathbf{n}}(\mathbf{x}') \chi_{\mathbf{n}'}^*(\mathbf{x})) t_{\mathbf{n}'}(\mathbf{k})$. Neglecting the nondiagonal elements in this basis only requires that the real part of the retarded selfenergy is much larger than its imaginary part, which is always fulfilled in our case because $k_c \Lambda_{\text{th}} \gg 1$.

Summarizing, the coherent and incoherent dynamics of the gas in the trap is for our toy model quite generally solved by

$$\langle \phi_{\mathbf{n}} \rangle(t) = \langle \phi_{\mathbf{n}} \rangle(0) e^{-i(\epsilon'_{\mathbf{n}} - \mu)t/\hbar} e^{-\Gamma_{\mathbf{n}} t/2} \quad (3.108)$$

and

$$N_{\mathbf{n}}(t) = N_{\mathbf{n}}(0)e^{-\Gamma_{\mathbf{n}}t} + N_{\mathbf{n}}(1 - e^{-\Gamma_{\mathbf{n}}t}), \quad (3.109)$$

respectively. In the limit $t \rightarrow \infty$, the average of the annihilation operators $\langle \phi_{\mathbf{n}} \rangle(t)$ thus always vanishes but the average occupation numbers $N_{\mathbf{n}}(t)$ relax to the equilibrium distribution $N_{\mathbf{n}} = (e^{\beta(\epsilon'_{\mathbf{n}} - \mu)} - 1)^{-1}$. Although this appears to be an immediately obvious result, its importance stems from the fact that it is also true if we tune the potential energy bias ΔV^{ex} such that at low temperatures the groundstate $\chi'_{\mathbf{0}}(\mathbf{x})$ acquires a macroscopic occupation, *i.e.*, $N_{\mathbf{0}} \gg 1$. The gas therefore never shows a spontaneous breaking of the $U(1)$ symmetry, in agreement with the notion that we are essentially dealing with an ideal Bose gas in the grand-canonical ensemble [90]. The reason of the absence of the spontaneous symmetry breaking can also be understood from our stationary solution of the Fokker-Planck equation in equation (3.104), which shows that the probability distribution for $|\phi_{\mathbf{0}}|$ is proportional to the Boltzmann factor $e^{-\beta(\epsilon'_{\mathbf{0}} - \mu)|\phi_{\mathbf{0}}|^2}$ in the degenerate regime of interest. Hence, the corresponding Landau free energy $F_L(|\phi_{\mathbf{0}}|) = (\epsilon'_{\mathbf{0}} - \mu)|\phi_{\mathbf{0}}|^2$ never shows an instability towards the formation of a nonzero average of $|\phi_{\mathbf{0}}|$ due to the fact that $\epsilon'_{\mathbf{0}} - \mu$ can never become less than zero. Once we introduce interactions between the atoms in the gas, this picture fully changes.

3.4 Condensate formation

We are now in a position to discuss an interacting Bose gas, because in an interacting Bose gas, the gas is roughly speaking its own thermal reservoir. The Fokker-Planck equation therefore turns out to be quite similar to the one presented in equation (3.103). To be more precise, however, we should mention that we aim in this section to describe the formation of a condensate in an interacting Bose gas under the conditions that have recently been realized in experiments with atomic rubidium, lithium, sodium and hydrogen gases. In these experiments the gas is cooled by means of evaporative cooling. Numerical solutions of the Boltzmann equation have shown that during evaporative cooling the energy distribution function is well described by an equilibrium distribution with time dependent temperature $T(t)$ and chemical potential $\mu(t)$, that is truncated at high energies due to the evaporation of the highest energetic atoms from the trap [91]. Moreover, in the experiments of interest the densities just above the critical temperature are essentially always such that the gas is in the weak-coupling limit, which implies in this context that the average interaction energy per atom is always much less than the energy splitting of the one-particle states in the harmonic trapping potential.

3.4.1 Weak-coupling limit

For a trapped atomic gas the appropriate one-particle states are the eigenstates $\chi_{\mathbf{n}}(\mathbf{x})$ of the external potential $V^{\text{ex}}(\mathbf{x})$. As a result the Fokker-Planck equation for the interacting gas will now quite generally be given by

$$\begin{aligned}
 i\hbar \frac{\partial}{\partial t} P[\phi^*, \phi; t] = & - \sum_{\mathbf{n}, \mathbf{n}'} \frac{\partial}{\partial \phi_{\mathbf{n}}} \left\{ \left((\epsilon_{\mathbf{n}} - \mu(t)) \delta_{\mathbf{n}, \mathbf{n}'} + \hbar \Sigma_{\mathbf{n}, \mathbf{n}'}^{(+)} \right) \phi_{\mathbf{n}'} \right. \\
 & + \sum_{\mathbf{m}, \mathbf{m}'} V_{\mathbf{n}, \mathbf{m}; \mathbf{n}', \mathbf{m}'}^{(+)} \phi_{\mathbf{m}}^* \phi_{\mathbf{m}'} \phi_{\mathbf{n}'} \left. \right\} P[\phi^*, \phi; t] \\
 & + \sum_{\mathbf{n}, \mathbf{n}'} \frac{\partial}{\partial \phi_{\mathbf{n}}^*} \left\{ \left((\epsilon_{\mathbf{n}} - \mu(t)) \delta_{\mathbf{n}, \mathbf{n}'} + \hbar \Sigma_{\mathbf{n}', \mathbf{n}}^{(-)} \right) \phi_{\mathbf{n}'}^* \right. \\
 & + \sum_{\mathbf{m}, \mathbf{m}'} V_{\mathbf{n}', \mathbf{m}'; \mathbf{n}, \mathbf{m}}^{(-)} \phi_{\mathbf{n}'}^* \phi_{\mathbf{m}'}^* \phi_{\mathbf{m}} \left. \right\} P[\phi^*, \phi; t] \\
 & - \frac{1}{2} \sum_{\mathbf{n}, \mathbf{n}'} \frac{\partial^2}{\partial \phi_{\mathbf{n}} \partial \phi_{\mathbf{n}'}^*} \left\{ \hbar \Sigma_{\mathbf{n}, \mathbf{n}'}^{\text{K}} \right. \\
 & + \sum_{\mathbf{m}, \mathbf{m}'} V_{\mathbf{n}, \mathbf{m}; \mathbf{n}', \mathbf{m}'}^{\text{K}} \phi_{\mathbf{m}}^* \phi_{\mathbf{m}'} \left. \right\} P[\phi^*, \phi; t]. \quad (3.110)
 \end{aligned}$$

For this equation to be useful, however, we need to determine the various selfenergies and interactions. To do so, let us for simplicity first consider the normal state of the gas which is usually in the weak-coupling limit $|\hbar \Sigma_{\mathbf{n}, \mathbf{n}'}^{(+)}| \ll |\epsilon_{\mathbf{n}} - \epsilon_{\mathbf{n}'}|$ for the experiments with atomic alkali gases that are of interest here. In this regime we can neglect the nondiagonal elements of the selfenergies and also the nonlinear terms in the right-hand side of equation (3.110). The Fokker-Planck equation then reduces to

$$\begin{aligned}
 i\hbar \frac{\partial}{\partial t} P[\phi^*, \phi; t] = & - \sum_{\mathbf{n}} \frac{\partial}{\partial \phi_{\mathbf{n}}} (\epsilon_{\mathbf{n}} + \hbar \Sigma_{\mathbf{n}}^{(+)} - \mu(t)) \phi_{\mathbf{n}} P[\phi^*, \phi; t] \\
 & + \sum_{\mathbf{n}} \frac{\partial}{\partial \phi_{\mathbf{n}}^*} (\epsilon_{\mathbf{n}} + \hbar \Sigma_{\mathbf{n}}^{(-)} - \mu(t)) \phi_{\mathbf{n}}^* P[\phi^*, \phi; t] \\
 & - \frac{1}{2} \sum_{\mathbf{n}} \frac{\partial^2}{\partial \phi_{\mathbf{n}}^* \partial \phi_{\mathbf{n}}} \hbar \Sigma_{\mathbf{n}}^{\text{K}} P[\phi^*, \phi; t], \quad (3.111)
 \end{aligned}$$

with $\hbar \Sigma_{\mathbf{n}}^{(\pm), \text{K}} = \hbar \Sigma_{\mathbf{n}, \mathbf{n}}^{(\pm), \text{K}}(\epsilon'_{\mathbf{n}} - \mu)$ and $\epsilon'_{\mathbf{n}} = \epsilon_{\mathbf{n}} + S_{\mathbf{n}}$. This equation looks identical to the one we derived for our Caldeira-Leggett toy model but describes in fact quite different physics because now the selfenergies are not

due to an interaction with a reservoir but due to the interactions between the atoms themselves. This is, however, completely hidden in the selfenergies as we show now explicitly. Performing the same manipulations as in Sections 2.5 and 2.8.2, we find in the many-body T-matrix approximation first of all that

$$\begin{aligned} \hbar\Sigma_{\mathbf{n}}^{(+)} &= \left(\hbar\Sigma_{\mathbf{n}}^{(-)}\right)^* = 2 \sum_{\mathbf{m}} V_{\mathbf{n},\mathbf{m};\mathbf{n},\mathbf{m}}^{(+)} (\epsilon'_{\mathbf{n}} + \epsilon'_{\mathbf{m}} - 2\mu) N_{\mathbf{m}} \\ &\quad + 2i \sum_{\mathbf{m}} \int \frac{d\epsilon}{2\pi\hbar} V_{\mathbf{n},\mathbf{m};\mathbf{n},\mathbf{m}}^{<}(\epsilon) \frac{\hbar}{\epsilon^- - (\epsilon'_{\mathbf{n}} + \epsilon'_{\mathbf{m}} - 2\mu)} \end{aligned} \quad (3.112)$$

and similarly that

$$\begin{aligned} \hbar\Sigma_{\mathbf{n}}^{\mathbf{K}} &= 2 \sum_{\mathbf{m}} V_{\mathbf{n},\mathbf{m};\mathbf{n},\mathbf{m}}^{\mathbf{K}} (\epsilon'_{\mathbf{n}} + \epsilon'_{\mathbf{m}} - 2\mu) N_{\mathbf{m}} \\ &\quad + 2 \sum_{\mathbf{m}} V_{\mathbf{n},\mathbf{m};\mathbf{n},\mathbf{m}}^{<} (\epsilon'_{\mathbf{n}} + \epsilon'_{\mathbf{m}} - 2\mu) (1 + 2N_{\mathbf{m}}). \end{aligned} \quad (3.113)$$

Our next task is therefore the evaluation of the various many-body T-matrix elements $V_{\mathbf{n},\mathbf{m};\mathbf{n}',\mathbf{m}'}^{(+),<,\mathbf{K}}(\epsilon) \equiv (T_{\mathbf{n},\mathbf{m};\mathbf{n}',\mathbf{m}'}^{(+),<,\mathbf{K}}(\epsilon) + T_{\mathbf{m},\mathbf{n};\mathbf{n}',\mathbf{m}'}^{(+),<,\mathbf{K}}(\epsilon))/2$ that occur in these expressions, which is easily carried out with our experience of the homogeneous gas and by noting that the Lippmann-Schwinger equation is in fact an operator equation that only needs to be expressed in a new basis. In terms of the appropriate matrix elements of the interatomic interaction, *i.e.*,

$$V_{\mathbf{n},\mathbf{m};\mathbf{n}',\mathbf{m}'} = \int d\mathbf{x} \int d\mathbf{x}' \chi_{\mathbf{n}}^*(\mathbf{x}) \chi_{\mathbf{m}}^*(\mathbf{x}') V(\mathbf{x} - \mathbf{x}') \chi_{\mathbf{n}'}(\mathbf{x}) \chi_{\mathbf{m}'}(\mathbf{x}'), \quad (3.114)$$

the retarded and advanced components of the many-body T matrix thus obey the Bethe-Salpeter equation [92]

$$\begin{aligned} T_{\mathbf{n},\mathbf{m};\mathbf{n}',\mathbf{m}'}^{(\pm)}(\epsilon) &= V_{\mathbf{n},\mathbf{m};\mathbf{n}',\mathbf{m}'} \\ &\quad + \sum_{\mathbf{n}'',\mathbf{m}''} V_{\mathbf{n},\mathbf{m};\mathbf{n}'',\mathbf{m}''} \frac{1 + N_{\mathbf{n}''} + N_{\mathbf{m}''}}{\epsilon^{\pm} - (\epsilon'_{\mathbf{n}''} + \epsilon'_{\mathbf{m}''} - 2\mu)} T_{\mathbf{n}'',\mathbf{m}'';\mathbf{n}',\mathbf{m}'}^{(\pm)}(\epsilon) \end{aligned} \quad (3.115)$$

and the optical theorem

$$\begin{aligned} T_{\mathbf{n},\mathbf{m};\mathbf{n}',\mathbf{m}'}^{(+)}(\epsilon) - T_{\mathbf{n},\mathbf{m};\mathbf{n}',\mathbf{m}'}^{(-)}(\epsilon) &= -2\pi i \sum_{\mathbf{n}'',\mathbf{m}''} \delta(\epsilon - (\epsilon'_{\mathbf{n}''} + \epsilon'_{\mathbf{m}''} - 2\mu)) \\ &\quad \times T_{\mathbf{n},\mathbf{m};\mathbf{n}'',\mathbf{m}''}^{(+)}(\epsilon) (1 + N_{\mathbf{n}''} + N_{\mathbf{m}''}) T_{\mathbf{n}'',\mathbf{m}'';\mathbf{n}',\mathbf{m}'}^{(-)}(\epsilon). \end{aligned} \quad (3.116)$$

Finally, we also need

$$\begin{aligned} T_{\mathbf{n},\mathbf{m};\mathbf{n}',\mathbf{m}'}^{<}(\epsilon) &= -2\pi i \sum_{\mathbf{n}'',\mathbf{m}''} \delta(\epsilon - (\epsilon'_{\mathbf{n}''} + \epsilon'_{\mathbf{m}''} - 2\mu)) \\ &\quad \times T_{\mathbf{n},\mathbf{m};\mathbf{n}'',\mathbf{m}''}^{(+)}(\epsilon) N_{\mathbf{n}''} N_{\mathbf{m}''} T_{\mathbf{n}'',\mathbf{m}'';\mathbf{n}',\mathbf{m}'}^{(-)}(\epsilon) \end{aligned} \quad (3.117)$$

and the Keldysh component

$$T_{\mathbf{n},\mathbf{m};\mathbf{n}',\mathbf{m}'}^{\mathbf{K}}(\epsilon) = -2\pi i \sum_{\mathbf{n}'',\mathbf{m}''} \delta(\epsilon - (\epsilon'_{\mathbf{n}''} + \epsilon'_{\mathbf{m}''} - 2\mu)) \\ \times T_{\mathbf{n},\mathbf{m};\mathbf{n}'',\mathbf{m}''}^{(+)}(\epsilon)(1 + N_{\mathbf{n}''} + N_{\mathbf{m}''} + 2N_{\mathbf{n}''}N_{\mathbf{m}''})T_{\mathbf{n}'',\mathbf{m}'';\mathbf{n}',\mathbf{m}'}^{(-)}(\epsilon). \quad (3.118)$$

Notice that the appearance of a δ function in the last three equations in practice never leads to any problems, because in the experiments with trapped atomic gases the number of particles is always so large that the critical temperature of the gas is much larger than the energy splitting of the trap and the discrete sum over states is well approximated by an integral over a continuous spectrum.

Making use of the above relations we find that for the states with thermal energies the renormalized energy is given by the pseudopotential result

$$\epsilon'_{\mathbf{n}}(t) = \epsilon_{\mathbf{n}} + \frac{8\pi a\hbar^2}{m} \int d\mathbf{x} \chi_{\mathbf{n}}^*(\mathbf{x})n(\mathbf{x},t)\chi_{\mathbf{n}}(\mathbf{x}), \quad (3.119)$$

with $n(\mathbf{x},t)$ the density profile of the gas cloud. For the states near the one-particle ground state there is, however, a correction given by

$$-2 \sum_{\mathbf{m}} \sum_{\mathbf{n}'',\mathbf{m}''} |V_{\mathbf{n},\mathbf{m};\mathbf{n}'',\mathbf{m}''}^{(+)}(t)|^2 N_{\mathbf{n}''}(t) N_{\mathbf{m}''}(t) \frac{\mathcal{P}}{\epsilon'_{\mathbf{n}}(t) + \epsilon'_{\mathbf{m}}(t) - \epsilon'_{\mathbf{n}''}(t) - \epsilon'_{\mathbf{m}''}(t)}$$

and $V_{\mathbf{n},\mathbf{m};\mathbf{n}'',\mathbf{m}''}^{(+)}(t) = V_{\mathbf{n},\mathbf{m};\mathbf{n}'',\mathbf{m}''}(\epsilon'_{\mathbf{n}''}(t) + \epsilon'_{\mathbf{m}''}(t) - 2\mu(t))$. In the weak-coupling limit, the renormalization of the one-particle energies plays by definition not such an important role and we are much more interested in the imaginary part of the retarded and advanced selfenergies. They are given by

$$R_{\mathbf{n}}(t) = 2\pi \sum_{\mathbf{m}} \sum_{\mathbf{n}'',\mathbf{m}''} \delta(\epsilon'_{\mathbf{n}''}(t) + \epsilon'_{\mathbf{m}''}(t) - \epsilon'_{\mathbf{n}}(t) - \epsilon'_{\mathbf{m}}(t)) \\ \times |V_{\mathbf{n},\mathbf{m};\mathbf{n}'',\mathbf{m}''}^{(+)}(t)|^2 [(1 + N_{\mathbf{n}''}(t) + N_{\mathbf{m}''}(t))N_{\mathbf{m}}(t) - N_{\mathbf{n}''}(t)N_{\mathbf{m}''}(t)]. \quad (3.120)$$

Furthermore, the Keldysh component of the selfenergies equals

$$\hbar\Sigma_{\mathbf{n}}^{\mathbf{K}}(t) = -4\pi \sum_{\mathbf{m}} \sum_{\mathbf{n}'',\mathbf{m}''} \delta(\epsilon'_{\mathbf{n}''}(t) + \epsilon'_{\mathbf{m}''}(t) - \epsilon'_{\mathbf{n}}(t) - \epsilon'_{\mathbf{m}}(t)) \\ \times |V_{\mathbf{n},\mathbf{m};\mathbf{n}'',\mathbf{m}''}^{(+)}(t)|^2 [(1 + N_{\mathbf{n}''}(t) + N_{\mathbf{m}''}(t))N_{\mathbf{m}}(t) \\ + N_{\mathbf{n}''}(t)N_{\mathbf{m}''}(t)(1 + 2N_{\mathbf{m}}(t))]. \quad (3.121)$$

As a result the quantum Boltzmann equation for the gas becomes

$$\frac{\partial}{\partial t} N_{\mathbf{n}}(t) = -\Gamma_{\mathbf{n}}^{\text{out}}(t)N_{\mathbf{n}}(t) + \Gamma_{\mathbf{n}}^{\text{in}}(t)(1 + N_{\mathbf{n}}(t)), \quad (3.122)$$

with the rate to scatter out of the state $\chi_{\mathbf{n}}(\mathbf{x})$ given by

$$\begin{aligned} \Gamma_{\mathbf{n}}^{\text{out}}(t) &= \frac{4\pi}{\hbar} \sum_{\mathbf{m}} \sum_{\mathbf{n}'', \mathbf{m}''} \delta(\epsilon'_{\mathbf{n}''}(t) + \epsilon'_{\mathbf{m}''}(t) - \epsilon'_{\mathbf{n}}(t) - \epsilon'_{\mathbf{m}}(t)) \\ &\quad \times |V_{\mathbf{n}, \mathbf{m}; \mathbf{n}'', \mathbf{m}''}^{(+)}(t)|^2 (1 + N_{\mathbf{n}''}(t))(1 + N_{\mathbf{m}''}(t))N_{\mathbf{m}}(t) \end{aligned} \quad (3.123)$$

and the rate to scatter into this state by

$$\begin{aligned} \Gamma_{\mathbf{n}}^{\text{in}}(t) &= \frac{4\pi}{\hbar} \sum_{\mathbf{m}} \sum_{\mathbf{n}'', \mathbf{m}''} \delta(\epsilon'_{\mathbf{n}''}(t) + \epsilon'_{\mathbf{m}''}(t) - \epsilon'_{\mathbf{n}}(t) - \epsilon'_{\mathbf{m}}(t)) \\ &\quad \times |V_{\mathbf{n}, \mathbf{m}; \mathbf{n}'', \mathbf{m}''}^{(+)}(t)|^2 N_{\mathbf{n}''}(t)N_{\mathbf{m}''}(t)(1 + N_{\mathbf{m}}(t)), \end{aligned} \quad (3.124)$$

as expected from Fermi's Golden Rule.

The quantum Boltzmann equation found above, in combination with the expressions for the shift in the energy levels, fully describes the dynamics of the gas in the normal state. However, close to the critical temperature when the occupation numbers of the one-particle groundstate $\chi_{\mathbf{0}}(\mathbf{x})$ start to become large, we are no longer allowed to neglect the nonlinear terms in the Fokker-Planck equation in equation (3.110). Applying again the Hartree-Fock approximation, which is essentially exact in the weak-coupling limit as we have seen in the equilibrium case, and substituting the ansatz $P[\phi^*, \phi; t] = P_0[\phi_{\mathbf{0}}^*, \phi_{\mathbf{0}}; t]P_1[\phi^*, \phi'; t]$ into equation (3.110), we obtain for the probability distribution of the condensate

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} P_0[\phi_{\mathbf{0}}^*, \phi_{\mathbf{0}}; t] &= -\frac{\partial}{\partial \phi_{\mathbf{0}}} \left(\epsilon_{\mathbf{0}} + \hbar \Sigma_{\mathbf{0}}^{(+)} - \mu(t) \right. \\ &\quad \left. + T_{\mathbf{0}, \mathbf{0}; \mathbf{0}, \mathbf{0}}^{(+)}(t) |\phi_{\mathbf{0}}|^2 \right) \phi_{\mathbf{0}} P_0[\phi_{\mathbf{0}}^*, \phi_{\mathbf{0}}; t] \\ &\quad + \frac{\partial}{\partial \phi_{\mathbf{0}}^*} \left(\epsilon_{\mathbf{0}} + \hbar \Sigma_{\mathbf{0}}^{(-)} - \mu(t) \right. \\ &\quad \left. + T_{\mathbf{0}, \mathbf{0}; \mathbf{0}, \mathbf{0}}^{(+)}(t) |\phi_{\mathbf{0}}|^2 \right) \phi_{\mathbf{0}}^* P_0[\phi_{\mathbf{0}}^*, \phi_{\mathbf{0}}; t] \\ &\quad - \frac{1}{2} \frac{\partial^2}{\partial \phi_{\mathbf{0}}^* \partial \phi_{\mathbf{0}}} \hbar \Sigma_{\mathbf{0}}^K P_0[\phi_{\mathbf{0}}^*, \phi_{\mathbf{0}}; t], \end{aligned} \quad (3.125)$$

where it should be remembered that for consistency reasons the selfenergies need to be evaluated at the energies $\epsilon_{\mathbf{0}}''(t) = \epsilon_{\mathbf{0}}'(t) + T_{\mathbf{0}, \mathbf{0}; \mathbf{0}, \mathbf{0}}^{(+)}(t) |\phi_{\mathbf{0}}|^2$. In equilibrium the fluctuation-dissipation theorem then reads

$$iR_{\mathbf{n}} = -\frac{\beta}{4} \hbar \Sigma_{\mathbf{0}}^K \left(\epsilon_{\mathbf{0}}' - \mu + T_{\mathbf{0}, \mathbf{0}; \mathbf{0}, \mathbf{0}}^{(+)} |\phi_{\mathbf{0}}|^2 \right), \quad (3.126)$$

which guarantees that the probability distribution for the condensate relaxes to the correct equilibrium distribution

$$P_0[\phi_0^*, \phi_0; \infty] \propto \exp \left\{ -\beta \left(\epsilon_0' - \mu + \frac{T_{0,0;0,0}^{(+)}}{2} |\phi_0|^2 \right) |\phi_0|^2 \right\}.$$

The Fokker-Planck equation, and hence the Boltzmann equation, for the noncondensed part of the gas is the same as in the normal state because for a discrete system the contributions from the condensate to the selfenergies is already included in our expressions for $\hbar \Sigma_{\mathbf{n}}^{(\pm),K}$ and needs not be separated out explicitly. This implies of course, that if we evaluate the rates $\Gamma_{\mathbf{n}}^{\text{out}}(t)$ and $\Gamma_{\mathbf{n}}^{\text{in}}(t)$ by replacing the sum over states by an integral over a continuum, we first need to separate the contribution from the condensate to obtain the correct result.

In summary we have thus found that in the weak-coupling limit the dynamics of Bose-Einstein condensation in an external trapping potential is described by the coupled equations in equation (3.122) and equation (3.125), *i.e.*, by a Boltzmann equation for the noncondensed part of the gas and a Fokker-Planck equation for the condensate, respectively. If we apply these equations to a Bose gas with a positive scattering length, we essentially arrive at the theory recently put forward by Gardiner *et al.* [93]. Indeed, neglecting the energy shifts and assuming that the noncondensed cloud is in equilibrium with a chemical potential $\mu > \epsilon_0$, our Fokker-Planck equation for a $U(1)$ invariant probability distribution of the condensate becomes

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} P_0[|\phi_0|; t] = & -\frac{\beta}{4} \hbar \Sigma_0^K \frac{\partial}{\partial \phi_0} \left(\epsilon_0 - \mu + T_{0,0;0,0}^{(+)} |\phi_0|^2 \right) \phi_0 P_0[|\phi_0|; t] \\ & -\frac{\beta}{4} \hbar \Sigma_0^K \frac{\partial}{\partial \phi_0^*} \left(\epsilon_0 - \mu + T_{0,0;0,0}^{(+)} |\phi_0|^2 \right) \phi_0^* P_0[|\phi_0|; t] \\ & -\frac{1}{2} \hbar \Sigma_0^K \frac{\partial^2}{\partial \phi_0^* \partial \phi_0} P_0[|\phi_0|; t]. \end{aligned} \quad (3.127)$$

It is equivalent to the Fokker-Planck equation for a single-mode laser, since introduction of the dimensionless time $\tau = t(i\Sigma_0^K/8)(2\beta T_{0,0;0,0}^{+})^{1/2}$, the dimensionless condensate number $I = |\phi_0|^2(2\beta T_{0,0;0,0}^{+})^{1/2}$, and the so-called “pump parameter” $a = 2\beta(\mu - \epsilon_0)/(2\beta T_{0,0;0,0}^{+})^{1/2}$ leads to the Fokker-Planck equation

$$\frac{\partial}{\partial \tau} P[I; \tau] = \frac{\partial}{\partial I} \left\{ 2(I - a)I + 4I \frac{\partial}{\partial I} \right\} P[I; \tau] \quad (3.128)$$

well-known from laser theory [94]. The typical behaviour of $P[I; \tau]$ during Bose-Einstein condensation is shown in Figure 17.

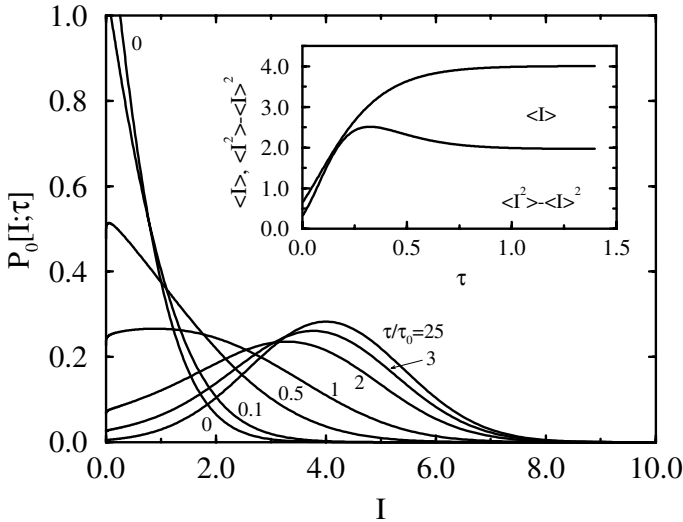


Fig. 17. Typical evolution of the condensate probability distribution during Bose-Einstein condensation. The slowest relaxation rate is $1/\tau_0 \simeq 5.7$. The inset shows the evolution of the average condensate number and its fluctuations.

Calculating $\langle I \rangle(\tau)$ from equation (3.128) by making use of the mean-field assumption $\langle I^2 \rangle(\tau) = (\langle I \rangle(\tau))^2$, precisely reproduces the theory of Gardiner *et al.* A comparison with the experiments of Miesner *et al.* shows that the theory of Gardiner and coworkers is unfortunately not fully satisfactory [95, 96]. The reason for this is presumably that these experiments are really in the strong-coupling limit, where the above theory does not apply. As mentioned previously, the theory is however applicable to gases with a negative scattering length. Since we know from our experience with homogeneous gases that the chemical potential will never be larger than ϵ'_0 in this case, we clearly see from the equilibrium probability distribution $P_0[\phi_0^*, \phi_0; \infty]$ that a condensate in a gas with effectively attractive interactions is only metastable and will ultimately collapse to a dense state after it has overcome an energy barrier, either by thermal fluctuations or by quantum mechanical tunneling. This is clearly in full agreement with the discussion in Section 3.1. Furthermore, we now also understand how the dynamics of the collapse must be treated. It requires the solution of a stochastic, dissipative nonlinear Schrödinger equation, in which the dissipative terms and the noise obey an appropriate fluctuation-dissipation theorem. Having arrived at this important result, we are finally left with a discussion of the strong-coupling limit.

3.4.2 Strong-coupling limit

The difficulty with the strong-coupling limit is that the appropriate one-particle states of the gas are no longer the states $\chi_{\mathbf{n}}(\mathbf{x})$ of the trapping potential because these states are now strongly coupled by the mean-field interaction. For our Caldeira-Leggett model this problem could be easily resolved by introducing the states $\chi'_{\mathbf{n}}(\mathbf{x})$ that incorporate the average interaction with the reservoir. However, for a trapped Bose gas the same procedure would lead to an expansion into states $\chi'_{\mathbf{n}}(\mathbf{x}; t)$ that parametrically depend on time since the mean-field interaction depends on time also. In principle, we thus have to deal with the situation that not only the occupation numbers vary with time but also the states to which these occupation numbers belong. This results in highly nontrivial dynamics since it is *a priori* clear that an adiabatic approximation, in which we neglect the nondiagonal matrix elements $\int d\mathbf{x} \chi'_{\mathbf{n}}^*(\mathbf{x}; t)(\partial/\partial t)\chi'_{\mathbf{n}'}(\mathbf{x}; t)$, is not valid, because of the lack of a separation of time scales. Notice that we were able to circumvent the above problems for a Bose gas with effectively attractive interactions due to the fact that on the one hand the growth of the condensate essentially takes place in the weak-coupling regime and that on the other hand the collapse, which certainly occurs in the strong-coupling regime, requires in first instance only knowledge of the collisionless dynamics of the condensate.

Notwithstanding the above remarks, we can make progress in the strong-coupling limit if we realize that in this limit the typical length scale on which the (noncondensate) density of the gas varies is always much larger than the trap size. We are therefore justified in performing a gradient expansion. To do so in a systematic fashion, it is convenient to express the various selfenergies and interactions in the coordinate representation, *i.e.*, by introducing

$$\hbar\Sigma^{(\pm),K}(\mathbf{x}, \mathbf{x}'; \epsilon) = \sum_{\mathbf{n}, \mathbf{n}'} \chi_{\mathbf{n}}(\mathbf{x}) \hbar\Sigma_{\mathbf{n}, \mathbf{n}'}^{(\pm),K}(\epsilon) \chi_{\mathbf{n}'}^*(\mathbf{x}') \quad (3.129)$$

and similarly

$$V^{(\pm),K}(\mathbf{x}, \mathbf{x}'; \mathbf{y}, \mathbf{y}'; \epsilon) = \sum_{\mathbf{n}, \mathbf{n}'} \sum_{\mathbf{m}, \mathbf{m}'} \chi_{\mathbf{n}}(\mathbf{x}) \chi_{\mathbf{m}}(\mathbf{y}) V_{\mathbf{n}, \mathbf{m}; \mathbf{n}', \mathbf{m}'}^{(\pm),K}(\epsilon) \chi_{\mathbf{n}'}^*(\mathbf{x}') \chi_{\mathbf{m}'}^*(\mathbf{y}'). \quad (3.130)$$

In this coordinate representation, our Fokker-Planck equation acquires in all generality the form

$$\begin{aligned}
i\hbar \frac{\partial}{\partial t} P[\phi^*, \phi; t] = & - \int d\mathbf{x} d\mathbf{x}' \frac{\delta}{\delta \phi(\mathbf{x})} \left\{ \left(\left(-\frac{\hbar^2 \nabla^2}{2m} + V^{\text{ex}}(\mathbf{x}) \right. \right. \right. \\
& \left. \left. \left. - \mu(t) \right) \delta(\mathbf{x} - \mathbf{x}') + \hbar \Sigma^{(+)}(\mathbf{x}, \mathbf{x}') \right) \phi(\mathbf{x}') \right. \\
& + \left. \int d\mathbf{y} d\mathbf{y}' V^{(+)}(\mathbf{x}, \mathbf{x}'; \mathbf{y}, \mathbf{y}') \phi^*(\mathbf{y}) \phi(\mathbf{y}') \phi(\mathbf{x}') \right\} P[\phi^*, \phi; t] \\
& + \int d\mathbf{x} d\mathbf{x}' \frac{\delta}{\delta \phi^*(\mathbf{x})} \left\{ \left(\left(-\frac{\hbar^2 \nabla^2}{2m} + V^{\text{ex}}(\mathbf{x}) \right. \right. \right. \\
& \left. \left. \left. - \mu(t) \right) \delta(\mathbf{x} - \mathbf{x}') + \hbar \Sigma^{(-)}(\mathbf{x}', \mathbf{x}) \right) \phi^*(\mathbf{x}') \right. \\
& + \left. \int d\mathbf{y} d\mathbf{y}' V^{(-)}(\mathbf{x}', \mathbf{x}; \mathbf{y}', \mathbf{y}) \phi^*(\mathbf{x}') \phi^*(\mathbf{y}') \phi(\mathbf{y}) \right\} P[\phi^*, \phi; t] \\
& - \frac{1}{2} \int d\mathbf{x} d\mathbf{x}' \frac{\delta^2}{\delta \phi(\mathbf{x}) \delta \phi^*(\mathbf{x}')} \left\{ \hbar \Sigma^K(\mathbf{x}, \mathbf{x}') \right. \\
& \left. + \int d\mathbf{y} d\mathbf{y}' V^K(\mathbf{x}, \mathbf{x}'; \mathbf{y}, \mathbf{y}') \phi^*(\mathbf{y}) \phi(\mathbf{y}') \right\} P[\phi^*, \phi; t].
\end{aligned} \tag{3.131}$$

To study its physical content and to familiarize ourselves with how to perform the desired gradient expansion, we first analyze again the normal state of the gas in which we can neglect the nonlinear terms representing the effect of the condensate.

In the normal state the condensate is absent and we are only interested in the behavior of the quantity $\langle \phi(\mathbf{x}) \phi^*(\mathbf{x}') \rangle(t)$. From the above Fokker-Planck equation we see that it obeys the equation of motion

$$\begin{aligned}
i\hbar \frac{\partial}{\partial t} \langle \phi(\mathbf{x}) \phi^*(\mathbf{x}') \rangle(t) = & \int d\mathbf{x}'' \left(\left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial \mathbf{x}^2} + V^{\text{ex}}(\mathbf{x}) - \mu(t) \right) \right. \\
& \times \left. \delta(\mathbf{x} - \mathbf{x}'') + \hbar \Sigma^{(+)}(\mathbf{x}, \mathbf{x}'') \right) \langle \phi(\mathbf{x}'') \phi^*(\mathbf{x}') \rangle(t) \\
& - \int d\mathbf{x}'' \left(\left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial \mathbf{x}'^2} + V^{\text{ex}}(\mathbf{x}') - \mu(t) \right) \right. \\
& \times \left. \delta(\mathbf{x}'' - \mathbf{x}') + \hbar \Sigma^{(-)}(\mathbf{x}'', \mathbf{x}') \right) \langle \phi(\mathbf{x}) \phi^*(\mathbf{x}'') \rangle(t) \\
& - \frac{1}{2} \hbar \Sigma^K(\mathbf{x}, \mathbf{x}').
\end{aligned} \tag{3.132}$$

Introducing now the Wigner distribution [97] by means of

$$N(\mathbf{x}, \mathbf{k}; t) + \frac{1}{2} = \int d\mathbf{x}' e^{-i\mathbf{k} \cdot \mathbf{x}'} \langle \phi(\mathbf{x} + \mathbf{x}'/2) \phi^*(\mathbf{x} - \mathbf{x}'/2) \rangle(t) \quad (3.133)$$

and similarly the selfenergies $\hbar\Sigma^{(\pm),K}(\mathbf{x}, \mathbf{k})$ by

$$\hbar\Sigma^{(\pm),K}(\mathbf{x}, \mathbf{k}) = \int d\mathbf{x}' e^{-i\mathbf{k} \cdot \mathbf{x}'} \hbar\Sigma^{(\pm),K}(\mathbf{x} + \mathbf{x}'/2, \mathbf{x} - \mathbf{x}'/2), \quad (3.134)$$

we find after substituting these relations in lowest nonvanishing order in the gradient $\partial/\partial\mathbf{x}$ the expected quantum Boltzmann equation [77, 83]

$$\begin{aligned} \frac{\partial}{\partial t} N(\mathbf{x}, \mathbf{k}; t) + \frac{1}{\hbar} \frac{\partial \epsilon'(\mathbf{x}, \mathbf{k}; t)}{\partial \mathbf{k}} \cdot \frac{\partial}{\partial \mathbf{x}} N(\mathbf{x}, \mathbf{k}; t) - \frac{1}{\hbar} \frac{\partial \epsilon'(\mathbf{x}, \mathbf{k}; t)}{\partial \mathbf{x}} \cdot \frac{\partial}{\partial \mathbf{k}} N(\mathbf{x}, \mathbf{k}; t) \\ = -\Gamma^{\text{out}}(\mathbf{x}, \mathbf{k}; t) N(\mathbf{x}, \mathbf{k}; t) + \Gamma^{\text{in}}(\mathbf{x}, \mathbf{k}; t) (1 + N(\mathbf{x}, \mathbf{k}; t)), \end{aligned} \quad (3.135)$$

where the energies of the atoms have to be determined selfconsistently from

$$\epsilon'(\mathbf{x}, \mathbf{k}; t) = \epsilon(\mathbf{k}) + V^{\text{ex}}(\mathbf{x}) + \text{Re}[\hbar\Sigma^{(+)}(\mathbf{x}, \mathbf{k}; \epsilon'(\mathbf{x}, \mathbf{k}; t) - \mu(t))]. \quad (3.136)$$

Moreover, the expressions for the retarded energy $\hbar\Sigma^{(+)}(\mathbf{x}, \mathbf{k}; \epsilon'(\mathbf{x}, \mathbf{k}; t) - \mu(t))$, and the collision rates $\Gamma^{\text{out}}(\mathbf{x}, \mathbf{k}; t)$ and $\Gamma^{\text{in}}(\mathbf{x}, \mathbf{k}; t)$ turn out to be identical to the ones for a homogeneous gas [91, 98, 99]. We only need to replace the one-particle energies $\epsilon'(\mathbf{k}; t)$ and occupation numbers $N(\mathbf{k}; t)$ by their local counterparts $\epsilon'(\mathbf{x}, \mathbf{k}; t)$ and $N(\mathbf{x}, \mathbf{k}; t)$, respectively. Notice also that the same substitution has to be made in the Bethe-Salpeter equation for the many-body T matrix, which implies that the effective interaction now implicitly depends both on the position $\mathbf{x}$ and the time t .

As an example, let us consider the gas not too close to the critical temperature. Then the effective interaction is well approximated by the two-body T matrix and we simply have

$$\epsilon'(\mathbf{x}, \mathbf{k}; t) = \epsilon(\mathbf{k}) + V^{\text{ex}}(\mathbf{x}) + \frac{8\pi n(\mathbf{x}, t) a \hbar^2}{m}. \quad (3.137)$$

As a result the equilibrium solution $N(\mathbf{x}, \mathbf{k}; \infty)$ of the quantum Boltzmann equation equals a Bose-Einstein distribution evaluated at the energy $\epsilon(\mathbf{k}) + V^{\text{ex}}(\mathbf{x}) + 8\pi n(\mathbf{x}) a \hbar^2 / m - \mu$. The equilibrium density profile $n(\mathbf{x}) = \int d\mathbf{k} N(\mathbf{x}, \mathbf{k}; \infty) / (2\pi)^3$ thus corresponds to a local-density approximation but is indeed very accurate for the atomic gases of interest. Apart from describing the relaxation of the gas towards equilibrium, the quantum Boltzmann equation can also be used to study the collective modes of the trapped gas above the critical temperature. Using the same methods that have recently been applied to inhomogeneous Bose gases by Zaremba

et al. [100], we can for example derive the hydrodynamic equations of motion for the gas. Moreover, the collisionless modes are obtained from

$$\begin{aligned} \frac{\partial}{\partial t} N(\mathbf{x}, \mathbf{k}; t) + \frac{\hbar \mathbf{k}}{m} \cdot \frac{\partial}{\partial \mathbf{x}} N(\mathbf{x}, \mathbf{k}; t) - \frac{1}{\hbar} \frac{\partial}{\partial \mathbf{x}} \left(V^{\text{ex}}(\mathbf{x}) \right. \\ \left. + \frac{8\pi n(\mathbf{x}, t) a \hbar^2}{m} \right) \cdot \frac{\partial}{\partial \mathbf{k}} N(\mathbf{x}, \mathbf{k}; t) = 0. \quad (3.138) \end{aligned}$$

Solving this equation is equivalent to the Generalized Random-Phase Approximation [83]. More important is that the above collisionless Boltzmann equation can be shown to satisfy the Kohn theorem [101] by substituting the shifted equilibrium profile $N(\mathbf{x} - \mathbf{x}_{\text{cm}}(t), \mathbf{k} - (m/\hbar) d\mathbf{x}_{\text{cm}}(t)/dt; \infty)$. For an harmonic external potential the center-of-mass of the gas cloud then precisely follows Newton's law $d^2 \mathbf{x}_{\text{cm}}(t)/dt^2 = -\nabla V^{\text{ex}}(\mathbf{x}_{\text{cm}}(t))$, which shows that the gas has three collisionless modes with frequencies that are equal to the three frequencies of the external trapping potential.

The full quantum Boltzmann equation in equation (3.135) also describes the relaxation of the gas towards equilibrium. It can thus be used to study forced evaporative cooling by adding an appropriate loss term to account for the escaping high-energetic atoms. In agreement with our previous picture we then expect that, if the evaporative cooling is performed slowly, the distribution function $N(\mathbf{x}, \mathbf{k}; t)$ can be well approximated by a truncated equilibrium distribution with a time-dependent temperature and chemical potential. As a result, we can use the results from the homogeneous gas to show that in the critical regime the gas again becomes unstable towards Bose-Einstein condensation. This is the case when $\epsilon'(\mathbf{x}, \mathbf{0}; t) < \mu(t)$ for positions near the center of the trap where the density of the gas is highest. If that happens we are no longer allowed to neglect the nonlinear terms in the Fokker-Planck equation and some corrections are necessary. Applying again the Hartree-Fock approximation, which is correct sufficiently close to the critical temperature where $k_B T \gg 4\pi n_0(\mathbf{x}, t) a \hbar^2 / m$, we find first of all that the quantum Boltzmann equation for the noncondensed part of the gas has the same form as in equation (3.135). We only have to add the by now familiar mean-field interaction $2n_0(\mathbf{x}, t) T^{(+)}(\mathbf{0}, 0)$ due to the condensate to the renormalized energy $\epsilon'(\mathbf{x}, \mathbf{k}; t)$. Finally, the scattering rates $\Gamma^{\text{out}}(\mathbf{x}, \mathbf{k}; t)$ and $\Gamma^{\text{in}}(\mathbf{x}, \mathbf{k}; t)$ have to be adjusted in precisely the same way as in the homogeneous case to account for the macroscopic occupation of the condensate [98, 102, 103].

In addition, the resulting quantum Boltzmann equation for the noncondensed atoms is coupled to a Fokker-Planck equation for the condensate.

After a gradient expansion the latter equals

$$\begin{aligned}
 i\hbar \frac{\partial}{\partial t} P_0[\phi_0^*, \phi_0; t] = & - \int d\mathbf{x} \frac{\delta}{\delta \phi_0(\mathbf{x})} \left(-\frac{\hbar^2 \nabla^2}{2m} + V^{\text{ex}}(\mathbf{x}) - \mu(t) \right. \\
 & \left. + \hbar \Sigma^{(+)}(\mathbf{x}, \mathbf{0}) + T^{(+)}(\mathbf{0}, 0) |\phi_0(\mathbf{x})|^2 \right) \phi_0(\mathbf{x}) P_0[\phi_0^*, \phi_0; t] \\
 & + \int d\mathbf{x} \frac{\delta}{\delta \phi_0^*(\mathbf{x})} \left(-\frac{\hbar^2 \nabla^2}{2m} + V^{\text{ex}}(\mathbf{x}) - \mu(t) \right. \\
 & \left. + \hbar \Sigma^{(-)}(\mathbf{x}, \mathbf{0}) + T^{(+)}(\mathbf{0}, 0) |\phi_0(\mathbf{x})|^2 \right) \phi_0^*(\mathbf{x}) P_0[\phi_0^*, \phi_0; t] \\
 & - \frac{1}{2} \int d\mathbf{x} \frac{\delta^2}{\delta \phi_0(\mathbf{x}) \delta \phi_0^*(\mathbf{x})} \hbar \Sigma^K(\mathbf{x}, \mathbf{0}) P_0[\phi_0^*, \phi_0; t],
 \end{aligned} \tag{3.139}$$

where $\hbar \Sigma^{(\pm),K}(\mathbf{x}, \mathbf{0})$ denotes $\hbar \Sigma^{(\pm),K}(\mathbf{x}, \mathbf{k} = \mathbf{0})$. In more detail we have for the real part of the retarded and advanced selfenergies that $S(\mathbf{x}, \mathbf{0}) = \text{Re}[\hbar \Sigma^{(\pm)}(\mathbf{x}, \mathbf{0}; \epsilon''(\mathbf{x}, \mathbf{0}; t) - \mu(t))]$ and $\epsilon''(\mathbf{x}, \mathbf{0}; t)$ the local energy of a condensate atom. Moreover, using our picture of the evaporative cooling of the gas, the imaginary parts follow most conveniently from the fluctuation-dissipation theorem

$$\begin{aligned}
 iR(\mathbf{x}, \mathbf{0}) = & -\frac{\beta(t)}{4} \hbar \Sigma^K(\mathbf{x}, \mathbf{0}) \\
 & \times \left(-\frac{\hbar^2 \nabla^2}{2m} + \epsilon'(\mathbf{x}, \mathbf{0}; t) - \mu(t) + T^{(+)}(\mathbf{0}, 0) |\phi_0(\mathbf{x})|^2 \right)
 \end{aligned} \tag{3.140}$$

where $\hbar \Sigma^K(\mathbf{x}, \mathbf{0}) = \hbar \Sigma^{(\pm),K}(\mathbf{x}, \mathbf{0}; \epsilon''(\mathbf{x}, \mathbf{0}; t) - \mu(t))$ can in a good approximation be considered as independent of $|\phi_0(\mathbf{x})|$. Near equilibrium the Fokker-Planck equation thus simplifies to

$$\begin{aligned}
 i\hbar \frac{\partial}{\partial t} P_0[|\phi_0|; t] = & -\frac{\beta}{4} \int d\mathbf{x} \hbar \Sigma^K(\mathbf{x}, \mathbf{0}) \frac{\delta}{\delta \phi_0(\mathbf{x})} \left(-\frac{\hbar^2 \nabla^2}{2m} + \epsilon'(\mathbf{x}, \mathbf{0}) \right. \\
 & \left. - \mu + T^{(+)}(\mathbf{0}, 0) |\phi_0(\mathbf{x})|^2 \right) \phi_0(\mathbf{x}) P_0[|\phi_0|; t] \\
 & - \frac{\beta}{4} \int d\mathbf{x} \hbar \Sigma^K(\mathbf{x}, \mathbf{0}) \frac{\delta}{\delta \phi_0^*(\mathbf{x})} \left(-\frac{\hbar^2 \nabla^2}{2m} + \epsilon'(\mathbf{x}, \mathbf{0}) \right. \\
 & \left. - \mu + T^{(+)}(\mathbf{0}, 0) |\phi_0(\mathbf{x})|^2 \right) \phi_0^*(\mathbf{x}) P_0[|\phi_0|; t] \\
 & - \frac{1}{2} \int d\mathbf{x} \hbar \Sigma^K(\mathbf{x}, \mathbf{0}) \frac{\delta^2}{\delta \phi_0(\mathbf{x}) \delta \phi_0^*(\mathbf{x})} P_0[|\phi_0|; t]
 \end{aligned} \tag{3.141}$$

and the probability distribution of the condensate relaxes to the expected stationary state

$$P_0[|\phi_0|; \infty] \propto \exp \left\{ -\beta \int d\mathbf{x} \phi_0^*(\mathbf{x}) \left(-\frac{\hbar^2 \nabla^2}{2m} + \epsilon'(\mathbf{x}, \mathbf{0}) - \mu + \frac{T^{(+)}(\mathbf{0}, 0)}{2} |\phi_0(\mathbf{x})|^2 \right) \phi_0(\mathbf{x}) \right\}. \quad (3.142)$$

From this result we conclude that equations (3.135) and (3.139) give an accurate description of the dynamics of Bose-Einstein condensation in the strong-coupling regime. Unfortunately, the solution of these coupled equations is not possible analytically and we therefore have to refer to future work for a numerical study and a comparison of this theory with experiment. We here only remark that the semiclassical approximation in this case amounts to the Thomas-Fermi result for the condensate density

$$n_0(\mathbf{x}; t) = \frac{1}{T^{(+)}(\mathbf{0}, 0)} (\mu(t) - \epsilon'(\mathbf{x}, \mathbf{0}; t)) \Theta(\mu(t) - \epsilon'(\mathbf{x}, \mathbf{0}; t)). \quad (3.143)$$

Such an approximation implicitly assumes, however, that the dominant mechanism for the formation of the condensate is by means of a coherent evolution and not by incoherent collisions. This might be expected not to be very accurate on the basis of the homogeneous result that the second mechanism only diverges logarithmically with the system size [90], whereas the first diverges linearly [104]. Nevertheless it seems that only a full solution of equations (3.135) and (3.139) can settle this important issue.

3.5 Collective modes

Although we have up to now primarily been focussed on the dynamics of Bose-Einstein condensation itself, it is interesting that we have in fact, similarly as for temperatures above the critical temperature, also arrived at an accurate description of the collective modes of a condensed gas at nonzero temperatures. Since these collective modes are receiving much attention at present, we now briefly want to discuss how such a description emerges from our Fokker-Planck equation. Since most experiments at present are performed in the collisionless limit, we consider only this limit here. It is in principle possible, however, to derive the hydrodynamic equations of motions as well [100]. Let us for simplicity first assume that the temperature of the gas is sufficiently far below the critical temperature that the many-body T matrix is well approximated by the two-body T matrix, but not so low that the Hartree-Fock approximation is no longer valid. In this regime we have that $\hbar \Sigma^{(\pm)}(\mathbf{x}, \mathbf{k}) = 8\pi n'(\mathbf{x}, t) a \hbar^2 / m$ and the dynamics of the non-condensed part of the gas is again determined by the collisionless quantum

Boltzmann equation given in equation (3.138), where the total density now consists of two contributions

$$n(\mathbf{x}, t) = n_0(\mathbf{x}, t) + n'(\mathbf{x}, t) \equiv |\langle \phi(\mathbf{x}) \rangle(t)|^2 + \int \frac{d\mathbf{k}}{(2\pi)^3} N(\mathbf{x}, \mathbf{k}; t). \quad (3.144)$$

The dynamics of the condensate follows again from the nonlinear Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \langle \phi(\mathbf{x}) \rangle(t) = \left\{ -\frac{\hbar^2 \nabla^2}{2m} + V^{\text{ex}}(\mathbf{x}) - \mu + \frac{4\pi a \hbar^2}{m} (2n'(\mathbf{x}, t) + n_0(\mathbf{x}, t)) \right\} \langle \phi(\mathbf{x}) \rangle(t), \quad (3.145)$$

which can be rewritten as the continuity equation

$$\frac{\partial}{\partial t} n_0(\mathbf{x}, t) = -\nabla \cdot (\mathbf{v}_s(\mathbf{x}, t) n_0(\mathbf{x}, t)) \quad (3.146)$$

together with the Josephson relation for the superfluid velocity

$$\begin{aligned} \frac{\partial}{\partial t} \mathbf{v}_s(\mathbf{x}, t) = & -\nabla \left(V^{\text{ex}}(\mathbf{x}) - \mu + \frac{4\pi a \hbar^2}{m} (2n'(\mathbf{x}, t) \right. \\ & \left. + n_0(\mathbf{x}, t)) + \frac{1}{2} m \mathbf{v}_s^2(\mathbf{x}, t) \right). \end{aligned} \quad (3.147)$$

Here, we used that $\langle \phi(\mathbf{x}) \rangle(t) = \sqrt{n_0(\mathbf{x}, t)} e^{i\theta(\mathbf{x}, t)}$, $\mathbf{v}_s(\mathbf{x}, t) = \hbar \nabla \theta(\mathbf{x}, t)/m$, and have applied the Thomas-Fermi approximation, which is appropriate in the strong-coupling limit. It will presumably not come as a surprise that these coupled equations for $N(\mathbf{x}, \mathbf{k}; t)$, $n_0(\mathbf{x}, t)$, and $\mathbf{v}_s(\mathbf{x}, t)$ can be shown to fulfill the Kohn theorem exactly. This is an important constraint on any theory for the collective modes of a trapped gas, as stressed recently by Zaremba *et al.* [100].

As a first step towards this goal we here consider the time-dependent Hartree-Fock theory for the collective modes of the Bose condensed gas, in which the collisionless Boltzmann equation in equation (3.138) is coupled to the nonlinear Schrödinger equation in equation (3.145). It turns out that a numerical determination of the eigenmodes of the collisionless Boltzmann equation is rather difficult. Therefore, we have recently proposed a variational approach to solve these coupled equations [105]. Denoting the anisotropic harmonic trapping potential used in the experiments [26, 27] by $V^{\text{ex}}(\mathbf{x}) = \sum_j m \omega_j^2 x_j^2 / 2$, we first of all take for the condensate wave function

the gaussian *ansatz*

$$\begin{aligned} \langle \phi(\mathbf{x}) \rangle(t) = & \sqrt{N_0} \prod_j \left(\frac{1}{\pi q_j^2(t)} \right)^{1/4} \\ & \times \exp \left\{ -\frac{x_j^2}{2q_j^2(t)} \left(1 - i \frac{m q_j(t)}{\hbar} \frac{d q_j(t)}{dt} \right) \right\}, \end{aligned} \quad (3.148)$$

with the functions $q_j(t)$ describing the “breathing” of the condensate in three independent directions. Clearly, this is the anisotropic generalization of the gaussian *ansatz* that we used in Section 3.1 to study the stability of a condensate with negative scattering length. Although it is not immediately obvious that such an *ansatz* is also appropriate in the strong-coupling regime of interest here, it has been shown by Perez-Garcia *et al.* [51] that at zero temperature the assumption of a gaussian density profile nevertheless leads to rather accurate results for the frequencies of the collective modes. We therefore anticipate that at nonzero temperatures the same will be the case.

Next we also need an *ansatz* for the distribution function $N(\mathbf{x}, \mathbf{k}; t)$ of the thermal cloud. Here, we consider the Bose distribution

$$\begin{aligned} N(\mathbf{x}, \mathbf{k}; t) = & N' \frac{1}{\zeta(3)} \left(\prod_j \frac{\hbar \omega_j}{k_B T \langle \alpha_j \rangle^2} \right) \\ & \times \left(\exp \left\{ \sum_j \frac{1}{k_B T \langle \alpha_j \rangle^2} \left(\frac{\hbar^2 \alpha_j^2(t)}{2m} \left(k_j - \frac{m x_j}{\hbar \alpha_j(t)} \frac{d \alpha_j(t)}{dt} \right)^2 \right. \right. \right. \\ & \left. \left. \left. + \frac{m \omega_j^2}{2} \frac{x_j^2}{\alpha_j^2(t)} \right) \right\} - 1 \right)^{-1}, \end{aligned} \quad (3.149)$$

where $\alpha_j(t)$ are again three scaling parameters, $N' = N - N_0$ is the number of noncondensed particles, $\langle \alpha_j \rangle$ denotes the equilibrium value of $\alpha_j(t)$ that in general is greater than 1 due to the repulsive interactions between the atoms, and $\zeta(3) \simeq 1.202$. The functional form of the distribution function is physically motivated by the following reasons. First, by integrating over the momentum $\hbar \mathbf{k}$ we see that the time-dependent density profile of the noncondensed cloud $n'(\mathbf{x}, t)$ is a time-independent function of $x_j/\alpha_j(t)$, as desired. Second, for such a density profile we must have that the local velocity $\hbar \langle k_j \rangle(\mathbf{x}, t)/m$ is given by $(x_j/\alpha_j(t)) d\alpha_j(t)/dt$. Third, we want the equilibrium distribution to be only anisotropic in coordinate space, and not in momentum space. This explains the appearance of the factor $1/\langle \alpha_j \rangle^2$ in the exponent.

Using the ideal gas result for the number of condensate particles and substituting the above *ansatz* for the condensate wave function and the

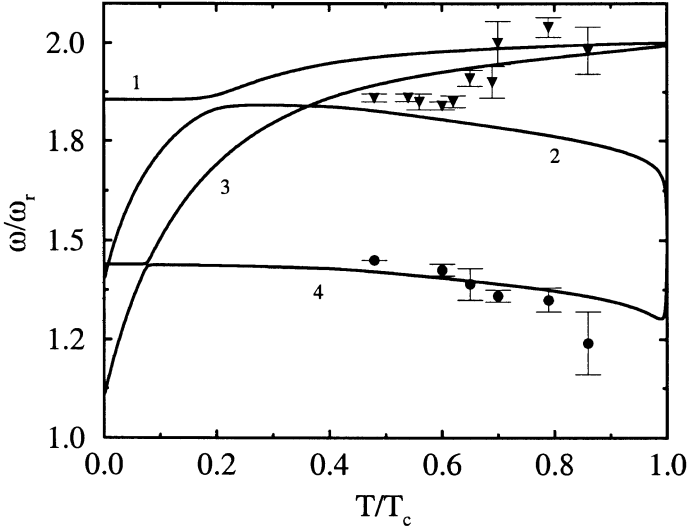


Fig. 18. Collisionless modes in a Bose condensed ^{87}Rb gas. The full lines give the results with a Bose distribution *ansatz* for the distribution function of the thermal cloud. Curves 1 and 2 correspond to the $m = 0$ in and out-of-phase modes, respectively. Similarly, curves 3 and 4 give the frequencies of the $m = 2$ in and out-of-phase modes. The experimental data is also shown. Triangles are for a $m = 0$ mode and circles for a $m = 2$ mode.

Wigner distribution function into the nonlinear Schrödinger and collisionless Boltzmann equations, it is straightforward but somewhat tedious to derive the six coupled equations of motion for the “breathing” parameters $q_j(t)$ and $\alpha_j(t)$. Linearizing these equations around the equilibrium solutions $\langle q_j \rangle$ and $\langle \alpha_j \rangle$, respectively, we can then also obtain the desired eigenmodes and eigenfrequencies. The results of this calculation for the trap parameters of Jin *et al.* [26] are shown in Figure 18 together with the experimental data. Note that the trap has a disk geometry with $\omega_x = \omega_y \equiv \omega_r$ and $\omega_z = \sqrt{8}\omega_r$. Due to the axial symmetry, the modes of the gas can be labeled by the usual quantum number m that describes the angular dependence around the z -axis. On the whole there appears to be a quite reasonable agreement between this simple theory and experiment. The only exceptions are the two data point almost halfway in between the in and out-of-phase $m = 0$ modes. A possible explanation for this discrepancy is that experimentally both modes are excited simultaneously [106]. To make sure of this, however, we need to determine the oscillator strength of the various modes and it appears that the in-phase mode indeed dominates the response for temperatures larger than about $0.6T_c$ [105].

4 Outlook

With the latter remark we end this course on the use of field-theoretical methods for the study of the equilibrium and nonequilibrium properties of trapped atomic gases. Although we have in principle illustrated all the necessary tools for an *ab initio* treatment of these new quantum systems, many interesting topics still need to be considered in detail. We already mentioned such topics as Fermi-Bose mixtures, the dynamics of condensate collapse, the strong-coupling theory for the formation of a condensate in either atomic Bose or Fermi gases, and the hydrodynamics of single or multicomponent atomic gases. Several other important areas of research, which can also be easily addressed within the context of quantum field theory, are atom lasers, the damping of collective modes, the behaviour of spinor condensates, the dynamics of topological excitations such as kinks, vortices and skyrmions, quantum critical phenomena, the optical properties of superfluid gases, and two-dimensional phase transitions. In view of these and many other possibilities that are now experimentally feasible, it appears certain that the physics of degenerate atomic gases will remain very exciting for years to come.

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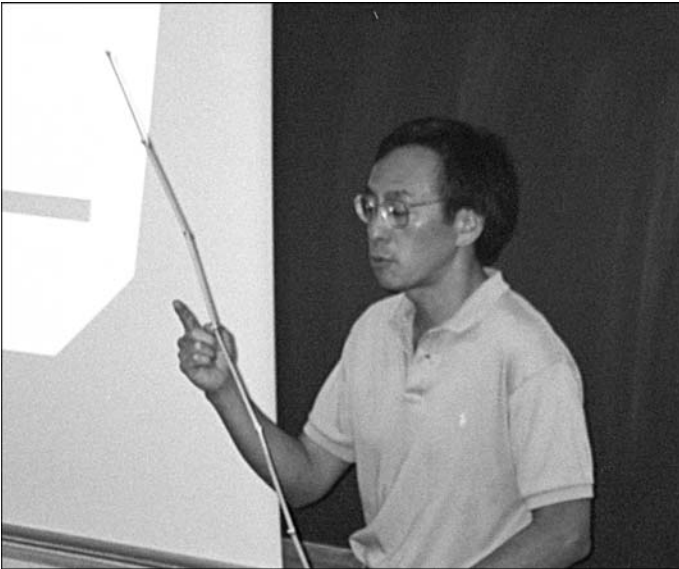
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COURSE 4

ATOM INTERFEROMETRY

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ATOM INTERFEROMETRY

S. Chu

1 Introduction

The first demonstrated atom interferometers, reported in 1991 by Carnal and Mlynek [1] and Keith *et al.* [2] were based on the diffraction of atoms with micro fabricated structures. This class of atom interferometers is analogous to optical interferometers, where slits or diffraction gratings have been used to divide and recombine beams of atoms. The gratings and slits can be either material structures or periodic light fields. Three months later, atom interferometers based on optical pulses of light were reported by Riehle *et al.* [3], and by Kasevich and Chu [4]. In this class of interferometers, the spatial separation of the atoms is accomplished by the momentum recoil induced by the electromagnetic field used to drive the atoms from one internal state to another. Thus, the internal and external degrees of freedom are intimately connected.

Atom interferometry has attracted significant interest for a number of reasons. (i) Atoms possess internal degrees of freedom so that the interferometers that combine interference effects from both the internal and external degrees of freedom can be constructed. (ii) Their internal states are easily manipulated by external magnetic, electric or electromagnetic fields. (iii) Different atoms possess a wide range of different properties that offer the experimentalist an opportunity to address a wide range of problems. (iv) The technologies of laser cooling and atom trapping allow extraordinarily long quantum measurement times so that atom interferometers of great precision can be constructed.

In this set of lectures, we will first present a development of the fundamental principles of atom interferometers. Next, we will discuss a few of the various methods now available to split and recombine atomic de Broglie waves, with special emphasis on atom interferometers based on optical pulses. These interferometers are the intellectual grandchildren of magnetic resonance methods that were later generalized to electronically excited states of atoms. Consequently, the wealth of theoretical and experimental techniques that have been developed for over a half century can be exploited

for atom interferometry. We will also be particularly concerned with high precision interferometers with long measurement times such as those made with atomic fountains. Some applications and the systematic effects encountered in those applications will also be covered. Finally, the outlook of future developments will be given.

2 Basic principles

We will be concerned with single particle interference in which each atom interferes with itself and only itself. Virtually all photon and matter wave interferometers demonstrated to date are of this type. Our quantum states may be described in terms of a set of pure states defined as a tensor product of the Hilbert space describing the internal energy state of the atom and the Hilbert space describing the external degrees of freedom,

$$|\Psi\rangle = \sum_n |n\rangle \otimes |c_n\rangle \quad (2.1)$$

where $|n\rangle$ and $|c_n\rangle$ are internal state and external state parts of the atom. The external state can be described by the center of mass position and $|\Psi\rangle$ will have an associated wave function $\Psi(\mathbf{x}, t)$. Alternatively, the external state can be described by momentum plane waves. This approach will be developed in Section (2.5).

2.1 Ramsey interference

An early example of an atom interference is the Ramsey method of separated oscillatory fields [6]. In this type of interferometer, only the internal states $|n\rangle$ contribute to the interference. An atom in an atomic beam initially in the ground state is placed into a superposition of states $|e\rangle$ and $|g\rangle$ as it passes through a microwave cavity. The atom then travels over some distance into a second microwave cavity where the atom is placed into another superposition state that depends on the phase of the atom superposition state relative to the phase of electromagnetic field in the second microwave cavity. Finally, the interference is measured by projecting the atomic state onto one of the quantum states, say $|g\rangle$, of the system. Interference requires that it is impossible to distinguish which path the atom took. Thus, the two alternate paths $|g\rangle \rightarrow |e\rangle \rightarrow |g\rangle$ and $|g\rangle \rightarrow |g\rangle \rightarrow |g\rangle$ should not have a measurable quantity that will allow one to differentiate the two trajectories. Since the small momentum recoil of an rf photon does not cause the two parts of the atom to spatially separate, the external degrees of freedom of the atom such as position and momentum can be assumed to be decoupled from the internal degrees of freedom. Later, when we generalize the treatment to include the recoil of an optical photon, we will have to consider the external state variables.

The time evolution of any quantum state¹

$$|\Psi(t)\rangle = a_e(t)|e\rangle + a_g(t)|g\rangle \Leftrightarrow \begin{bmatrix} a_e(t) \\ a_g(t) \end{bmatrix} \quad (2.2)$$

is given by the Schrödinger equation

$$i\hbar \frac{d}{dt} |\Psi(t)\rangle = \hat{H} |\Psi(t)\rangle. \quad (2.3)$$

The Hamiltonian for a two-level atom coupled to an electromagnetic field, in the absence of spontaneous emission, is

$$\begin{aligned} \hat{H} &= \hbar\omega_e |e\rangle\langle e| + \hbar\omega_g |g\rangle\langle g| - \mathbf{d} \cdot \mathbf{E} \\ &= \begin{bmatrix} \hbar\omega_e & V_{eg} \\ V_{eg}^* & \hbar\omega_g \end{bmatrix} \end{aligned} \quad (2.4)$$

where the electromagnetic field operator is

$$\mathbf{E} = \mathbf{E}_0 \cos(\omega_L t + \phi), \quad (2.5)$$

couples to the atom *via* an electric dipole coupling term $V = -\mathbf{d} \cdot \mathbf{E} = |e|\mathbf{r} \cdot \mathbf{E}$, where $\mathbf{r}$ is defined as the vector from the nucleus of the atom to the electron position. The eigenfrequencies ω_e and ω_g represent the *total* energy of the atom, both internal and external, but if the kinetic energy of the atom is decoupled from the internal states, one may take these frequencies as the internal state energies. The matrix element V_{eg} is defined to be

$$\begin{aligned} V_{eg} &= \langle e|V|g\rangle \\ &= \hbar\Omega_{eg} \left(\frac{e^{i(\omega_L t + \phi)} + e^{-i(\omega_L t + \phi)}}{2} \right), \end{aligned} \quad (2.6)$$

and the Rabi frequency is defined as

$$\Omega_{eg} \equiv -\frac{\langle e|\mathbf{d} \cdot \mathbf{E}_0|g\rangle}{\hbar}. \quad (2.7)$$

For simplicity, we will assume that the amplitude of the electric field $\mathbf{E}_0$ is constant when the light is on.

It is often convenient to go to a new interaction basis where $c_e(t)$ and $c_g(t)$ are slowly varying functions

¹The double arrow denotes the correspondence between the state vector description and a particular representation given by the two-spinor. Henceforth, we will use the two descriptions interchangeably.

$$|\Psi(t)\rangle = \begin{bmatrix} c_e(t)e^{-i\omega_e(t)/2} \\ c_g(t)e^{-i\omega_g(t)/2} \end{bmatrix}. \quad (2.8)$$

We also make the “rotating wave approximation” where the near resonant terms $e^{i(\omega_{eg}-\omega)t'}$ are taken to be much larger than the off resonant terms $e^{i(\omega_{eg}+\omega)t'}$, with $\omega_{eg} \equiv \omega_e - \omega_g$ and $\delta \equiv \omega_L - \omega_{eg}$.

The Hamiltonian in this transformed frame becomes [8]

$$\hat{H}_R = \frac{\hbar}{2} \begin{bmatrix} 0 & \Omega_{eg}e^{-i(\delta t+\phi)} \\ \Omega_{eg}^*e^{i(\delta t+\phi)} & 0 \end{bmatrix}. \quad (2.9)$$

For nonzero detunings, the weakly *time-dependent* Hamiltonian can be turned into a *time-independent* Hamiltonian by the transformation of variables $c_e(t) = d_e(t)e^{-i\delta t/2}$ and $c_g(t) = d_g(t)e^{i\delta t/2}$. Physically, this transformation describes the quantum states in terms of a frame rotating about the $\mathbf{z}$ -axis with frequency δ . (Similarly, the transformation from the Schrödinger picture to the interaction picture can be viewed as a transformation to a frame rotating at ω_{eg} .) This transformation is analogous to the magnetic resonance transformation to the rotating frame in which the oscillating magnetic field inducing a transition on a spin- $\frac{1}{2}$ system appears as a static torque [7].

The transformation of a ket $|\Psi\rangle$ to a ket $|\Psi\rangle_R$ in a frame rotated through an angle $-\delta t$ about the $\hat{\mathbf{z}}$ -axis is given by

$$D(\hat{\mathbf{z}}, -\delta t)|\Psi\rangle = |\Psi\rangle_R, \quad (2.10)$$

where the rotation operator $D(\hat{\mathbf{z}}, -\delta t)$ has the representation

$$D(\hat{\mathbf{z}}, -\delta t) \Leftrightarrow e^{i\sigma_z \delta t/2} = \begin{bmatrix} e^{i\delta t/2} & 0 \\ 0 & e^{-i\delta t/2} \end{bmatrix} \quad (2.11)$$

where σ_z is a Pauli spin matrix [84].

The description of Schrödinger’s equation in the rotating frame is found by starting with

$$i\hbar \frac{d}{dt} (D^\dagger |\Psi\rangle_R) = \hat{H} (D^\dagger |\Psi\rangle_R). \quad (2.12)$$

Operating on the left with D , we get

$$i\hbar \frac{d}{dt} |\Psi\rangle_R = \left[D \hat{H} D^\dagger - i\hbar D \left(\frac{dD^\dagger}{dt} \right) \right] |\Psi\rangle_R. \quad (2.13)$$

The term in brackets defines $\hat{H}_R$, which when evaluated becomes

$$\hat{H}_R = \frac{\hbar}{2} \begin{bmatrix} -\delta & \Omega_{eg} e^{-i\phi} \\ \Omega_{eg}^* e^{i\phi} & \delta \end{bmatrix}. \quad (2.14)$$

The eigenvalues $\lambda_{\pm}$ of $\hat{H}_R$ are

$$\lambda_{\pm} = \pm \frac{\hbar \Omega_r}{2}, \quad (2.15)$$

where the off-resonant Rabi frequency is defined as $\Omega_r \equiv \sqrt{|\Omega_{eg}|^2 + \delta^2}$.

Since the overall phase of the quantum state is arbitrary, the initial phase ϕ is assumed to be combined with the phase of Ω_{eg} to make Ω_{eg} real and positive. Then the eigenstates of $\hat{H}_R$ are given by (see, for example, Cohen-Tannoudji *et al.* [9])

$$\begin{aligned} |\lambda_+\rangle &= \cos(\tfrac{\theta}{2})|e\rangle_R e^{-i\phi/2} + \sin(\tfrac{\theta}{2})|g\rangle_R e^{i\phi/2} \\ |\lambda_-\rangle &= -\sin(\tfrac{\theta}{2})|e\rangle_R e^{-i\phi/2} + \cos(\tfrac{\theta}{2})|g\rangle_R e^{i\phi/2}, \end{aligned} \quad (2.16)$$

where θ is defined by the relations

$$\sin \theta = \Omega_{eg}/\Omega_r, \quad \cos \theta = -\delta/\Omega_r, \quad 0 \leq \theta \leq \pi. \quad (2.17)$$

With the Hamiltonian (2.9) the time evolution of the atom in the presence of the light is calculated by solving the eigenvector-eigenvalue problem and then writing the initial state in terms of a projection onto the new basis states, *i.e.*, the new eigenvectors. The time evolution of each of the eigenvectors is particularly simple: if $|\lambda_+\rangle$ is the eigenvector, then the time evolution is given by an oscillation about the eigenfrequency, $e^{-i\lambda_+\tau/\hbar}|\lambda_+\rangle$. Thus, if at time t_0 , the quantum state *in the rotating frame* is $|\Psi(t_0)\rangle_R$, then

$$|\Psi(t_0 + \tau)\rangle_R = \left(e^{-i\lambda_+\tau/\hbar} |\lambda_+\rangle \langle \lambda_+| + e^{-i\lambda_-\tau/\hbar} |\lambda_-\rangle \langle \lambda_-| \right) |\Psi(t_0)\rangle_R. \quad (2.18)$$

The time evolution for the general case of non-zero detuning $\delta \neq 0$ but constant laser amplitude has been worked out elsewhere [6, 8]. For the special case of $\delta = 0$, the effect of a pulse of light of duration τ on the atom is described by a simple 2×2 matrix

$$\hat{U}_R = \begin{bmatrix} \cos(\tfrac{\Omega_r \tau}{2}) & -ie^{-i\phi} \sin(\tfrac{\Omega_r \tau}{2}) \\ -ie^{i\phi} \sin(\tfrac{\Omega_r \tau}{2}) & \cos(\tfrac{\Omega_r \tau}{2}) \end{bmatrix}. \quad (2.19)$$

From the form of the matrix $\hat{U}_R$, one can readily see that an atom initially in the ground state, and exposed to two pulses of “area” $\int \Omega_r(t) dt = \Omega_r \tau =$

$\pi/2$ will undergo the transformations

$$|\Psi\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \rightarrow \begin{bmatrix} -i/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix} \rightarrow \begin{bmatrix} -i \\ 0 \end{bmatrix}. \quad (2.20)$$

If the atomic oscillation during the drift time T in between the two $\pi/2$ pulses is the same as the microwave oscillator, the atom will be put into the excited state. If the number of oscillations differs by a π radians, the atom is left in the ground state. Thus, the interference creates an oscillation between the ground and excited state with an effective resonance linewidth of $\delta_{\text{FWHM}} = \pi/T$. Note that this interference is strictly between two internal states of the atom.

The mathematical description of a two-level atom is identical to the description of a spin 1/2 system, where an atom in the ground state is depicted as a spin down Bloch vector aligned along the minus z -axis and an atom in the excited state is a spin up vector. The transformation given by equation (2.10) is equivalent to transforming into a frame of reference rotating at the laser frequency ω_L . In this frame of reference, if the laser frequency $\omega_L = \omega_{eg}$, the excitation of an atom is depicted as a static torque in the $x-y$ plane. An excitation from the ground state to the excited state is depicted as a torque applied for a time needed to cause the Bloch vector to rotate by π radians from the spin down state to the spin up state. The relative phase of the atom with respect to the driving electric field is given by the angle between the projection of the Bloch vector and the torque vector on to the $x-y$ plane. This geometric picture is often very useful in developing intuition about two-level atoms [7].

2.2 Interference due to different physical paths

We will now take the other extreme position and assume that the atom remains in one internal state and the interference is between parts of the atom that have taken two or more separate paths. Just as optical waves can be diffracted from matter gratings, matter waves can be diffracted from an optical grating defined as the periodic variations in the intensity of light field.

We again begin with the Schrödinger equation

$$-\left[\frac{\hbar^2}{2M}\nabla^2 - V(\mathbf{x}, t)\right]\Psi(\mathbf{x}, t) = i\hbar\frac{\partial\Psi}{\partial t}(\mathbf{x}, t). \quad (2.21)$$

For $V(\mathbf{x}, t) = V(\mathbf{x})$ independent of time, $\Psi(\mathbf{x}, t) = \Psi(\mathbf{x}) \exp(-iEt/\hbar)$ and the total energy $E = T + V$ is constant. Thus, we obtain the Helmholtz equation,

$$\nabla^2\Psi(\mathbf{x}, t) + k^2\Psi(\mathbf{x}, t) = 0, \quad (2.22)$$

with

$$k(\mathbf{x}) = \sqrt{\frac{2M}{\hbar^2} [E - V(\mathbf{x})]}. \quad (2.23)$$

We seek a solution to the Helmholtz equation of the form $\Psi(\mathbf{x}) \sim e^{i\psi(\mathbf{x})}$. Thus, $\psi(\mathbf{x})$ will satisfy

$$-(\nabla\psi)^2 + i\nabla^2\psi + k^2 = 0. \quad (2.24)$$

If the potential $V(r)$ is slowly varying relative to $1/k(r)$, then it is possible to define a local de Broglie wavelength $\lambda_{dB} = 2\pi/k(\mathbf{x})$, and the solution of (2.24) may be approximated by expanding about the local position $\mathbf{x} = 0$

$$\psi(\mathbf{x}) = \psi(0) + \mathbf{k}(0) \cdot \mathbf{x} + \nabla k(0) \frac{x^2}{2} + \dots \quad (2.25)$$

In the WKB approximation, we take only the first order term in the Taylor series expansion. By direct substitution, one can readily see that $\Psi(\mathbf{x}) \sim e^{i\mathbf{k} \cdot \mathbf{x}}$. Adding the explicit time dependence, the local wave function for the external motion becomes a plane wave

$$\Psi(\mathbf{x}, t) = e^{i(\mathbf{k}(\mathbf{x}) \cdot \mathbf{x} - \omega t)}, \quad (2.26)$$

where the de Broglie energy $E = \hbar\omega$ is defined as the total energy of the atom. More generally, the external motion part of the wave function at two positions $(\mathbf{x}_a, t_a)$ and $(\mathbf{x}_b, t_b)$ are related by

$$\Psi(\mathbf{x}_b, t_b) = e^{i \int (\mathbf{k} \cdot d\mathbf{x} - \omega dt)} \Psi(\mathbf{x}_a, t_a). \quad (2.27)$$

2.3 Path integral description of interference

Feynman's path integral approach to quantum mechanics [10], provides a natural framework for analyzing atom interferometers [12]. The time evolution of a state vector is described by a unitary operator

$$|\Psi(t_b)\rangle = U(t_b, t_a) |\Psi(t_a)\rangle. \quad (2.28)$$

The wave function is the projection of this state vector onto the position basis and can then be written as

$$\begin{aligned} \Psi(x_b, t_b) &= \langle x_b | \Psi(t_b) \rangle = \langle x_b | U(t_b, t_a) | \Psi(t_a) \rangle \\ &= \int dx_a \langle x_b | U(t_b, t_a) | x_a \rangle \langle x_a | \Psi(t_a) \rangle \\ &= \int dx_a K(x_b, t_b; x_a, t_a) \Psi(x_a, t_a), \end{aligned} \quad (2.29)$$

where the function K is quantum propagator

$$K(z_b, t_b; x_a, t_a) \equiv \langle x_b | U(t_b, t_a) | x_a \rangle \quad (2.30)$$

that gives the amplitude for the particle starting at point (x_a, t_a) ending at point (x_b, t_b) . Note that the wave function $\Psi(x_b, t_b)$ at the space time point (x_b, t_b) is due to the contributions from *all* points $(x_a, t_a), (x'_a, t'_a), (x''_a, t''_a, \dots)$ that end up at point (x_b, t_b) , and is analogous to Huygens principle in optics.

Feynman showed that the quantum propagator can be written as

$$K(x_b, t_b; x_a, t_a) = \mathcal{N} \sum_{\Gamma} e^{-iS/\hbar}, \quad (2.31)$$

where S is the action given by

$$S = \int_{t_a}^{t_b} L(x, \dot{x}) dt. \quad (2.32)$$

$L(x, \dot{x})$ is the Lagrangian of the atomic path, $\mathcal{N}$ is the normalization factor, and the sum is over *all* paths connecting point (x_a, t_a) to point (x_b, t_b) . In the sum over all states, if $S_{Cl} \gg \hbar$, then slight changes in the path will give an amplitude with a wildly different phase. Only the paths near an extremum, *i.e.*, the classical trajectory, will allow the phases to add constructively. In the limit of a large action, the sum in (2.31) simplifies and the wavefunction is simply

$$\Psi(x_b, t_b) = e^{iS_{Cl}/\hbar} \Psi(x_a, t_a). \quad (2.33)$$

In classical Lagrangian dynamics, the Hamiltonian is defined as

$$H_{Cl} \equiv p\dot{x} - L_{Cl}. \quad (2.34)$$

By substituting (2.34) into (2.32), we recover (2.27).

2.4 Atom optics

Atom optics and photon optics both satisfy the Helmholtz equation and their phase properties are described by strikingly similar equations. To push the analogy further, equations (2.22) and (2.23), tell us that a static potential acts as a medium with an effective refractive index of

$$n(\mathbf{x}) = \frac{k(\mathbf{x})}{k_0} = \sqrt{\left(1 - \frac{V(\mathbf{x})}{E}\right)} \quad (2.35)$$

where $k_0 = \sqrt{(2ME/\hbar^2)}$.

There are some important differences. For example, atomic de Broglie waves are inherently dispersive, whereas photons propagate in vacuum non-dispersively. Using the definitions for phase velocity, $k \equiv \omega/v_P$ and $v_G \equiv \partial\omega/\partial k$, we have

$$v_P = \frac{1}{\hbar} \frac{E}{k} = \frac{\hbar k_0^2}{2Mk} = \frac{1}{n} \sqrt{\frac{E}{2M}}, \quad (2.36)$$

$$v_G = \frac{1}{\hbar} \frac{\partial E}{\partial k} = \frac{\hbar k}{M} = n \sqrt{\frac{2E}{M}}. \quad (2.37)$$

The group velocity v_G is identified with the wave packet velocity while the velocity of the phase fronts v_P are associated with (2.33). Note that the product $v_P v_G$ is independent of n .

As a simple application of the atom optics formalism, consider a wave packet moving along the z -direction and incident onto a parabolic potential along the x -axis. If $V < 0$, the index of refraction $n > 1$, and the potential focuses the wave packet. Using the Feynman propagator description of quantum mechanics, one traces out each of trajectories for each space time point $(\mathbf{x}, t)$. As each part of the wave packet traverses through the “thin lens” defined by this potential, each path receives an impulse $F\delta t$ that is linearly proportional to the lateral displacement from the center of the lens. In the paraxial approximation, these impulses cause all of the particle trajectories to converge at the “focal point” of the lens.

One can also understand why the de Broglie wave has to be dispersive. Since $k > k_0$ in the region where $V < 0$, the shorter wavelength delays the number of cycles of phase at some point past the potential. Similarly, the part of the atom that goes through the center of the lens will arrive sooner since particles increase their speed when they roll into a potential well.

In real experiments, we do not have plane waves and one must consider wave packets with a finite velocity spread. For many types of atom interferometers, this velocity spread poses serious limitations on the fringe visibility analogous to finite longitudinal and spatial coherence of a light source in optical interferometers [11]. As an example, consider a Young’s double slit interferometer. Assume a single slit (or series of slits) creates a beam of atoms propagating in the x -direction with negligible spatial incoherence, but the thermal beam has a momentum spread

$$\Psi(\mathbf{x}, t) = \int_{-\infty}^{+\infty} \frac{d\mathbf{k}}{(2\pi)^3} a_k \exp[i(\mathbf{k} \cdot \mathbf{x} - E_k t/\hbar)]. \quad (2.38)$$

We are implicitly assuming that the atomic system can be described by a coherent wave packet, and take as an example, a_k as given by

$$a_k = \frac{(4\pi)^{1/4}}{\sigma_k^{1/2}} \exp[-(k - k_0)^2/2\sigma_k^2]. \quad (2.39)$$

The wave packet will move with a group velocity $v_G = \hbar k_0/M$ and expand with a free space dispersion given by $E_k = \hbar^2 k^2/2M$. After a time t , it will have expanded to

$$\sigma_x^2(t) = \frac{1}{\sigma_k^2} + \frac{\hbar^2 t^2}{M^2} \sigma_k^2. \quad (2.40)$$

At a distance L further down stream from the double slit, a detector records the arrival of atoms at different positions y normal to the slits. At the slit, the phases of the two wave packets overlap perfectly, but at a position y the wave packets are longitudinally displaced from each other by $\pm l = d/\text{Ly}$. The probability to detect an atom at position y is proportional to

$$\int |\Psi(x-l, t) + \Psi(x+l, t)|^2 dx. \quad (2.41)$$

For our Gaussian wave packet, the interference term is

$$\int \Psi^*(x-l, t) \Psi(x+l, t) dx = \frac{1}{4} \exp(-\sigma_k^2 l^2) \exp(2ik_0 l). \quad (2.42)$$

Note that there is no time dependence in (2.42), so that the quantum spreading wave packet does not affect the interference pattern.

This result is general and holds even if the atomic source is a statistical mixture of random phases. The reason is because any pair of wavefunctions that time evolve together undergo the same unitary transformation $U(t) = e^{-iHt/\hbar}$ and

$$\langle \Psi_1(t) | \Psi_2(t) \rangle = \langle \Psi_1(0) | U(t)^\dagger U(t) | \Psi_2(0) \rangle = \langle \Psi_1(0) | \Psi_2(0) \rangle. \quad (2.43)$$

The intensity at the position y is then proportional to

$$I(y) = |\Psi_{\Gamma_1} + \Psi_{\Gamma_2}|^2 = \frac{I_0}{2} \left[1 + \exp\left(-\frac{\sigma_k^2 d^2}{4L^2} y^2\right) \cos\left(\frac{k_0 d}{L} y\right) \right]. \quad (2.44)$$

The fringe visibility fades with the longitudinal separation of the two wave packets $\pm \delta x = d/(2 \text{Ly})$

$$\mathcal{V}(\delta x) \equiv \frac{I_{\max} - I_{\min}}{I_{\max} + I_{\min}} = \exp(-\sigma_k^2 \delta x^2). \quad (2.45)$$

Thus, the interference fringes will begin to disappear as soon as the center of mass wave packet separation begins to exceed the coherence length $l_{\text{coh}} = 1/\sigma$. While the spatial overlap arising from dispersion is a necessary condition for observing interference, it is not sufficient. We shall see that optical pulse beam splitters do not have this limitation and are far more tolerant of both spatial and longitudinal coherence.

2.5 Interference with combined internal and external degrees of freedom

The formalism presented in Section 2.1 was originally developed for rf and microwave excitation. In those cases, the lateral dimensions of an atomic beam are much smaller than the wavelength of the electromagnetic waves. Consequently, all atoms passing through two traveling microwave fields will interact with nearly the same relative phase. Furthermore, the position of the atoms can be decoupled from the internal states and is considered to be a classical variable.

If one applies the Ramsey technique to the optical domain, the spatial variation of the electric field and the momentum recoil of the atom when it absorbs a photon has to be considered. Also, the spatial extent of the atomic source and the spread of transverse momenta have to be included. For example, imagine an atomic wave packet irradiated by a $\pi/2$ pulse that generates two packets. The two packets will begin to diverge with some recoil velocity, and at some later time, the two wave packets may no longer overlap when the second $\pi/2$ pulse is applied. If this is the case, Ramsey fringes will not be observed. Alternatively, an atomic source with very low transverse velocity spread would have atoms with de Broglie wavelengths that exceed the wavelength of the light. In this case, the semiclassical approximation breaks down and the “position of the atom” relative to a particular crest of the wave has no meaning.

One approach to analyzing atom interferometers is to consider explicitly the propagation of spatial wave packets as in Section 2.2. In this approach, the interferometer phase shifts are calculated combining a set of phase-shift rules for the atom-light interaction points with the phase shifts associated with the free-space propagation [4, 13, 14, 16]. These results have been generalized to account for AC Stark shifts in two-photon transitions by Weiss *et al.* [15].

As an alternate approach to the wave-packet description of the atomic trajectories, one can begin with a quantum treatment where the atomic wave packets are taken to be the sum of momentum plane-wave states. The momentum transfer due to the interaction of the electromagnetic field (*e.g.*, single-photon absorption, stimulated Raman transition, or adiabatic transfer) are calculated for a given plane-wave component and the integral over all of the momentum states in the atomic ensemble is performed last. In this basis, each of the atomic states is described in terms of a tensor product of the Hilbert space describing the internal energy state of the atom and the Hilbert space describing the external degrees of freedom,

$$\begin{aligned} |e, \mathbf{p}_e\rangle &= |e\rangle \otimes |\mathbf{p}_e\rangle, \\ |g, \mathbf{p}_g\rangle &= |g\rangle \otimes |\mathbf{p}_g\rangle. \end{aligned} \quad (2.46)$$

The Hamiltonian becomes

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} + \hbar\omega_e|e\rangle\langle e| + \hbar\omega_g|g\rangle\langle g| - \mathbf{d} \cdot \mathbf{E} \quad (2.47)$$

where $\hat{\mathbf{p}}$ operates on the momentum portion of the basis states. The interaction term is modified to include the spatial dependence of the electric field

$$\mathbf{E} = \mathbf{E}_0 \cos(\mathbf{k} \cdot \mathbf{x} - \omega_L t + \phi). \quad (2.48)$$

The new terms of the electric field operator, $e^{i\mathbf{k} \cdot \mathbf{x}}$ can be rewritten with the closure relation

$$\begin{aligned} 1 \cdot e^{\pm i\mathbf{k}_L \cdot \mathbf{x}} &= \int d^3\mathbf{p} e^{\pm i\mathbf{k}_L \cdot \mathbf{x}} |\mathbf{p}\rangle\langle\mathbf{p}| \\ &= \int d^3\mathbf{p} |\mathbf{p} \pm \hbar\mathbf{k}_L\rangle\langle\mathbf{p}|. \end{aligned} \quad (2.49)$$

The last step in equation (2.49) uses the fact that $e^{\pm i\mathbf{k}_L \cdot \mathbf{x}}$ is the translation operator of the momentum eigenstate $|\mathbf{p}\rangle$. We see explicitly how the spatial dependence of the electric field in the momentum basis formally gives us the well known result: the absorption or emission of a photon of wave vector $\mathbf{k}$ changes the atom's total momentum from $\mathbf{p}$ to $\mathbf{p} + \hbar\mathbf{k}_L$. This one-to-one correspondence between the internal and external degrees of freedom implies that the basis states simplify to $|g, \mathbf{p}\rangle$ and $|e, \mathbf{p} + \hbar\mathbf{k}_L\rangle$ for each momentum $\mathbf{p}$.

Following the development of the Ramsey case without photon recoil, equation (2.9), we transform into the rotating frame and use the rotating wave approximation (different “rotations”!), to get the Hamiltonian

$$\hat{H}_R = \left\{ \frac{\hat{\mathbf{p}}^2}{2M} + \frac{\hbar}{2} \begin{bmatrix} -\delta & \Omega_{eg} e^{i(\mathbf{k}_L \cdot \mathbf{x} - \phi)} \\ \Omega_{eg}^* e^{-i(\mathbf{k}_L \cdot \mathbf{x} - \phi)} & \delta \end{bmatrix} \right\}. \quad (2.50)$$

The time evolution of the ket can be written in terms of slowly varying coefficients $c_{e, \mathbf{p} + \hbar\mathbf{k}}(t)$ and $c_{g, \mathbf{p}}(t)$

$$|\Psi(t)\rangle = \begin{bmatrix} c_{e, \mathbf{p} + \hbar\mathbf{k}}(t) e^{-i\left(\omega_e + \frac{|\mathbf{p} + \hbar\mathbf{k}|^2}{2M\hbar}\right)t} \\ c_{g, \mathbf{p}}(t) e^{-i\left(\omega_g + \frac{|\mathbf{p}|^2}{2M\hbar}\right)t} \end{bmatrix}. \quad (2.51)$$

The detuning now has additional terms

$$\delta = \omega_L - \left(\omega_{eg} + \frac{\mathbf{p} \cdot \mathbf{k}}{M} + \frac{\hbar|\mathbf{k}|^2}{2M} \right) \quad (2.52)$$

corresponding to the Doppler shift $\mathbf{p} \cdot \mathbf{k}_L/M$ and the photon-recoil shift $\hbar|\mathbf{k}_L|^2/2M$.

When a photon of momentum $\hbar\mathbf{k}$ puts an atom into a coherent superposition of two energy states, the recoil will cause the parts of the atom in each of its internal states $|g\rangle$ and $|e\rangle$ to separate with a velocity $\mathbf{v}_r = \hbar\mathbf{k}_L/M$. If these two wave packets are to interfere at some later time, they must be made to spatially overlap. If optical photons are used in an atomic fountain, the recoil distance can approach a centimeter, much larger than the spatial coherence of the atomic source. Thus, the application of equations (2.9) as modified by equations (2.51) and (2.52) must also consider the spatial overlap of wave packets. As a simple example, the simple Ramsey $\pi/2 - \pi/2$ pulse sequence will not produce interference fringes.

More complicated pulse sequences are needed to bring the parts of the atom, which separate during the first $\pi/2$ pulse, back together again at some later time. The simplest optical pulse sequence that recombines the atomic wave packets is the $\pi/2 - \pi - \pi/2$ pulse sequences shown in Figure 1a, and first demonstrated by Kasevich and Chu [4, 17]. The first $\pi/2$ pulse acts as a beam splitter, introducing a velocity difference $\mathbf{v}_r = \hbar\mathbf{k}/m$ between the two wave packets. After a time T , the π pulse acts as a mirror and redirects the two wave packets so that they overlap at the time $2T$ of the second $\pi/2$ pulse. The momentum states making an atomic transition will receive that same momentum transfer and thus register the same net interferometer phase shift for this pulse sequence. This is true even if the inhomogeneous velocity distribution is sufficiently broad that the spectral width of the π pulse ($\delta\omega \simeq 1/\tau$) is less than the Doppler-broadened linewidth.

This statement is proved rigorously using the formalism presented here. We use equation (2.50) to analyze a $\pi/2 - \pi - \pi/2$ pulse sequence. The result for $\delta = 0$ is that we recover equation (2.19). To generalize the result slightly, we now take $0 < |\delta| \ll \Omega_r$, so that $\cos\theta \simeq 0$ and $\sin\theta \simeq 1$. For a more complete treatment including small deviations from ideal pulse areas and detunings that cause AC Stark shifts, see Weiss *et al.* [15]. The unitary Bloch rotation operator $\hat{U}$ becomes

$$\hat{U}_R = \begin{bmatrix} e^{-i\delta\tau/2} \cos\left(\frac{\Omega_r\tau}{2}\right) & -ie^{-i\delta\tau/2}e^{-i(\delta t_0+\phi)} \sin\left(\frac{\Omega_r\tau}{2}\right) \\ -ie^{i\delta\tau/2}e^{i(\delta t_0+\phi)} \sin\left(\frac{\Omega_r\tau}{2}\right) & e^{i\delta\tau/2} \cos\left(\frac{\Omega_r\tau}{2}\right) \end{bmatrix}. \quad (2.53)$$

Consider an atom initially in $|g, \mathbf{p}\rangle$. A crucial component of light-pulse atom interferometers is the phase of the atom relative to the driving fields. Suppose that the laser detuning δ is constant for the entire pulse sequence and phase ϕ for each pulse may vary. We will later show in Section 3.2.2 that phase shifts accrued during the time the light is off are the same for each path. Successive applications of (2.53) for a $\pi/2$ pulse at t_1 , a π pulse

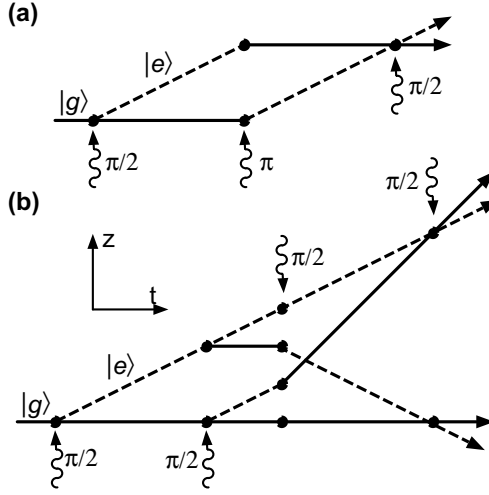


Fig. 1. Recoil diagrams for two optical pulse atom interferometers. The vertical axis is the position z of an atom relative to a reference frame freely falling along the initial trajectory of the atom. Solid and dashed lines indicate paths for which the atom is in $|g\rangle$ and $|e\rangle$, respectively. The vertices are points of interaction with light pulses, with $\mathbf{k}_{\text{eff}}$ indicated by the direction of the arrows. (a) The $\pi/2 - \pi - \pi/2$ geometry used for the g measurement. (b) The Ramsey-Bordé sequence used for the photon recoil measurement. Note that the orientation of $\mathbf{k}_{\text{eff}}$ is reversed for the second pair of $\pi/2$ pulses.

at $t_2 = T + \tau/2 + t_1$ and a $\pi/2$ pulse at $t_3 = 2T + 3\tau/2 + t_1$ yields

$$c_{e,\mathbf{p}+\hbar\mathbf{k}}(t_3 + \tau/2) = -\frac{i}{2}e^{-i\delta\tau/2}e^{-i[\delta t_2 + \phi(t_2)]}\left(1 - e^{i\delta\tau/2}e^{-i\Delta\phi}\right), \quad (2.54)$$

where

$$\Delta\phi = \phi(t_1) - 2\phi(t_2) + \phi(t_3). \quad (2.55)$$

At each time t_i , $\phi(t_i)$ is the phase of the light relative to the atom, referenced to the phase at some fixed time point. The probability of finding the atom in the excited state is

$$|c_{e,\mathbf{p}+\hbar\mathbf{k}}(2T + 2\tau)|^2 = \frac{1}{2}[1 - \cos(\Delta\phi - \delta\tau/2)]. \quad (2.56)$$

Note that $\Delta\Phi \equiv \Delta\phi - \delta\tau/2$ is not a function of the momentum so that atoms (or parts of one atom) in different momentum states will contribute coherently to the interference signal. Consequently, the phase shift of a sum over a large number of momentum states (*i.e.*, a wave packet), will be

given by this equation. For the pulse times given above, if the atoms see a constant detuning and if the phase of the driving light field is not changed, then $\Delta\Phi = \delta\tau/2$, so by equation (2.56), the atom will be found in the ground state after the last pulse. The atomic population will be modulated if the relative phase of the pulses relative to the atoms is changed. This effect is the basis for inertial force measurements and the photon recoil measurement described in the following sections.

This pulse sequence was first used in nuclear magnetic resonance (NMR) studies to compensate for the inhomogeneous spread of resonance frequencies in the NMR sample. Nuclear spins sitting at different sites of a solid have different resonance frequencies. If a $\pi/2 - \pi/2$ pulse sequence is used, the inhomogeneous spread of frequencies would wash out the fringes. On the other hand, a π pulse sandwiched in between the two $\pi/2$ pulses would cause the spins to re-phase. In the absence of the second $\pi/2$ pulse, a pulse would be emitted from the sample in the form of a “spin echo”. When applied to atom interferometry, this pulse sequence does an equivalently beautiful thing: it compensates for the inhomogeneous velocity width of the atomic sample so that the fringe visibility does not require exceptionally high longitudinal or spatial coherence.

In terms of the Feynman formulation of quantum mechanics, a sample of atoms with a spread of momentum states will have many wavefunctions at space-time points $\Psi(\mathbf{x}_a, t_a), \Psi(\mathbf{x}'_a, t'_a), \dots$ contributing to the wavefunction $\Psi(\mathbf{x}_b, t_b)$, since each of the different space time points $(\mathbf{x}_a, t_a), (\mathbf{x}'_a, t'_a), \dots$ with different momenta can end up at point $(\mathbf{x}_b, t_b)$. The phase difference of all of these paths are the same, even in the presence of a uniform gravitational field. Thus, this type of atom interferometer can produce almost 100% fringe visibility, even with mediocre longitudinal coherence. As compared with interferometers based on microstructures which require high longitudinal coherence, optical pulse interferometers have higher fringe contrast with simultaneously higher atom fluxes.

The first optical pulse interferometer considered used a pulse sequence consisting of one pair of $\pi/2$ pulses followed by a pair of oppositely directed $\pi/2$ pulses as shown in Figure 1b is another pulse scheme used to redirect the trajectories of the atoms [18,19]. This pulse sequence was originally used to extend the Ramsey separated oscillatory field technique to the optical domain for the purpose of constructing an optical clock. Eight years later, Bordé realized that this pulse sequence generates an atom interferometer with spatially separated wave packets [20]. We have used this pulse sequence to measure the recoil velocity of an atom which then yields a value for $\hbar/m$ [15,21]. The analysis of this pulse sequence is very similar to the analysis for the $\pi/2 - \pi - \pi/2$ sequence. The details of this type of interferometer will be discussed in Section 5.

3 Beam splitters and interferometers

The heart of any interferometer are the beam splitters. These components have to divide each atom into a superposition of (at least) two coherent states and then return the two parts back together while maintaining the quantum coherence. A number of coherent beam splitters have been demonstrated, ranging from micro fabricated structures, crystalline or magnetically patterned surfaces, standing waves and optical pulses of light.

3.1 Interferometers based on microfabricated structures

A key technology used in the demonstration of these types of interferometers was the ability to fabricate free-standing diffraction gratings. Silicon nitride gratings (now commercially available) on the order of 100–200 nm thick and with a 200 nm period can be made with better than 10 nm accuracy over an area of 0.8 mm $\times$ 0.8 mm. The primary advantage of an interferometer based on physical transmissions gratings is that the same gratings will work for any atom or molecule.

A serious disadvantage is the low atom throughput. The theoretical maximum fringe contrast for an atom interferometer using three equally spaced transmission diffraction gratings (obtained by optimizing the open fraction of the gratings) is 67%, provided one uses a very well collimated atomic beam. Up to 50% fringe contrast has been observed, but in order to achieve this contrast, the aperture sizes have to be chosen so that only $\leq 1\%$ of collimated atomic beam detected [22]. This disadvantage has prompted Clauser [23] and to consider another class of interferometers that use physical gratings, but depend on the so-called “Talbot-Lau” effect instead of the better-known Fraunhofer diffraction. In a first version of the Talbot interferometer, the atomic current was demonstrated to be orders of magnitude higher for a given source brightness [23].

In the case of transmission gratings, the atom is either adsorbed by the grating or left alone, so that the sole effect of the grating is to impress a spatial modulation on the wave function that only modifies the external degrees of freedom of the state vector. In the case of an optical potential, the atom can make a transition to another internal quantum state. (This aspect of atom interferometry is not an issue with photons, electrons or neutrons.)

Since matter waves and optical waves are both described by the same Helmholtz equation (2.22) with k -vector defined as (2.23), the diffraction of matter waves and light by microstructures are essentially equivalent. However, we will use a description of matter wave interferometer [24] that departs from the usual description found in standard electromagnetic text books in order to introduce the Talbot-Lau effect.

Consider an atom wave propagating in the z direction that is partially masked by a diffraction grating with some periodic structure $\eta(x) = \eta(x+a)$, where a is the period of the grating. Immediately after passing through the grating, the wavefunction $\Psi(x) = \eta(x)$, which can be written as the sum of plane wave states

$$\Psi(x) = \eta(x) = \sum_k \eta_k e^{-ikx}. \quad (3.1)$$

Translational symmetry $\eta(x) = \eta(x \pm na)$ with n an integer demands that

$$\sum_k \eta_k e^{-ikx} = \sum_k \eta_k e^{-ik(x+na)} = \sum_k \eta_k e^{-ikx} e^{-inka}. \quad (3.2)$$

For this statement to be true for all x and $\pm na$, k must take on integer values $k = nG = (2\pi/a)n$. $G = 2\pi/a \sim k_L$ is sometimes referred to as the “reciprocal lattice vector”. Thus,

$$\eta(x) = \sum_n \eta_n e^{in k_L x}. \quad (3.3)$$

We rewrite this expression by multiplying both sides by $e^{-ikx}/\sqrt{2\pi}$ and integrating over all space to get

$$\begin{aligned} \tilde{\Psi}(p) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \eta(x) e^{-ikx} dx \\ &= \frac{1}{\sqrt{2\pi}} \sum_n \eta_n \int_{-\infty}^{+\infty} e^{i(n k_L - k)x} dx \\ &= \frac{1}{\sqrt{2\pi}} \sum_n \eta_n [2\pi \delta(n k_L - k)] \\ &= \sqrt{2\pi} \eta_k. \end{aligned} \quad (3.4)$$

Equation (3.4) tells us that the momentum distribution and hence, the diffraction pattern at infinity, is the Fourier transform of the aperture transmission function. This result is the well-known Fraunhofer approximation to the Fresnel-Kirchhoff diffraction integrals.

Note that we assumed the periodic lattice only changed the momentum component along x , normal to the atomic beam and the momentum component in the z direction remains unchanged and $k_z \gg k_x$. This approximation is sometimes referred to as the “Raman Nath” or “thin grating” regime. It is valid if the interaction time τ_{int} with the beam splitter is short and energy has to be conserved to the extent that $\Delta E \leq \hbar/\tau_{\text{int}}$. Equation (3.4) tells us that a large number of momentum states are populated after the interaction. For long interaction times, energy must be conserved

and the atoms scatter predominantly into one diffraction order. This “thick grating” regime is also known as Bragg scattering.

Combining (3.1) and (3.4), the Fourier transform of $\Psi(x)$ is given by

$$\tilde{\Psi}(p) = \sqrt{2\pi\hbar} \sum_n \eta_n \delta(p - m\hbar k), \quad (3.5)$$

where

$$\eta_n = \int \frac{dx}{a} e^{-imkx} \eta(x) \quad (3.6)$$

is the Fourier coefficient.

One way to derive an expression for the interference pattern some distance downstream from the microstructure grating is convert displacement into a time evolution of the system expressed in a convenient basis set. The classical motion of the atoms in the z direction gives us the needed correspondence between distance and the time.

$$t = z/u, \quad (3.7)$$

where $u = p_z/M$ and M is the atomic mass. For each u , we use equation (3.4) to get the time evolution of the momentum space wave function

$$\tilde{\Psi}(p, t) = e^{-i\epsilon_p t/\hbar} \tilde{\Psi}(p) = \sqrt{2\pi\hbar} \sum_m \eta_m \exp[-im^2\omega_k t] \delta(p - m\hbar k), \quad (3.8)$$

where $\epsilon_p = p^2/2M$ is the kinetic energy of an atom with momentum p . We see that the periodic grating constraints the time evolution to occur as multiples of m^2 of the recoil frequency $\omega_r = \hbar k^2/2M$.

In the space representation,

$$\begin{aligned} \Psi(x, t) &= \int_{-\infty}^{+\infty} \frac{dk}{\sqrt{2\pi}} e^{ikx} \tilde{\Psi}(p, t) \\ &= \sum_m \eta_m \exp[imkx - im^2\omega_r t]. \end{aligned} \quad (3.9)$$

The interference of the various amplitudes in (3.9) as a function of the time t or the distance x was first predicted by Chebotayev *et al.* [25] and observed by Chapman *et al.* [26].

After a “Talbot” time $t_T \equiv 2\pi/\omega_r$ or “Talbot” distance $L_T \equiv ut_T = 2d^2/\lambda_{dB}$, the atomic wave function rephases to produce an image of the amplitude function of the transmission grating. This effect is discovered in optics by Talbot in 1836. One can also show [24] that a self-image of the grating, shifted along x by half a period, appears at distances $L_T/2$. At distances L_T/n higher order atomic gratings are formed.

So far our analysis of these diffraction effects tacitly assumed that the angular divergence θ_b of the atomic beam is less than a/L_T , where a is the grating period. Otherwise the diffraction patterns associated with the different velocity sub-groups would wash out the overall diffraction pattern. For typical beams, this corresponds to $\theta_b < 10^{-4} - 10^{-5}$ rad. It is possible to circumvent this restriction and increase the usable beam flux by employing an “echo-like” technique analogous to the spin echo techniques used in NMR.

The “spin-echo” technique is based on an atomic beam passing through two identical diffraction gratings separated by a distance L . It turns out that the combined quantum diffraction and geometrical shadowing give a dephasing and rephasing which are unchanged from the classical case. Thus, this type of interferometer should be able to allow a less collimated (and hence higher flux) beam to be used [27]. The higher periodicities increase the interferometer sensitivity, but at the expense of fringe contrast. For further details, the reader is referred to the references cited in this section.

3.2 Interferometers based on light-induced potentials

3.2.1 Diffraction from an optical standing wave

Next, we consider an atomic beam propagating along the $\mathbf{z}$ -axis entering an optical standing wave

$$E_L = E_0(z) \cos(k_L x + \pi/4) \cos \omega_L t. \quad (3.10)$$

As in Section 3.1, we will assume that the atomic kinetic energy is large compared with the atom-light interaction energy. Under these conditions, the group velocity of the packet remains constant and the change in z is turned into a time dependence $t = u/z$. The interaction Hamiltonian (2.50) then becomes

$$\hat{H}_R = \frac{\hbar}{2} \begin{bmatrix} -\delta & \Omega_{eg}(t) \cos(k_L x + \pi/4) \\ \Omega_{eg}(t)^* \cos(k_L x + \pi/4) & \delta \end{bmatrix}. \quad (3.11)$$

Analogous to (2.15), the new eigenstates (“dressed states”) have energies

$$\begin{aligned} U_{\pm}(x, t) &= \pm \frac{\hbar}{2} \sqrt{\delta^2 + \Omega_{eg}^2(t) \cos^2(k_L x + \pi/4)} \\ &\sim \pm \frac{\delta}{2} \pm \frac{\Omega_{eg}^2(t)}{4\delta} (1 - \sin 2k_L x), \end{aligned} \quad (3.12)$$

where the last step is for detunings where $\delta \gg \Omega_{eg}$. Under these circumstances, an atom in the ground state $|g\rangle$ will evolve adiabatically into one of the dressed states $|\pm, n(\mathbf{x})\rangle$ which now has its de Broglie frequency ω modulated by the optical potential. After the atom passes through the standing

wave potential, its wave function acquires a phase shift given by

$$\begin{aligned}\Psi(x) &= \Psi_0 \exp\left(-i \int_t U_{+,n}(x, t') dt' / \hbar\right) \\ &\sim \Psi'_0 \exp\left(i \frac{\Omega_{eg}^2}{4\delta} \sin(2k_L z t)\right).\end{aligned}\quad (3.13)$$

Once we know the real space wave function $\Psi(x)$, the momentum distribution (or in the real space amplitude in the Fraunhofer diffraction limit) is given by the Fourier transform of $\Psi(x)$. This type of diffraction was first demonstrated by Pritchard and collaborators [22, 28].

3.2.2 Interaction of atoms with light in the sudden approximation

In the previous section, we saw how a plane wave incident on a standing wave will have its phase spatially modulated by an optical potential. The differences in the phase were caused by the adiabatic evolution (3.13) of an atom from $|g\rangle$, to the dressed state $|+, n\rangle$, and then back to the initial state $|g\rangle$.

Beamsplitters based on optical pulses can be considered to be at the other extreme: the application of a potential in the sudden approximation. An atom in state $|g\rangle$ is suddenly irradiated with an optical field. In order to calculate the time evolution of the system, we project the initial state onto the new eigenstates (the dressed states) of the system, which in turn evolve in time as described in equations (2.18) and (2.19). The Rabi oscillations between excited and ground states are due to the interference between the two dressed states which experience different potentials and propagate with different phase and group velocities.

In atom interferometry, the motion of the atom with respect to the phase of the light inducing the transition is at the heart of the calculation of the fringe pattern. At the most basic level, consider a fixed atom irradiated by two Ramsey pulses separated by a time t . The atomic phase that accrues during that time is $\phi_{\text{atom}} = \phi_e - \phi_g = \omega_{eg}t$. In the Ramsey technique, one compares this phase with the optical phase ϕ_L . If the atom has moved by a distance Δz in the same direction as the radiation, the number of cycles of phase the atom will see will be decreased by an amount $\Delta\phi_L = k_L \Delta x$.

We account for this change in phase due to the motion of the atom in the Feynman description quite easily since one evaluates the interaction at each space time point. By applying equations (2.19) and (2.53), the phase term ϕ includes the position (x_1, t_1) of the interaction by adding a phase term $k_L x_1 - \omega_L t_1$. Thus, we derive a simple rule for each interaction with an optical pulse: the atomic wave function is multiplied by one of four factors

depending on the transition.

transition	multiplying factor	
$ g\rangle \rightarrow e\rangle$	$U_{eg} \exp[-i(k_L x_1 - \omega_L t_1 - \phi)]$	
$ e\rangle \rightarrow g\rangle$	$U_{ge} \exp[+i(k_L x_1 - \omega_L t_1 - \phi)]$	(3.14)
$ g\rangle \rightarrow g\rangle$	U_{gg}	
$ e\rangle \rightarrow e\rangle$	U_{ee}	

The transition amplitudes U_{eg} , U_{ge} , U_{ee} and U_{gg} are determined by the pulse areas as given in unitary operator (2.53).

As an example of how one calculates the interference fringe pattern for an optical pulse interferometer, explicitly including the displacement of the atom, we calculate the phase shift for a $\pi/2 - \pi - \pi/2$ pulse sequence. It is clear that the phase shifts due to the free propagation

$$\delta\phi = S_{Cl}/\hbar = \frac{1}{\hbar} \int_{\Gamma} dt \left[\frac{1}{2} M v^2 \right] \quad (3.15)$$

are the same for both paths, due to the symmetry of the interferometer.

Referring to Figure 2 we apply the transition rules to path I to calculate the amplitude for being in the state $|g\rangle$ at time t_3 :

$$\begin{aligned} \Psi(x_3, t_3)|_{\Gamma_I} &= U_{gg} U_{ge} \exp \{ +i[k_L x_{2,I} - \omega t_2 - \phi_2] \} \\ &\times U_{eg} \exp \{ -i[k_L x_1 - \phi_1] \} \Psi(x_1, t_1). \end{aligned} \quad (3.16)$$

Similarly, for path II, the amplitude is

$$\begin{aligned} \Psi(x_3, t_3)|_{\Gamma_{II}} &= U_{ge} \exp \{ +i[k_L x_3 - \omega t_3 - \phi_3] \} \\ &\times U_{eg} \exp \{ -i[k_L x_{2,II} - \omega t_2 - \phi_2] \} \\ &\times U_{gg} \Psi(x_1, t_1). \end{aligned} \quad (3.17)$$

Since

$$k_L(x_3 - x_{2,II}) = k_L(x_{2,I} - x_1), \quad (3.18)$$

the net phase shift for each of the paths due to the light-atom interactions is also zero, provided $\phi_1 = \phi_2 = \phi_3$. At the end of the pulse sequence, the atom is then returned back to the ground state $|g\rangle$.

4 An atom interferometry measurement of the acceleration due to gravity

Now let us consider the phase shift of the interferometer in the presence of gravity. The action along the classical path is now given by

$$\delta\phi = S_{Cl}/\hbar = \frac{1}{\hbar} \int_{\Gamma} dt \left[\frac{1}{2} M v^2 - M g x \right]. \quad (4.1)$$

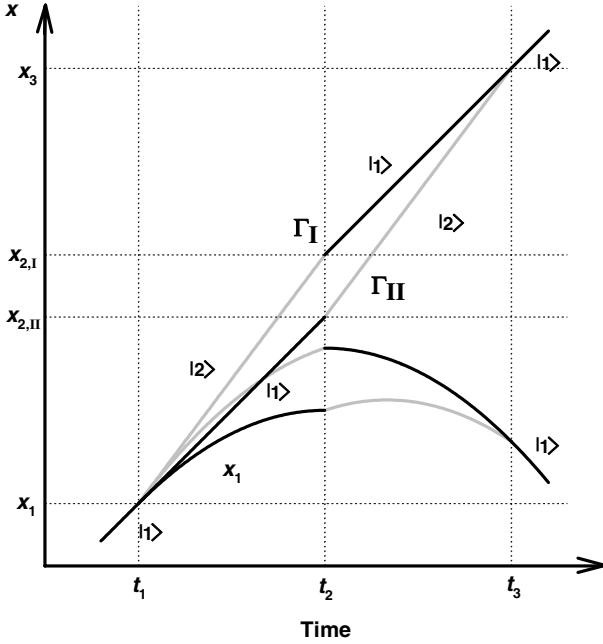


Fig. 2. Phase space diagram of the atom interferometer based on the $\pi/2-\pi-\pi/2$ pulse sequence, showing paths in both absence and presence of gravity. The momentum pulses due to the off-resonant Raman pulses are assumed to be directed upwards. The pulse timing is chosen so that the π pulse is applied near the top of the fountain.

It is a straight forward exercise to show that the evaluation of the action (4.1) for each of the paths is again identical.

There is a non-zero phase difference due to the interaction of the atom with the light. The easiest way to see this is to note that the phase of the optical field only enters into the atomic phase when there is a transition between internal states as given in equations (3.15). Setting $t_2 - t_1 = t_3 - t_2 \equiv \Delta t$, the change in phase shifts relative to (3.18) for each of the two paths is

$$\Delta\phi_I = \Delta\phi_I|_{\text{no gravity}} + k_L \Delta x|_I = +k_L \left(\frac{1}{2} g \Delta t^2 \right) - (\phi_2 - \phi_1) \quad (4.2)$$

$$\Delta\phi_{II} = \Delta\phi_I|_{\text{no gravity}} + k_L \Delta x|_{II} = +k_L \left(2g\Delta t^2 - \frac{1}{2} g \Delta t^2 \right) - (\phi_2 - \phi_3), \quad (4.3)$$

and

$$\Delta\phi \equiv \Delta\phi_{\text{II}} - \Delta\phi_{\text{I}} = k_L g \Delta t^2 + (\phi_1 - \phi_2) - (\phi_2 - \phi_3). \quad (4.4)$$

The origin of the phase shift given by (4.4) is clear from the derivation. An atom at rest will see $\omega_L \Delta t / 2\pi$ oscillations of the applied field during the time interval Δt . On the other hand, if the atom moves a distance Δx in the same direction as the light during the same time Δt , it will see $k_L \Delta x / 2\pi$ fewer oscillations. The interferometer measurement of g compares the phase shift $k_L \Delta x$ an atom experiences during the first part of the free fall time with the phase shift during the second interval of time. The phase shift can also be interpreted in terms of a Doppler shift where the precision of the measurement given by equation (4.4) increases quadratically in Δt . One power of Δt comes from the fact that $\Delta v \sim g \Delta t$ and the other power comes from the fact that the linewidth of the transition varies inversely as the quantum measurement time, $\Delta t \sim 1/(\Delta \nu_{\text{Ramsey}})$.

This analysis also shows that the interferometric measurement of g is a differential measurement: the phase shift of one part of the atom in the second half of the fall is compared to the phase shift of the other part of the atom in the first half of the fall. Thus, a number of potentially troublesome effects such as the AC Stark shift generated by the optical fields as well as phase shifts due to the rf filters, amplifiers, electro-optic and acousto-optic modulators are greatly suppressed by this pulse sequence.

Note that the phase shift is independent of the quantum scale factor $\hbar/M$. This might lead one to think of the phase shift measured by this atom interferometer as “classical” and different from the “quantum” measurement made by a neutron interferometer. We will now show that both the neutron and atom interferometer measurements of g result from the same basic quantum physics. However, an absolute measurement of g with an atom interferometer has the advantage that the interaction of an atom with a laser field is inherently better understood than the interaction of a neutron with a crystal.

In the neutron interferometer literature, the phase shift is usually calculated by dividing the Lagrangian into two terms $L = L_0 + L_1$, where $L_1(t) = Mg z(t)$ is a small perturbation. (See, for example, Greenberger and Overhauser) [29]. To first order, the action can be calculated as the integral of the perturbative action along the unperturbed path determined by L_0 . Evaluation of this integral leads to a net phase shift given by

$$S' \equiv \int_{t_a}^{t_b} L_1 dt \quad (4.5)$$

along the unperturbed path determined by L_0 . (In this simplified treatment, we ignore the complications due to the dynamical scattering of neutrons in a

crystal, the multiple interferometer paths taken by the neutrons and possible mass shifts.) A straightforward evaluation of this integral leads to a net phase shift $\Delta\phi = -(Mg/\hbar) \times (\text{phase space area})$ where the interferometer phase space area is given by $\Delta x \times \Delta t$. The product of $M/\hbar$ and the phase space area are often cited as a measure of the sensitivity of the device.

People who work with neutron interferometers have stressed the significance of a formula where both g and $\hbar$ appear in the same equation. Although this formula explicitly contains g and $\hbar/M$, the area can be written in terms of the momentum transferred by the lattice of wavevector $k_{\text{Latt}} = 2\pi/a$, where a is the interatomic spacing of the lattice plane causing the Bragg scattering. The area is $\Delta x \times \Delta t = (\hbar k_{\text{Latt}}/M)\Delta t \times \Delta t$ so that $\Delta\phi = -k_{\text{Latt}}g\Delta t^2$. Since the neutrons scatter from three portions of the same single crystal of silicon, the relative phases of the three lattice planes $(\phi_1 - \phi_2) - (\phi_2 - \phi_3) = 0$. Thus, this method of calculating the phase shift also gives equation (4.4). Alternatively, the same phase shift can be obtained by the exact calculation where the free evolution is calculated along the true (gravitationally perturbed) path. With this analysis, the $\Delta\phi$ is seen as the phase slip of the neutron with respect to the lattice caused by gravity and is completely analogous to the optical pulse interferometer of Kasevich and Chu [4].

4.1 *Circumventing experimental obstacles*

The above analysis has been over simplified since we assumed that the frequency of the light is constant. In practice, this type of interferometer has been used in an atomic fountain of cold atoms with free fall times up to 2×0.16 seconds, corresponding to a Doppler shift $k_{\text{L}}gt^2$ of several Megahertz. Unless the frequency of the light is changed, atoms that are in resonance with the first laser pulse will be far out of resonance with the remaining pulses. Also, during this time, the states $|1\rangle$ and $|2\rangle$ must be stable against radiative decay. Also, if the frequency of the optical field is not stable during the drift time of the interferometer, the fringes will wash out. Since the measurement time is so long, a change in the optical frequency of a few Hertz will cause the interferometer to cycle through 2π radians. Currently, lasers with this frequency stability do not exist.

Both of these requirements are satisfied if we use stimulated transitions between two (magnetic field insensitive) ground states of the atom separated by a hyperfine splitting. If the two laser beams k_1 and k_2 are counter propagating, the phase shift seen by the atom is given by $(k_1 + k_2) \times \Delta x$, approximately twice the shift relative to a single beam. On the other hand, only the frequency difference of the two beams is critical for the measurement. While it is difficult to control the absolute frequency of light, it is relatively easy to phase lock two laser beams relative to each other, either by generating the second frequency with an electro-optic or acousto-optic

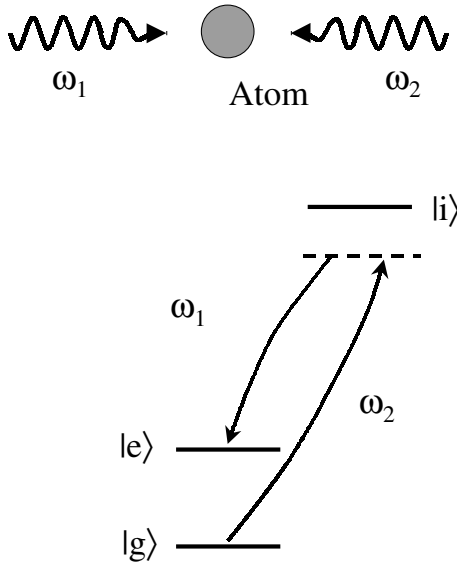


Fig. 3. An atom undergoes a stimulated Raman transition. It absorbs a photon of frequency ω_2 and emits another one (via a stimulated emission) of frequency ω_1 . Since both photons carry momentum, and because momentum has to be conserved in the process, the atom receives a recoil momentum kick.

device or by phase locking two independent lasers to a stable microwave reference. Thus, by inducing a two-photon transition with counter propagating beams, the extraordinary requirement of sub-Hertz optical stability is reduced to the much more modest demand of sub-Hertz microwave stability. This measurement of the acceleration due to gravity converts the measurement of an optical phase change into a microwave measurement relative to a stable microwave reference. The introduction of Raman transitions to induce velocity changes is the closest thing to a free lunch that this physicist has ever encountered.

4.2 Stimulated Raman transitions

In this section, we introduce some of the formalism needed to analyze the atom interferometer phase shifts using Raman transitions. Consider the three-level atom in Figure 3 consisting of two ground-state hyperfine levels $|g\rangle$ and $|e\rangle$ with rf splitting ω_{eg} coupled by optical transitions to an intermediate state $|i\rangle$. Assume the atom is initially prepared in state $|g\rangle$. Two counter propagating beams of frequency ω_1 and ω_2 induce stimulated Raman transitions to level $|e\rangle$ if $\omega_1 - \omega_2 - \Delta\omega_D \simeq \omega_{eg}$, where

$\Delta\omega_D = (\mathbf{k}_1 - \mathbf{k}_2) \cdot \mathbf{v}$. When the beams counter propagate, $\Delta\omega_D \simeq 2\mathbf{k}_1 \cdot \mathbf{v}$, so the transition has a Doppler sensitivity twice that of a single-photon optical transition. For Cs, the two-photon Raman transition has a Doppler sensitivity of 23.5 kHz/(cm/s) when the Raman beams are nearly resonant with the 852 nm optical transition.

We present a brief summary of the theory underlying the two-photon, velocity-sensitive Raman transition. The essential results are: (1) in certain regimes the three-level system can be viewed as a two-level system coupled with an effective Rabi frequency given by the two-photon transition rate; (2) the internal state of the atom is correlated with its momentum; and (3) the two-photon Raman excitation can be modeled by a traveling-wave excitation of frequency $\omega_1 - \omega_2 \simeq \omega_{eg}$ and effective propagation vector $\mathbf{k}_{\text{eff}} \equiv \mathbf{k}_1 - \mathbf{k}_2 \simeq 2\mathbf{k}_1$ for counter propagating beams.

The key assumption in the treatment which follows is that the detuning of the frequencies ω_1 and ω_2 from the optical resonance is large enough that spontaneous emission from the intermediate level $|i\rangle$ can be neglected. When the detuning from the intermediate level is large, the intermediate level can be adiabatically eliminated from the interaction picture Schrödinger equations and the dynamics of the three-level system reduce to those of a two-level system.

The Hamiltonian for the three-level system is

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} + \hbar\omega_e|e\rangle\langle e| + \hbar\omega_i|i\rangle\langle i| + \hbar\omega_g|g\rangle\langle g| - \mathbf{d} \cdot \mathbf{E}. \quad (4.6)$$

In this case the driving electric field contains two frequency components:

$$\mathbf{E} = \mathbf{E}_1 \cos(\mathbf{k}_1 \cdot \mathbf{x} - \omega_1 t + \phi_1) + \mathbf{E}_2 \cos(\mathbf{k}_2 \cdot \mathbf{x} - \omega_2 t + \phi_2). \quad (4.7)$$

The frequencies $\omega_1 \simeq \omega_i - \omega_g$ and $\omega_2 \simeq \omega_i - \omega_e$ while the difference frequency $\omega_1 - \omega_2 \simeq \omega_{eg}$. For counter propagating beams $\mathbf{k}_1 \simeq -\mathbf{k}_2$. We have explicitly neglected spontaneous emission from the off-resonant excitation of the optical transition.

Following the procedure given in Section 2.5 while using the interaction coefficients from equation (2.51) along with an additional coefficient for the corresponding intermediate state $|i, \mathbf{p} + \hbar\mathbf{k}_1\rangle$, one obtains a set of coupled first-order differential equations for $c_{g,\mathbf{p}}$, $c_{i,\mathbf{p}+\hbar\mathbf{k}_1}$, and $c_{e,\mathbf{p}+\hbar\mathbf{k}_{\text{eff}}}$. In the limit where the detunings $\omega_1 - (\omega_i - \omega_g)$ and $\omega_2 - (\omega_i - \omega_e)$ are much larger than the Rabi frequencies, the coefficients $c(t)$ vary slowly compared to the explicitly time-dependent terms. Thus, we can adiabatically eliminate all coefficients for the intermediate states. We are then left with coupled equations for a two-level system in an external driving field. In the spinor representation for $|e, \mathbf{p} + \hbar\mathbf{k}_{\text{eff}}\rangle$ and $|g, \mathbf{p}\rangle$, the Hamiltonian describing this

time evolution is

$$\hat{H} = \frac{\hbar}{2} \begin{bmatrix} \Omega_e^{\text{AC}} & (\Omega_{\text{eff}})e^{-i(\delta_{12}t + \phi_{\text{eff}})} \\ (\Omega_{\text{eff}})e^{i(\delta_{12}t + \phi_{\text{eff}})} & \Omega_g^{\text{AC}} \end{bmatrix}, \quad (4.8)$$

where we define

$$\Omega_e^{\text{AC}} \equiv \frac{|\Omega_e|^2}{2\Delta}, \quad \Omega_g^{\text{AC}} \equiv \frac{|\Omega_g|^2}{2\Delta}, \quad (4.9)$$

$$\delta_{12} \equiv (\omega_1 - \omega_2) - \left(\omega_{eg} + \frac{\mathbf{p} \cdot \mathbf{k}_{\text{eff}}}{m} + \frac{\hbar |\mathbf{k}_{\text{eff}}|^2}{2m} \right), \quad (4.10)$$

$$\Omega_e \equiv -\frac{\langle i | \mathbf{d} \cdot \mathbf{E}_2 | e \rangle}{\hbar}, \quad \Omega_g \equiv -\frac{\langle i | \mathbf{d} \cdot \mathbf{E}_1 | g \rangle}{\hbar}, \quad (4.11)$$

$$\Omega_{\text{eff}} e^{-i\phi_{\text{eff}}} \equiv \frac{\Omega_e^* \Omega_g}{2\Delta} e^{i(\phi_1 - \phi_2)}, \quad (4.12)$$

with the real angle ϕ_{eff} chosen to make Ω_{eff} a positive real number.

Here $\Delta \simeq \omega_1 - (\omega_i - \omega_g)$ is the detuning from the optical resonance as illustrated in Figure 4. As expected, momentum recoil explicitly shows up in the one-to-one correlation between the atom's internal state and its momentum for the two states $|e, \mathbf{p} + \hbar \mathbf{k}_{\text{eff}}\rangle$ and $|g, \mathbf{p}\rangle$ coupled by this Hamiltonian, and the dynamics are governed by the difference frequency $\omega_1 - \omega_2$. The effective detuning δ_{12} from the Raman resonance contains the expected Doppler-shift and recoil-shift terms. The main diagonal elements of the Hamiltonian are the AC Stark shifts of levels $|e\rangle$ and $|g\rangle$. The relative shift of the two levels caused by AC Stark shifts is

$$\delta^{\text{AC}} \equiv (\Omega_e^{\text{AC}} - \Omega_g^{\text{AC}}). \quad (4.13)$$

For simplicity we have neglected contributions to the AC Stark shift from the couplings shown in Figure 4 by the dotted lines. These additional terms can be found in Weiss *et al.* [15].

This Hamiltonian is similar in form to equation (2.9) for a two-level atom except for the AC Stark shift terms on the main diagonal. Given one additional step, it is possible to transform it into a time-independent Hamiltonian of the exact form of $\hat{H}_R$ in equation (2.50) so that the solution for a two-level atom can be directly applied. This extra step is to first make a uniform shift of the energy scale by $-\hbar(\Omega_e^{\text{AC}} + \Omega_g^{\text{AC}})/2$. This anti symmetrizes the main diagonal elements to $\pm \hbar \delta^{\text{AC}}/2$, which can be combined with the $\mp \hbar \delta_{12}/2$ terms that arise in the transformation to the rotating frame. For further details, the reader is referred to Young *et al.* [8].

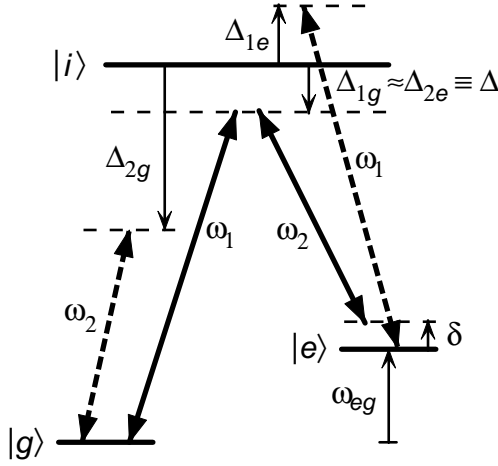


Fig. 4. Schematic representation for a three-level atom. Two light fields at frequencies ω_1 and ω_2 couple states $|g\rangle$ and $|e\rangle$ via the intermediate state $|i\rangle$. The one- and two-photon detunings are Δ and δ , respectively. Additional AC Stark shifts are caused by the interaction of ω_1 and ω_2 with the wrong levels, as indicated by the dashed arrows.

4.3 Frequency sweep and stability issues

Typical free-fall times of an atomic fountain-based atom interferometer is 0.3 seconds. The corresponding velocity change $g\Delta t = 300$ cm/s give a Doppler shift of ~ 4 MHz. Since the linewidth of the transition $\sim 1/\Omega_{\text{eff}} \sim 20$ kHz, the laser frequency $\omega_1 - \omega_2$ of the Raman pulses must be changed in a phase stable manner in order to keep in resonance with the atoms. At the time of our initial experiment, inexpensive rf oscillators did not remain phase locked when the frequency was swept.

Our initial solution [4] was to use three inexpensive digital frequency synthesizers (Stanford Research Systems) running at fixed frequencies ω_1, ω_2 and ω_3 driven by the same master clock signal derived from a Loran-C receiver. An rf switch mixes each of the frequencies with a phase stable high frequency oscillator at 1.77 GHz that then drives an electro-optic modulator. Laser light at frequency ω_L passing through the modulator has rf sidebands at ω_{rf} added to the carrier frequency ω_L . An acousto-optic modulator is used to switch the light onto the atoms at the appropriate time. Note that the Ramsey method is insensitive to the slight amount of timing jitter that may occur in the AO modulator. For the cesium experiment, we used two independent diode lasers that were phased locked to an rf signal constructed by mixing a phase stable 9.2 GHz oscillator with a low frequency digital sweep oscillator. The details of how the feedback loop locked to the correct

frequency were not important as long as the lock was established before the light was turned onto the atoms.

4.4 *Vibration isolation*

The phase shift measurements described above require control of the optical frequencies to a small fraction of one optical cycle during the free-fall time. Vibrations in the laboratory do not affect the motion of the falling atoms, but vibrations of the Raman beam mirrors can perturb the phase of the light field in the interaction region. We have employed two methods for insuring sufficient phase stability of the light field incident on the atoms.

The simplest technique for obtaining phase-stable light fields applies when the two Raman beams at frequencies ω_1 and ω_2 can be allowed to copropagate through all of the same optics until they pass through the interaction region. Since $\mathbf{k}_1$ and $\mathbf{k}_2$ only differ at the $\sim 10^{-5}$ level, the Doppler shifts from vibrations of these mirrors are nearly identical for the two beams, so they cancel with high accuracy in the Raman frequency difference. All of the experiments described in the previous section use velocity-sensitive transitions, which require counter propagating beams. Consequently, a final mirror is used after the interaction region to retro reflect both beams back through the interaction region. If the atoms are moving at a nonzero velocity along the direction of $\mathbf{k}_{\text{eff}}$, then the Doppler shift of the two-photon detuning can be used to select which pair of velocity-sensitive beams drives the transition. Thus, the problem of obtaining stable phase-fronts reduces to vibrationally isolating the final retro-reflection mirror and the motion of an atom is measured relative to the retro-reflecting mirror.

An active vibration isolation system is used to stabilize this mirror. A sensitive, low frequency accelerometer rigidly connected to the reference mirror measures the acceleration of the mirror/accelerometer assembly suspended passively by springs. The acceleration signal is processed through a digital feedback loop to produce a signal to a transducer that reduces the amplitude of the accelerations. The reduction of the accelerometer error signal with the feedback loop closed is reduced by up to a factor of 200 in the frequency range from $\sim 0.01 - 100$ Hz. To actually achieve this level of isolation along $\mathbf{k}_{\text{eff}}$ requires a ~ 1 mrad alignment of the sensor axis to $\mathbf{k}_{\text{eff}}$, and a similarly good alignment of the atomic trajectory below the sensor to avoid problems due to tilt [30].

Although mechanically and electronically easier to implement, the retro-reflection approach has the drawback that extra beams are present in the interaction region. These beams may introduce spurious phase shifts in the atomic coherence due to, for example, the AC Stark effect or mechanical effects from standing-wave potentials. Furthermore, this approach is completely unacceptable when using adiabatic transfer instead of stimulated Raman transitions. In that case, the Doppler shift of the atoms can be

large enough to detune the two-photon resonance for the undesired beam pair, but not the single-photon resonance, so the atoms will incoherently scatter photons from those beams. Consequently, for interferometers using adiabatic transfer, or those using stimulated Raman transitions either near zero velocity or for which the undesired light shifts are unacceptable, ω_1 and ω_2 must be independently directed to the interaction region.

Since the photon recoil measurement uses an atom interferometer based on adiabatic passage, ω_1 and ω_2 must reflect off of several mirrors that are not shared by the two beams, so there is no common-mode cancelation of vibrations. Rather than trying to vibrationally isolate all of these mirrors, we built a stable reference platform suspended immediately above the vacuum chamber on which we measure the beat note of the two Raman laser beams. The Raman frequency difference is then locked to a stable rf source. Since the phase of the light must be stable from the instant that it is pulsed on, it is not sufficient to measure the vibrations by detecting the beatnote between the Raman beams. Instead, we overlap with the Raman beams a cw tracer beam detuned 8 nm from the atomic resonance.

The observed improvement of the g measurement signal-to-noise with active vibration isolation matches to within a factor of two the optimum performance expected from the reduction of the accelerometer error signal. The effect of vibration isolation on fringe contrast has been observed for the photon recoil measurement that is described below. Without vibration corrections, the fringe contrast falls 50% as T is increased to about 1 ms. When vibrations are canceled using the tracer beams, with the active platform isolation disabled, the contrast drops 50% by $T \approx 30$ ms. With the active isolation enabled, the contrast is still over 60% of its initial value at $T = 150$ ms.

4.5 *Experimental results*

Each cycle of the experiment begins by capturing cesium atoms in a magneto-optical trap in a low density vapor cell. After ~ 0.6 seconds, the atoms are further cooled in polarization gradient molasses by shifting the frequencies of the molasses beams from a detuning of 20 MHz to 60 MHz, and then launched upwards by shifting the relative frequencies of the molasses beams. In the final stages of the launch, the light intensity is ramped down in 300 μ s so that the atoms can be adiabatically cooled to still colder temperatures (1.3–1.5 μ K). Since our experiment is not shot noise limited, atoms in the $|F = 3, m_F = 0\rangle$ state within a narrow slice of the initial velocity distribution are selected through a series of stimulated microwave and optical pulses in order to increase the interferometer contrast. Stimulated Raman pulses generated by two phase-locked diode lasers are used to produce the interferometer pulses when the atoms are inside a quadruple magnetic shielded region with a bias field of 2 mG. The population of atoms

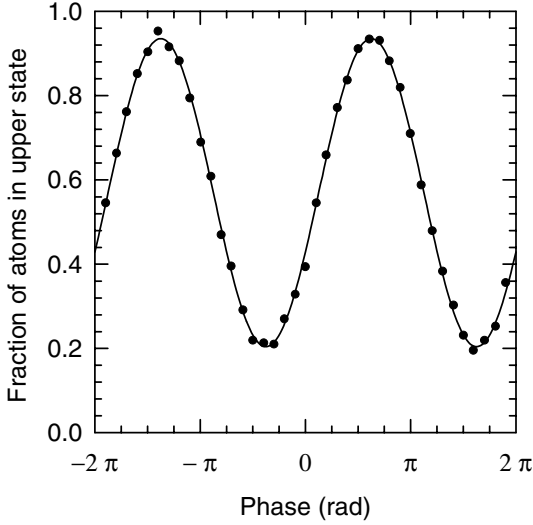


Fig. 5. Typical Doppler sensitive interferometer fringe for $T = 160$ ms. The data shown was taken in one minute and a least squares fit determines the local gravity to an uncertainty of 3×10^{-9} g.

in the $|4, 0\rangle$ state is measured for each launch by recording the fluorescence from the atoms illuminated by circularly polarized light tuned to $F = 4$ ground state to $F' = 5$ excited state transition. Next, the remaining atoms in the $F = 3$ state are transferred to the $F = 4$ state and the fluorescence measurement is repeated in order to measure the total number of atoms that have made it to the detection region.

Figure 5 shows the interferometer fringes for an interferometer time $2T$ of 0.32 seconds. Each data point represents a single launch of atoms. We emphasize the equivalent of 5.9×10^5 cycles of phase have accumulated during the measurement time. The short term stability of the interferometer is $\Delta g/g \sim 3 \times 10^{-9}$ after one minute of data taking. Figure 6 shows the results of over 2 days of continuous data taken with our atom interferometer. The data is plotted with a tidal model that includes only the elastic deformation of the earth and another model that also adds ocean loading effects. Figure 7 shows the difference between the data and the two tidal models. Each data point corresponds to an integration time of 1 minute. The statistical uncertainty for this data is $\Delta g/g \leq 1 \times 10^{-10}$. The long term stability of this interferometer has been demonstrated out to $\sim 10^4$ seconds.

During the course of our experiment we ran a Micro-g Solutions FG5 absolute gravimeter for three days to measure the absolute value of g . This instrument is a Michelson optical interferometer with one arm defined by a

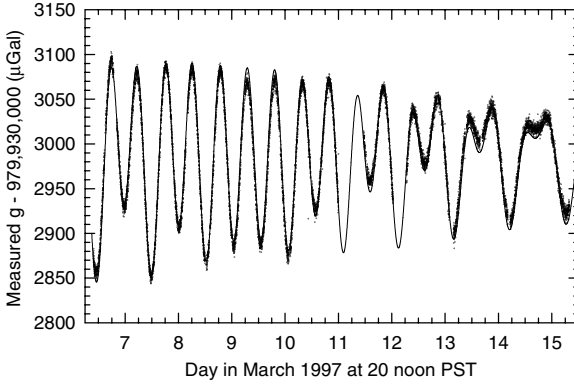


Fig. 6. Gravity data taken over a period of 9 days. The data points correspond to approximately one minute of integration time shown in Figure 5. The solid line is a single parameter fit using a theoretical model of the gravity tides at our measurement site, Stanford, California.

freely falling corner-cube and has a quoted relative uncertainty of 2 parts per billion (ppb). A comparison with the value of g we obtained in a 2-day run shows a difference of (7 ± 7) ppb. This comparison was limited mostly by a 5 ppb uncertainty in our measurement of the local gravity gradient which produces a 3 ppb correction per cm vertical displacement. Direct comparison of the noise of both instruments also showed that our atom interferometer has 4 times higher resolution than the falling corner cube gravimeter.

Table 1 shows the most important identified systematic effects and their associated uncertainties. Other effects, such as magnetic field gradients, wavefront curvature, speckle, dispersion in the air and windows, timing and switching errors in the optical pulses, etc., were experimentally found to be below the 0.1 ppb level and are not listed. We have also estimated relativistic corrections (< 0.1 ppb) and the effect of a changing effective wavevector due to different propagation delays during the interferometer sequence (corrected to an uncertainty of < 0.1 ppb). A summary of the systematic effects can be found in [31].

We have varied the time of the $\pi/2 - \pi - \pi/2$ pulses relative to the time of the launch. We observe a variation in g that quantitatively agrees with a calculated change due to the gravity gradient and the change in the magnitude of the k -vectors of the light. The fit of our data to the calculated curve (residual $\ll 1$ ppb) allows us to set an upper limit to a systematic effect due to any “trajectory effect”. This test also states that the presence of both Raman frequencies ω_1 and ω_2 in the downward and upward traveling beams, which could excite off-resonant coherences that would affect the measured

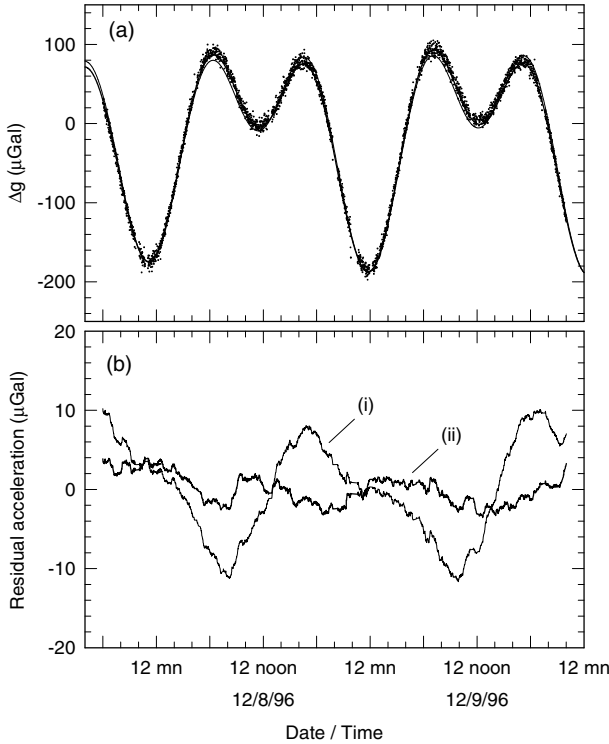


Fig. 7. (a) A measurement of g taken over another two day period. Here we plot two tidal models. (b) The residuals of the data with respect to a tidal model where (i) the Earth is modeled as a solid elastic object, and (ii) where the effects of ocean loading of the Earth is taken into account.

phase shift, is not a significant problem. This potential problem becomes especially acute when the π -pulse is applied when the atoms are near the apogee of their trajectory and would appear as an unaccounted phase shift as the trajectory is varied.

At ppb levels, uncertainties due to environmental effects become significant. The major uncertainties are listed in Table 1. However, these effects are not part of the instrumental uncertainty. The measurement presented here is a million-fold increase in absolute accuracy obtained by atom interferometers. From our study of the systematic effects of this measurement, we feel that further improvements in the control of Coriolis effect, *e.g.*, by rotating the whole system, and ensuring that there is no synchronized noise on the vibration isolator, should lead to a relative uncertainty on the order of one part in 10^{10} .

Table 1. Major known potential systematic effects. Major sources of potential systematic effects are tabulated. Systematic effects that are 0.1 ppb or less are not listed including timing, switching and chirping of pulses, Zeeman and DC Stark shifts, dispersion of light in air, Cs vapor and windows, tilt of Raman beam with respect to the vertical, standing waves effect, leakage light, wavefront curvature and speckle, Berry phase, second order Doppler shift, gravitational redshift and other relativistic effects. Environmental effects, while not part of our instrumental uncertainty, are important for comparing g measured at different times. Other environmental effects include water table correction.

Systematic Error	Uncertainty (ppb)
Instrumental	
RF phase shift	2
Coriolis Effect	2
ac Stark shift	1
Synchronous noise	1
Dependence on pulse timing	1
Retro reflection	0.6
Laser lock offset	0.4
Cs Wavelength	0.3
Gravity gradient	0.2
Cold collision	0.2
Synchronous vibration	0.2
Synchronous fields	0.2
Changing k-vector	0.1
Overall instrumental uncertainty	3.4
Environment	
Pressure correction	1
Ocean loading	1
Other environmental effects	2

5 Interferometry based on adiabatic transfer

The first atom interferometers were constructed using stimulated Raman transitions, which have the many advantages discussed above. Disadvantages of this technique in precision measurements include its sensitivity to spatial inhomogeneity of the laser beams and laser intensity fluctuations, and the systematic errors that can arise from ac Stark shifts. Also, several atom interferometer experiments have sensitivities that can be greatly enhanced by applying multiple light pulses to deliver a large number of photon recoils, but adding more pulses also increases the sensitivity of the interferometer to intensity variations. For a laser beam with a Gaussian

intensity profile, different atoms will sample different intensities so that the π pulse condition cannot be simultaneously met for atoms at all locations in the beam. Increasing the laser beam waist reduces this problem, but also decreases the Rabi frequency (for fixed laser power), which reduces the atom signal size for typical experimental parameters. In the first version of the photon recoil experiment, spatial variation of the beam intensity limited the π pulse transfer efficiency to 85%.

Fluctuations of the beam intensities also cause deviations from the desired π pulse condition. This effect is second order in the fractional intensity noise, but if several pulses are applied, it can still become a significant noise source unless the laser intensities are actively controlled. The most pernicious effects of intensity fluctuations, however, involve ac Stark shifts. With stimulated Raman transitions, ac Stark shifts can make sizable contributions to the atom interferometer phase. Typically, the ac Stark shift of the two-photon transition Ω^{AC} is of the same size as the effective Rabi frequency Ω_{eff} . Consequently, for a single π pulse, the ac Stark shift can cause a phase shift that is a sizable fraction of a complete cycle. The average Stark shift can generally be zeroed by properly adjusting the ratio of beam intensities, but the phase shift remains linearly sensitive to intensity variations and inhomogeneities around the set values. For example, a major source of systematic error in the first photon recoil measurement made by the Stanford group [15] was the ac Stark shift caused by standing waves. The average ac Stark shift had been zeroed in this experiment, but the presence of standing waves caused a strong modulation of the ac Stark shift along the direction of the beam, which caused a systematic shift of the interferometer phase.

An alternate technique for changing the states of atoms and molecules is adiabatic passage, which was first used in magnetic spin resonance [85]. In our current photon recoil experiment, we use an adiabatic passage technique first introduced by Gaubatz *et al.* [32]. In this form of adiabatic passage, time-delayed, on-resonant light fields efficiently transfer atoms between two states. The atoms adiabatically follow an eigenstate of the atom-field interaction Hamiltonian that is never coupled to the excited state. This method yields two important benefits: (1) despite the use of on-resonant light, spontaneous emission can be nearly completely avoided, and (2) the atoms experience very low ac Stark shifts [40]. Population transfer with adiabatic passage was first demonstrated in the optical regime by passing a molecular beam through two displaced Gaussian beams [32]. The possibility of using counterpropagating beams to obtain momentum transfer for use in atom interferometry was quickly pointed out by Marte *et al.* (1991) [34] and by Bordé (1992) [60]. Momentum transfer *via* adiabatic passage was quickly demonstrated by Pillet *et al.* (1993) [36], Lawall and Prentiss (1994) [37], and Goldner *et al.* (1994) [35]. More recently, we have demonstrated

an atom interferometer using adiabatic passage to split, redirect, and recombine the atomic wave packets [39].

5.1 Theory of adiabatic passage with time-delayed pulses

Consider the three-level atom of Figure 4 interacting with counterpropagating laser beams of frequencies ω_1 and ω_2 . For adiabatic passage the single-photon detuning is generally set near zero, so the relaxation rate Γ of the intermediate state $|i\rangle$ cannot be neglected. Its effect can be included by adding to the Hamiltonian of equation (4.6) a non-Hermitian term, as in Oreg *et al.* [38]. The total Hamiltonian is then

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} + \hbar\omega_e|e\rangle\langle e| + \hbar(\omega_i - i\Gamma/2)|i\rangle\langle i| + \hbar\omega_g|g\rangle\langle g| - \mathbf{d} \cdot \mathbf{E}, \quad (5.1)$$

where the electric field is given by equation (4.7). We will neglect here the off-resonant couplings of $|e\rangle$ and $|i\rangle$ by ω_1 , and $|g\rangle$ and $|i\rangle$ by ω_2 , as shown by the dashed lines in Figure 4. (In a real experiment, these couplings are important since they can limit the transfer efficiency and can be the dominant source of ac Stark shifts. The numerical simulations by Weitz *et al.* include these couplings [39]).

We again use the interaction picture. For adiabatic passage, we cannot adiabatically eliminate the population of the excited state as with the off-resonant Raman case, so the interaction state vector has the form

$$|\psi\rangle = \begin{pmatrix} c_{e,\mathbf{p}+\hbar\mathbf{k}_{\text{eff}}}(t) \\ c_{i,\mathbf{p}+\hbar\mathbf{k}_1}(t) \\ c_{g,\mathbf{p}}(t) \end{pmatrix}, \quad (5.2)$$

where $\mathbf{k}_{\text{eff}}$ is the effective wave vector for the two-photon transition. The interaction Hamiltonian is

$$\hat{H}_{\text{int}} = \frac{\hbar}{2} \begin{pmatrix} 0 & \Omega_e^* e^{i(\Delta_2 t - \phi_2)} & 0 \\ \Omega_e e^{-i(\Delta_2 t - \phi_2)} & -i\Gamma & \Omega_g e^{-i(\Delta_1 t - \phi_1)} \\ 0 & \Omega_g e^{i(\Delta_1 t - \phi_1)} & 0 \end{pmatrix}, \quad (5.3)$$

where the single-photon detunings of ω_1 and ω_2 are

$$\begin{aligned} \Delta_1 &= \omega_1 - (\omega_i - \omega_g) + \frac{|\mathbf{p}|^2 - |\mathbf{p} + \hbar\mathbf{k}_1|^2}{2m\hbar}, \\ \Delta_2 &= \omega_2 - (\omega_i - \omega_e) + \frac{|\mathbf{p} + \hbar\mathbf{k}_{\text{eff}}|^2 - |\mathbf{p} + \hbar\mathbf{k}_1|^2}{2m\hbar}, \end{aligned} \quad (5.4)$$

the Rabi frequencies Ω_e and Ω_g are given by equations (4.11), and the two-photon detuning $\delta_{12} = \Delta_1 - \Delta_2$ agrees with the definition given in

equation (4.10). In the zero-detuning case $\Delta_1 = \Delta_2 = 0$, the Hamiltonian of equation (5.3) simplifies to

$$\hat{H}_{\text{int}} = \frac{\hbar}{2} \begin{pmatrix} 0 & \Omega_e^* e^{-i\phi_2} & 0 \\ \Omega_e e^{i\phi_2} & -i\Gamma & \Omega_g e^{i\phi_1} \\ 0 & \Omega_g^* e^{-i\phi_1} & 0 \end{pmatrix}. \quad (5.5)$$

Then for any Ω_e and Ω_g , there exists an eigenvector of $\hat{H}_{\text{int}}$ with eigenvalue zero, given by

$$|\Psi_D\rangle = \begin{pmatrix} \sin\theta e^{-i\phi} \\ 0 \\ \cos\theta \end{pmatrix}, \quad (5.6)$$

where the real angles θ and ϕ are defined by the relation

$$\tan\theta e^{-i\phi} = -\frac{\Omega_g}{\Omega_e} e^{i(\phi_1 - \phi_2)}. \quad (5.7)$$

This eigenvector has two amplitudes for excitation from the two lower levels to the excited state that cancel. Consequently, despite the presence of on-resonance light, an atom in $|\Psi_D\rangle$ will not experience spontaneous emission. This state is consequently referred to as the non coupled, or “dark” state. Since the single-photon detuning is zero, the ac Stark shift for a three-level system is zero even if the transfer is not completely adiabatic [40]. The presence of additional energy levels introduces an ac Stark shift, but if the detuning of these states is sufficient, the ac Stark shift can still contribute much less than one cycle of phase shift to an interferometer during the time of the light pulse. Numerical calculations of transfer efficiencies and ac Stark shifts for realistic experimental parameters have been performed by integrating the time-dependent Schrödinger equation showing that adiabatic transfer using the cesium $P_{1/2}$ excited state is superior to stimulated Raman transitions for both transfer efficiency and ac Stark shifts [40].

If $\Omega_e = \Omega_e(t)$ and $\Omega_g = \Omega_g(t)$, but the variation with time is sufficiently slow that the system can evolve adiabatically, then the steady-state solution of equation (5.6) still applies [41]. To characterize the requirements for adiabaticity, we define an effective Rabi frequency

$$\Omega_0 = \sqrt{\Omega_e^2 + \Omega_g^2}. \quad (5.8)$$

If an atom is in the dark state defined by the light fields at one time, and the dark-state parameters θ and ϕ are varied gradually over a time $\tau \gg 1/\Omega_0$ for $\Omega_0 \gg \Gamma$, or $\tau \gg \Gamma/\Omega_0^2$ for $\Omega_0 \ll \Gamma$, then the atom will follow along in the dark state defined by the light, without undergoing excitation into $|i\rangle$. Note that this adiabaticity criterion does not preclude turning on a single

beam instantaneously, nor suddenly turning both beams on or off together, since none of these operations forces a rapid change of θ or ϕ . On the other hand, if both beams are turned on or off together, care must be taken so that the ratio of two Rabi frequencies in equation (5.6) is maintained.

The population transfer achieved with adiabatic passage is qualitatively very different from the transfer achieved with stimulated Raman transitions. For stimulated Raman transitions, the atomic state vector evolves coherently regardless of the initial state of the system when the light pulse is applied. Consequently, light pulses that take an atom from $|g\rangle$ to $|e\rangle$ will also take an atom from $|e\rangle$ to $|g\rangle$. The effects of adiabatic transfer pulses, however, depend strongly on the initial state of the system. For example, if an atom starts out in $|g\rangle$, then Ω_e must be turned on alone at the beginning of the adiabatic pulse sequence in order to avoid spontaneous emission. If Ω_e alone were applied to an atom initially in $|e\rangle$, then the atom would scatter photons, eventually resulting in an incoherent transfer into $|g\rangle$ *via* optical pumping.

More generally, suppose the state of the atom at time $t = 0^-$ is $|\psi(0^-)\rangle$, and that the laser beams are turned on at time $t = 0$ with phases and intensities defining a dark state $|\Psi_D(0^+)\rangle$. The projection $|\Psi_D(0^+)\rangle\langle\Psi_D(0^+)|\psi(0^-)\rangle$ of the initial atomic state onto the dark state gives the fraction of the initial state that will not scatter photons, and will adiabatically follow the dark state as it slowly changes to $|\Psi_D(t)\rangle$. Assuming that the beam intensities are varied sufficiently slowly that the transfer is completely adiabatic, the coherently transferred part of the wave function immediately after the end of an adiabatic transfer pulse of duration τ is

$$|\psi(\tau^+)\rangle = |\Psi_D(\tau^-)\rangle\langle\Psi_D(0^+)|\psi(0^-)\rangle. \quad (5.9)$$

5.2 Atom interferometry using adiabatic transfer

We now have the tools to construct an atom interferometer based on adiabatic transfer. Figure 8 shows the pulse sequences that, along with their complements formed by interchanging Ω_e and Ω_g , are the basis for constructing atom interferometers using adiabatic passage. The dark state at any time during the sequences is determined by substituting the laser phases and Rabi frequencies into equations (5.6) and (5.7). The net effect of each of these sequences can be determined from equation (5.9), using the dark states $|\Psi_D(0^+)\rangle$ and $|\Psi_D(\tau^-)\rangle$ corresponding to the beam phases and intensities at the beginning and end of the pulse sequence, respectively. In Figure 8a, the initial and final dark states are $|\Psi_D(0^+)\rangle = |g\rangle$ and $|\Psi_D(\tau^-)\rangle = |e\rangle$, so an atom initially in $|g\rangle$ is completely transferred to $|e\rangle$. Reversing the roles of Ω_e and Ω_g provides for the opposite transfer. In Figure 8b, the initial dark state is still $|g\rangle$, but the final dark state is $(|g\rangle + |e\rangle)/\sqrt{2}$, so this sequence transfers an atom in $|g\rangle$ into an equal coherent superposition

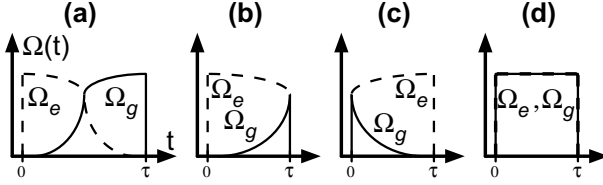


Fig. 8. Pulse shapes used to construct an atom interferometer using adiabatic transfer. Changing the field amplitudes Ω_g and Ω_e with time (a) transfers an atom from $|g\rangle$ to $|e\rangle$, (b) transfers an atom from $|g\rangle$ to $(|g\rangle + |e\rangle)/\sqrt{2}$, (c) transfers an atom from $(|g\rangle + |e\rangle)/\sqrt{2}$ to $|g\rangle$, and (d) projects an atom onto $(|g\rangle + |e\rangle)/\sqrt{2}$, and then leaves it off in that state.

of $|g\rangle$ and $|e\rangle$. A pulse of this type splits a single path into two paths for an atom interferometer. Figure 8c is the time reversal of Figure 8b, so it projects the initial state of the atom onto the equal coherent superposition with phase defined by $|\Psi_D(0^+)\rangle$, and then transfers that fraction of the wave function into $|g\rangle$. This sequence combines or redirects paths in an atom interferometer. Similarly, Figure 8d projects the initial state onto the superposition state defined by $|\Psi_D(0^+)\rangle$, but then leaves the atom still in that superposition state. This pulse sequence is used to split interferometer paths when the atom must start and remain in a superposition state.

The pulse sequences of Figures 8a-d require tailored pulse shapes. These shapes were produced by independently controlling beam intensities using acousto-optic modulators. Figure 9 shows a standard Ramsey-Bordé interferometer and its implementation using the adiabatic transfer pulses from Figure 8 [39]. The first pulse splits the initial state into a coherent superposition of $|g\rangle$ and $|e\rangle$. After the atom is allowed to freely evolve for a time T , a second pulse is applied that projects the atomic wave function onto the dark superposition state $|\Psi_D(t_2^+)\rangle$, where t_2 is the start time of the second pulse, as shown in Figure 9b. Then Ω_g is turned off so that the atom is left in $|g\rangle$. (Turning off Ω_e instead also leads to a valid interferometer, which is the upper interferometer of Fig. 1b for the photon recoil measurement.) The fraction of the wave packet that is out of phase with $|\Psi_D\rangle$ will undergo spontaneous emission, and thus lose coherence. It may contribute to the background signal of the interferometer, but will not cause a systematic shift of the fringes. The third pulse splits each of the two paths in state $|g\rangle$ into superposition states. After waiting again for a time T , two of the paths overlap spatially. A final pulse applied at this time projects the wave function onto the superposition state $|\Psi_D(t_4^+)\rangle$, again evaluated at the start of the pulse. This final pulse is tailored to force the atoms to exit in whichever state is preferable for detection, in this case $|g\rangle$. If the phase of the atomic coherence at the overlap point matches the phase of the dark

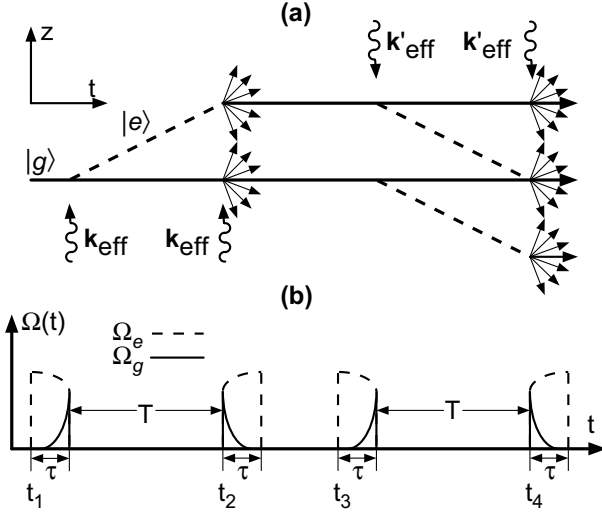


Fig. 9. Ramsey-Bordé interferometer based on adiabatic transfer. (a) Recoil diagram. At the second and fourth interactions, the multiple arrows indicate atoms that spontaneously emit because they are in the coupled state. For a three-level system, all of these atoms are optically pumped into $|g\rangle$, so they contribute to the background signal of the interferometer. In our actual experiment, we use circularly polarized light to induce transitions between the two $m_F = 0$ Zeeman levels of the ground state. Atoms that undergo spontaneous emission tend to optically pump into the high angular momentum states. The diagram omits the spreading of the wave packets that occurs for nonzero τ . Neglecting ac Stark shifts, the interferometer phase shift depends only on T , not on τ . (b) The adiabatic passage pulse sequence required for implementing the interferometer shown in (a).

state, then the atom signal will be at a maximum. Scanning δ_{12} changes the relative phase of the atomic coherence and the field, allowing observation of fringes in the atom populations.

Creating an analog of the three pulse $\pi/2 - \pi - \pi/2$ interferometer using adiabatic transfer presents special difficulty due to the lack of a substitute for the π pulse. Similar problems limit the use of adiabatic transfer for creating large-area interferometers in which multiple stimulated Raman π pulses are used to further separate the arms of an interferometer. These limitations are discussed in an earlier work [42].

The atom interferometer geometry in Figure 8 modified to include a number of π -pulses sandwiched between times t_2 and t_3 can be easily implemented using adiabatic transfer since for either the upper or lower interferometer, the atoms are in the same internal state when the π pulses

are applied. This is the approach presently used for the photon recoil measurement, which provides a factor of $N + 1$ enhancement of the sensitivity.

Another possible route for achieving large-area interferometers using adiabatic transfer is to apply a single adiabatic transfer pulse that involves the interchange of multiple photons, *e.g.*, using $\sigma^+ - \sigma^-$ beams to transfer an atom between the $m_F = -F$ to $m_F = +F$ ground state sublevels of an atom [35, 43]. For a valid dark state, the frequency width of the dark state must be larger than the total recoil splitting between the two states, which can require considerable laser powers for typical beam diameters. Also, these approaches generally involve the use of magnetic-field sensitive transitions. For most precision measurement experiments, magnetic-field inhomogeneities can not be controlled to the level that such transitions can be used.

A final consideration regarding the use of adiabatic transfer for atom interferometry is the level of background atoms that appear in the interferometer signal. In the present case of a collection of three-level systems, it would be difficult to distinguish the atoms transferred by adiabatic transfer from those transferred by optical pumping. On average, the momentum transfer would be smaller for optical pumping, but this would be hard to distinguish without sub recoil initial cooling of the atoms. Incorporating an adiabatic transfer pulse into an atom interferometer would reveal a loss of fringe contrast corresponding to the fraction of optically pumped atoms. In more complex systems, careful selection of beam polarizations allow optical pumping predominantly into states other than the states used for the adiabatic transfer. This allows the coherently and incoherently transferred atoms to be distinguished in the detection stage, so that the optical pumping does not cause a severe degradation of fringe contrast [39].

5.3 A measurement of the photon recoil and $\hbar/M$

In its simplest form, the photon recoil measurement records the Doppler shift of an atomic resonance caused by the momentum recoil from an absorbed photon. Consider the two-level atomic system of Figure 10a with two stable states $|a\rangle$ and $|b\rangle$. If the atom interacts with two counterpropagating, on-resonance fields, as in Figure 10b, then the difference $\omega_B - \omega_A$ contains a contribution from the momentum recoil of the photon absorbed in the first interaction. We use the differential measurement of Figure 10c. The first field puts the atom into a superposition of both momentum states. Two resonances exist for the second field frequency ω_B —one for each of the momentum states. The two pairs of momentum states coupled by ω_B have a velocity difference of $\Delta v = \frac{z\hbar k}{M_A}$, where $\hbar$ is the Planck constant, M_A is the atomic mass, and $k \sim k_A \sim k_B$ is the wave number of the light field. Ignoring the second- and higher-order Doppler shifts, which are insignificant for our experimental parameters, this velocity difference creates a Doppler-shift

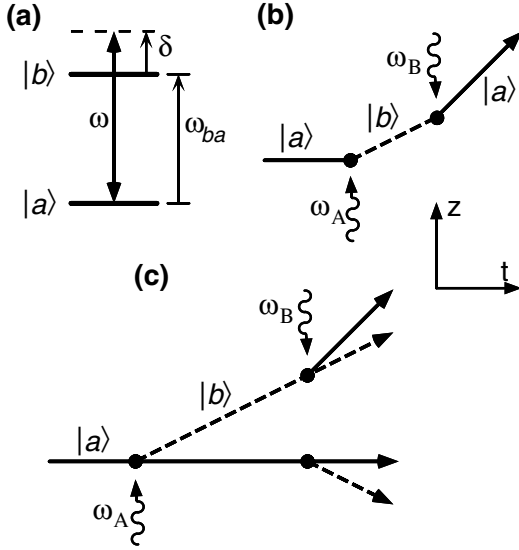


Fig. 10. Simplified version of the photon recoil measurement. The experiment is performed using the two-level atom in (a). The position of the atom relative to the initial unperturbed trajectory is shown as a function of time. The two field frequencies ω_A and ω_B are centered on resonance. (b) The difference $\omega_B - \omega_A$ includes a contribution from the momentum recoil caused by the absorption of a photon from the first interaction. (c) A simple modification converts this into a differential measurement which cancels out the contribution from the initial atomic velocity.

frequency difference between the two resonances of

$$\Delta f = \frac{k\Delta v}{2\pi} = \frac{2h\nu^2}{M_A c^2}, \quad (5.10)$$

where c is the speed of light and $\nu = ck/2\pi$ is the frequency of the light field.

The measurement can be further improved if we use a pair of $\pi/2$ pulses instead of single π pulses, ω_1 and ω_2 in much the same way that a Ramsey pulse pair is superior to a single Rabi pulse. Thus, we are naturally led to the Ramsey-Bordé interferometer shown in Figure 8a. The differential measurement is enhanced by maximizing the distance between the two interferometers as indicated schematically in Figure 8.

The fine structure constant α can be determined from the photon recoil measurement using the relation

$$\alpha^2 = \frac{2\text{Ry}_\infty}{c} \frac{h}{m_e}, \quad (5.11)$$

where Ry_∞ is the infinite-mass Rydberg constant and m_e is the electron mass. In our h/M_{Cs} experiment, we measure the frequency shift Δf for cesium atoms using light on resonance with the D_1 line. Assuming that ν is known accurately, equation (5.10) gives with high precision the ratio

$$\frac{h}{M_{\text{Cs}}} = \frac{c^2 \Delta f}{2\nu^2}. \quad (5.12)$$

Since Ry_∞ is known to 0.028 ppb [78] and c is defined, the uncertainty in the ratio of h/m_e limits the calculation of α from this relation. Expanding equation (5.11) using mass ratios, then substituting h/M_{Cs} from equation (5.12) gives

$$\alpha^2 = \frac{2\text{Ry}_\infty}{c} \left(\frac{m_p}{m_e} \right) \left(\frac{M_{\text{Cs}}}{m_p} \right) \frac{h}{M_{\text{Cs}}}. \quad (5.13)$$

The proton-electron mass ratio has been measured to 2.2 ppb [64]. The cesium-proton mass ratio is presently known only to 34 ppb [86], but may be improved in the near future to ~ 1 ppb [81]. We stabilize the laser frequency relative to the cesium D_1 line with an accuracy of about 0.3 ppb. The absolute frequency of this transition was known to 45 ppb [88] at the start of this measurement. However, this work prompted Udem, *et al.*, to measure the D_1 line to an accuracy of 12 parts in 10^{10} [76]. Consequently, an accurate measurement of Δf could determine α with an uncertainty below 1 ppb.

Presently the anomalous magnetic moment of the electron $a_e \equiv (g-2)/2$ provides the most precise determination of the fine-structure constant α , with an uncertainty of 4.2 ppb (parts per billion). This approach equates the experimental value of a_e [87] with the quantum electrodynamics (QED) calculation of a_e as a power series in α [74] to determine a value for α . Consequently, the currently accepted value for α assumes the validity of QED. Improved precision in a QED-independent measurement of α thereby constitutes a test of QED. The goal of this work is a precision measurement of the recoil of an atom caused by the absorption of a photon. This result, when combined with an absolute frequency measurement and mass-ratio measurements, determines a value for α which does not require QED.

The most precise measurements of α , including this work at the time of Brent Young's thesis [55], with precision better than 100 ppb are shown in Figure 11. In addition to the a_e determination, these include measurements based on the quantum Hall effect [61], neutron diffraction [75], and

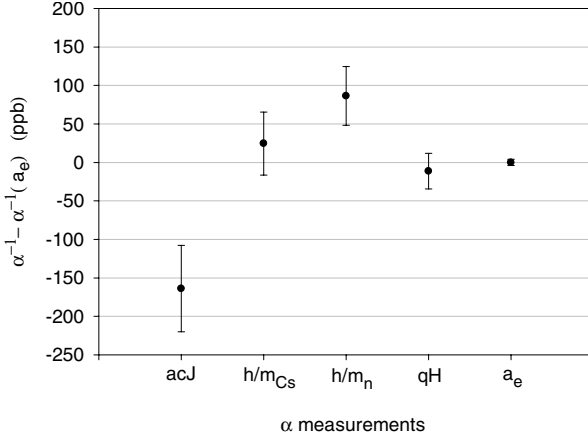


Fig. 11. Measurements of α better than 100 ppb. The values are plotted relative to $\alpha^{-1}(a_e) = 137.035\,999\,44(57)$ determined from the electron anomalous magnetic moment. These include results from the ac Josephson effect (acJ), this measurement (h/M_{Cs}), neutron diffraction (h/m_n), the quantum Hall effect (qH), and a_e .

the ac Josephson effect [92] with relative uncertainties of 24 ppb, 39 ppb, and 56 ppb, respectively. These measurements have statistically significant differences between them, and have considerably higher uncertainties than the a_e value, so another independent measurement of α would be of interest. Even the very precise a_e value recently changed 10σ because of a correction to the theory [74].

The neutron diffraction and photon recoil measurements, on the other hand, are independent of electrical definitions. The neutron diffraction and photon recoil measurements are conceptually very similar—the former measuring h/m_n and the latter h/m_{Cs} . Both approaches use quantum interference of neutral particles, so that they can easily be isolated from perturbing forces, and their interactions with matter are well understood. For neutron diffraction, the interferometer is generated by interactions of the neutrons with silicon crystals, the lattice spacing of which must be calibrated interferometrically. In the photon recoil measurement, the matter-wave interferometers are created by interactions with light fields propagating in vacuum. Accurate stabilization of the laser frequency provides an absolute calibration for the impulses created by the interferometer interactions. Reference [74] provides a comprehensive review of fine-structure constant measurements.

Many of the details of our h/M_{Cs} experiment have been described in the thesis of Brent Young [55]. The current level of precision in α is ~ 4 ppb after 5 hours of integration time. At the present time, we are still searching

for systematic effects and hope to report a measurement with an absolute uncertainty in this range.

6 Atom gyroscopes

Consider an atom interferometer in an inertial (Galilean) frame of reference (x', y') . In this inertial frame, the atom goes in straight line trajectories. However, in a rotating laboratory frame, we see a distorted path. We use the Feynman formulation of quantum mechanics to calculate the phase-shift $\Psi(x_b, t_b) = e^{S_{\text{Cl}}/\hbar} \Psi(x_a, t_a)$ for the two paths Γ_{I} and Γ_{II} and follow the treatment given by Storey and Cohen-Tannoudji [16]. As before, S_{Cl} is the classical action, and in the inertial frame, it is given by

$$S_{\text{Cl}} = \int_{\Gamma'} L'(\mathbf{x}', \dot{\mathbf{x}}') dt \quad (6.1)$$

$$= \int_{\Gamma'} \frac{1}{2} M \mathbf{v}'^2 dt. \quad (6.2)$$

If we transform to the rotating (un-primed) frame a point a distance $\mathbf{r}$ from the axis of rotation will have velocity given by $\mathbf{v}' = \mathbf{v} + \boldsymbol{\Omega} \times \mathbf{r}$. The Lagrangian in the rotating frame is

$$L(\mathbf{r}, \mathbf{v}) = L'(\mathbf{r}', \mathbf{v}') = \frac{1}{2} M [\mathbf{v} + (\boldsymbol{\Omega} \times \mathbf{r})]^2 \quad (6.3)$$

$$= \frac{1}{2} M \mathbf{v}^2 + M \boldsymbol{\Omega} \cdot (\mathbf{r} \times \mathbf{v}) + \frac{1}{2} M (\boldsymbol{\Omega} \times \mathbf{r})^2. \quad (6.4)$$

For an angular velocity Ω slow enough so that $\Omega \Delta t \ll 1$, where Δt is that transit time of the atoms through the interferometer, the rotation can be taken as a small perturbation.

$$L = L_0 + L_1 \quad (6.5)$$

$$= \frac{1}{2} M \mathbf{v}^2 + M \boldsymbol{\Omega} \cdot (\mathbf{r} \times \mathbf{v}) \quad (6.6)$$

where only the term to first order in Ω was kept. Thus, the phase difference between the two paths is then given by the action of the perturbing Lagrangian *integrated along the unperturbed (straight-line) paths*

$$\delta\phi = \frac{1}{\hbar} \int_{t_a}^{t_b} L_1 dt \quad (6.7)$$

$$= \frac{M\Omega}{\hbar} \int_{t_a}^{t_b} [\mathbf{r}(t) \times \mathbf{v}(t)] dt. \quad (6.8)$$

Using $d\mathbf{r}/dt = \mathbf{v}(t)$,

$$\delta\phi = \frac{M\Omega}{\hbar} \int_{t_a}^{t_b} [\mathbf{r}(t) \times d\mathbf{r}(t)] \quad (6.9)$$

$$= \frac{M\Omega}{\hbar} \int_{t_a}^{t_b} 2d(\text{Area})\hat{\mathbf{z}} \quad (6.10)$$

$$= \frac{2M\Omega}{\hbar} A_0, \quad (6.11)$$

where A_0 is the total area of the triangle formed by the origin and the beginning and ending points $\mathbf{r}_a$ and $\mathbf{r}_b$. Each interferometer path Γ_I and Γ_{II} consists of two straight-line segments. The phase difference between the two paths is given by

$$\Delta\phi = \Delta\phi|_{\Gamma_I} - \Delta\phi|_{\Gamma_{II}} \quad (6.12)$$

$$= \oint L_1(\mathbf{x}, \dot{\mathbf{x}}) dt \quad (6.13)$$

$$= \frac{2M\Omega}{\hbar} (\text{Enclosed area}). \quad (6.14)$$

This simple result could have been derived by considering a Mach-Zender interferometers in the shape of a circle. One calculates the difference in the number of oscillations of phase of the atom de Broglie wave going in circular clockwise and counter-clockwise directions. The atoms split by the first beamsplitter are rejoined after going halfway around the circle. However, if the apparatus is rotating during the transit time of the atoms, the second beamsplitter will have moved so as to introduce a path length difference. The phase difference is proportional to the area of the circle, the rotation rate and the mass of the atom. By considering infinitesimal changes in the shape of the paths, one can show that the formula applies to gyroscopes of arbitrary path shapes. The velocity and hence the de Broglie wavelength of the atom is not a factor: the shorter wavelength of faster moving atoms is counter-balanced by the shorter transit time of the atom through the apparatus.

6.1 A comparison of atom interferometers

Several matter wave gyroscopes have been constructed using cw optical beams [3, 46], nanofabricated gratings [44, 49], and micro fabricated shadow gratings [45, 50]. To date, the most sensitive instrument is the one constructed using off-resonant Raman pulses [46]. This interferometer uses a 2 meter long path with an enclosed area of 0.22 cm^2 . Recent improvements such as the use of a transversely laser cooled atomic beam with a flux of 2×10^{10} atoms/s. Two beams, counterpropagating through the Mach-Zender path produce significant “common-mode” rejection by measuring

$|\Omega_{\text{rot},+} - \Omega_{\text{rot},-}| = |2\Omega_{\text{rot},+}|$, where $\Omega_{\text{rot},+}$ and $\Omega_{\text{rot},-}$ are the rotations measured by the two opposing atomic beams. With these improvements, the sensitivity of the atom interferometer gyroscope was increased to 6×10^{-10} rad/s/ $\sqrt{\text{Hz}}$, or 8×10^{-6} of Earth's rotation per $\sqrt{\text{Hz}}$ [47].

The relative performance of the various atom interferometers reflects a combination of inherent differences in the technologies and the experimental execution ("engineering") of the apparatus. Interferometers based on optical π and $\pi/2$ pulses have less stringent requirements on the velocity spread and divergence of the atom beam source as discussed in Section 3.1. It also may be intrinsically easier to compensate for vibrations since the optical phase of the light can be controlled with high bandwidth feedback systems and either acousto-optic, electro-optic or direct modulation of the laser frequencies. The error signal must still be referenced to a stable inertial platform. Atom interferometers based on material objects require mechanical isolation of all gratings and beamsplitters. Finally, Chu's Second Golden Rule states that a frequency or frequency-shift measurement is invariably superior to another measurement. However, interferometers as the one introduced by Kasevich and Chu [4], are phase measurements tied to the wavelength of light. A strictly *time-domain* measurement would be more accurate.

A comparison of atom interferometry measurements of gravity and rotations is listed in Table 2. The short term sensitivity of atom gyroscopes are now competitive with the best ring laser gyroscopes despite their short engineering time. There are no studies on the absolute accuracy and long term drift of atom interferometer gyroscopes. Work is now underway to study the long term stability of the instrument. So far, no work has been done trying to establish the absolute accuracy of these devices. Current drift rates produce a noise floor comparable to the short term stability. By contrast, the sensitivity of an atom interferometer gravimeter continues to improve out to integration times approaching 10^4 seconds.

Cryogenic gravimeters (a superconducting sphere levitated in a magnetic field) drift at the level of 2×10^{-10} g/day due to the changing mass of the sphere due to cryo-pumping. It is possible to calibrate these devices with an instrument that can measure an absolute value for g , but quantum flux jumps induced by vibrations prevent the device from being moved, once calibrated. Conventional spring/mass instruments, the current workhorse device used in oil and mineral exploration, have a drift of 3×10^{-8} g/day due to aging and thermal drift of the mechanical spring.

6.2 Future prospects

Atom interferometers are still in their infancy and one can expect significant improvements in sensitivity in the near future. Work has begun on atom interferometers based on multiple beam interference [52–54].

Table 2. Comparison of atom interferometer inertial sensors.

Rotation	Short term sensitivity rad/sec/ $\sqrt{\text{Hz}}$	
Raman Pulse [47]	6×10^{-10}	
Moiré classical fringes [50]	2.25×10^{-9}	
Nanofabricated gratings [49]	3.6×10^{-6}	
Ring Laser gyro [48]	13×10^{-10}	
Superfluid helium [44]	2×10^{-7}	
Fiber optic gyro (commercial)	$\sim 3 \times 10^{-7}$	

Acceleration due to gravity	Short term sensitivity g/ $\sqrt{\text{Hz}}$	Accuracy
Raman pulse [31]	2×10^{-8}	5×10^{-9}
Moiré [50]	1.2×10^{-7}	not meas.
Spring/mass system	1×10^{-10}	not appl.
Cryogenic gravimeter	$< 10^{-12}$	not appl.
Falling corner cube	5×10^{-8}	2×10^{-9}

The basic idea is that optical resolution scales as the number of lines illuminated on a diffraction grating or as the effective number of bounces between the mirrors of a Fabry-Perot cavity. The hope is that multiple beam interference in atom interferometry will lead to a similar increase in resolution. Although these type of interferometers have yet to surpass the off-resonant Raman [31, 47], or adiabatic interferometers [55], excellent signals with as many as 160 interfering beams have been obtained [52].

Considerable attention is being paid to improving the atom beam source. However, it is worth remarking that the current state-of-the-art interferometers are not limited by the brightness of the source of atoms. For example, the short term sensitivity of the atomic fountain *g*-meter is *two orders of magnitude below the shot noise limit* imposed by the 3×10^6 atoms detected per launch cycle and four orders of magnitude below what is possible with high flux cold atom sources. Major noise sources in our instrument include high frequency phase noise (11 ppb), background fluctuations (7 ppb), residual vibration and rotation noise (5 ppb), Raman laser intensity noise (3.5 ppb), and the frequency stability of the Loran-C receiver (3.0 ppb).

There are several groups working to develop atom interferometers based on Bose-condensed atoms. The reasons for this push include (1) the higher

brightness of a Bose condensate would mean less transverse spreading during long atomic fountain times (2) the spatial distribution of the cloud of atoms would be better characterized (useful for understanding potential systematic effects), and (3) the well-defined momentum distribution would allow well-separated transitions between the same internal state but different momentum states (*e.g.* $|g, \mathbf{p}\rangle \leftrightarrow |g, \mathbf{p} + 2\hbar\mathbf{k}_{\text{eff}}\rangle$) [56].

There are also a number of groups working towards the demonstration of atom waveguides suitable for atom interferometers.

Acknowledgements

This work was supported in part from grants by the NSF, AFOSR. The author also wishes to thank K.Y. Chung for assistance in the preparation of the figures for this manuscript.

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COURSE 5

MESOSCOPIC LIGHT SCATTERING IN ATOMIC PHYSICS

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MESOSCOPIC LIGHT SCATTERING IN ATOMIC PHYSICS

B.A. van Tiggelen

Waves always behave in a similar way
(Léon Brillouin, in: *Wave Propagation and Group Velocity*, 1960)

1 Introduction

The recognition of wave propagation in daily life goes back a long time ago. The first serious mathematical descriptions - put forward in the context of light propagation - were due to Huygens (1690), who formulated the famous Huygens' principle and Fresnel (1810) who derived this principle from a wave equation. With the formulation of Maxwell's equations for electromagnetic waves by the end of the 19th century, the wave concept found its first spectacular application in physics.

This century may again be called the century of the wave. During the last century, quantum-mechanical wave behavior of first electrons and later atoms and even entire macroscopic material objects, such as superconductors, superfluids and Bose-Einstein condensates, has been established. The wave concept has undoubtedly become the most important concept in physics. This statement implies that wave mechanics - the theory of wave propagation in space-time - is the most important formalism in physics. The wave concept is what this lecture has in common with other themes of this summer school. The aim of this lecture is to introduce "mesoscopic" scattering theory in atomic physics, using knowledge gathered from classical waves [1], keeping the citation above in mind. Other lectures with regard to this subject have been given [2,3] with an approach more from the atomic physics point of view, though recognizing the importance of mesoscopic scattering. Mesoscopic physics has been the subject of a Les Houches summer school in 1994 [4]. It has seen a considerable breakthrough in the last 10 years, especially in the context of quantum transport, with the development of its own language of random matrix theory [5].

Only after I had decided to use Brillouin's openings phrase of his famous book as a slogan for my lectures, I realized the highly nontrivial nature of

Table 1. Waves and their behavior.

WAVE	WAVE EQUATION
Non-interacting Matter Waves Schrödinger equation	$[-\hbar^2\nabla^2/2m + V(\mathbf{r})]\psi = i\hbar\partial_t\psi$ ψ : complex probability amplitude
Linear Electromagnetic Waves Helmholtz equation	$c_0^{-2}\varepsilon(\mathbf{r})\partial_t^2\mathbf{E} + \nabla \times \nabla \times \mathbf{E} = 0$ $\mathbf{E}$: electric field
Mechanical Waves Elastic wave equation	$\rho\partial_t^2\mathbf{s} = (\lambda + 2\mu)\nabla\nabla \cdot \mathbf{s}$ $\quad - \mu\nabla \times \nabla \times \mathbf{s}$ $\mathbf{s}$: displacement vector
Flexural waves Euler-Bernouli equation	$\nabla^4\phi + \kappa(\mathbf{r})\partial_t^2\phi = 0$ ϕ : transverse displacement

its message. It led me to pose three pertinent questions, namely

- 1. What is a wave?
- 2. What means “behave”?
- 3. What exactly is meant by “similar”?

Mathematically, any object described by a complex number $\psi(A, \phi) = A\exp(i\phi)$ can be called a “wave”, its phase in the complex plane ϕ called the phase of the wave, and the absolute value A related to some density $\rho \sim A^2$ of the wave. Complex numbers have the properties that we believe characterize “waves”, namely *superposition* (the sum of two waves is again a wave, but the phases do not add), *interference* (the joint density A^2 of two waves is not equal to the sum of the densities, and can actually vanish, *i.e.* interfere destructively) and periodicity: $\psi(\phi) = \psi(\phi + 2\pi)$.

The answer to the second question refers to a set of rules that govern the propagation of waves in space-time $(\mathbf{r}, t)$. This brings us to the physical aspects of waves, finding applications in almost all domains of physics. In general, the answer depends on the nature of the waves, such as electromagnetic waves, acoustic or elastic (mechanical) waves, De Broglie (matter) waves, or flexural waves (Tab. 1). In principle, the behavior of a wave is completely described by the solution of its wave equation, the density A^2 in all cases proportional to some “conserved quantity” in time. The “similarity” of wave behavior, conjectured by Brillouin, is not evident by looking at Table 1.

Despite early successes in the understanding of wave behavior, most of our present knowledge on wave mechanics - scattering theory in particular - was developed during the development of quantum mechanics in the

beginning of the 20th century. One crucial property of a wave, the wave number $\mathbf{k}$, describing the phase evolution in space, was related to the momentum $\mathbf{p} = m\mathbf{v}$ of a particle, according to the famous De Broglie relation $\mathbf{p} = \hbar\mathbf{k}$. The phase evolution in time was, *via* the Schrödinger equation, related to nothing less than the Hamiltonian of the particle. The success of quantum mechanics has been so impressive that some people think that wave mechanics and quantum mechanics are actually synonymous (note the word “quantum” in Ref. [4]). Many results in quantum mechanics are mere consequences of wave mechanics, and are not “quantum” at all. Real quantum results are related to the specific interpretation of the Schrödinger wave function as a probability distribution and its consequences for the measurement problem, as well as most results of second quantification, where “wave-particle duality” emerges.

The universality of wave mechanics is often obscured by details required to solve a specific problem. In atomic physics one wishes to understand how light interacts with atoms. From the point of view of wave mechanics this problem can be cast into a well-defined scattering problem, creating a “light-in-light-out” set-up. One has in that case integrated out the material degrees of freedom that have been hidden in a S-matrix of the light, a situation that is actually close to the way atomic physics is done experimentally. However, the usual approach in theoretical atomic physics is different, and prefers to integrate out the light waves, leaving us with “dressed” material degrees of freedom, involving electrical polarization, spontaneous emission and Lamb shifts. Even the incident light is transformed into a material property called the Rabi frequency! In general, both pictures are complementary, but to do mesoscopic physics the scattering theory is highly favorite. Many ideas in this course have already been written down in a 1996 review paper [6]. This contribution intends to introduce scattering theory in atomic systems.

2 Mesoscopic wave physics

Wave mechanics is the formalism to describe wave propagation in space and time. Before discussing mathematical details of this theory, it is important to oversee its limitations and universality, and to identify the differences. We can then decide under what conditions waves behave “similarly”.

2.1 Mesoscopic quantum mechanics

Central in quantum mechanics is a complex wave field $\psi(\mathbf{r}, t)$. The time-evolution is governed by the “energy operator” or Hamiltonian H . The Schrödinger equation of motion and its formal solution are given by,

$$i\hbar\partial_t\psi = H\psi \Rightarrow \psi(t) = \exp(-iHt/\hbar)\psi(0). \quad (2.1)$$

From the formal solution it is clear that the phase evolution of the wave in time is directly related to the Hamiltonian. The phase is a crucial property for waves because it is at the base of interference phenomena. Two reasons exist why the “exact” solution really only is a formal solution in practice: decoherence and randomness. A clear distinction of both aspects is crucial for a comparison of classical waves and “quantum” waves.

The first point is that, for equation (2.1) to apply, H must be the *total* Hamiltonian of the system. The hermitean nature of H guarantees that, at all times

$$\langle \psi(t) | \psi(t) \rangle = \int d\mathbf{r} |\psi(\mathbf{r}, t)|^2 = 1, \quad (2.2)$$

or equivalently, that the density matrix has total trace of unity. In practice, H always contains an unknown coupling to some large system, the “environment”, with many degrees of freedom which are, due to lack of knowledge, described by a statistical mixture. In the world whose H we know and whose properties we want to study, energy is not conserved, and processes are inelastic. Because equation (2.1) relates the energy directly to the phase evolution in time, a characteristic *inelastic time* τ_ϕ exists, beyond which all interference phenomena will be destroyed by dephasing inelastic effects. A possible definition of the inelastic time is,

$$\frac{\langle \psi(\mathbf{r}, t) \psi^*(\mathbf{r}, t + \tau) \rangle}{\langle \psi(\mathbf{r}, t) \psi^*(\mathbf{r}, t) \rangle} \sim \exp(-\tau/\tau_\phi). \quad (2.3)$$

In atomic physics the left hand side of this definition is known as the *first order coherence function* $g_1(\tau)$ [16]. The averaging carried out in definition (2.3) addresses the unknown degrees of freedom, such as vacuum fluctuations, randomly passing phonons, or atomic collisions, that have been integrated out (“traced over”). Beyond the time τ_ϕ there is no point doing quantum mechanics anymore: the phase is scrambled and only phase-insensitive, classical effects remain. The “reduced” density matrix, obtained after having integrated out the unknowns, *remains normalized to unity*, when traced over the known degrees of freedom. The destruction of phase (more technically speaking off-diagonal elements in the density matrix) by the coupling with a large environment is called *decoherence* [7]. It is discussed in detail by Zurek and Paz in this book.

To give an order of magnitude, $\tau_\phi \approx 10^{-11}$ s for a copper wire at $T = 1$ K. With a Fermi velocity of 10^6 m/s this corresponds to a dephasing length of $\ell_\phi = 10$ μm . This length explains immediately why phase plays no role for normal ohmic conduction. On the other hand, this dephasing length is still large enough compared to the lattice spacing for the electrons to benefit from constructive Bloch interferences. Since $\tau_\phi \sim 1/\delta E$, with δE typical fluctuations of system energy, we estimate that $\tau_\phi \sim 1/kT$ at temperature

T , which is typically what is found for electron-phonon coupling [8]. Hence, cooling down is the way to enter the regime where the phase comes in.

The role of disorder is less dramatic, but nevertheless as important. The known part of the Hamiltonian is often only known in a statistical way. For instance, it describes s -wave impurities in a semi-conductor, whose exact locations we do not know. Yet, they are *not* integrated out, but treated in a probabilistic way. No inelastic scattering exists and the phase is not destroyed, just randomized in a way that we should be able to figure out. This means that interference phenomena can still persist on all length scales, although the wave number is no longer a conserved quantity as it was in a homogeneous medium. The dephasing caused by randomization of the wavenumber is described by another length scale, called the *extinction mean free path* ℓ . In terms of a solution at energy E it can be defined as,

$$\langle \psi(\mathbf{r}, E) \psi(\mathbf{r} + \mathbf{x}, E)^* \rangle \sim \exp(-x/2\ell(E)). \quad (2.4)$$

The averaging is now performed over random variables in the known Hamiltonian. The *extinction mean free time* τ is readily defined as $\tau = \ell/v$ with v the wave velocity. The factor of 2 in equation (2.4) is included to guarantee that for a source at $\mathbf{r}$ the density $|\langle \psi(\mathbf{r} + \mathbf{x}) \rangle|^2$ decays as $\exp(-x/\ell)$, a law that is in optics referred to as Beer's law. In a copper wire at 1 K, The mean free path caused by electron-impurity scattering amounts to $\ell \approx 5$ nm, much smaller than the inelastic length, but only one order of magnitude bigger than the De Broglie wavelength λ_B .

The confusion between dephasing processes caused by decoherence and randomness is due to bad but unfortunately irreversible terminology. For instance, classical light scattered from a random medium like Teflon or fog is regularly called "incoherent" by optical physicists, because the phase is randomized. However, this "incoherent" signal is as coherent as the incident light, according to the proper definition in atomic physics, using the coherence function $g_1(\tau)$. The phase is just a random variable. By studying for instance "speckles" (intensity fluctuations) a lot of information on randomness can be retrieved. This is much more difficult - if not impossible - for decoherence processes.

If Δt is the typical time the wave spends in the medium, the regime,

$$\frac{\hbar}{E} < \tau < \Delta t < \tau_\phi \quad (\text{De Broglie waves}) \quad (2.5)$$

is called the *mesoscopic regime* for matter waves, a regime located in between "macroscopic" ($\Delta t > \tau_\phi$) and "microscopic" ($\Delta t < \tau$), but with best of both worlds [4]. The time scales Δt , τ_ϕ and τ can be called "*the good, the bad and the ugly*", after a famous Eastwood western: Δt is "good" because it is under control experimentally; τ_ϕ is bad for it destroys something beautiful; finally, τ is ugly because multiple scattering and disorder are often a

nuisance, but they are just a nuisance. The last inequality sign guarantees the pertinence of phase throughout the sample. The second inequality implies that the system is sufficiently disordered to have multiple scattering. The first inequality is a rough criterion for Anderson localization (in three dimensions) to set in, and locates a completely different regime in wave propagation, which I - contrary to others [4] - wish to exclude from the mesoscopic regime. In this regime, the phase has induced a genuine phase transition, called Anderson localization. Localization of waves has been discussed in a former Les Houches lecture [9], where all important references can be found.

2.2 Phenomenological radiative transfer

For almost one entire century, the standard way to describe multiple scattering of light has been by means of the *equation of radiative transfer*. This equation ignores any possible interference, treating waves as classical particles, and reads [10]

$$\frac{1}{c} \partial_t I_{\mathbf{k}}(\mathbf{r}, t) + \hat{\mathbf{k}} \cdot \nabla I_{\mathbf{k}}(\mathbf{r}, t) + \left(\frac{1}{\ell} + \frac{1}{\ell_a} \right) I_{\mathbf{k}}(\mathbf{r}, t) = \frac{\varepsilon(\mathbf{r}, t)}{4\pi} + n \int d\hat{\mathbf{k}}' \frac{d\sigma}{d\Omega}(\mathbf{k}' \rightarrow \mathbf{k}) I_{\mathbf{k}'}(\mathbf{r}, t), \quad (2.6)$$

featuring the local *specific intensity* $I_{\mathbf{k}}(\mathbf{r}, t)$, *i.e.* the local energy flux density propagating in direction $\mathbf{k}$. Equation (2.6) is a book-keeping and treats a number of processes in a phenomenological way. The first two terms describe a volume element “co-moving with the light”. The third “loss” term contains two parts. The *coherent* loss term $1/\ell$ describes light that is scattered elastically out of the forward beam, featuring the scattering mean free ℓ ; the *incoherent term* $1/\ell_a$ is a genuine sink term and describes loss of light. Similarly, the righthand side contains two “gain” terms. The term ε represents a source term that creates light (*i.e.* by inelastic atomic transitions). Finally, the last term describes the amount of light (per unit volume) that is scattered elastically into the direction $\mathbf{k}$, with n the number density of scatterers. Two extreme cases can be considered.

If scattering can be neglected, the equation of radiative transfer contains a sink term $1/\ell_a$ and a source term ε . If both are constant in space, and if energy flow is stationary, this simplified case can be solved easily by introducing the so-called source function $S = \varepsilon \ell_a / 4\pi$. In (local) thermal equilibrium, absorption and emission can be related, with the result that S is essentially equal to the Planck function $B_\lambda(T)$. This is the celebrated *Kirchoff theorem*. The solution to equation (2.6) is in good approximation,

$$I_{\mathbf{k}}(\mathbf{r}) \approx B_\lambda[T(\mathbf{r} - \hat{\mathbf{k}}\ell_a)], \quad (2.7)$$

i.e. it equals the Planck function corresponding to the local temperature of the spot one mean free path away along the line of light. This simple notion explains why stars radiate more or less as black bodies. It also explains why most atomic transitions in the Solar atmosphere are observed *in absorption*: these transitions have a relatively small mean free path so that emerging photons originate from relatively cool layers of the Sun, for which $B_\lambda(T)$ is relatively small.

On the other hand, if absorption and emission are negligible, all light is scattered elastically. The resulting equation is still very complex, and its solutions have been studied numerically in great detail [11]. It is this situation for which the neglect of phase is not necessarily legitimate. In the next section I will address this question in more detail.

2.3 Mesoscopic physics with classical waves

The classical, macroscopic Maxwell equations contain constitutive constants such as the dielectric constant and the electric conductivity, and should describe the electromagnetic field on scales much bigger than atomic scales. These “constants” do not contain *all* information. Especially in the solid state, where the density of the atoms is high, radiative oscillators couple to a large number of non-radiative decay channels, giving rise to loss of energy. These losses are bigger than $\hbar\omega$ so that photons really disappear in great numbers, in an entirely classical way. In classical wave equations, “energy” is not directly related to time evolution of phase, as we have seen for De Broglie waves. Hence, no reason exists that the phase of a classical wave should be scrambled. I emphasize the importance of “classical” to this statement. As soon as classical waves are “quantized”, the energy takes over again the role of time evolution. Classically, a phase relation persists between incident and elastically scattered light (*i.e.* the scattered light is “phase locked” to the incident wave), and phase can be measured as long as the amplitude is still large enough for detection. If the time τ_a is the typical absorption time, the mesoscopic regime for classical waves with circular frequency ω can now be defined as,

$$\frac{2\pi}{\omega} < \tau < \Delta t < \tau_a \quad (\text{classical waves}). \quad (2.8)$$

The last inequality guarantees the wave to survive. For classical waves the relation

$$\int d\mathbf{r} W(\mathbf{r}, t) = \exp(-t/\tau_a), \quad (2.9)$$

holds, where the energy density $W(\mathbf{r}, t) \sim |\psi(\mathbf{r}, t)|^2$ is proportional to the classical field amplitude squared. This relation is to be contrasted against

relation (2.2) for De Broglie waves. Equation (2.9) expresses the fact that *non-radiative decay channels have not been included at all* into the equation. They have not even been integrated out as was done in equation (2.2) with the unknown degrees of freedom for matter waves, for that would have led to conservation of W in time. Classically, the simple discard of non-radiative degrees of freedom is possible, since W is not interpreted as “probability density”.

In general, matter waves and classical waves seem to be much less “similar” than Brillouin wanted us to make believe. Research in the last decades established that only in the regimes described by the criteria (2.5) and (2.8), classical waves and matter waves behave in a surprisingly universal, so-called “mesoscopic” way. The similarity of wave propagation in the mesoscopic regime makes studies with classical waves and matter waves *complementary*, for “similar” does not mean “identical”. Dispersion laws are still different, and also charge and spin constitute notable differences, with large impact even in the mesoscopic regime.

The mesoscopic regime is much easier to enter with classical waves. For light propagation in semiconductors (and with frequencies inside the electronic gap to avoid electronic transitions) the absorption length can be as large as centimeters, whereas at the same time the mean free path can be submicron, just at room temperature. This leaves us with four (!) orders of magnitude for the path length $c \times \Delta t$ to do mesoscopic physics. The present world record for the mean free path is $\ell = 0.17 \mu\text{m}$ for infrared light in GaAs powders [12]. This small value actually violates the first inequality of criterion (2.8), which offers the possibility of Anderson localization in this system.

In Figure 1 I show the outcome of a recent mesoscopic experiment, demonstrating the pertinent role of phase in the multiple scattering regime [13]. Another typical experiment (see Fig. 9), where the phase itself is monitored in the multiple scattering regime - involving coherent backscattering - will be discussed in Section 4. These mesoscopic experiments confirm that the phase is not destroyed by multiple scattering, but just randomized. Microwaves and acoustic waves facilitate a direct measurement of the phase. The high frequencies of light enable only indirect phase studies, focusing on flux or energy density.

2.4 Mesoscopic light scattering in atomic gases

The first study of multiple light scattering in resonant atomic systems is due to Compton in 1922 [14] and was refined in 1947 by Holstein [15] in a really outstanding paper. The question raised by Compton and Holstein was how light will propagate in a gas with atoms more or less resonant with the light. If the medium is bigger than the mean free path, emitted photons will be rapidly recaptured by other atoms. As a result, Compton argued,

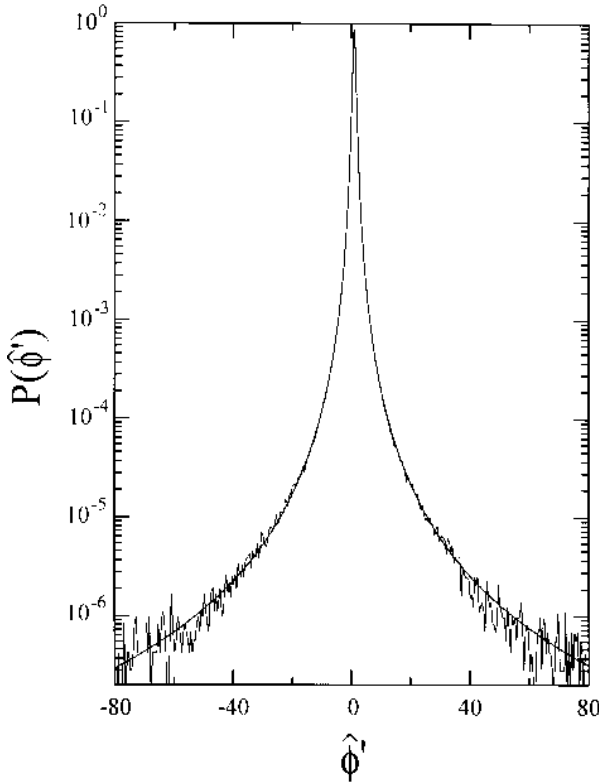


Fig. 1. A recent experiment with classical waves, demonstrating the pertinence of phase in the mesoscopic regime, despite multiple scattering. Microwaves experiments have direct access to the wave. The figure shows the probability distribution of the frequency derivative of the phase shift of microwaves (wavelength 1.5 cm) in transmission from a tube of 1 meter in length, containing 0.5-inch polystyrene spheres (mean free path of 5 cm). Note the high accuracy of more than 1 ppm. The frequency derivative of phase shift is intimately related to “delay time” of the waves in the medium, as explained in Section 3. Taken from Genack *et al.* (1999) [13], with thanks to Genack.

the photons actually perform a random walk, satisfying a diffusion equation, rather than escaping ballistically. The escape time for diffuse propagation is larger than the one for ballistic propagation. Hence the name “radiation trapping”.

The good news for atomic gases is that most transitions are radiative, because of the relatively low density of atoms. This implies that no light is lost. However, the matter is quantum mechanical and couples to

degrees of freedom over which we have no control. This gives rise to inelastic line broadening, at low temperatures and pressures caused by vacuum fluctuations, and at normal (room) temperatures dominated by atomic collisions and Doppler broadening [16]. The amount of light that is still scattered elastically - the “Rayleigh component” [16] - can be quantified by the albedo defined as the ratio of natural and total line width: $a = \Delta\omega_{\text{nat}}/\Delta\omega_{\text{tot}} < 1$ [6]. Inelastic line broadening is a specific complication for atomic systems in obeying criterion (2.5). Suppose the light wave travels through the atomic gas, by means of a random walk with diffusion constant D , as envisaged by Compton. One total scattering event takes one atomic life time τ_0 plus one mean free time to travel to the next atom, which is often much smaller. The diffusion constant is thus estimated to be $D \approx r^2/t \approx \ell^2/\tau_0$. The total time to traverse a distance L - the sample size - is $\Delta t \approx L^2/D \approx (L/\ell)^2\tau_0$. Criterion (2.5) imposes that

$$\left(\frac{L}{\ell}\right)^2 \tau_0 < \tau_\phi \quad (2.10)$$

for the photons to behave mesoscopically. But at the same time we want the medium to be sufficiently inhomogeneous to have multiple scattering, *i.e.* $L > \ell$. The large factor $(L/\ell)^2$ in criterion (2.10) shows that *dephasing is much more sensitive in multiple scattering than it is in single scattering*. In the last case we would simply impose the natural decay time to be less than the inelastic time or, equivalently, the natural line width to exceed the inelastic line width. Since $\tau_0 \approx \tau_\phi \approx 10^{-8}$ s and $L/\ell > 50$, radiation trapping is far from being mesoscopic. Indeed, Holstein started out with the transport equation (2.6), describing the light waves in the atomic gas as if they were soccer balls in a forest.

The inelastic nature of the light is responsible for one very anomalous feature in multiple light scattering. For purely elastic light scattering it is well known that the step length distribution $P(r)$ of a wave between two successive scattering events is given by an exponential distribution [17]

$$P(r) = \frac{1}{\ell(\omega)} \exp\left(-\frac{r}{\ell(\omega)}\right), \quad (2.11)$$

featuring the mean free path ℓ at frequency ω . However, an inelastic spectral distribution $F(\omega)$ exists around the resonant frequency. For incoherent light we are allowed to add intensities so that equation (2.11) generalizes to,

$$P(r) = \int d\omega \frac{F(\omega)}{\ell(\omega)} \exp\left(-\frac{r}{\ell(\omega)}\right). \quad (2.12)$$

Since $F(\omega)$ and the total atomic cross-section $\sigma(\omega)$ are both Lorentzian around the resonant frequency, we anticipate $F(\omega) \times \ell(\omega) = F(\omega)/n\sigma(\omega) \approx$

to be constant around the resonant transition. It easily follows [15]

$$P(r) \sim 1/r^{3/2}. \quad (2.13)$$

This law is recognized as a *Lévy distribution*. Its long range makes the radiation trapping problem fundamentally different from light diffusion in fog or paint, and its important role in the interpretation of radiation trapping experiments was first discussed by Holstein [15]. In particular, its first moment - defined as *the* mean free path- diverges. Its second moment - related to the diffusion constant [17] - diverges as well. Photon transport in atomic gases is thus not Brownian after all.

A contemporary challenge is to obey criterion (2.5) with an atomic gas, and to establish the coherence of the light despite the randomness in the locations of the atoms. Among all line broadening mechanisms, radiative line broadening is the only one that can be 100% elastic and coherent ($\tau_\phi = \infty$), as is the case for a two level system at not too large radiation intensities [16, 18]. Genuine inelastic mechanisms, such as Doppler broadening and collisional broadening can be suppressed by cooling down, now a state-of-the-art technique. For purely elastic scattering one may expect normal diffusion of waves, but now with giant resonant cross-sections and particles (and perhaps even the light) that must be described quantum-mechanically. Unfortunately, a genuine two-level system is not always at hand (Rubidium has degenerated ground and excited states), and one has to cope with Raman contributions. The first result has recently been obtained by the group in Nice [19], who measured coherent backscattering of light from a cold Rubidium gas, deducing a mean free path of $\ell \approx 2$ mm. Coherent backscattering is one of the pilot effects in mesoscopic wave physics, and has been observed with light (see Fig. 9), ultrasound [20], and indirectly in the conductance of electronic conductors [21, 22].

I hope that this experiment will set a new trend for mesoscopic wave mechanics in atomic gases. It was mentioned in the former section that once in the mesoscopic regime, wave mechanics is a universal formalism, insensitive to small specific details of the system. Once in this regime, scattering theory is the most powerful formalism. In the rest of this lecture I will discuss a semi-classical elastic scattering theory for two-level systems, where mesoscopic effects are most apparent.

3 Light scattering from simple atoms

In this section I will introduce classical wave mechanics, and apply it to light scattering from atoms, without actually doing atomic physics. My aim is to establish the vital link between scattering theory and atomic physics, not to do better than atomic physicists. Many familiar concepts will emerge

from this classical approach, such as superradiance, excited energy, dipole-dipole coupling, polarizability. This emphasizes the pertinent role of wave mechanics in problems that are sometimes believed to be truly quantum-mechanical.

3.1 Vector Green's function

The wave equation for classical electromagnetic propagation was shown earlier in Table 1. In this equation, $\varepsilon(\mathbf{r})$ is the dielectric constant that can vary in space. Outside scattering objects it is supposed to take its vacuum value $\varepsilon = 1$. Denoting by $\mathbf{p}$ the operator $-i\nabla$, it is customary in wave mechanics to consider first the following inhomogeneous equation,

$$\frac{\varepsilon(\mathbf{r})}{c_0^2} \partial_t^2 \mathbf{G}(\mathbf{r}, \mathbf{p}, t, t') - \mathbf{p} \times \mathbf{p} \times \mathbf{G}(\mathbf{r}, \mathbf{p}, t, t') = \mathbf{I} \delta(t - t'). \quad (3.1)$$

This equation defines the vector Green's operator $\mathbf{G}(\mathbf{r}, \mathbf{p}, t, t')$. Its importance for wave mechanics cannot be underestimated, although especially experimentalists often consider this object as a technical element to be avoided. Bad news for them since *the Green's function is wave mechanics*, and I shall discuss its properties in a nut shell.

The vector nature of the electric field makes $\mathbf{G}$ a second-rank tensor in polarization space. Causality imposes it to vanish for $t' < t$, since no waves can exist before the source emits. This favors a Laplace transform, introducing the complex frequency z . Causality makes $G(\mathbf{r}, \mathbf{p}, z)$ an analytic operator in the "physical" Riemann sheet $\text{Im } z > 0$ ¹. Resonant excitations in wave propagation must appear as complex poles in $\mathbf{G}(z)$, when continued analytically into the second sheet $\text{Im } z < 0$. This can be made more explicit for light propagation in vacuum ($\varepsilon \equiv 1$). Laplace transforming $t - t'$ to z in the physical sheet, yields

$$\mathbf{G}_0(\mathbf{p}, z) = \frac{1}{z^2/c_0^2 - \mathbf{p}^2 + \mathbf{p}\mathbf{p}}, \quad (3.2)$$

with $\mathbf{p}\mathbf{p}$ the second rank tensor with components $p_i p_j$. For $z = \omega + i\epsilon$ we conclude that poles occur for $\omega/c_0 = \pm p - i\epsilon$ and for $\omega = -i\epsilon$, all located in the lower half sheet, but infinitely close to the real axis, showing that these are real excitations, with infinite lifetime.

Formally, $\mathbf{G}_0(\mathbf{r}, \mathbf{p}, z)$ is still an operator, containing the canonical operators $\mathbf{r}$ and $\mathbf{p}$. The matrix element in momentum representation takes the

¹Strictly speaking this statement is only true in the rotating wave approximation, and a second "physical sheet" with $\text{Im } z < 0$ can be identified for counter-rotating waves.

form $\mathbf{G}_0(\mathbf{p}, \mathbf{p}', \omega) = \mathbf{G}_0(\mathbf{p}, \omega) \delta(\mathbf{p} - \mathbf{p}')$, with

$$\mathbf{G}_0(\mathbf{p}, \omega) = \frac{\hat{\mathbf{p}}\hat{\mathbf{p}}}{(\omega + i\epsilon)^2/c_0^2} + \frac{\mathbf{I} - \hat{\mathbf{p}}\hat{\mathbf{p}}}{(\omega + i\epsilon)^2/c_0^2 - p^2}. \quad (3.3)$$

The above poles at $\omega/c_0 = \pm p - i\epsilon$ are oppositely propagating plane wave excitations with speed c_0 and arbitrary transverse polarization vector. The pole at $\omega/c_0 = -i\epsilon$ is a purely longitudinal and *static* excitation.

The matrix element in real space,

$$\mathbf{G}(\mathbf{r}, \mathbf{r}', \omega) = \langle \mathbf{r} | \mathbf{G}(\omega + i\epsilon) | \mathbf{r}' \rangle \quad (3.4)$$

describes the propagation of a spherical wave at frequency ω from $\mathbf{r}$ to $\mathbf{r}'$ in real space. This interpretation gives many complicated expressions in wave mechanics a relatively easy interpretation. In vacuum, $\mathbf{G}_0(\mathbf{r}, \mathbf{r}', \omega)$ depends on the difference $\mathbf{r} - \mathbf{r}'$ only, and can be calculated by Fourier transforming equation (3.3). It has a longitudinal part Q , a transverse part P , and a contact term according to,

$$\mathbf{G}_0(\mathbf{r}, \omega) = \frac{\omega}{4\pi c_0} \left[Q \left(\frac{\omega r}{c_0} \right) \hat{\mathbf{r}}\hat{\mathbf{r}} + P \left(\frac{\omega r}{c_0} \right) (\mathbf{I} - \hat{\mathbf{r}}\hat{\mathbf{r}}) \right] + \frac{c_0^2 \delta(\mathbf{r})}{3\omega^2} \quad (3.5)$$

with $P(y) = -\exp(iy)[1/y - 1/iy^2 - 1/y^3]$ and $Q(y) = -2\exp(iy)[1/iy^2 + 1/y^3]$. This expression has two important limits. The static regime is defined by $\omega r/c_0 < 1$, whereas the far-field has $\omega r/c_0 > 1$. It can be checked that

$$\mathbf{G}_0(\mathbf{r}, \omega) \rightarrow \begin{cases} c_0^2(4\pi\omega^2 r^3)^{-1} [\mathbf{I} - 3\hat{\mathbf{r}}\hat{\mathbf{r}}] + c_0^2\delta(\mathbf{r})/3\omega^2 & \text{near field} \\ -(4\pi r)^{-1} [\mathbf{I} - \hat{\mathbf{r}}\hat{\mathbf{r}}] \exp(i\omega r/c_0) & \text{far field.} \end{cases} \quad (3.6)$$

In the near field, $\mathbf{G}_0(\mathbf{r}, \omega)$ equals the familiar static $1/r^3$ dipole-dipole interaction. The somewhat subtle contact term plays an important role in multiple scattering, as we shall see in Section 4. In the far field, the phase $\omega r/c_0$ denotes retardation of the wave. In both regimes, the imaginary part of the Green's function behaves nonsingular, and is - for future purposes - shown in Figure 2.

3.2 An atom as a point scatterer

An atom is very small compared to the resonant wavelength of the light, its “size parameter” $k_0 a_0$ being equal to $1/137$, so we assert the dielectric constant of the atom to be given by the point interaction $\varepsilon(\mathbf{r}) = 1 + \alpha \delta(\mathbf{r} - \mathbf{r}_a)$, where $\mathbf{r}_a$ is the position of the atom. The polarization α has the dimension of a volume. Point scatterers for classical waves and their applications have been reviewed recently by De Vries *et al.* [23].

We can insert $\mathbf{E}(\mathbf{r}, t) = \mathbf{E}(\mathbf{r})e^{-i\omega t}$ into the Helmholtz equation, and compare the result to the ordinary Schrödinger eigenvalue problem $[p^2 +$

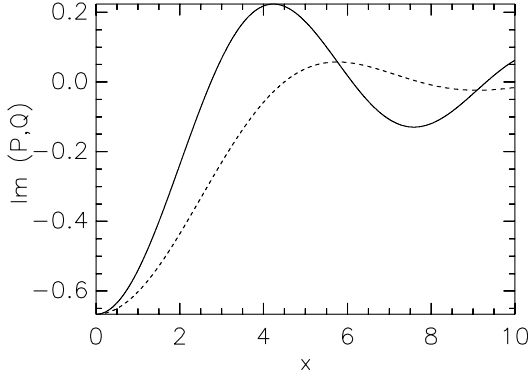


Fig. 2. Imaginary parts of the transverse Green's function P (solid) and the longitudinal Green's function Q (dashed) as a function of distance $x = r\omega/c_0$.

$V(\mathbf{r})\psi(\mathbf{r}) = E\psi(\mathbf{r})$. This comparison identifies ω^2/c_0^2 as the energy E , $[1 - \varepsilon(\mathbf{r})]\omega^2/c_0^2 \equiv V(\mathbf{r}, \omega)$ as the “electromagnetic potential” and seen to be “energy dependent”. Finally, the kinetic operator p^2 is identified with the second rank operator $-\mathbf{p} \times \mathbf{p} \times = \mathbf{p}^2 - \mathbf{p}\mathbf{p}$. This comparison is purely mathematical, and just avoids solving the same equation twice. A well-known “solved” result in wave mechanics is the expression for the scattering operator T in terms of the Born series in the potential [24]. Upon carrying out the above modifications for electromagnetic waves, the electromagnetic scattering operator becomes,

$$\mathbf{T}(\omega) = \mathbf{V}(\mathbf{r}, \omega) + \mathbf{V}(\mathbf{r}, \omega) \cdot \mathbf{G}_0(\mathbf{p}, \omega) \cdot \mathbf{V}(\mathbf{r}, \omega) + \cdots, \quad (3.7)$$

where $\mathbf{G}_0$ is the vector Green's function in vacuum, introduced in the previous section. The Born series can be interpreted in terms of multiple scattering inside the particle. The series (3.7) are easy to evaluate for the above point interaction. The result is the scattering amplitude is

$$\mathbf{t}_{\mathbf{k}\mathbf{k}'}(\omega) \equiv \langle \mathbf{k} | \mathbf{T}(\omega) | \mathbf{k}' \rangle = - \left[\frac{1}{\alpha} \frac{c_0^2}{\omega^2} + \sum_{\mathbf{p}} \mathbf{G}_0(\mathbf{p}, \omega) \right]^{-1}. \quad (3.8)$$

The momentum integral $\sum_{\mathbf{p}} \equiv \int d\mathbf{p}/(2\pi)^3$ in this expression diverges. The longitudinal catastrophe scales like $c_0^2/\omega^2 \sum_{\mathbf{p}} \mathbf{p}\mathbf{p}/p^2$ and contributes an infinite value to the static polarizability α . We will discard this divergence and say that $\alpha(0)$ is just the measured static polarizability. The transverse catastrophe $\sum_{\mathbf{p}} 1/p^2$ has the dimension of an inverse length scale. Regularizing it by $1/\Gamma$ gives the final form [25],

$$\mathbf{t}_{\mathbf{k}\mathbf{k}'}(\omega) = - \frac{4\pi\Gamma\omega^2}{\omega_0^2 - \omega^2 - \frac{2}{3}i\Gamma\omega^3/c_0}, \quad (3.9)$$

where the resonant frequency is defined as $\omega_0^2 \equiv 4\pi\Gamma c_0^2/\alpha(0)$. Expression (3.9) is recognized as the scattering amplitude for a classical radiating dipole [26], provided $\Gamma = r_e$. Thus, the transverse regularization involves the classical electron radius, which is the smallest length scale that can be constructed from classical natural constants, *i.e.* free from $\hbar$. For this reason, the Bohr radius of the atom disqualifies. In the next section it is established that the lifetime of the excited state equals $(\frac{2}{3}\Gamma\omega_0^2/c_0)^{-1}$. The cross-section for a polarization transition $\mathbf{e} \rightarrow \mathbf{e}'$ is proportional to $|\mathbf{e}^* \cdot \mathbf{t}_{\mathbf{k}\mathbf{k}'} \cdot \mathbf{e}'|^2 \sim |\mathbf{e}^* \cdot \mathbf{e}'|^2$, and by adding the in-plane ($\mathbf{e}^* \cdot \mathbf{e}' = \cos\theta$) and out-of plane transitions ($\mathbf{e}^* \cdot \mathbf{e}' = 1$) yields the familiar $1 + \cos^2\theta$ dipole radiation.

3.3 Polarization, cross-section and stored energy

The best known property that can be calculated from the T -matrix is the extinction cross-section, stating how much light flux is captured by the particle and scattered in some direction, and given by $-\text{Im } \mathbf{T}_{\mathbf{k}\mathbf{k}}/k$ [6], with $k = \omega/c_0$. Less well known is how material properties are expressed in terms of the T -matrix (3.7) featuring in light scattering theory: the total induced polarization and the totally stored energy of the particle inside a radiation field.

The operator $\varepsilon(\mathbf{r}) - 1$ denotes the polarizability density of the particle and is expressed in terms of the potential as $-\mathbf{V}(\mathbf{r}, \omega)c_0^2/\omega^2$. Let $|\mathbf{E}_{\mathbf{k}}^+(\omega)\rangle$ be the exact “outgoing” eigenfunction of the scattering eigenvalue problem for a normalized incident plane wave $|\mathbf{k}\rangle$ at frequency ω and wave vector $\mathbf{k}$ and some unspecified polarization vector. The induced polarization density is assumed local and linear in the applied electric field, according to the constitutive equation,

$$|\mathbf{P}_{\mathbf{k}}^+(\omega)\rangle = -\frac{c_0^2}{\omega^2} \mathbf{V}(\mathbf{r}, \omega) |\mathbf{E}_{\mathbf{k}}^+(\omega)\rangle. \quad (3.10)$$

The total polarizability tensor $\alpha_{\mathbf{k}}(\omega)$ is obtained by integrating the polarization density over the whole particle,

$$\begin{aligned} \alpha(\omega, \mathbf{k}) &\equiv \int d\mathbf{r} \langle \mathbf{r} | \mathbf{P}_{\mathbf{k}}^+(\omega) \rangle = -\frac{c_0^2}{\omega^2} \langle \mathbf{p} = 0 | \mathbf{T}(\omega) | \mathbf{k} \rangle \\ &= -\frac{c_0^2}{\omega^2} \mathbf{T}_{\mathbf{0}, \mathbf{k}}(\omega). \end{aligned} \quad (3.11)$$

We have inserted equation (3.10) and used the relation $\mathbf{V}|\mathbf{E}_{\mathbf{k}}^+\rangle = \mathbf{T}|\mathbf{k}\rangle$, which is a general result of scattering theory [24]. This equation establishes the link between polarizability α of an arbitrary dielectric particle and its *off-shell* T -matrix. The absorption cross-section, being a property of the far

field, involves only the *on-shell* T -matrix, for which $p = k = \omega/c_0$,

$$\sigma(\omega, \mathbf{k}) = -\frac{c_0}{\omega_0} \operatorname{Im} T_{i\mathbf{k}i\mathbf{k}}(\omega). \quad (3.12)$$

Upon comparing equations (3.11) and (3.12) we conclude that the familiar relation $\sigma \sim \operatorname{Im} \alpha$ between polarizability α and absorption cross-section σ breaks down for any finite-size scatterer.

The third property of interest is the stored potential energy V_{stored} inside the scatterer during scattering. Standard methods in atomic physics calculate the vibrational energy of the oscillating dipole [27] or obtain - for a two-level atom - the excited-state density matrix element $\rho_{22}(\omega)$ from the optical Bloch equations [16]. Scattering theory provides rigorous expressions, which have been successfully applied to Mie scatterers (dielectric spheres) [6]. The method of finding the totally accumulated energy around a dielectric scatterer follows a similar one, originally due to Friedel, applied to the accumulation of charge around an impurity in the solid state [28]. For an incident plane wave with wavenumber $\mathbf{k}$ and polarization i , the totally stored electromagnetic energy around the scatterer is defined as

$$V_{\text{stored}}(\omega) = \int d\mathbf{r} [\varepsilon(\mathbf{r}) |\mathbf{E}_{i\mathbf{k}}(\omega)|^2 - 1]. \quad (3.13)$$

The “ -1 ” subtracts the normalized incident energy density of the plane wave. In stationary situations, total electric and total magnetic energy can be shown to be equal, as has been supposed in equation (3.13).

Scattering theory relates the stored energy to the (far-field) scattering amplitude, and in particular to its phase shift ϕ [29], according to

$$V_{\text{stored}}(\omega) = -\frac{c_0^2}{2\omega^2} \frac{d}{d\omega} \omega \operatorname{Re} T_{i\mathbf{k}i\mathbf{k}} + c_0 \sum_j \int d\Omega' \frac{d\sigma}{d\Omega}(i\mathbf{k} \rightarrow j\mathbf{k}') \frac{d\phi}{d\omega}. \quad (3.14)$$

Herein, $d\sigma/d\Omega = |T_{i\mathbf{k} \rightarrow j\mathbf{k}'}|^2 / (4\pi)^2$ is the differential cross-section for a scattering event from polarization i and wave number $\mathbf{k}$ to j and $\mathbf{k}'$ [24]; ϕ denotes the phase shift of the scattering amplitude for the same transition. The first term in equation (3.14) is a somewhat subtle contribution from the forward channel that does not really scatter. The stored energy allows to estimate the typical time scale of the scattering process. Since σc_0 is the energy leaving the particle per unit of time, we can define the (Wigner) *time delay* in the scattering process as,

$$\tau_d(\omega) \equiv \frac{V_{\text{stored}}(\omega)}{\sigma(\omega)c_0}. \quad (3.15)$$

This relation can actually serve to get a heuristic explanation for equation (3.14) [6].

For the “atom”, whose t -matrix is given by equation (3.9), no difference exists between on-shell and off-shell t -matrix. Hence,

$$\alpha(\omega) = -\frac{c_0^2}{\omega^2} t(\omega), \quad (3.16)$$

and we recover the well-known relation between scattering amplitude and polarization of the harmonic oscillator. Similarly, insertion of equation (3.9) into equation (3.14) yields,

$$V_{\text{stored}}(\omega) = \frac{c_0^4}{\alpha(0)} \frac{(4\pi\Gamma)^2}{(\omega_0^2 - \omega^2)^2 + (\frac{2}{3}\Gamma\omega^3/c_0)^2}. \quad (3.17)$$

This result coincides with the one obtained for the matrix element $\rho_{22}(\omega)$ using the optical Bloch equations [16] in the case of pure radiation line broadening. The total atomic cross-section being $\sigma = |t|^2/6\pi$, the delay time becomes,

$$\tau_d = \frac{6\pi c_0^3}{\alpha(0)\omega^4}. \quad (3.18)$$

This time is essentially *constant* in the region $\omega_0 \pm \Delta\omega$ around the resonant frequency. The relation to the spontaneous emission time can be established inserting $\alpha(0)/4\pi = 2|\mathbf{d}|^2/\hbar\omega_0$ [30] in terms of the atomic dipole matrix element $\mathbf{d}$. Hence,

$$\frac{1}{\tau_d} = \frac{4}{3} \frac{|\mathbf{d}|^2\omega_0^3}{\hbar c_0^3} = A. \quad (3.19)$$

This is the standard expression for the spontaneous emission coefficient A of a two-level atom in vacuum [27]. Spontaneous emission and time delay near resonance thus coincide numerically for pointlike atoms. In the next section I confirm this statement even for two atoms. Physically however, spontaneous emission and resonant time delay are *not at all* equal, since spontaneous emission is an inelastic process and completely incoherent, triggered by vacuum fluctuations, whereas equation (3.19) describes the mesoscopic time delay of an *elastically scattered* wave, and is - contrary to A , also defined far away from resonance.

3.4 Two atoms: Dipole-dipole coupling

When two resonant scatterers are located in each others near field, their collective scattering cross-section can be different from the sum of the individual cross-sections. This phenomenon is known as *dependent scattering*. In multiple scattering situations it is an important mechanism for the experimental fact that the scattering mean free path is underestimated by

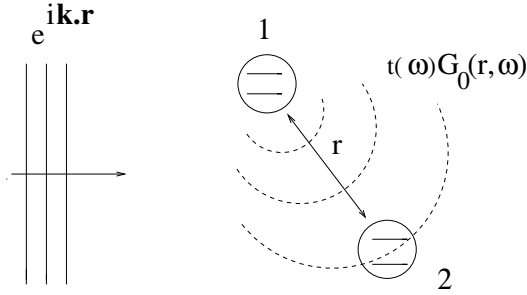


Fig. 3. A plane wave incident on a pair of “two-level” atoms, separated by a distance r . The dashed line denotes a spherical wave scattered by atom 1 towards atom 2 and is given mathematically by $t(\omega)\mathbf{G}_0(\mathbf{r}, \omega)$. The scattering amplitude of the two particle system contains all orders in this scattered wave, which induces new scattering resonances.

the well-known formula $\ell = 1/n\sigma$, where n is the number density of the particles.

Consider Figure 3, showing a plane electromagnetic wave incident on two “atoms”. Apart from being scattered into the far field, both particles act as point sources for their neighbors. As a result, the T-operator of the total system can be written down as,

$$\mathbf{T} = \frac{t|1\rangle\langle 1| + t|2\rangle\langle 2| + t^2\mathbf{G}_0(\mathbf{r})(|1\rangle\langle 2| + |2\rangle\langle 1|)}{1 - t^2\mathbf{G}_0^2(\mathbf{r})}. \quad (3.20)$$

In this equation, $\mathbf{r}$ is the interparticle axis, $\mathbf{G}_0(\mathbf{r})$ is a spherical wave propagating from one particle to the other as explained earlier, t is the isotropic scattering amplitude for one particle, as defined in equation (3.9), and $|1\rangle, |2\rangle$ denote the positions of the two pointlike atoms. The denominator $1 - t^2\mathbf{G}_0^2(\mathbf{r})$ signifies all orders of recurrent scattering between the two particles. If $|t^2\mathbf{G}_0^2(\mathbf{r})| > 1$ this factor reduces the scattering amplitude considerably. Since the total scattering cross-section equals $\sigma = |t|^2/6\pi$ and typically $|\mathbf{G}_0| \approx 1/4\pi r$ for not too closely separated atoms, we infer that dependent scattering sets in when $r^2 < \sigma$, *i.e.* when the optical volumes overlap. Near resonance the optical volume is much bigger than the atomic size.

Dependent scattering induces new frequency poles of the scattering amplitude in the complex plane. As customary in atomic physics I define a detuning parameter $\delta = \omega_0 - \omega$. The detuning normalized by the line width $\gamma = \Gamma\omega_0^2/c_0$ I will call Δ . Hence,

$$t(\Delta) = -\frac{4\pi c_0}{\omega_0} \frac{1}{\Delta - \frac{2}{3}i}. \quad (3.21)$$

For finite $\omega_0 r/c_0$ the pole at $\Delta = \frac{2}{3}i$ of a single atom splits up into four different poles,

$$\begin{cases} \Delta = \frac{2}{3}i \pm P(\omega_0 r/c_0) \\ \Delta = \frac{2}{3}i \pm Q(\omega_0 r/c_0). \end{cases} \quad (3.22)$$

The quantities P and Q were introduced earlier in equation (3.5). Figure 2 shows that $\text{Im}(P, Q) \geq -\frac{2}{3}$, so that all poles ly in the “unphysical Riemann sheet” $\text{Im} \omega < 0$, as was argued earlier on the basis of causality. The Q -resonances correspond to dressed Σ states with both atomic polarizations along the $\mathbf{r}$ -axis. The P solutions have both atomic polarizations perpendicular to the $\mathbf{r}$ -axis, and are referred to as the Π -states.

The 4 above poles are reminiscent of the four optical transitions in the famous Dicke problem addressing spontaneous emission from two coupled two-level systems, two of which are “subradiant”, and two of which are “superradiant” [31]. The poles that approach the real axis are called *subradiant*. These poles show up as narrow resonances in the joint cross-section, with large delay time. For $\omega_0 r/c_0 \ll 1$, the subradiant poles correspond to the “+” sign in equation (3.22) and tend to genuine bound states. In this regime the Green’s function is typically equal to the static dipole-dipole interaction which has $Q \approx -2/y^3$ and $P \approx 1/y^3$, so that subradiant poles occur for $\Delta \approx -2/y^3$, i.e. $\omega = \omega_0[1 + 2\alpha(0)/4\pi r^3]$, and $\Delta \approx 1/y^3$, i.e. $\omega = \omega_0[1 - \alpha(0)/4\pi r^3]$, located at both sides of the resonance ω_0 . This outcome is confirmed by the (quantum-mechanical) theory of the resonant Van der Waals interaction between one atom in the ground state and one in the excited state [34].

Poles that move away from the real axis are called *superradiant*. They have a line width twice as large as the one for one atom, reminiscent of the Dicke problem. For large $\omega_0 r/c_0$, all poles finally merge onto the pole at ω_0 , with a dominant contribution from the Π -states, for which $\text{Im} \omega = -A(1 \pm \frac{3}{2} \sin k_0 r/k_0 r)$. Again, this result also emerges in superradiance from two atoms that are many optical wavelengths apart [32].

In view of the former section, three quantities are of interest: the total cross-section, the total polarization and the stored energy by two atoms, which I shall now obtain. The absorption cross-section is obtained from the forward scattering amplitude using equations (3.20) and (3.12) which I shall average over interparticle direction. This averaging can easily be carried out analytically, and the result is shown in Figure 4 for $\omega_0 r/c_0 = 1$. The two narrow subradiant resonances at both sides of the original resonance ω_0 are clearly visible. Near the atomic resonance ω_0 , dependent scattering suppresses the total cross-section of the two particles significantly.

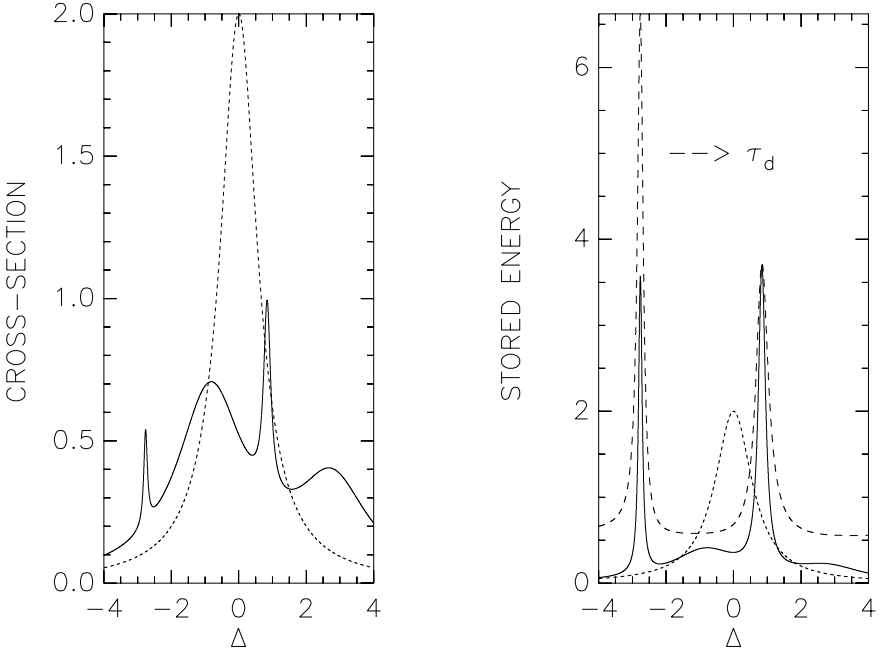


Fig. 4. Total scattering cross-section (left, in units of $6\pi c_0^2/\omega_0^2$, *i.e.* the resonant cross-section of one atom) and stored energy (right, in units of the resonant value for one atom) for two atoms separated by a distance $r = c_0/\omega_0$. The dotted line in both graphs denotes the Lorentzian profile of two independent atoms far apart. The two subradiant poles are clearly visible. The two superradiant poles give rise to a much broader lobe. Near the original resonance ($\Delta \approx 0$) the collective cross-section is suppressed by dependent scattering. The stored energy is very large only near the two subradiant resonances. The line labeled τ_d denotes the delay time defined as $V_{\text{stored}}/\sigma c_0$, in units of the spontaneous emission time for one atom. Away from the subradiant poles it has the constant superradiant value $0.5A^{-1}$.

The polarization tensor α of the two particles is readily obtained from equation (3.11). Since $\langle \mathbf{p} = 0 | 1, 2 \rangle = 1$ it follows that,

$$\alpha_{\mathbf{k}}(\Delta, \mathbf{r}) = \frac{8\pi}{k_0^3} \frac{2 \cos(\frac{1}{2} \mathbf{k} \cdot \mathbf{r})}{\Delta - \frac{2}{3}i + Q(k_0 r) \hat{\mathbf{r}} \hat{\mathbf{r}} + P(k_0 r) [\mathbf{I} - \hat{\mathbf{r}} \hat{\mathbf{r}}]} . \quad (3.23)$$

The polarization tensor is anisotropic, different along and parallel to the interparticle axis. It contains only two poles. For $k_0 r \ll 1$ they are both maximally superradiant. In this classical picture “superradiance” refers to an increased collective radiation damping. The two subradiant transitions

hardly suffer from radiation damping since they involve no net excitation of polarization.

The stored energy by the two atoms in an optical radiation field is defined in equation (3.13). Also in this case, scattering theory provides a rigorous expression in terms of the forward scattering amplitude $\mathbf{T}_{\mathbf{pp}}$ [33]

$$V_{\text{stored}}(\omega) = -\frac{2\pi W_0(\omega)c_0^3}{\omega^3} \times \text{Im Tr} \sum_{\mathbf{p}} (p^2 - \mathbf{pp}) \cdot \mathbf{G}_0(\mathbf{p}, \omega) \cdot \mathbf{T}_{\mathbf{pp}}(\omega) \cdot \mathbf{G}_0(\mathbf{p}, \omega). \quad (3.24)$$

$W_0(\omega)$ denotes the energy density of the background radiation which has been assumed isotropic. Tr denotes a trace over polarization, the tensor $(p^2 - \mathbf{pp})$ guaranteeing that only transverse polarizations come in. Like we saw for the polarization (3.11), evaluation of the above formula requires knowledge of the *off-shell* scattering amplitude. This information is provided by equation (3.20) for the atom pair. Straightforward insertion, thereby consistently applying the regularization procedure of the previous section, yields the relatively simple expression,

$$V_{\text{stored}}(\mathbf{r}) = \frac{\pi W_0(\omega)c_0^3}{\omega^2} \text{Im Tr} \frac{d}{d\omega} [2\text{Log } t(\omega) - \text{Log}(1 - t^2 \mathbf{G}_0^2(\mathbf{r}, \omega))]. \quad (3.25)$$

The first term just reproduces the stored energy (3.17) of two independent atoms. The second term is the *induced dipole-dipole binding energy* $V_{\text{dd}}(\mathbf{r})$. In atomic physics, this binding energy is often described in terms of a “virtual” exchange of a photon between two atoms in the ground state [34]. In equation (3.25) this exchange is made explicit by the term $t^2 \mathbf{G}_0^2(\mathbf{r})$. It is the first term in a series where high order recurrences are accounted for by the complex logarithm.

In Figure 4 (right) the stored energy has been evaluated near resonance. Near the subradiant resonances, the delay time τ_d (indicated as a dashed line) becomes very large and would tend to the infinite subradiant value if $\omega_0 r/c_0 \ll 1$. Elsewhere, near the superradiant resonances in particular, the delay time is constant, and equal to the familiar superradiant value of $0.5A^{-1}$.

3.5 Induced dipole force between two simple atoms

By means of the induced dipole-dipole force, an external radiation field can be expected to affect the interaction between two atoms in their ground state. Fedichev *et al.* [35] calculated how the *s*-wave scattering length is modified by light nearly resonant with a vibrational resonance of two ^7Li

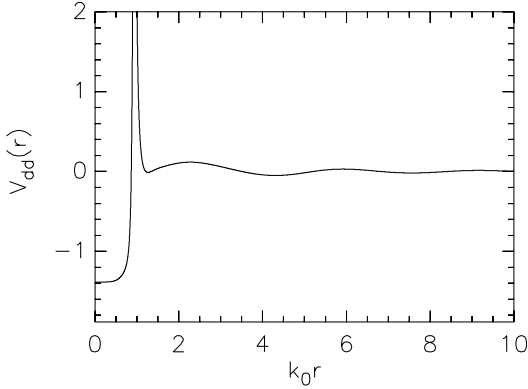


Fig. 5. Induced dipole-dipole energy between two two-level systems tuned one linewidth off-resonance ($\Delta = 1$) in an isotropic radiation field with energy density W_0 , as a function of their separation r . Energy unit is $W_0/k_0^3 \times 1/\Gamma k_0$, whose order of magnitude is discussed in the text. The potential is attractive at small distances, reaches a strongly repulsive maximum when a subradiant pole at $k_0 r \approx \Delta^{1/3}$ is excited and asymptotically oscillates as $\sin(2k_0 r)/r^2$.

atoms. I will here estimate the typical interaction strengths involved for a pair of two-level systems with *pure* radiative broadening, and light nearly resonant with the optical transition at ω_0 . For an (assumed isotropic) *purely* monochromatic radiation density W_0 , equation (3.25) yields, around the resonance ω_0 ,

$$V_{\text{dd}}(\mathbf{r}) = -\frac{W_0 c_0^3}{\Gamma \omega_0^3} \text{Im Tr} \frac{t^3(\Delta) \mathbf{G}_0^2(\mathbf{r}, \omega_0)}{1 - t^2(\Delta) \mathbf{G}_0^2(\mathbf{r}, \omega_0)}. \quad (3.26)$$

This potential energy is shown in Figure 5. Asymptotically, *i.e.* for $k_0 r > 1$, this potential decays as

$$V_{\text{dd}}(\mathbf{r}) \approx \frac{W_0}{k_0^3} \times \frac{1}{\Gamma k_0} \times \frac{1}{(\Delta^2 + \frac{4}{9})^{3/2}} \frac{\sin(2k_0 r + \phi)}{(k_0 r)^2}. \quad (3.27)$$

The oscillation factor with wavenumber $2k_0$ is, mostly in the context of impurity screening in the solid state, known as a Friedel oscillation [28]. The factor $1/\Gamma k_0$ denotes the quality factor $\omega_0/\Delta\omega$ of the oscillator. Its large value, 6×10^7 for the optical transition in Rubidium [3], makes the induced dipole energy large. For a typical radiation density $W_0 \approx 10^{-2} \text{ J/cm}^3$, corresponding to a radiation intensity $I \approx 1 \text{ mW/cm}^2$ and small enough to avoid saturation effects in Rubidium, we find that $V_{\text{dd}} \approx 88 \text{ K}$, 6 orders of magnitude larger than the typical $100 \text{ } \mu\text{K}$ associated with the kinetic energy of the atoms! For detunings far off-resonance, and for densities

$n \approx 10^{14} \text{ cm}^{-3}$ we can check that the average distance between the atoms is less than the strong repulsive peak in the dipole-dipole potential, located at $r \approx \Delta^{1/3}/k_0$.

Nearly resonant light has the disadvantage that recoil effects, caused by radiation pressure, are largest [3]. They can be suppressed by lowering the flux density of the incident light. The dipole-dipole energy is proportional to the light flux as well but can, in view of the large quality factor, still largely exceed the kinetic energy of the atoms.

3.6 Van der Waals interaction

In this section I discuss the Van der Waals force from the uncustomary point of view of scattering theory, facilitated by the induced dipole-dipole coupling, obtained in equation (3.25). In standard textbooks [34], the Van der Waals Interaction is obtained by perturbing the Hamiltonian of two atoms in their ground state, separated by a distance r , by the standard dipole-dipole interaction varying as $1/r^3$. Second-order perturbation theory leads to a shift of the order of $-1/r^6$ in the energy levels, identified as the attractive Van der Waals potential.

Equation (3.25) provides the binding energy of two (classical) atoms at distance r , for a incident plane wave with normalized energy density. The second term is identified as the dipole-dipole energy. For a general radiation energy density $W(\omega)$, assumed to be isotropic, the total dipole-dipole energy is readily seen to be,

$$V_{\text{dd}}(\mathbf{r}) = \pi c_0^3 \int_0^\infty d\omega \frac{d}{d\omega} \left(\frac{W(\omega)}{\omega^2} \right) \text{Im Tr Log} [1 - t^2 \mathbf{G}_0^2(\mathbf{r}, \omega)], \quad (3.28)$$

where one partial integration has been carried out. This formula illustrates that a radiation field $W(\omega) \propto \omega^2$ - the case for (classical) thermal radiation at very high temperatures [36] - does not induce a net force. In the absence of any (thermal) background radiation, vacuum fluctuations still contribute an energy density $W(\omega) = \frac{1}{2} \hbar \omega \times \omega^2 / \pi^2 c_0^3$, so that

$$V_{\text{dd}}(\mathbf{r}) = \frac{\hbar}{2\pi} \int_0^\infty d\omega \text{Im Tr Log} [1 - t^2 \mathbf{G}_0^2(\mathbf{r}, \omega)] . \quad (3.29)$$

A formal series expansion of the complex logarithm shows how subsequent high orders in recurrent scattering contribute to the Van der Waals potential. Only for the simple two-level system it is possible to sum the whole series of recurrent exchange. The far-field corresponds to $r > 1/k_0$, with $k_0 = \omega_0/c_0$. A straightforward asymptotic analysis shows that low frequencies dominate in equation (3.29). Since $t(\omega) \mathbf{G}_0 \sim \omega^3$ this notion also

guarantees high orders to be negligible, and

$$V_{\text{dd}}(\mathbf{r}) = -\frac{\hbar}{2\pi} \left(\frac{\alpha(0)}{4\pi} \right)^2 \text{Im} \int_0^\infty d\omega \frac{\omega^6}{c_0^6} \left[2P \left(\frac{r\omega}{c_0} \right)^2 + Q \left(\frac{r\omega}{c_0} \right)^2 \right] \\ \sim -\frac{\hbar c_0}{\pi r^7} \left(\frac{\alpha(0)}{4\pi} \right)^2. \quad (3.30)$$

This is recognized as the retarded Casimir-Polder interaction [37]. The retardation is contained in the phase of the Green's functions P and Q in the far field.

In the near field $r < 1/k_0$ retarding phase factors in the Green's function and t -matrix can be neglected. One obtains,

$$V_{\text{dd}}(\mathbf{r}) = \frac{\hbar}{2\pi} \int_0^\infty d\omega \, 2 \log \left[1 - \left(\frac{\alpha(0)}{4\pi r^3} \right)^2 \left(\frac{\omega_0^2}{\omega_0^2 - \omega^2 + i\epsilon} \right)^2 \right] \\ + \log \left[1 - \left(\frac{\alpha(0)}{4\pi r^3} \right)^2 \left(\frac{2\omega_0^2}{\omega_0^2 - \omega^2 + i\epsilon} \right)^2 \right].$$

This result is valid for $\alpha(0)/4\pi r^3 < 1$, where $\alpha(0) \approx 4\pi a_0^3/3$. Since $k_0 a_0 \approx 1/137$, there is still a considerable regime $a_0 < r < 1/k_0$ where the nonretarded version of the potential applies. The integration can be carried out using contour integration and

$$V_{\text{dd}}(\mathbf{r}) = -\hbar\omega_0 \left(2\sqrt{\frac{1 + \sqrt{1 + \xi^2}}{2}} + \sqrt{\frac{1 + \sqrt{1 + 4\xi^2}}{2}} - 3 \right). \quad (3.31)$$

I abbreviated $\xi \equiv \alpha(0)/4\pi r^3$. For $\xi \ll 1$ this result coincides with the standard Van der Waals potential $V_{\text{dd}}(\mathbf{r}) \sim -K(e^2/r)(a_0/r)^5$ [34]. In the regime $a_0 < r < 1/k_0$ the front factor K changes by only a factor of two. When $r < a_0$ the overlap of the atomic orbitals, not described here, leads to a strong repulsion of the atoms, as made explicit in the Lennard-Jones potential.

4 Applications in multiple scattering

Let us consider a random collection of semi-classical two-level atoms. I assume all “atoms” to be identical and neglect any source of inhomogeneous line broadening. The number density of the “atoms” is denoted by n , and their polarizability is $\alpha(\omega)$. For a point particle, the latter relates directly to the scattering amplitude $t(\omega)$, as shown in equation (3.16).

4.1 Effective medium

The first aspect of multiple scattering is the dielectric constant ε_e of the effective medium. This parameter relates the average, macroscopic polarization to the applied electric field, according to,

$$\langle \mathbf{P}(\omega) \rangle = (\varepsilon_e - 1) \langle \mathbf{E}(\omega) \rangle . \quad (4.1)$$

The brackets denote an ensemble averaging over all positions of the atoms. The “textbook” result [38],

$$\varepsilon_e = 1 + \frac{n\alpha(\omega)}{1 - \frac{1}{3}n\alpha(\omega)} . \quad (4.2)$$

is the celebrated *Lorentz-Lorenz formula*. A number of very critical comments are in order.

Equation (4.2) is often obtained by adding the microscopic polarizations of the individual atoms inside a big sphere, thereby dealing with the surface charges on the boundary of this sphere, generating the “local field factor” $1/(1 - \frac{1}{3}n\alpha)$ [39]. This treatment is correct for $\omega = 0$, *i.e.* in electrostatics. For $\omega \neq 0$, in particular at optical frequencies, one is obliged to consider retardation. The exact propagation of light at any frequency between two particles is described by the Green’s function (3.5). It is possible to derive the Lorentz-Lorenz formula from rigorous microscopic scattering theory. An elegant though difficult proof can be found in the standard work by Born and Wolf [38], later modified by Felderhof *et al.* [40] and Lagendijk *et al.* [41]. The recent proofs establish that the local field factor in equation (4.2) can be seen as a direct consequence of the subtle contact term in equation (3.5). They also show that the Lorentz-Lorenz formula applies *provided* that all dependent scattering is ignored. In the former section I showed that these effects become significant when the optical volumes start to overlap. When that happens, the Lorentz-Lorenz relation is a bad approximation. Morice *et al.* [42] and Ruostekoski and Javanainen [43] calculated dependent scattering corrections to ε_e for resonant two-level atoms. As we will see, these corrections are sensitive to the statistics of the atoms and may enable to monitor a Bose-Einstein transition or the formation of a Fermi gas.

The second critical remark relevant to relation (4.2) involves the exact role of ε_e in the context of mesoscopic wave physics. This role can only be elucidated with scattering theory. The effective-medium dielectric constant describes the ensemble-averaged field. It is readily checked that ε_e is complex-valued, with *positive* imaginary part. Thus, the average electromagnetic field suffers from *extinction*. Inserting the constitutive relation (4.1) into Maxwell’s equations provides a complex dispersion law, relating wave number k and frequency ω of an excitation by a point source

$$\exp(-i\omega t) \exp(iKr)/r,$$

$$K^2 \equiv \left(k + \frac{i}{2\ell}\right)^2 = \varepsilon_e(\omega) \frac{\omega^2}{c_0^2}. \quad (4.3)$$

As shown by Loudon [2], the resonant frequency dependence of the real part of the complex wave number K , $k(\omega)$, leads to a familiar polariton behavior, with a pseudo-gap opening up near the resonant frequency. The positive imaginary part of K is translated to an *extinction length* ℓ and is a good example of the discussion on “decoherence”, “randomness” and “absorption” in Section 2. All three mechanisms contribute to extinction, and by looking at ε_e *alone* no distinction can be made. The parameter ε_e is *not* associated with the (ensemble-averaged) energy density W , and $\text{Im } \varepsilon_e$ does not necessarily imply absorption. The extra knowledge that we started out with, a harmonic oscillator with pure radiative line broadening, leads us to conclude that here, the positive imaginary part must be due to “randomness”, making the phase a random variable, and described by the mean free path introduced earlier in equation (2.4). On the contrary, in strongly condensed matter, $\text{Im } \varepsilon_e$ refers to genuine absorption, expressed by the absorption time τ_a defined in equation (2.9). In radiation trapping, the extinction mean free path refers to pure inelastic scattering, as expressed by equation (2.12). It is very important to keep this confusing, double role of ε_e in mesoscopic wave mechanics in mind.

4.2 Group and energy velocity

The dispersion relation $\omega(k)$ deduced from equation (4.3) defines the group velocity,

$$\begin{aligned} v_g(\omega) &\equiv \frac{d\omega}{dk} = \frac{c_0^2}{v_p} \left[1 - \frac{nc_0^2}{2\omega} \frac{d}{d\omega} \text{Re } t(\omega) + \mathcal{O}(n^2) \right]^{-1} \\ &\approx c_0 \left[1 + \frac{4\pi n c_0^4}{\omega_0^4 \Gamma} \frac{\Delta^2 - \frac{4}{9}}{(\Delta^2 + \frac{4}{9})^2} \right]^{-1}. \end{aligned} \quad (4.4)$$

The last approximation applies close to the resonant frequency ω_0 ; $v_p = \omega/k$ is the phase velocity.

It is well-known that the group velocity describes the speed of the *maximum* of a wave packet, provided that the pulse distortion is not too big [38]. This is a particularly interesting statement in view of formula (4.4). The factor $4\pi n c_0^4 / \omega_0^4 \Gamma$ can be rewritten as $(4\pi n / k_0^3) \times (\omega_0 / \Delta\omega) \equiv P$. The first factor is basically the number of atoms per optical volume at resonance. A typical atomic density in Bose-Einstein experiments is $n = 10^{14} \text{ cm}^{-3}$ so that $4\pi n / k_0^3 \approx 0.7$. The second factor is the quality factor of the resonance. It can be large for atomic resonators. Already when the front factor

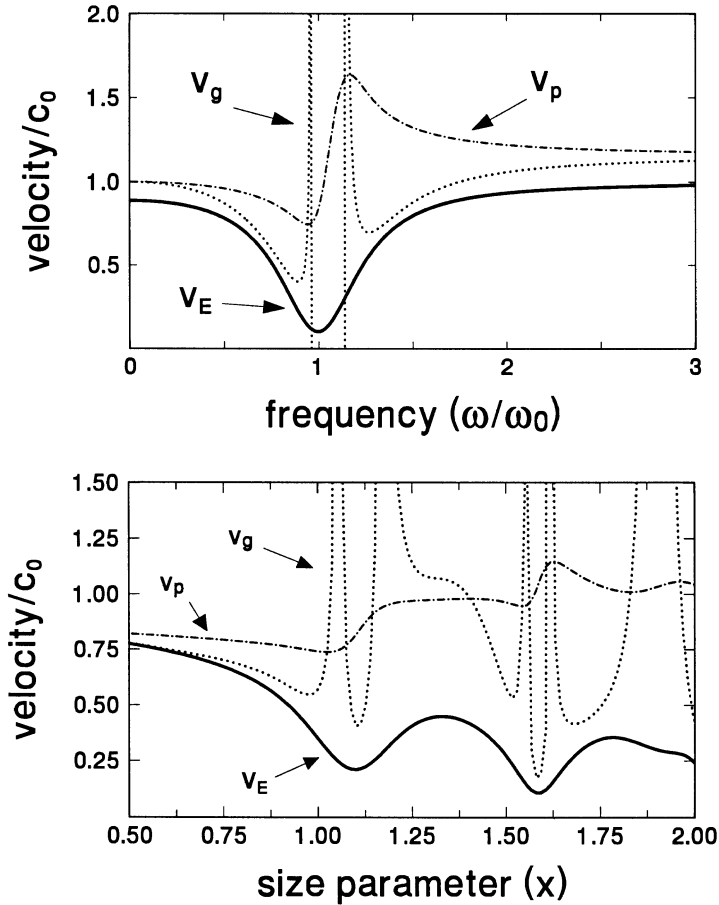


Fig. 6. Phase velocity $v_p = \omega/k$, group velocity $v_g = d\omega/dk$ and energy velocity v_E as a function of frequency. Top figure applies to a polariton with resonant frequency ω_0 and atom density $4\pi n/k_0^3 = 1.5$; bottom figure applies to a random collection of dielectric spheres with index of refraction $m = 2.7$ and volume fraction of 20%. The parameter $x = a\omega/c_0$ scales the frequency with the size a of the spheres. For simplicity, only the absolute value $|v_g|$ has been plotted. Taken from Lagendijk and Van Tiggelen [6], with thanks to Lagendijk.

$P > 0.5$, the group velocity has two singular points where it diverges, taking *negative values* in between (see Fig. 6). This criterion is easily satisfied with atomic resonators.

The validity of “group velocity” in this anomalous regime is often questioned. However, the anomalous value of the group velocity is not

necessarily violating Einstein causality, which imposes that energy transport cannot be faster than c_0 . It has been remarked earlier that the effective-medium dielectric constant ε_e , and hence all quantities constructed from it, have no relation to energy transport. Hence, the group velocity does not describe energy transport and Einstein causality cannot be discussed, and no first principle exists why $0 < v_g < c_0$. Negative group velocities were first discussed by Garret and McCumber [44], later followed by an experiment by Chu *et al.* [45], reporting group velocities $v_g \approx -10^6$ m/s. They occur when the peak of the Gaussian pulse emerges from the sample before the peak of the pulse actually enters. Group velocities have recently achieved new interest in acoustic wave propagation [46].

To show that near resonance no causality problems occur, Brillouin [47] and Loudon [16, 48] introduced the energy velocity v_E . This velocity is defined as the ratio of the average Poynting vector $\langle S \rangle$ and the average electromagnetic energy density $\langle W \rangle$,

$$v_E(\omega) = \frac{\langle S(\omega) \rangle}{\langle W(\omega) \rangle}. \quad (4.5)$$

The crucial point is that, near a resonance, the energy density achieves a significant and even dominating matter component, signifying the strong delay of light in the scattering process. Inclusion of the matter energy, easily calculated for the harmonic oscillator, confirms that $v_E < c_0$ (Fig. 6).

Since 1990, a derivation of the energy velocity v_E exist using mesoscopic scattering theory [49]. Phenomenological treatments are inadequate if one wishes to keep track of all the phases. As a bonus, this treatment elucidates what exactly propagates with the energy velocity, something that is not directly clear from the work of Brillouin and Loudon. Nevertheless, scattering theory confirms in great detail the physics behind v_E as it was put forward by Brillouin and Loudon. Quite recently, an asymptotic analysis was published, showing that the peak velocity of the attenuated beam actually approaches the energy velocity when the sample is much larger (typically a hundred times bigger) than the mean free path [52].

The easiest “mesoscopic” derivation of v_E uses arguments of the former sections, and is closest to the original arguments of Brillouin and Loudon. Without the explicit consideration of scattering, the group velocity would equal $v_g = c_0^2 k / \omega = c_0^2 / v_p$. Next we must treat the scattering, including the subtle forward scattering, which alone would lead to the group velocity (4.4). The delay time for waves scattered in arbitrary direction has been given in equation (3.15). An elementary argument shows that during multiple scattering, the effective velocity along one mean free path is renormalized by the factor $(\ell/c_0)/[\ell/(c_0^2/v_p) + \tau_d]$. Since $\ell = 1/n\sigma(\omega)$ in terms of the total cross-section $\sigma(\omega)$ of the particles, and using equation (3.15) for the

delay time, one obtains for the energy velocity,

$$v_E(\omega) = \frac{c_0^2}{v_p} \frac{1}{v_p/c_0 + nV_{\text{stored}}(\omega)} . \quad (4.6)$$

By using relation (3.14) for V_{stored} in terms of the scattering matrix, one basically recovers the expression for v_E that was originally obtained from transport theory [49], involving the phase-shifts. It applies when dependent scattering can be neglected. Equation (3.14) for the stored energy shows explicitly how the anomalous group velocity term in equation (4.4) is compensated by a scattering term, *i.e.* the group velocity does not count the scattering but that seems to be where most of the energy finally goes near resonant scattering.

Despite the strong similarity of v_E to earlier work, the scattering theory for v_E for classical waves has been subject of a significant and rather technical controversy in literature [50, 51]. It was initiated by a field-theoretical “Ward” identity, valid for electron waves in impurity scattering, stating that the nominator of equation (4.6) equals *unity*. It is now known that classical waves do not obey this identity [51], which has to do with their somewhat different conserved quantity. This difference is best be elucidated by splitting the energy V_{stored} stored in one particle up according to

$$V_{\text{stored}}(\omega) = \int d\mathbf{r} [|\mathbf{E}(\mathbf{r}, \omega)|^2 - 1] + \int d\mathbf{r} \mathbf{E}(\mathbf{r}, \omega) \cdot \mathbf{P}^*(\mathbf{r}, \omega), \quad (4.7)$$

where $\mathbf{P}(\mathbf{r}, \omega) = [\varepsilon(\mathbf{r}, \omega) - 1]\mathbf{E}(\mathbf{r}, \omega)$ has been inserted for the local polarization density at frequency ω . The second term signifies stored potential energy inside the scatterer, but does not exist for De Broglie waves. The first term *cancels* against the term v_p/c_0 in equation (3.14) by the “Ward” identity [28], to give 1. The remainder, the potential energy in equation (4.7), makes the desired link with the approaches by Loudon and Brillouin, who calculated the vibrational energy of the radiating dipole. Near scattering resonances, V_{stored} becomes large and the velocity v_E small. In Figure 6 I show group and energy velocity for the polariton discussed by Loudon and Brillouin, as well as for an ensemble of Mie scatterers.

The above argument to obtain v_E reveals the role of v_E in the mesoscopic regime. It is the velocity of light measured along *any* long scattering sequence. Long scattering sequences are typically described by a diffusion process, involving a diffusion constant $D(\omega)$. The classical expression for this transport coefficient involves the product of a velocity and a mean free path, the step length of the random walk. The former discussion favors the energy velocity, so that [6, 49],

$$D(\omega) = \frac{1}{3} v_E(\omega) \ell^*(\omega). \quad (4.8)$$

This deceptively simple expression hides the highly mesoscopic nature of v_E and ℓ^* , both subject to interferences. The same equation was derived by Compton back in 1922 [14] for the phenomenon of radiation trapping. In this case, the time delay is just the time it takes for an atom to re-radiate a captured photon inelastically, and also much larger than the mean free time between two captures. The “transport mean free path” ℓ^* differs from the extinction length ℓ if the scattering is anisotropic [53], but for the two-level atom they are just equal. The diffusion coefficient is an experimentally accessible quantity, at least for classical waves, and it is in this way that v_E should be and has been measured directly [49, 54]. The energy velocity also shows up as a typical velocity in *self-induced transparency*, a nonlinear phenomenon due to saturation of the excited level of a two-level system [27], and with a recent report of $v_E \approx 17$ m/s [55].

Values $v_E \approx c_0/10$ have been confirmed by diffusion experiments with visible light [49] and microwaves [54]. The values for v_E measured for classical scatterers are quite smaller than velocities in transparent homogeneous materials, but are still much larger than the ones expected for atomic oscillators. At resonance, the value $v_E/c_0 = 1/[1 + 9\pi n/k_0^3 \times \omega_0/\Delta\omega]$ is obtained, which can become very small due to the large atomic quality factor. It must be noted that inhomogeneous line broadening decreases the quality factor significantly. In classical wave propagation, a broad size distribution of the particles is often an important source of inhomogeneous line broadening. Cold atoms do not suffer from this. With a atomic density of $n \approx 10^9 \text{ cm}^{-3}$ and an atomic quality factor $\omega_0/\Delta\omega \approx 6 \times 10^7$ (Rubidium) a velocity $v_E \approx 3 \times 10^{-4} c_0$ may be achieved.

4.3 Dipole–dipole coupling in the medium

In Section 3.4 I discussed the dipole-dipole energy between two atoms at a fixed distance. The question I address here is how much dipole-dipole binding energy will be stored in a random medium with atom density n . This binding energy provides the leading “dependent scattering” correction to the energy velocity v_E given in equation (4.6).

For completely randomly distributed atoms and background radiation with unit energy density, the stored energy density is directly obtained from equation (3.25),

$$\langle W_{\text{dd}} \rangle = -\frac{1}{2}n^2 \times \frac{\pi c_0^3}{\omega^2} \int d\mathbf{r} \text{Im} \text{Tr} \frac{d}{d\omega} \text{Log} (1 - t^2 \mathbf{G}_0^2(\mathbf{r}, \omega)) . \quad (4.9)$$

Similarly, it is possible to obtain the “dependent scattering” correction to the total “absorption” cross-section, using equations (3.20) and (3.12),

$$\langle \delta\sigma_{\text{dd}} \rangle = -\frac{c_0}{\omega} n \int d\mathbf{r} \text{Im} \left(\frac{t^3 \mathbf{G}_0^2(\mathbf{r}, \omega) + t^4 \mathbf{G}_0^3(\mathbf{r}, \omega) e^{i\mathbf{k} \cdot \mathbf{r}}}{1 - t^2 \mathbf{G}_0^2(\mathbf{r}, \omega)} \right)_{ii} . \quad (4.10)$$

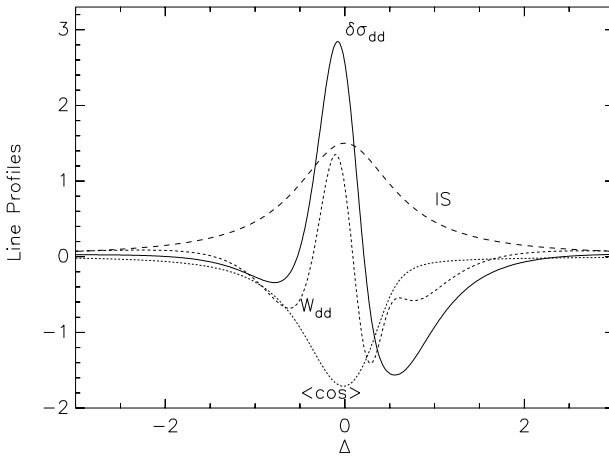


Fig. 7. Dependent scattering corrections (DSC) around the resonant frequency ω_0 , due to recurrent scattering from uncorrelated pairs of two-level systems. The corrections have been drawn for an atomic density $4\pi n/k_0^3 = 1$. The curve labeled $\delta\sigma_{dd}$ represents DSC to the absorption cross-section of the atoms (in units of the resonant scattering cross-section $6\pi c_0^2/\omega_0^2$), the curve labeled W_{dd} denotes the dipole-dipole energy density (in units of the quality factor $c_0/\omega_0\Gamma$ of one atom). The curve labeled $\langle \cos \rangle$ measures the anisotropy in scattering from pairs, mainly due to weak localization, as discussed in the text. The curve “IS” represents the Lorentzian homogeneous line shape for a single atom, both for stored energy and cross-section.

The first term describes recurrent scatterings back and forth (“loops”) to the same atom, averaged over neighbor atoms. The second term has begun and end points on different particles.

Dependent scattering becomes significant when $4\pi n/k_0^3 > 1^2$. At optical frequencies this requires an atomic density $n > 10^{14} \text{ cm}^{-3}$, close to the typical density required for Bose-Einstein condensation. In Figure 7 I show the dependent scattering contributions to stored energy (dashed) and scattering cross-section (solid). A number of features can be remarked. First, both quantities are enhanced on one side ($\Delta < 0$ so $\omega > \omega_0$) and suppressed on the other ($\omega < \omega_0$), leading to a line narrowing. In fact, sumrules imposed by causality impose the frequency integral of both dependent scattering corrections to vanish [56]. This implies that inhomogeneous line broadening will seriously hamper these modifications to the line shape. The structure

²This can be seen by working out the first term of equation (4.10), thereby neglecting the denominator, and inserting the far-field expression for the Green’s function, given in Section 3.1.

is caused by the shifts of the subradiant poles in Figure 4 as the distance r is varied.

It was observed by that the Kurchatov group [57, 58] that an analytical solution is possible for detunings Δ far off-resonance. In this regime the scattering matrix is $t \approx -4\pi c_0/\omega_0 \Delta$. Large detunings have been popular for non-destructive observation of BEC's, since absorption is small. The so-called *quasi-static approximation* assumes that the optical transitions in the atoms are modified by static dipole-dipole interactions with atoms around. In that case the Green's function is approximated by the familiar $1/r^3$ dipolar form, given in equation (3.6). The radial integrals in equations (4.9) and (4.10) can be done with the result [59]

$$W_{\text{dd}}(\Delta) \sim \left(\frac{4\pi n}{k_0^3} \right)^2 \times \frac{1}{\Gamma k_0} \times \frac{1}{\Delta^2}, \quad (4.11)$$

$$\Delta\sigma_{\text{dd}}(\Delta) \sim \frac{4\pi n}{k_0^3} \times \frac{4\pi}{k_0^2} \times \frac{1}{\Delta^2}. \quad (4.12)$$

Since optical absorption and stored energy both scale like $1/\Delta^2$ for independent scatterers as well at large detunings, dipole-dipole interactions start to dominate the wings of the line shape when $4\pi n/k_0^3 > 1$ [60].

4.4 Coherent backscattering

Constructive interferences of waves scattered by two atoms modify the angular distribution of the scattered light. The most important contribution is drawn in Figure 8a. It describes the constructive interference between two waves scattered from the two particles in opposite order. This phenomenon involves a mesoscopic effect, so-called *coherent backscattering*, that has been extremely well studied with classical waves, most often involving much more particles [20]. For only two atoms, this contribution is easily written down in terms of Green's functions and transition matrices defined in previous sections. A great simplification occurs by supposing that recurrent scattering does not play a role. Then the scattering cross-section for coherent backscattering becomes,

$$\frac{d\sigma}{d\Omega}(\mathbf{k} \rightarrow \mathbf{k}') = \frac{\text{Tr}}{(4\pi)^2} n \int d\mathbf{r} |t|^4 \Delta_{\mathbf{k}'} \cdot \mathbf{G}_0(\mathbf{r}) \cdot \Delta_{\mathbf{k}} \cdot \mathbf{G}_0(\mathbf{r})^* \exp[i(\mathbf{k} + \mathbf{k}') \cdot \mathbf{r}]. \quad (4.13)$$

The factor $|t|^4$ represents the 4 scattering events, the two Green's functions denote the two waves propagating oppositely from one atom to the other. The two transverse tensors $\Delta_{\mathbf{k}} = \mathbf{1} - \hat{\mathbf{k}}\hat{\mathbf{k}}$ guarantee polarizations of incident and outgoing electric field to be transverse, the trace summing over all possible polarizations. The last exponential signifies the constructive

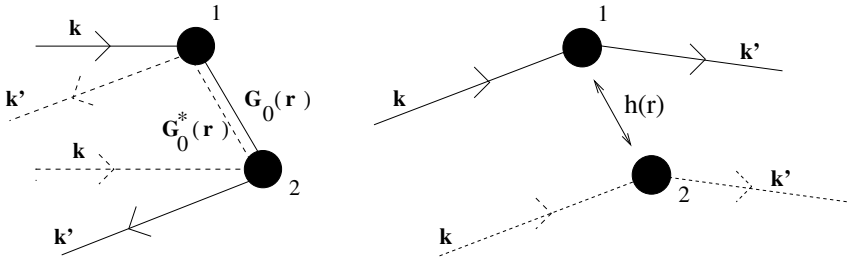


Fig. 8. Two scattering events that modify the angular distribution of the scattered light. Left: coherent backscattering from two particles. This is a contribution to the scattering cross-section involving at least two particles, and two time-reversed sequences of scattering. The dashed path denotes the path of the complex conjugate wave. The interference between $\psi(1 \rightarrow 2)$ and $\psi^*(2 \rightarrow 1)$ is constructive at backscattering $\mathbf{k} = -\mathbf{k}'$, and survives any averaging over the positions of particles 1 and 2. Right: correlation between two particles, with a positive pair correlation function $h(r)$, tends to favor forward scattering.

interference between the scattered waves, and which is perfect at backscattering. An average has been carried out over all neighbor particles 2 that surround particle 1 with number density n . Equation (4.13) contains two complications.

First, the integral in equation (4.13) diverges when the atoms are close. This catastrophe is an artifact of having discarded the recurrent scatterings in equation (3.20). They introduce a lower cut-off $r \approx \sqrt{\sigma} \leq 1/k$. The phase factor is then of order unity in all directions, and this near-field regime is not expected to be relevant for coherent backscattering. The problem is eliminated by using the far-field expression (3.6) for $\mathbf{G}_0$. For two atoms far apart, the phase factor in equation (4.13) is constructive when $(\mathbf{k} + \mathbf{k}') \cdot \mathbf{r} < 1$, *i.e.* very near backscattering.

Second, the integral diverges at large distances exactly at backscattering. Inserting the far-field amplitude, yields

$$\begin{aligned} \frac{d\sigma}{d\Omega}(\mathbf{k} \rightarrow \mathbf{k}') &\sim \frac{1}{(4\pi)^2} n \int d\mathbf{r} \frac{|t|^4}{(4\pi r)^2} \exp(i(\mathbf{k} + \mathbf{k}') \cdot \mathbf{r}) \\ &= \frac{d\sigma}{d\Omega}(1) \times \frac{3\pi}{4\ell} \frac{1}{|\mathbf{k} + \mathbf{k}'|} . \end{aligned} \quad (4.14)$$

The first factor is just the differential cross-section of one atom. Very near back scattering is $|\mathbf{k} + \mathbf{k}'| = 2k \sin \theta/2$ and we obtain a θ^{-1} behavior of the phase function near backscattering. The singularity is integrable and does not lead to a singular total cross-section. Very near backscattering, one should realize that when two atoms are separated by more than than one mean free path ℓ , the coherent backscattering involving only two

particles in Figure 8 is seriously hampered. Mathematically this amounts to replacing the Green's function by $\mathbf{G} \sim \exp(ikr) \exp(-r/2\ell)/4\pi r$, with finite extinction. This solves the catastrophe at $\theta = 0$ and reproduces a perfectly well defined line shape with $FWHM \approx 8/k\ell$. For comparison, coherent backscattering from a semi-infinite medium (with all orders of scattering) is known to have the much smaller value $FWHM \approx 0.7/k\ell$ [61, 62]. The reason is that sequences involving n scatterings give much narrower contributions to the cone, because begin and end points are farther apart, typically $\sqrt{n} \times \ell$.

Coherent backscattering from Rubidium has recently been reported for a cold Rubidium gas by Labeyrie *et al.* [19]. The known mean free path is $\ell = 1.8$ mm and the wavelength $\lambda \approx 800$ nm leads to $k\ell = 14\,500$. The two-atom prediction is $FWHM \approx 0.5$ mrad, very close to the measured value. Since the density is only 10^{10} cm $^{-3}$, the value $4\pi n/k_0^3 \approx 10^{-4}$ shows that dependent scattering is completely negligible in this experiment. However, coherent backscattering is *not* negligible, because of the extra factor $k\ell$ that is gained by the above regularization of the $1/\theta$ phase function.

The above arguments are quite technical. More rigorous reciprocity arguments show that the coherent enhancement factor must always be of the order of the “background” (*i.e.* a factor of two enhancement). The basic reciprocity relation for a general T -matrix is [63],

$$T_{\sigma\mathbf{k}\sigma'\mathbf{k}'}(\omega, \mathbf{B}) = T_{\sigma'-\mathbf{k}'\sigma-\mathbf{k}}(\omega, -\mathbf{B}). \quad (4.15)$$

In the absence of a magnetic field $\mathbf{B}$, this relation guarantees direct and inverse scattering sequence to interfere constructively for $\mathbf{k} = -\mathbf{k}'$, *i.e.* guarantees an enhancement factor of *exactly* 2, provided that $\sigma = \sigma'$, *i.e.* when input and output deal with the same helicity of the wave.

Several trivial reasons exist why the observed enhancement factor is sometimes less than the one imposed by reciprocity. First, very long orders of scattering lead to a narrow cone, impossible to resolve. Secondly, single scattering does not contribute to the cone, but contributes some 10% to the background reflection of linearly polarized light. Both effects decrease the enhancement factor. For off-diagonal polarization channels, no symmetry argument exists, and the scrambling of polarization leads to an enhancement factor much smaller than 2 [61, 62, 64]. The possible presence of absorption - or stimulated emission [65] - does *not* affect the reciprocity relation and does therefore in principle not affect the enhancement factor either, although in practice it may come in indirectly *via* the relative amount of single scattering.

The non-trivial mechanisms that affect coherent backscattering are much more interesting. According to the reciprocity principle (4.15), an external magnetic field destroys coherent backscattering *via* Faraday rotation of the electromagnetic polarization vector, an effect predicted theoretically

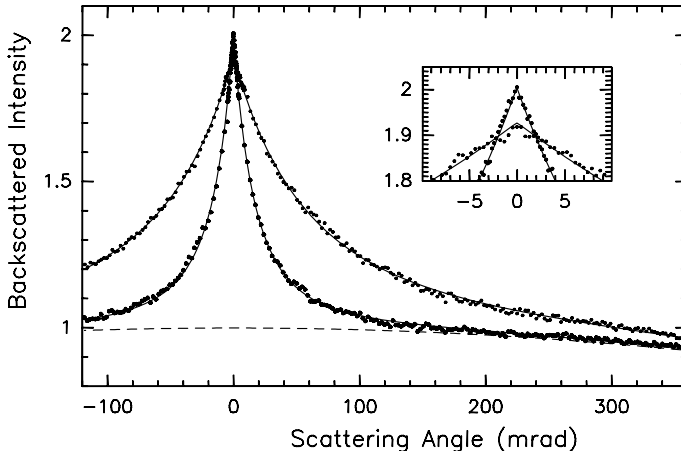


Fig. 9. Coherent backscattering of red light from a disordered slab containing a powder of BaSO_4 , with a mean free path $\ell = 0.6 \mu\text{m}$ (broad curve) and $\ell = 2.1 \mu\text{m}$ (narrow curve). Taken from Wiersma *et al.* (1995) [69], with thanks to Wiersma.

by John *et al.* [66] and confirmed experimentally by Maret *et al.* [67]. Dephasing mechanisms and selection rules in Raman transitions are now under study in relation to coherent backscattering in atomic systems [68].

In Figure 9, a cone is presented that was measured with a very accurate angular technique [69]. The used helicity preserving channel has the convenient property that, at least for spherical scatterers, single scattering vanishes. Thus, the experimental enhancement should be exactly two. The inset of Figure 9 confirms the value of two only for $k\ell \gg 1$. The somewhat smaller value for $k\ell \approx 6$ is explained in terms of recurrent scattering. The absence of single scattering in the helicity preserving channel - due to rotational symmetry of the scatterers - does no longer apply to recurrent scattering from two spheres, which break this symmetry. The importance of recurrent scattering is quantified by the value of $4\pi n/k_0^3 \approx 1/k\ell$. The inset of Figure 9 also visualizes the non-analytic line shape at backscattering, as first predicted by Akkermans *et al.* [61, 62] on the basis of the diffusion equation.

The coherent backscattering from two particles demonstrates the collective scattering to become anisotropic. One single two-level system has as much scattering in the forward direction as it has in the backward direction. The angular asymmetry parameter $\langle \cos \theta \rangle$ denotes $\cos \theta$ averaged over the angular phase function, and measures the amount of forward scattering. For individual two-level atoms one has $\langle \cos \theta \rangle = 0$. The curve labeled $\langle \cos \rangle$ in Figure 7 is the result of an exact calculation of the modification by dependent scattering of the angular differential cross-section of two atoms. We

notice that $\langle \cos \theta \rangle \approx -4\pi n/k_0^3$ near resonance. The negative value is due to the coherent backscattering effect [56]. It can be expected to suppress diffuse propagation, *i.e.* lower the diffusion constant.

4.5 Dependent scattering with quantum correlation

Dependent scattering is sensitive to the positions of the two atoms and will change when the positions of the two atoms are correlated, as is for instance the case close to the Bose-Einstein transition. As pointed out in references [42, 57, 58], a measurement of the optical absorption may provide insight into quantum correlations between atoms. Dependent scattering becomes important when $4\pi n/k_0^3 > 1$, making them relevant near Bose-Einstein condensation ($n \approx 10^{14} \text{ cm}^{-3}$). The simplest correlations are described by a pair correlation $h(\mathbf{r})$, related to the two-atom distribution function according to $\rho(\mathbf{r}_1, \mathbf{r}_2) = n^2[1 + h(\mathbf{r})]$.

I will illustrate the previous statements for the ideal, homogeneous Bose gas, whose quantum pair function is given by [70],

$$h(\mathbf{r}) = \frac{2n_0}{n} F(\mathbf{r}) + |F(\mathbf{r})|^2, \quad (4.16)$$

$$F(\mathbf{r}) = \frac{\sum_{\mathbf{k}} n_{\mathbf{k}} \exp(i\mathbf{k} \cdot \mathbf{r})}{n_0 + \sum_{\mathbf{k}} n_{\mathbf{k}}}. \quad (4.17)$$

Here n_0 denotes the number density of atoms in the condensate, and $n_{\mathbf{k}}$ the density in the excited levels. We deduce that $h(0) = 1 - (n_0/n)^2$, *i.e.* beyond the critical temperature it is twice as probable as expected classically to find two atoms on top of each other, but this value decreases below the critical temperature. Far away from the critical temperature, it is easily found that $h(r) = \exp(-\pi r^2/\lambda_B^2)$, with λ_B the De Broglie wavelength. At the critical temperature, it can be checked that $F(r) \approx \lambda_B/r$ so that $h(r) \approx \lambda_B^2/r^2$. For $k_0\lambda_B \approx 1$ and $4\pi n/k_0^3 > 1$, quantum correlations significantly influence line profiles *via* dependent scattering. Both equalities are obeyed. For Rubidium at $T = 100 \text{ } \mu\text{K}$ we find that $\lambda_B = 0.2 \text{ } \mu\text{m}$ so that $k_0\lambda_B \approx 2.5$, and $4\pi n_c/k_0^3 \approx 2$.

Figure 10 shows stored dipole-dipole energy, dependent scattering cross-section and $\langle \cos \theta \rangle$, displayed earlier in Figure 7, but now for correlated atoms. We have adopted a correlation function $h(r) = 1/(1 + r^2/a^2)$ using $k_0 a = 1$. This correlation function resembles the more complicated one in equation (4.17). Upon comparing to Figure 7 the impact of quantum correlations can be estimated. In particular, the line profile of the stored energy is modified. We notice that for $4\pi n/k_0^3 = 1$, these corrections are no longer small, and dependent scattering involving more than only pairs of atoms should be considered.

Bose correlations lead to a *positive* contribution to the angular asymmetry factor $\langle \cos \theta \rangle$, even dominating the negative weak localization correction

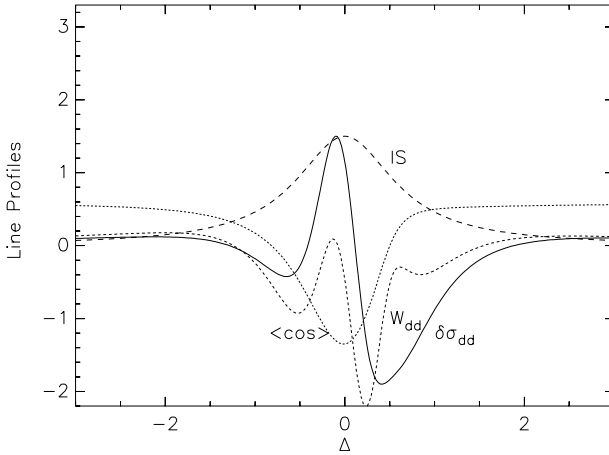


Fig. 10. Dependent scattering corrections (DSC) around the resonant frequency ω_0 , due to recurrent scattering from *correlated* pairs of two-level systems (compare to Fig. 7, drawn on the same scale). The correction has been calculated for an atomic density $4\pi n/k_0^3 = 1$, and a pair correlation typical at the BEC transition of free bosons. The curve “IS” represents the Lorentzian homogeneous line shape for a single atom, both for stored energy and cross-section.

for detunings beyond one line width. Indeed, particle correlations induce an angular anisotropy in the collective phase function. This contribution is shown in Figure 8b and reads,

$$\frac{d\sigma}{d\Omega}(\mathbf{k} \rightarrow \mathbf{k}') = \frac{d\sigma}{d\Omega}(1) \times n \int d\mathbf{r} h(r) \exp(i(\mathbf{k} - \mathbf{k}') \cdot \mathbf{r}). \quad (4.18)$$

For a pair correlation $h(r)$ that slowly decays as a^2/r^2 this yields - like was seen in equation (4.14) for coherent backscattering - a diverging cross-section θ^{-1} , but now in the *forward* direction. Hence, $\langle \cos \theta \rangle > 0$, independent of Δ . This is confirmed in Figure 10.

Equations (4.17) and (4.18) can be combined to express pair correlations in terms of the Bose distribution $n_{\mathbf{k}}$ in phase space. If we add the “independent scattering result, we obtain for the collective cross-section,

$$\frac{d\sigma}{d\Omega}(\mathbf{k} \rightarrow \mathbf{k}') = \frac{d\sigma}{d\Omega}(1) \times \sum_{\mathbf{p}_n} n_{\mathbf{p}} [1 + n_{\mathbf{p}-\mathbf{k}'+\mathbf{k}}]. \quad (4.19)$$

The factor $1 + n_{\mathbf{p}-\mathbf{k}'+\mathbf{k}}$ signifies pair correlation but can alternatively be regarded as a *stimulated emission* of a boson from a state $\mathbf{p}$ to an already occupied state $\mathbf{p} - \mathbf{k}' + \mathbf{k}$, while the photon is scattered from $\mathbf{k}$ to $\mathbf{k}'$. It was shown by Javanainen [71] that his notion implies that, in the condensed

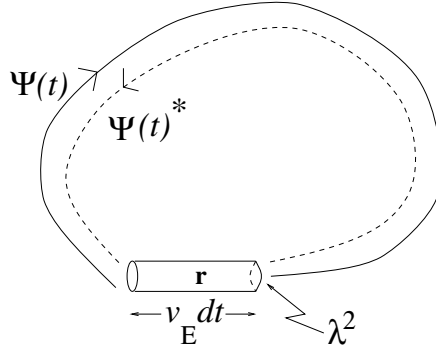


Fig. 11. Schematic representation of constructive interference between two counter-propagating wave paths, long compared to the mean free path. Within a time interval dt , and after a time t they interfere constructively in the small volume element, which enhances the return probability, and lowers the diffusion constant.

phase, inelastic recoil components show up in the scattered light at both $\omega + \omega_r$ and $\omega - \omega_r$, where $\omega_r = \hbar \Delta \mathbf{k}^2 / 2m$ is the recoil frequency, and not only at $\omega - \omega_r$.

In the presence of a condensate, the large occupation of the state $\mathbf{p} = 0$ yields a cross-section similar to $n_{\mathbf{k}-\mathbf{k}'} \sim 1/\Delta \mathbf{k}^2$. In real space, this corresponds to very long-range $1/r$ behavior in the pair correlation function. Repulsive interactions between the bosons modify this feature somewhat [72], but the consequences for light scattering have so far not been investigated. Recent theoretical research also concentrates on the optics of Fermi-Dirac gazes [73], in which case the stimulated emission factor in equation (4.19) achieves a minus sign.

4.6 From weak towards strong localization

The modification of transport coefficients by constructive interferences is called *weak localization*, and is one of the most important effects in mesoscopic wave physics. They become even more significant when high orders in scattering start to contribute. We shall rely on the following semi-heuristic, but highly mesoscopic argument (Fig. 11). Long paths are described by a diffusion equation. The diffusion Green's function $G_D(\mathbf{r}, \mathbf{r}', t)$ satisfies,

$$[\partial_t - D \nabla^2] G_D(\mathbf{r}, \mathbf{r}', t) = \delta(\mathbf{r} - \mathbf{r}') \delta(t), \quad (4.20)$$

and describes how much wave energy arrives at time t at $\mathbf{r}$ per unit volume after having left $\mathbf{r}$ at time $t = 0$. The return probability $G_D(\mathbf{r}, \mathbf{r}, t)$ can be seen to be inversely proportional to the diffusion constant D . By the

reciprocity principle (4.15), the same amount of energy must return due to constructive interference of time reversed waves. This extra term *enhances* the return probability, and should thus lead to a smaller diffusion constant. The typical transverse width of a wave path is of order λ so that during a small interval dt the relevant volume element to consider is $v_E dt \times \lambda^2$, with v_E the transport velocity. Upon summing over paths of all lengths, one finds

$$\frac{D_0}{D} \approx 1 + \lambda^2 v_E \int_0^\infty dt G_D(\mathbf{r}, \mathbf{r}, t). \quad (4.21)$$

This result is confirmed by sophisticated transport theories [74], and has been widely used as a starting point for many mesoscopic phenomena [21, 22]. It is a nontrivial outcome as G_D still depends on D by means of equation (4.20). For an infinite medium, equation (4.20) is easily solved with the result that,

$$\int_0^\infty dt G_D(\mathbf{r}, \mathbf{r}, t) = \int \frac{d^3 \mathbf{q}}{(2\pi)^3} \frac{1}{Dq^2} \approx \frac{1}{(2\pi)^2 D \ell}. \quad (4.22)$$

The $\mathbf{q}$ -integral diverged for large q , but a cut-off $1/\ell$ has been adopted to avoid low orders of scattering, for which the diffusion equation is not valid. Since $D_0 \sim v_E \ell$ we arrive at,

$$\frac{D}{D_0} \approx 1 - \frac{\text{constant}}{(k\ell)^2}, \quad (4.23)$$

with the constant of order unity. Extrapolating optimistically equation (4.23), offers the possibility of a vanishing diffusion constant. This is the weakest among the (many) definitions of *strong localization* [9]. In three dimensions, it is expected to set in when $k\ell \approx 1$, known as the *Ioffe-Regel criterion* of waves. For matter waves at low energy, the cross-section σ reaches the finite value πa^2 , with a the s -wave scattering length of the impurity potentials. Thus, localization can be expected at “low energies”. For conducting electrons, for which the concept of localization was devised in the first place, the Ioffe-Regel criterion favors the location of the Fermi level near the band edges of the conduction band.

Classical waves have the property that $\sigma \sim \omega^4$ at low frequencies which makes localization very unlikely. For light scattering from nearly resonant atoms, the Ioffe-Regel criterion asserts that $4\pi n/k_0^3 > 1$ to have localization of light, making it an interesting challenge for future experiments with cold gases. A cold Rubidium gas with $n = 10^{14} \text{ cm}^{-3}$ gives $k\ell \approx 0.28$ at resonance. However, in this strongly scattering regime, dependent scattering must be considered. As evident from Figure 7, dependent scattering may in fact help to *increase* the scattering cross-section somewhat more.

And why not think of the inverse problem of localization of Bose condensed matter waves in a disordered light potential? After all, for such matter waves we should expect $k\ell < 1$ as $k \approx 0$. At present, strong localization has been reported for microwaves and infrared light, as well as for bending waves and acoustic waves (see Ref. [9] for references).

Acknowledgements

Most of this work has been carried out with Ad Lagendijk, who I would like to thank for his continuous input. I thank Robin Kaiser, Rodney Loudon, and Ad Lagendijk for the many critical remarks on earlier versions of the manuscript. Discussions with Yvan Castin, Jean Dalibard, Dominique Delande, David Lacoste, Christian Miniatura, Janne Ruostekoski, Rudolf Sprik, Pedro de Vries and Diederik Wiersma are highly appreciated.

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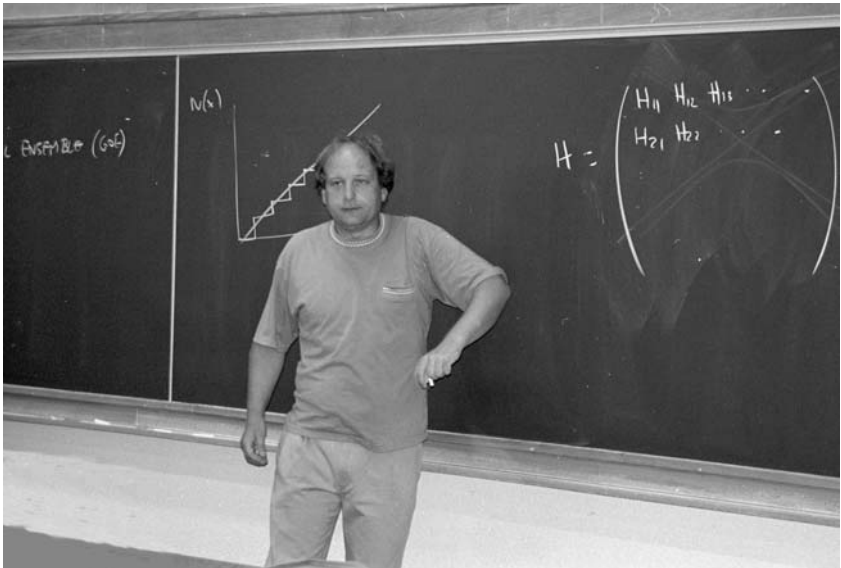
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COURSE 6

QUANTUM CHAOS IN ATOMIC PHYSICS

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QUANTUM CHAOS IN ATOMIC PHYSICS

D. Delande

Abstract

How classical chaos manifests itself in microscopic systems where a quantum description must be used, is the subject of quantum chaos. In these lectures, I present the concepts and tools used in quantum chaos – random matrix theory, periodic orbit theory, localization theory – and show their relevance for studying complex atomic systems.

1 What is quantum chaos?

Our understanding of chaos considerably improved during the last 40 years. It is now well known that, for a typical system with several strongly coupled degrees of freedom, chaos is the rule and regularity the exception. The dynamics of chaotic systems often looks erratic giving the false impression that most variables behave randomly. In fact, there usually exists an underlying well organized robust non trivial structure (for example, a strange attractor).

For microscopic systems such as atoms, the standard concepts used for chaotic systems cannot be applied because quantum – and not classical – mechanics must be used. How chaos manifests itself in quantum systems is the subject of Quantum Chaos¹. In these lectures, I present our current understanding of Quantum Chaos, which uses various theoretical tools, and show its relevance for atomic systems. Of course, it also has applications in other domains of physics, especially for mesoscopic systems [3]. As a matter of fact, the key difference between classical and quantum physics is the existence of quantum *interferences* between various paths. As soon as interferences are present in complex systems, the concepts used for Quantum Chaos may be useful. This is for example the case for complex disordered systems [4, 5].

¹Good introductions to Quantum Chaos can be found in [1] and [2].

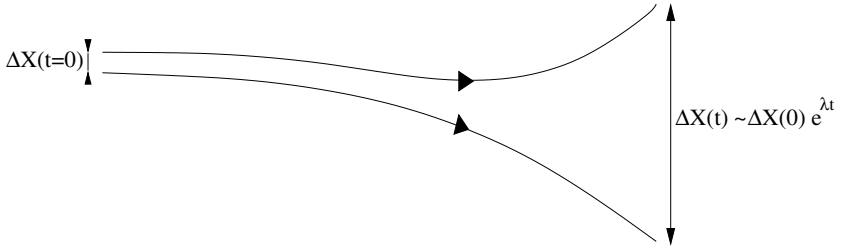


Fig. 1. Classical chaos is characterized by exponential sensitivity on initial conditions, that is exponential divergence of neighbouring trajectories. The rate of divergence is the Lyapounov exponent λ .

1.1 Classical chaos

Chaos is usually defined for classical systems, *i.e.* systems whose dynamics can be described by deterministic equations of evolution in some phase space. In the specific case of a time-independent Hamiltonian system for a single particle, the phase space coordinates are the position $\mathbf{q}$ and momentum $\mathbf{p}$, and the equations of motion can be expressed using the Hamilton function $H(\mathbf{q}, \mathbf{p})$ as [6]:

$$\frac{dq_i}{dt} = \frac{\partial H}{\partial p_i} \quad (1.1)$$

$$\frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i}, \quad \text{for } 1 \leq i \leq d. \quad (1.2)$$

where d is the number of degrees of freedom. Basically, classical chaos is exponential sensitivity on initial conditions: two neighbouring trajectories diverge exponentially with time (see Fig. 1), *i.e.* the distance between the two trajectories generically increases as $\exp(\lambda t)$ where λ is the Lyapounov exponent of the system [7]. Sensitivity on initial conditions is responsible for the decrease of correlations over long times, loss of memory of the initial conditions and ultimately for deterministic unpredictability of the long time behaviour of the system. Most often, when the system is sensitive on initial conditions, it is also mixing and ergodic [7], *i.e.* a typical trajectory uniformly fills up a finite volume of the phase space at long time.

For low-dimensional systems, the dynamics is often a mixed regular-chaotic one, depending on the initial conditions; also, when a parameter is changed in the Hamilton function, the transition from regularity to chaos is usually smooth with intermediate mixed dynamics. Such mixed systems

are rather complicated and not too well understood² – at least for quantum effects to be discussed in these lectures – and we will here restrict to the two extreme simple situations where the motion is almost fully integrable or almost fully chaotic.

It should be emphasized that the systems considered in these lectures are completely deterministic, without any randomness. Nevertheless, concepts inherited from statistical physics, *e.g.* Random Matrix Theory, will be very useful.

1.2 Quantum dynamics

In quantum mechanics, there is neither any phase space, nor anything looking like a trajectory. Hence, the notions of classical chaos cannot be simply extended to quantum physics. Quantum mechanics uses completely different notions, like the state vector $|\psi\rangle$ belonging to some Hilbert space, which describes all the physical properties of the system. Its evolution is given by the Schrödinger equation³:

$$i\hbar \frac{d|\psi(t)\rangle}{dt} = H(t) |\psi(t)\rangle \quad (1.3)$$

where $\hbar$ is the Planck's constant and $H(t)$ the Hamiltonian.

$|\psi\rangle$ is not directly observable in quantum mechanics. In general – according to the standard interpretation of quantum mechanics – the result of a measure is some diagonal element of an Hermitean operator, something like $\langle\psi|O|\psi\rangle$. The physical processes involved in an experimental measurement are quite subtle, difficult and interesting, but beyond the subject of these lectures. It is also the subject of a vast literature [8, 9]. I will not consider this problem and restrict to a purely Hamiltonian evolution.

The time-evolution operator $U(t', t)$ is the linear operator mapping the state $|\psi(t)\rangle$ onto the state $|\psi(t')\rangle$. It obeys the following equation (which is equivalent to Schrödinger equation):

$$i\hbar \frac{\partial U(t', t)}{\partial t'} = H(t') U(t', t). \quad (1.4)$$

Because H is an Hermitean operator, $U(t', t)$ is a linear unitary operator. An immediate consequence is that the overlap between two states is preserved during the time evolution. Indeed, one has:

$$\langle\psi_1(t')|\psi_2(t')\rangle = \langle\psi_1(t)|U^\dagger(t', t)U(t', t)|\psi_2(t)\rangle = \langle\psi_1(t)|\psi_2(t)\rangle \quad (1.5)$$

²In a very rough approximation, a mixed system can be seen as composed of non-interacting regular and chaotic components.

³I here restrict the analysis to systems isolated from their environment. As discussed in this book [9], the (quantum) dynamics may be significantly affected by the environment. This problem is also discussed in Sections 2.4 and 5.6.

which implies that two “neighbouring” states will remain neighbors forever. Because of linearity and unitarity, quantum mechanics cannot display any sensitivity on initial conditions, hence cannot be chaotic in the ordinary sense!

However, the previous statement must be considered with care. Indeed, classical mechanics can also be seen as a linear theory if one considers the evolution of a classical phase space density $\rho(\mathbf{q}, \mathbf{p}, t)$ given by the Liouville equation [6]:

$$\frac{\partial \rho}{\partial t} = \{\rho, H\} \quad (1.6)$$

where $\{, \}$ denotes the Poisson bracket. The fact that we obtain both in classical and quantum mechanics a linear equation of evolution in some space just implies that the above argument on linearity in quantum mechanics is irrelevant. Discussions on subjects like “Is there any quantum chaos?” are in my opinion completely uninteresting because they focus on the formal aspects of the mathematical apparatus used.

We will here define quantum chaos as the study of quantum systems whose classical dynamics is chaotic. The questions we would like to answer are thus:

- What are the appropriate observables to detect the regular or chaotic *classical* behavior of the system?
- More precisely, how the chaotic or regular behaviour expresses in the energy levels and eigenstates of the quantum system? (see Sect. 3)
- What kind of semiclassical approximations can be used? (see Sect. 4)
- What is the long-time behaviour of a quantum system? (see Sect. 5).

These are the questions discussed in these lectures. I will only present selected topics, forgetting lots of interesting questions and relevant references.

These questions of course go towards an intrinsic definition of quantum chaos not referring to the classical dynamics [10]. Thus, the problem of quantum chaos is essentially related to the correspondance between classical and quantum dynamics, the subject of *semiclassical* physics.

More generally, classical chaos is an example of *complexity*. The dynamics of complex systems is usually so complicated that a fully detailed analysis is of no relevance for a global understanding. For example, for classically chaotic systems, we are not interested in the knowledge of each individual trajectory, but rather in the statistical properties of the motion like the Lyapounov exponents. The same is true for the quantum properties: the most interesting ones have to be robust *versus* a small change in the parameters describing the system. A good example is to consider

how localization effects affect the global transport properties of the system (Sect. 5). In chaotic systems, the phase space structure – although rather complicated – is partly well known which makes it possible to derive and use some sophisticated semiclassical approaches, as will be shown in Section 4. It is reasonable to think that similar treatments are possible for complex systems [4].

1.3 Semiclassical dynamics

The whole idea of a semiclassical analysis is to obtain approximate solutions of the quantum equation of motion (the Schrödinger equation) using only classical ingredients (trajectories...) and the Planck's constant $\hbar$. For a macroscopic object, our common knowledge is that an approximate semiclassical solution should be very accurate. Technically, this is true because $\hbar$ is much smaller than any classical quantity of interest (such as the classical action of the particle). One often refers to the “correspondance principle” as an explanation. However, this is a *very vague* concept which is usually not clearly stated. Part of these lectures are devoted to a serious scientific discussion of this issue, using the modern knowledge on classical chaos.

In order to make the connection between classical and quantum quantities, it is useful to define the Wigner representation [11]:

$$W(\mathbf{q}, \mathbf{p}) = \frac{1}{(2\pi\hbar)^N} \int \psi\left(\mathbf{q} - \frac{\mathbf{x}}{2}\right) \psi^*\left(\mathbf{q} + \frac{\mathbf{x}}{2}\right) \exp\left(i\frac{\mathbf{p}\cdot\mathbf{x}}{\hbar}\right) d\mathbf{x}. \quad (1.7)$$

This is a real phase space density probability, or rather quasi-probability because it can be either positive or negative. It evolves according to [11]:

$$\frac{\partial W}{\partial t} = -\frac{2}{\hbar} H(\mathbf{q}, \mathbf{p}) \sin\left(\frac{\hbar\Lambda}{2}\right) W(\mathbf{q}, \mathbf{p}) \quad (1.8)$$

with:

$$\Lambda = \sum_i \frac{\overleftarrow{\partial}}{\partial p_i} \frac{\overrightarrow{\partial}}{\partial q_i} - \frac{\overleftarrow{\partial}}{\partial q_i} \frac{\overrightarrow{\partial}}{\partial p_i} \quad (1.9)$$

where the left (resp. right) arrow indicates action on the quantity on the left (resp. right) side.

An explicit power expansion of the sine function is possible. This is in fact a power expansion in $\hbar$, hence well suited for a semiclassical approximation. At lowest (zeroth) order, one finds *exactly* the classical Liouville equation (1.6), thus establishing a link between the quantum and classical dynamics. At next order in $\hbar$ (actually $\hbar^2$), one finds terms involving third partial derivatives of the Hamiltonian. For example, for a one-dimensional

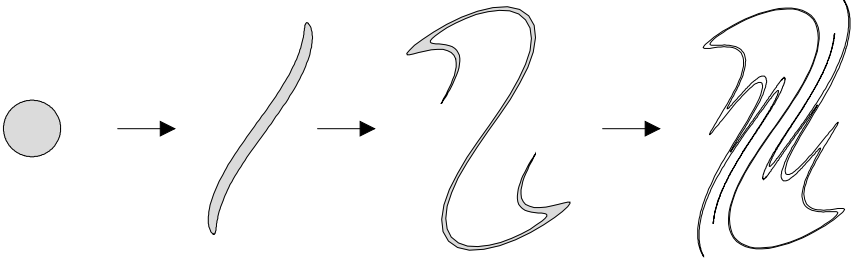


Fig. 2. Classical temporal evolution of an initially localized phase space density for a chaotic system. Because of sensitivity on initial conditions, the density stretches along the unstable direction, generating whorls and tendrils. Because of the finiteness of the Planck’s constant $\hbar$, the quantum system cannot develop such rapid spatial variations: after some time, the classical and quantum dynamics have to differ.

particle in a potential $V(q)$, one gets:

$$\frac{\partial W}{\partial t} = \{W, H\} - \frac{\hbar^2}{24} \frac{\partial^3 V}{\partial q^3} \frac{\partial^3 W}{\partial p^3} + O(\hbar^4). \quad (1.10)$$

For harmonic systems, the corrective terms vanish, proving that the classical and quantum phase space dynamics completely coincide. For non-harmonic systems, they produce a spreading of wavepackets. For chaotic systems, the classical solutions of the Liouville equations tend to stretch and fold along (exponentially) unstable directions and – because of conservation of volume in phase space – to shrink along (exponentially) attractive directions. As shown in Figure 2, this rapidly creates “whorls” and “tendrils” in the classical phase space density, which in turn implies more and more rapid spatial changes of the density. Thus, as time goes on, one expects some higher order partial derivatives to grow exponentially. Although the corresponding terms in the quantum equation of evolution are multiplied by $\hbar^2$, they will unavoidably overcome the classical Liouville term. Hence, after some “break time”, the detailed quantum evolution will differ from the classical one (see Sect. 2 and Refs. [8–10] for a more detailed discussion).

Of course, for smaller $\hbar$, the higher order terms are smaller and it requires a longer time for them to perturb the dynamics. Hence, the break time has to tend to infinity in the semiclassical limit $\hbar \rightarrow 0$. For a fixed time interval, one can always find a sufficiently small $\hbar$ such that the quantum and classical dynamics are almost identical. In other words, over a finite time range, the quantum dynamics tends to the classical one as $\hbar \rightarrow 0$. However, this limit is not *uniform*. For fixed $\hbar$, there is always a finite time after which the quantum dynamics differs from the classical one. In other words, the two

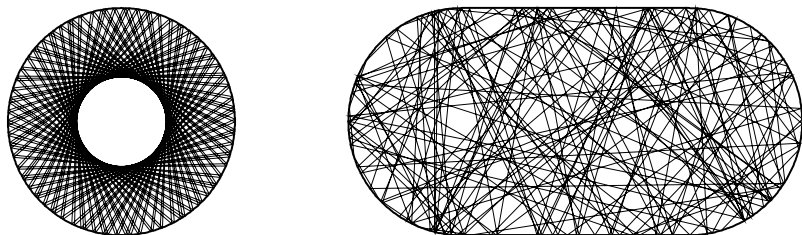


Fig. 3. Typical trajectories for the circular billiard (left) and the stadium billiard (right). The former case is completely regular and integrable because – beside energy – the angular momentum is a constant of motion. The latter case is completely chaotic and trajectories look disordered without any visible regular pattern.

limits $t \rightarrow \infty$ and $\hbar \rightarrow 0$ do not commute. Taking first $\hbar \rightarrow 0$, then $t \rightarrow \infty$ is studying the long time classical dynamics, *i.e.* classical chaos. The other limit $t \rightarrow \infty$, then $\hbar \rightarrow 0$, is what we are interested in, namely quantum (and semiclassical) chaos.

1.4 Physical situations of interest

Simple equations of motion may produce a chaotic behaviour. A rather non-intuitive result is that chaos may take place in low dimensional systems. On the other hand, classical chaos can only exist in systems where different degrees of freedom are *strongly* coupled [7]. This implies that a small perturbation added to a regular system cannot make it chaotic.

The simplest possible chaotic systems are thus time-independent 2-dimensional systems. It is also simpler to consider bound systems with a discrete energy spectrum. Various model systems have been studied, among which billiards are the simplest ones. A billiard is a compact area in the plane containing a point particle bouncing elastically on the walls. Depending on the shape of the boundary, the motion may be regular or chaotic, see Figure 3. From the quantum point of view, one has to find the eigenstates of the Laplace operator whose wavefunction vanishes on the boundary [12].

Open (*i.e.* not bound) systems have also been studied. The simplest example is the “three disks system” which is an open billiard with three identical circular obstacles centered on a equilateral triangle. This is an example of “chaotic scattering” [13], where the chaotic behaviour comes from the existence of arbitrarily long and complex trajectories bouncing off the 3 disks without escaping. From the quantum point of view, there are no longer discrete bound states, but rather resonances with complex energies which are poles of the S -matrix or of the Green’s function.

In an open system, the classical dynamics is not bound and often shows some similarity with a diffusive motion (although it is perfectly deterministic) with the average excursion increasing as the square root of time. Quantum interferences between various paths may modify the transport properties, leading to partial (weak) or complete (strong) localization, as discussed in Section 5.

If we now turn to “experimental” systems, it is obvious that quantum effects are likely to be noticeable only for microscopic systems. The dynamics of nucleons in an atomic nucleus might be chaotic – at least at sufficiently large energy – and the experimental results on highly excited states played a major role in the early developments of quantum chaos [12]. The drawback is the existence of complex collective effects and the fact that the interaction is not perfectly well known.

Atoms are among the best available prototypes for studying quantum chaos and I will use them as examples in these lectures. Compared with other microscopic complex systems (nuclei, atomic clusters, mesoscopic devices...), atoms have the great advantage that all the basic components are well understood: these are essentially point particles (electrons and nucleus) interacting through a Coulomb static field, and interacting with the external world through electromagnetic forces. Hence, it is possible to write down an explicit expression of the Hamiltonian. A second major advantage is that the coupling with the environment can be more or less controlled. Atomic media are usually very dilute media composed of almost independent identical atoms. Collisions and, more generally inelastic processes (for example spontaneous emission) are rare.

Another crucial advantage of atomic systems is that they can be studied theoretically and *experimentally*. The word “experiment” must here be understood as traditional laboratory experiments, but also as “numerical experiments”. Indeed, currently available computers make it possible to compute properties of complex systems described by simple Hamiltonians. During the last fifteen years, the constant interplay between the experimental results and the numerical simulations led to major advances in the field of quantum chaos.

Depending on the energy scale involved, different parts of the atomic dynamics are relevant. At “large” energy – in the range [1 meV – 1 eV] – it is the internal dynamics of the atomic electrons (their motion around the nucleus) which may be chaotic. The typical time scale involved in the internal dynamics is picosecond.

At much lower energy – 1 μ eV – it is the external dynamics of the center of mass of the atom (considered as a single particle) which may display a chaotic behavior under the influence of an external electromagnetic field [14]. The latter case has been made possible because of the impressive recent improvements on the control of cold atomic gases using quasi-resonant laser

beams [15, 16]. I discuss recent beautiful experimental results on quantum chaos using cold atoms in Section 5.

In molecules, the dynamics of the electrons may also be chaotic. In some cases, the motion of the nuclei in the effective potential created by the electrons (which follow the nuclei adiabatically) is chaotic. Some interesting results have been obtained [17].

At the microscopic level, the dynamics of electrons in a solid state sample may present a chaotic dynamics in, for example, suitable combinations of external fields. This has lead to dramatic results showing very clearly the relevance of periodic orbits for understanding the quantum chaotic dynamics [18]. Another possibility is to build microscopic cavities of various shapes where an electron may propagate ballistically: it is an experimental realization of an open quantum billiard. In the last few years, an increasing number of experiments on *mesoscopic* physics have been realized [3, 19–21], some of them related to quantum chaos. The key point and the main difficulty of mesoscopic physics is to keep the phase coherence of the electronic wavefunction, killed by electron-electron interaction and electron-phonon scattering. Another drawback of solid state samples is that it is impossible to prepare selectively the system. The only measurable quantities are global transport coefficients from a gas of electrons at the thermodynamic equilibrium.

Another possibility exists for experimental study of quantum chaos. One can consider wave equations – similar to the Schrödinger equation – describing some other physical phenomena. As what we are interested in is in fact “wave chaos” (properties of eigenmodes for example) whatever the waves themselves are, this opens a wide variety of possible experiments. The best example is provided by flat microwave cavities where solving the Maxwell equations is equivalent to calculating the eigenstates of the corresponding two-dimensional Schrödinger billiard [1, 22]. The advantage is that a measure of the “wavefunction” is possible. Alternatively, quantum chaos can be simulated using acoustic waves [23].

I now work out in some detail the simplest atomic prototype, which will be discussed as an example in the following.

1.5 A simple example: The hydrogen atom in a magnetic field

1.5.1 Hamiltonian

We consider the simplest atom – hydrogen – exposed to a strong external uniform magnetic field directed along the z -axis.

Using the symmetric gauge $\mathbf{A} = \frac{1}{2}\mathbf{r} \times \mathbf{B}$ for the vector potential, the Hamiltonian is given by (q is the charge of the electron):

$$H = \frac{\mathbf{p}^2}{2m} - \frac{q^2}{4\pi\epsilon_0 r} - \frac{qB}{2m}L_z + \frac{q^2 B^2 \rho^2}{8m} \quad (1.11)$$

where L_z is the z -component of the angular momentum. In atomic units ($\hbar = m = |q| = 4\pi\epsilon_0 = 1$), it reads:

$$H = \frac{\mathbf{p}^2}{2} - \frac{1}{r} + \frac{\gamma}{2}L_z + \frac{\gamma^2 \rho^2}{8} \quad (1.12)$$

where γ denotes the magnetic field in atomic units of 2.35×10^5 T.

Because of the azimuthal symmetry around the magnetic field axis, the paramagnetic term $\gamma L_z/2$, responsible for the usual Zeeman effect, is just a constant. The diamagnetic term, $\gamma^2 \rho^2/8$, is directly responsible for the onset of chaos in the system. The competition between the Coulomb potential with spherical symmetry and the diamagnetic potential with cylindrical symmetry governs the dynamics. As a crude criterion, chaos is most developed when these two terms have the same order of magnitude. This can be realized in a laboratory experiment with Rydberg states $n \simeq 40 - 150$ [24–26].

When written in cylindrical coordinates, the Hamiltonian (1.12) describes a time-independent two-dimensional system belonging to the simplest class of chaotic systems [7]. This makes this system an almost ideal prototype for quantum chaos [27, 28].

1.5.2 Classical scaling

There is a convenient scaling of all variables and external fields which leave the equations of motion invariant [27]:

$$\begin{cases} \mathbf{r} \rightarrow \lambda^{-1}\mathbf{r}, \\ \mathbf{p} \rightarrow \lambda^{1/2}\mathbf{p}, \\ H \rightarrow \lambda H, \\ \gamma \rightarrow \lambda^{3/2}\gamma, \end{cases} \quad (1.13)$$

where λ is any positive real number.

This means that different initial conditions with different external fields may have exactly the same classical dynamics. Because of the scaling law, the classical dynamics, instead of depending both on E and γ , actually depends only on the scaled energy:

$$\epsilon = E\gamma^{-2/3}. \quad (1.14)$$

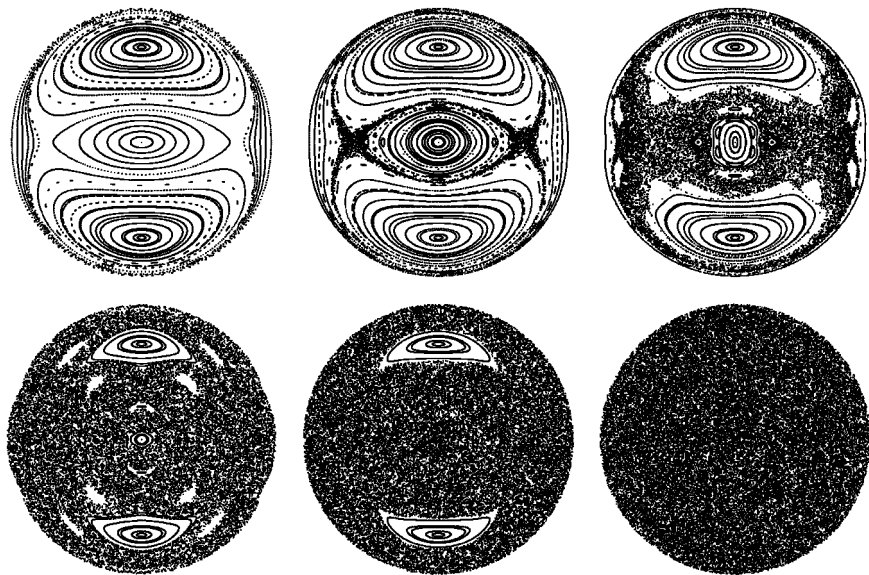


Fig. 4. Poincaré surfaces of section for the classical dynamics of a Rydberg electron of the hydrogen atom in a magnetic field. The various plots are for increasing values of the scaled energy, equation (1.14). From left to right, $\epsilon = -1, -0.5, -0.4$ (top), $-0.3, -0.2, -0.1$ (bottom). The dynamics is almost fully integrable for $\epsilon = -1$, some small chaotic region appears around $\epsilon = -0.5$ and progressively invades the phase space which is almost completely chaotic for $\epsilon > -0.13$.

1.5.3 Classical dynamics

Figure 4 shows a series of Poincaré surfaces of section for this system at increasing values of the scaled energy. At low scaled energy (roughly $\epsilon < -0.5$), the classical dynamics is mainly regular: this is the low field limit where the magnetic field is a small perturbation and where a complete quantitative analysis is possible [27]. Increasing ϵ from -0.5 , the system smoothly evolves to a fully chaotic situation reached above $\epsilon = -0.13$. Finally, the phase space opens to infinity at $\epsilon = 0$.

The corresponding trajectories in configuration space also clearly display a qualitative change when chaos is present. Figure 5 shows two trajectories at $\epsilon = -0.2$ differing only by the initial conditions. The first one (on the left side) starts on an invariant torus visible in Figure 4 and looks very regular. The second one (on the right side) lives in the chaotic sea and has a much more erratic aspect.

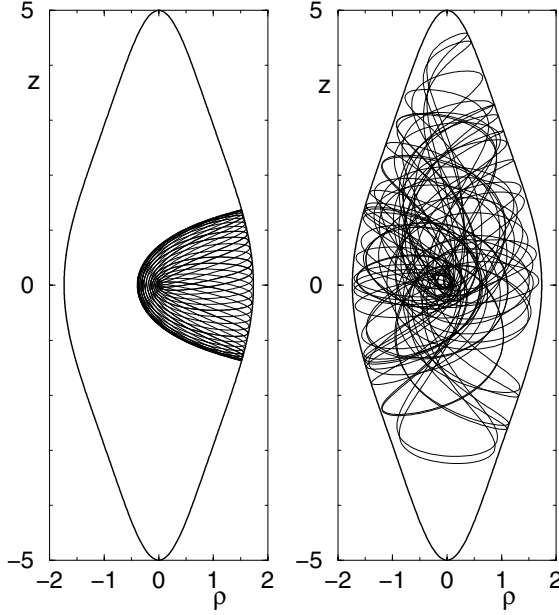


Fig. 5. Two typical classical trajectories of the Rydberg electron of an hydrogen atom in a magnetic field at scaled energy $\epsilon = -0.2$. The nucleus is at the origin, at the center of the figures. The outer solid line represents the part of space allowed by energy conservation. The left trajectory is regular with a well organized structure whereas the right trajectory is chaotic. Below $\epsilon = -0.5$, all trajectories look like the left one, above $\epsilon = -0.13$, they all look like the right trajectory. Note that the two trajectories differ only by the initial conditions. At $\epsilon = -0.2$, the dynamics is thus mixed regular-chaotic.

1.5.4 Quantum scaling – Scaled spectroscopy

The scaling law is no longer valid in quantum mechanics, since there is an absolute scale imposed by the Planck's constant $\hbar$. Hence, quantum properties depend *a priori* on both E and γ . However, this offers a unique opportunity to study *experimentally* the semiclassical limit $\hbar \rightarrow 0$. Indeed, in rescaled coordinates, equation (1.13), the Schrödinger equation can be written as:

$$\left(-\frac{\gamma^{2/3}}{2} \Delta - \frac{1}{r} + \frac{\rho^2}{8} - \epsilon \right) |\psi\rangle = 0 \quad (1.15)$$

where Δ is the Laplace operator. This shows that $\gamma^{1/3}$ plays the role of an effective Planck's constant.

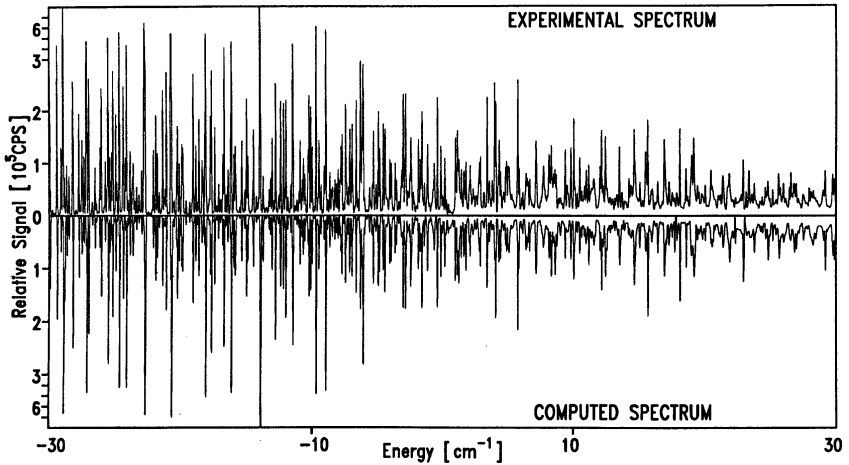


Fig. 6. Comparison between the experimental spectrum of Rydberg states of the Lithium atom in a magnetic field of 6T and the *ab initio* numerical calculation shown as a mirror image. The agreement is clearly excellent, with several hundred lines perfectly reproduced. This implies that numerical calculations can be safely used in complement with real experiments.

Hence, in a real (or numerical) experiment, the semiclassical limit $\hbar \rightarrow 0$ can be studied, just by tuning simultaneously the energy and the magnetic field according to equation (1.13) – keeping the scaled energy constant – towards lower magnetic field $\gamma^{1/3} \rightarrow 0$ and higher excited states. This possibility is known as “scaled spectroscopy” and has revealed extremely important for understanding the classical-quantal correspondence [25]. The dream of the theorist – doing quantum mechanics at an arbitrary tunable value of $\hbar$ – became a reality thanks to the tunability of laser and magnetic field sources.

From the experimental point of view, the highly excited chaotic Rydberg states are prepared by optical excitation from the ground or a low-excited state. The high monochromaticity of a laser makes it possible to selectively excite the various states. A detailed high resolution spectroscopic analysis is thus possible [24–26].

From the theoretical point of view, the use of group theory allows extremely efficient numerical experiments [27, 28], making the accurate computation of very highly excited energy levels and wavefunctions possible. This is illustrated in Figure 6 which shows an experimental spectrum obtained at 6T on the Rydberg states of the lithium atom compared to the *ab initio* numerical calculation without any adjustable parameter. Although

the spectrum looks extremely complicated (a manifestation of chaos!) with several hundred lines, the calculation reproduces exactly all of them. In fact, a Rydberg atom in a magnetic field is one of the very rare systems (if not the only one...) where one can calculate the thousandth excited state and find it experimentally exactly at the predicted position! This makes us confident that numerical experiments are excellent approximations to the real world.

2 Time scales – Energy scales

For a correct understanding of the connections between the quantum and classical properties of a chaotic system, it is crucial to know the relevant time and energy scales – of classical or quantum origin – of the problem.

2.1 Shortest periodic orbit

The shortest time scale is simply the period of the shortest periodic orbit T_{Min} . A slightly longer time scale is given by the time taken for chaos to manifest, that is the inverse of the typical Lyapounov exponent. The larger the sensitivity on initial conditions, the shorter this time scale. In a typical chaotic system – far from a bifurcation and far from the onset of chaos – the product λT_{Min} is of the order of unity. Hence, these two time scales coincide. The corresponding energy scale, $2\pi\hbar/T_{\text{Min}}$, see Figure 7, is the largest energy scale of interest in the problem.

2.2 Ehrenfest time

The Ehrenfest time is the shortest time scale of pure quantum origin. It is the time it takes for a minimum wave-packet to significantly spread over a macroscopic part of phase space. It can be estimated as follows⁴: the extension of a minimum wave-packet is typically:

$$\Delta q_0 \sim \sqrt{\frac{\hbar}{m\omega}} \quad \Delta p_0 \sim \sqrt{\hbar m\omega} \quad (2.1)$$

where m is the mass of the particle and ω the typical frequency of the system (of the order of $2\pi/T_{\text{Min}}$).

For a non-linear system, the typical size of the configuration space is:

$$\chi \sim \sqrt{\frac{\partial_q V}{\partial_q^3 V}}. \quad (2.2)$$

⁴See also the similar discussion in the lecture notes of W. Zurek in this book.

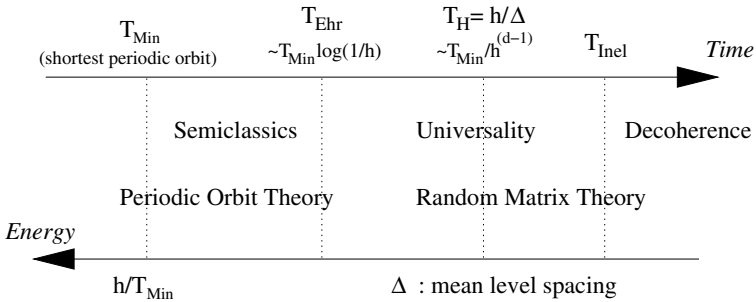


Fig. 7. The important time and energy scales for a chaotic quantum system. The shortest relevant time scale is T_{Min} , the period of the shortest periodic orbit. The Ehrenfest time T_{Ehr} is a quantum time scale after which the details of the quantum and classical evolution have to differ. The most important quantum time scale is the Heisenberg time T_{H} , associated the mean energy level spacing. In the semiclassical limit, T_{H} is much larger than T_{Min} . One expects a universal behaviour at long times, thus universal statistical properties of the energy levels, described in Section 3. At short times (long energy range), the specificities of the system appear to be related to the periodic orbits of the system, as explained in Section 4. At very long time, characterized by the inelastic time T_{Inel} , the system cannot be considered as isolated from its environment; phase coherence and quantum interferences are lost. The system eventually behaves classically.

If λ is the mean Lyapounov exponent, the size of the wave-packet typically grows in the unstable direction as $\Delta q_0 \exp(\lambda t)$ and reaches the macroscopic size of the configuration space at the Ehrenfest time:

$$T_{\text{Ehr}} = \frac{1}{\lambda} \log \frac{\chi \Delta p_0}{\hbar}. \quad (2.3)$$

Although the Ehrenfest time tends to infinity in the semiclassical limit, it depends only logarithmically on $\hbar$, and is typically only slightly longer than T_{Min} .

Alternatively, the Ehrenfest time can be seen as the time scale after which the Wigner distribution of a quantum system cannot evolve classically. Indeed, in a chaotic system, any initially localized distribution spreads along the unstable directions, but also shrinks along stable directions at a rate given by the Lyapounov exponent. Hence, the typical size of the smallest classical structures will decrease as $\exp(-\lambda t)$. This also implies that the spatial derivatives of the phase space density have to increase exponentially with time. Thus, the corrective terms in equation (1.10) will unavoidably *increase* exponentially with time. After the Ehrenfest time, they will be larger than the terms driving the classical evolution, equation (1.6) and the quantum evolution has to differ from the classical one.

By comparing the classical and quantum evolutions of phase space densities (calculated numerically), W. Zurek shows in his lectures (in this book) that they actually differ after the Ehrenfest time. However, a warning is here necessary. After the Ehrenfest time, the quantum interference effects have to manifest themselves through fringes in the Wigner distribution and similar non-classical phenomena. This means that the details of the classical and quantum dynamics certainly differ. However, when more global quantities are considered – for example expectation values of operators or transport coefficients – the differences may be completely smoothed out. There are rather strong indications that this happens and that the Ehrenfest time is rather irrelevant for the global dynamics: firstly, the semiclassical approximation for chaotic systems discussed in Section 4 shows that the only relevant global time scales are T_{Min} and the Heisenberg time discussed below. Secondly, the experimental results obtained on quantum transport, discussed in Section 5, do not show any change at the Ehrenfest time. Thus, in my opinion, the Ehrenfest time is not a fully relevant time scale for quantum chaotic systems, except for analysis of the finest details.

2.3 Heisenberg time

This is another basic quantum time scale. To understand its origin, let us consider a time-independent bound quantum system with Hamiltonian H , in an arbitrary initial state $|\psi(t=0)\rangle$. Its evolution can be expressed using the discrete eigenstates and eigenvalues of the Hamiltonian H

$$H|\phi_i\rangle = E_i|\phi_i\rangle \quad (2.4)$$

with the following expression:

$$|\psi(t)\rangle = \sum_i c_i \exp\left(-i\frac{E_i t}{\hbar}\right) |\phi_i\rangle, \quad (2.5)$$

where the constant coefficients c_i are computed from the initial state using:

$$c_i = \langle \phi_i | \psi(0) \rangle. \quad (2.6)$$

The autocorrelation function of the quantum system is a diagonal element of the time-evolution operator:

$$C(t) = \langle \psi(0) | \psi(t) \rangle = \langle \psi(0) | U(t, 0) | \psi(0) \rangle = \sum_i |c_i|^2 \exp\left(-i\frac{E_i t}{\hbar}\right). \quad (2.7)$$

It is a discrete sum of oscillating terms, and, consequently, a quasi-periodic function of time. This is *extremely different* from a classical autocorrelation function for a chaotic system which decreases over the characteristic time scale T_{Min} and does not show any revival at longer time [7].

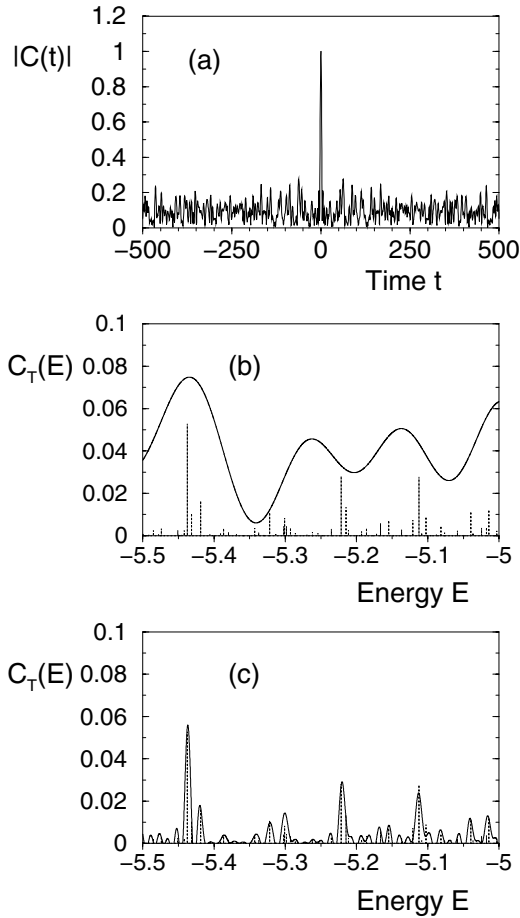


Fig. 8. (a): The typical behaviour of a quantum autocorrelation function $C(t) = \langle \psi(0) | \psi(t) \rangle$; it is of course unity at time $t = 0$ and rapidly decreases further from 0. Its Fourier transform is a series of δ -peaks centered at the positions of the energy levels, see equation (2.8), and shown as dashed lines in (b) and (c). When the Fourier transform of $C(t)$ is limited to a finite time interval, the δ -peaks are smoothed. Over a short time interval (b), the individual energy levels are not resolved. Over a time interval comparable to the Heisenberg time T_H , the individual peaks are resolved (c).

The Fourier transform of the autocorrelation function is:

$$\tilde{C}(E) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} e^{iEt/\hbar} C(t) dt = \sum_i |c_i|^2 \delta(E - E_i), \quad (2.8)$$

that is a sum of δ -peaks at the positions of the energy levels.

If we now consider the Fourier transform not over the whole range of time from $-\infty$ to $+\infty$, but over a finite time interval, we obtain a smoothed version of the quantum spectrum:

$$\tilde{C}_T(E) = \frac{1}{T} \int_{-T/2}^{T/2} e^{iEt/\hbar} C(t) dt = \sum_i |c_i|^2 \frac{\sin \frac{T(E-E_i)}{2\hbar}}{\frac{T(E-E_i)}{2\hbar}}, \quad (2.9)$$

where all the peaks are smoothed δ -peaks of width $2\pi\hbar/T$. For short T , the different broadened peaks centered at the energy levels E_i overlap, and $\tilde{C}_T(E)$ is a globally smooth function, like its classical counterpart. In such a situation, it is possible (although nothing proves that is always the case) that the quantum $\tilde{C}_T(E)$ mimics the classical chaotic behaviour. The important point is that, for large T , the different peaks do not overlap and the discrete nature of the energy spectrum **must** appear in $\tilde{C}_T(E)$, whatever the initial state. The typical time needed for resolving individual quantum energy levels is called the Heisenberg time and is simply related to the mean level spacing Δ through:

$$T_H = \frac{2\pi\hbar}{\Delta}. \quad (2.10)$$

After this time, the quantum system *cannot* mimic the classical chaotic behaviour which has a continuous spectrum. Since T_H depends on $\hbar$, one can understand how quantum tends to classical dynamics as $\hbar$ goes to zero. The mean level spacing is given by the Weyl's rule and scales as $\hbar^d$, with d the number of degrees of freedom (see Eq. (3.3)). For two- (or higher) dimensional systems, T_H tends to infinity as $\hbar \rightarrow 0$, see Figure 7.

In some sense, after the Heisenberg time, the quantum system “knows” that the energy spectrum is discrete, it has resolved all individual peaks and the future evolution cannot bring any new information. As a consequence, the system cannot explore a new part of the phase space, it freezes its evolution, repeating forever the same type of dynamics.

2.4 Inelastic time

At very long time, the system cannot be considered as isolated, but the coupling to its environment has to be taken into account. The subtle phase coherences between the different parts of the wavefunction are rapidly destroyed by this coupling as explained in [8, 9]. Such a decoherence phenomenon – a typically inelastic process – is responsible for the loss of quantum phase coherence and makes the system to behave classically, as shown by W. Zurek in the lectures (in this book). The typical time scale for this phenomenon, T_{Inel} , has to be longer than the previous quantum time scales; otherwise, quantum effects are killed by the coupling to the environment.

Other time scales may exist in specific systems. For example, in an open Hamiltonian system, the typical time scale for escaping the chaotic region is obviously important. Also, in mixed chaotic-regular systems, different time scales coexist in the different regions of phase space (and at their boundaries) making general statements extremely difficult.

As explained above, the Ehrenfest time is only relevant for very detailed properties of the quantum dynamics. In any case, because of its logarithmic dependence with $\hbar$, it lies between T_{Min} and T_{H} , see Figure 7. For the sake of simplicity, we will first consider the case where the inelastic time T_{Inel} is much longer than the Heisenberg time T_{H} , the situation shown in Figure 7. It means that typical quantum effects appear before the coupling with the environment significantly affects the system. This is typically what happens for Rydberg atoms in an external field. There, T_{Min} is of the order of picoseconds to nanoseconds while T_{H} is about 10 to 100 times longer. On the other hand, the lifetime T_{Inel} of a Rydberg atom *versus* spontaneous emission is of the order of microseconds to milliseconds. Hence, we are in a situation where the various time scales are well separated.

For the external dynamics of cold atoms in a laser field, the situation may be different. In Section 5.6, I discuss what happens when T_{Inel} becomes comparable to T_{H} .

In the semiclassical limit $\hbar \rightarrow 0$, the energy scales $2\pi\hbar/T_{\text{Min}}$ and $\Delta = 2\pi\hbar/T_{\text{H}}$ are small compared to the energy itself. This means that we will always look at relative small changes in the energy, such that the classical dynamics does not substantially change over the energy range considered. This is of course possible in the semiclassical regime thanks to the large density of states.

3 Statistical properties of energy levels – Random Matrix Theory

3.1 Level dynamics

The goal of traditional spectroscopy is to assign quantum numbers to the different energy levels in order to obtain a complete classification of the spectrum. When little is known about the system, it is difficult to identify the good quantum numbers and their physical interpretation, or even to know whether they exist or not. A simple tool is to look at the level dynamics, that is the evolution of the various energy levels as a function of a parameter. As good quantum numbers are associated with conserved quantities, *i.e.* operators commuting with the Hamiltonian, energy levels with different sets of good quantum numbers are not coupled and thus generically cross each other [29]. On the contrary, if two states are coupled, the energy levels will repel each other, producing an avoided crossing. The width of the avoided crossing, *i.e.* the minimum energy difference between the two energy curves, is a direct measure of the strength of the coupling.

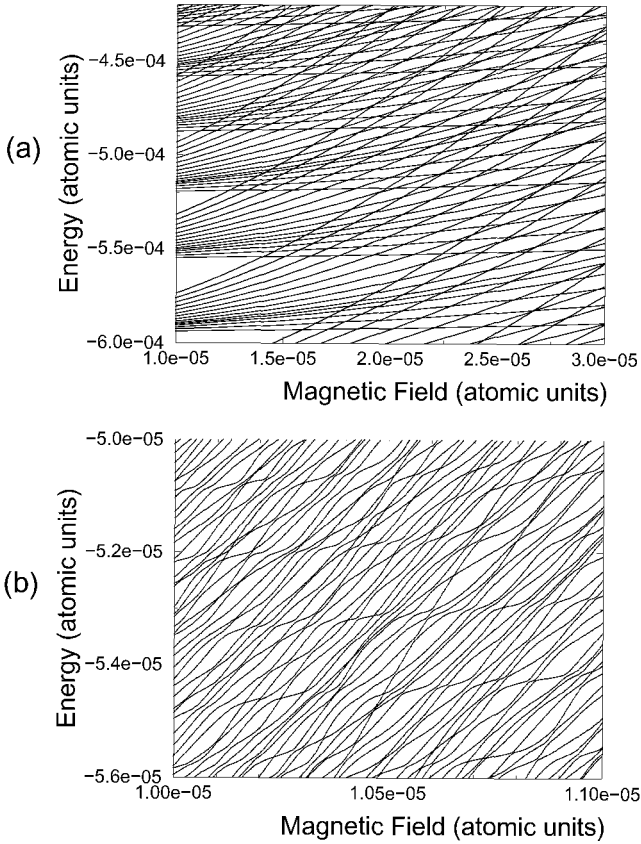


Fig. 9. Map of the energy levels of a hydrogen atom *versus* magnetic field for typical Rydberg states of the ($L_z = 0$, even parity) series. At low energy (a), the classical dynamics is regular and the energy levels (quasi-) cross. The quantum eigenstates are defined by a set of good quantum numbers. At high energy (b), the classical dynamics is chaotic, the good quantum numbers are lost and the energy levels strongly repel each other. The strong fluctuations in the energy levels are characteristic of a chaotic behaviour.

Thus, looking at the level dynamics gives some qualitative information on the properties of the system. This is illustrated in Figure 9 which shows the evolution of the energy levels of a hydrogen atom as a function of the magnetic field strength. At low magnetic field, Figure 9a, there are only level crossings. A given eigenstate can be unambiguously followed in a wide range of field strength, since it crosses (or has very small avoided crossings with) the other energy levels, which proves that there are at least approximate

good quantum numbers. At higher magnetic field, Figure 9b, the sizes of the avoided crossings increase and individual states progressively lose their identities. In other words, the good quantum numbers are destroyed.

A crucial observation is that the transition from crossings (or tiny avoided crossings) to large crossings takes place *precisely* where the classical dynamics evolves from regular to chaotic. The transition is smooth – with the proportion of large avoided crossings progressively increasing – and there is a large intermediate region where crossings and large avoided crossings coexist. This corresponds to the range of scaled energies $\epsilon \in [-0.5, -0.13]$, in complete agreement with the classical transition from regularity to chaos, see Section 1.5. From a pure quantum point of view, this phenomenon is extremely difficult to understand: when the magnetic field strength increases, the only change in the matrix representing the Hamiltonian, equation (1.11), in any basis, is a global multiplication of all the matrix elements of ρ^2 by a constant factor. The dramatic effect on the energy level dynamics is a direct manifestation of chaos in the quantum properties of the system. In Section 4, I give an explanation of this transition from the regular region where good quantum numbers, *i.e.* conserved quantities, exist to the chaotic region where they are destroyed.

In the fully chaotic regime, the energy levels and the eigenstates strongly *fluctuate* when the magnetic field is changed. In that sense, the quantum system shows a high sensitivity on a small perturbation, like its classical equivalent. The energy spectrum of a classically chaotic system displays an extreme *intrinsic* complication, which means the death of traditional spectroscopy. Such extremely complex spectra have been observed experimentally in atomic systems in external fields [30], on the eigenmodes of microwave billiards (when a parameter of the billiard shape is varied) [22] and numerically on virtually all chaotic systems [1, 12, 29]. It should be emphasized that level dynamics in the chaotic regime looks similar whatever the system is, as long as its classical dynamics is chaotic. It is probably the simplest and most universal property.

3.2 Statistical analysis of the spectral fluctuations

This qualitative property has been put on a firm ground by the study of the statistical properties of energy levels [12, 29, 31]. The idea is the following: there are too many levels and their evolution is too complicated to deserve a detailed explanation, level by level. In complete similarity classical with a gas of interacting particles where the detailed positions of the particles do not really carry the relevant information which is rather contained in some *statistical* properties, we must use a statistical approach for the description of the energy levels of a chaotic quantum system. In order to compare different systems and characterize the *spectral fluctuations*, we must first define proper quantities. For a complete description, see [12, 29].

3.2.1 Density of states

The density of states is:

$$d(E) = \sum_i \delta(E - E_i) \quad (3.1)$$

where the E_i are the energy levels of the system. The cumulative density of states counts the number of energy levels below energy E . It is thus:

$$n(E) = \int_{-\infty}^E d(\epsilon) d\epsilon = \sum_i \Theta(E - E_i). \quad (3.2)$$

This is a step function with unit steps at each energy level. When there is a large number of levels, one can define the averaged cumulative density of states $\bar{n}(E)$, a function interpolating $n(E)$ by smoothing the steps. Its derivative is the averaged density of states $\bar{d}(E)$. There are situations when this is the only relevant physical quantity. For example, in a large semiconductor sample, the averaged density of states at the Fermi level is what determines the contribution of electrons to the specific heat at low temperature [3].

The averaged density of states can be determined in the semiclassical approximation (see Sect. 4) by the Weyl's rule (also known as the Thomas-Fermi approximation):

$$\bar{d}(E) = \frac{1}{(2\pi\hbar)^d} \int d\mathbf{p} d\mathbf{q} \delta(H(\mathbf{q}, \mathbf{p}) - E). \quad (3.3)$$

It only depends on the classical Hamilton function H and not on the regular or chaotic nature of the dynamics. As shown in Figure 10 in the specific case of the hydrogen atom in a magnetic field, the difference between the exact cumulative density of states $n(E)$ and the semiclassical approximation $\bar{n}(E)$ is extremely small. Typical fluctuations of $n(E) - \bar{n}(E)$ are only 1 or 2 units. This means that the spectrum is rather rigid over a long range.

3.2.2 Unfolding the spectrum

The next step is to eliminate the slow changes in the averaged density of states by defining an unfolded spectrum through the following quantity:

$$\hat{N}(x) = n(\bar{n}^{-1}(x)) \quad (3.4)$$

which is nothing but the cumulative density of states represented as a function of a rescaled variable such that the “energy levels” now appear equally spaced by one unit. By construction, the rescaled energy levels $x_i = \bar{n}(E_i)$ have a density of states equal to one. It allows to compare spectra got for different parameters or even for completely different systems.

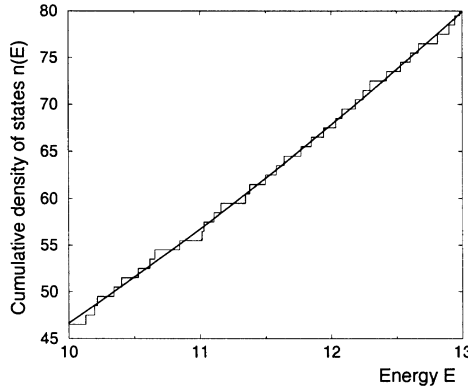


Fig. 10. Comparison between the exact cumulative density of states $n(E)$ which counts the number of energy levels below energy E (this is the step function) and its semiclassical approximation – the smooth function $\bar{n}(E)$ – proportional to the phase space volume, equation (3.3). The agreement is excellent with only short range fluctuations of the order of one mean level spacing.

3.2.3 Nearest-neighbor spacing distribution

The simplest quantity is the distribution of nearest neighbour spacings, *i.e.* of energy difference between two consecutive levels $s_i = x_{i+1} - x_i$. This distribution is traditionally denoted $P(s)$. By virtue of the unfolding procedure, the average spacing is one. Its behaviour near $s = 0$ measures the fraction of very small spacings (quasi-degeneracies), hence the degree of level repulsion.

3.2.4 Number variance

The use of the nearest neighbor spacing distribution is simple, but not very logical from the statistical physics point of view. Indeed, $P(s)$ involves *all* correlation functions among the energy levels. It is simpler to consider separately the two-point, three-point, etc. correlation functions. The two-point correlation function R_2 depends only on the energy difference if the spectrum is stationary (*i.e.* statistically invariant by a global translation, which is likely for a large unfolded spectrum). Near 0, it again measures the degree of level repulsion. A more global quantity is the number variance $\Sigma^2(L)$ which is the variance of the number of levels contained in an energy interval of length L . It is related to the two-point correlation by [12]:

$$\Sigma^2(L) = L + 2 \int_0^L (L - x)(R_2(x) - 1) dx. \quad (3.5)$$

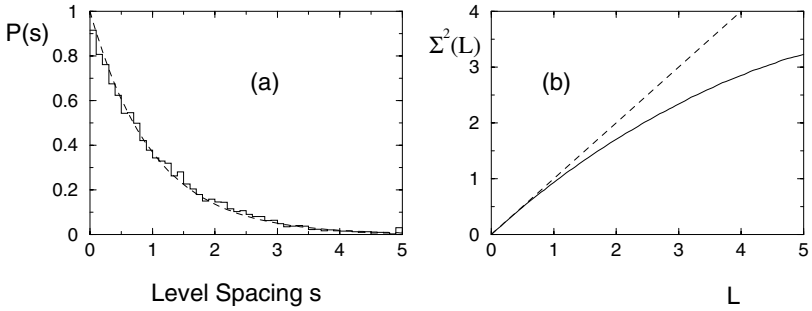


Fig. 11. Statistical properties of energy levels for the hydrogen atom in a magnetic field, obtained from numerical diagonalization of the Hamiltonian in the regular regime. (a) Nearest neighbor spacing distribution. The distribution is maximum at 0 and well fitted by a Poisson distribution (dashed line). (b) Number variance. Again, the Poisson prediction (dashed line) works quite well. The saturation at large L is due to the residual effects of periodic orbits and is well understood.

It is a measure of the rigidity of the spectrum, that is, it measures how the spectrum deviates from a uniform spectrum of equally spaced levels.

A related quantity is the so-called spectral rigidity $\Delta_3(L)$ which measures how much the cumulative density of states differs from its best linear fit on an energy interval of length L . It is another alternative to the two-point correlation function. Its advantage is that it is very robust against imperfections such as spurious or missing energy levels and can be determined rather safely from a limited number of energy levels. This is of major importance for example in analyzing experimental atomic [32,33] or nuclear spectra [12].

3.3 Regular regime

In the regular regime, Figure 9a, consecutive energy levels generally do not interact. Thus, from the statistical point of view, they can be considered as independent random variables. The distribution of spacings is the one of uncorrelated levels, that is a Poisson distribution:

$$P(s) = \exp(-s), \quad (3.6)$$

which nicely reproduces the numerical results obtained on different systems (see Fig. 11a) and also several experimental results [22,34]. Note that the maximum of the distribution is near $s = 0$ which shows that quasi-degeneracies are very probable and that level repulsion is absent.

This is a *universal* result which applies generically to regular systems. Other statistical quantities can be described as well. The two-point

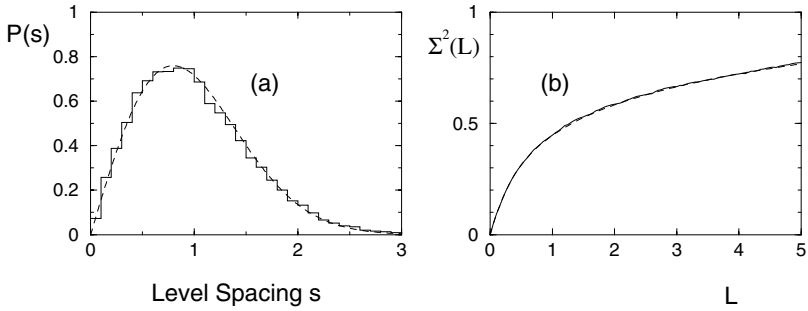


Fig. 12. Same as Figure 11, but in the classically chaotic regime. (a) The probability of finding almost degenerate levels is very small (level repulsion). The results are well reproduced by the Wigner distribution (dashed line) and Random Matrix Theory. (b) The number variance is much smaller than in the regular case, showing the rigidity of the energy spectrum. It agrees perfectly with the prediction of Random Matrix Theory (dashed line).

correlation function is simply $R_2(x) = 1$ and the number variance is:

$$\Sigma^2(L) = L. \quad (3.7)$$

Figure 11b shows the numerical result for the hydrogen atom in a magnetic field in the regular regime. The agreement with the prediction is good, at least for low L . The saturation at large L can be quantitatively understood using periodic orbit theory [35]. In simple words, it is due to long range correlations in the spectrum induced by periodic orbits.

3.4 Chaotic regime – Random Matrix Theory

In the chaotic regime, the strong level repulsion induces a completely different result for the spacing distribution – see Figure 12a – with practically no small spacing, and also a lack of large spacings.

A simple model is able to predict the statistical properties of energy levels. It assumes a maximum disorder in the system and that – from a statistical point of view – all basis sets are equivalently good (or bad). It therefore models the Hamiltonian by a set of random matrices which couple any basis state to all the other ones. Depending on the symmetry properties of the Hamiltonian (especially with respect to time reversal, see below), different ensembles of random matrices have to be considered. Let us assume for the moment that the system is time-reversal invariant and thus can be represented by a real symmetric matrix H_{ij} in some basis.

If the matrix size is N (not to be confused with the number of degrees of freedom), this leaves $N(N+1)/2$ real independent random variables.

The natural metric in the space of real symmetric matrices is:

$$ds^2 = \text{Tr}(dH \, dH^+). \quad (3.8)$$

The corresponding (unnormalized) measure over the matrix space is:

$$dH = \prod_{1 \leq i \leq N} dH_{ii} \prod_{1 \leq i < j \leq N} dH_{ij} \quad (3.9)$$

which is invariant by any orthogonal transformation and thus puts all the orthonormal basis on the same footing. As a consequence, the probability density $P(H)$ itself must be invariant by any orthogonal transformation.

For simplicity, we will assume that the various matrix elements are *independent* random variables⁵.

With these basic assumptions, it is tedious but rather easy to show that the probability density can be written as [29]:

$$P(H) \propto \exp\left(-\frac{\text{Tr}(H^2)}{4\sigma^2}\right) \quad (3.10)$$

where σ is the only remaining free parameter.

From this equation and expanding the trace of H^2 as a function of the matrix elements H_{ij} , one obtains easily that all matrix elements have a Gaussian distribution with zero average and variance:

$$\langle H_{ij}^2 \rangle = (1 + \delta_{ij})\sigma^2. \quad (3.11)$$

These properties define the Gaussian Orthogonal Ensemble (GOE) of random matrices⁶.

Knowing the probability density, we can extract the statistical properties of the eigenvalues. The first step is to calculate the joint probability density of the eigenvalues. Indeed, it is natural to change from the $N(N+1)/2$ variables H_{ij} to the N eigenvalues of H and the $N(N-1)/2$ parameters of the orthogonal transformation which diagonalizes H . The only important factor is the Jacobian of this transformation. Because of the orthogonal invariance of the eigenvalues, the Jacobian depends only on the eigenvalues and the integration over the orthogonal group is trivial. The Jacobian can be easily calculated for $N=2$ (it is left to the reader as an exercise): it is

⁵This hypothesis is not at all crucial. It can be easily relaxed, generating other ensemble of random matrices with similar statistical properties [29,31].

⁶An alternative derivation of the GOE is based on information theory. If we look for the probability density which maximizes the entropy $-\int P(H) \ln P(H) dH$ with the constraint that the average value of $\text{Tr}(H^2)$ is fixed, one rediscovers the GOE. The idea behind this derivation is that we know nothing about the distribution and have to take it as general as possible.

proportional to the difference $|E_1 - E_2|$ between the two eigenvalues. Hence, the probability of getting two degenerate eigenvalues is zero! This is the very origin of level repulsion. It is a statistical effect induced by the geometry of the GOE: matrices with quasi-degenerate eigenvalues are just much less probable. Generalization to an arbitrary value of N is simple. The Jacobian is a polynomial function of the eigenvalues with degree $N(N-1)/2$ and must vanish as soon as two eigenvalues are equal. This gives the joint probability density:

$$P(E_1 \dots E_N) \propto \left(\prod_{1 \leq i < j \leq N} |E_i - E_j| \right) \exp \left(-\frac{\sum_{i=1}^N E_i^2}{4\sigma^2} \right). \quad (3.12)$$

Although the rest of the calculation – *i.e.* extracting the various correlation functions – looks easy when the joint probability is known, it turns out that the calculation is feasible only for small N and in the $N \rightarrow \infty$ limit. It involves the use of either beautiful old-fashioned mathematics [31] or almost incomprehensible supersymmetry techniques [36]. Most formulas are explicit but not very illuminating; they can be found in [12, 31].

The spacing distribution cannot be calculated in closed form, but it is very close to the so-called Wigner distribution:

$$P(s) = \frac{\pi s}{2} \exp \left(-\frac{\pi s^2}{4} \right). \quad (3.13)$$

This distribution, shown in Figure 12a, agrees extremely well with the numerical results got on the hydrogen atom in a magnetic field, but also with the experimental results shown in Figure 13. These are not easy to obtain, because they require an excellent resolution in the chaotic regime where the density of states is large and a good signal to noise ratio to make sure that all energy levels are observed and that no stray line is present.

Similar results have been obtained on dozens of quantum chaotic systems, both numerically and experimentally. Experimental examples are the energy levels of highly excited nuclei [12], rovibrational levels of the NO_2 molecules [17] and electromagnetic eigenmodes of microwave cavities [22].

The transition from a Poisson distribution in the classically regular regime to a Wigner distribution in the chaotic regime gives a **characterization** of quantum chaos, at least for highly excited states.

Other statistical properties have been studied and are found in good agreement with the predictions of Random Matrix Theory [32]. For example, the number variance, shown in Figure 12b, is in perfect agreement with the GOE prediction which, for large L , is

$$\Sigma^2(L) \simeq \frac{1}{\pi^2} \ln 2\pi L. \quad (3.14)$$

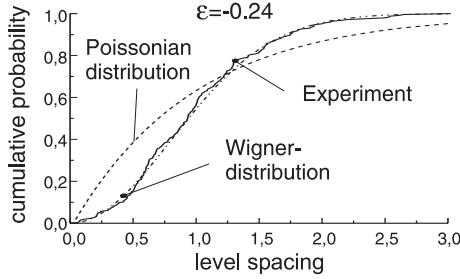


Fig. 13. Cumulative nearest neighbor spacing distribution $N(s) = \int_0^s P(x) dx$ experimentally observed for Rubidium Rydberg states in a strong magnetic field (scaled energy $\varepsilon = -0.24$, in a mainly chaotic regime) compared with the Wigner distribution (prediction of Random Matrix Theory) and the Poisson distribution (courtesy of H. Held).

Note that the number variance is much smaller here than in the regular case. The spectrum is *extremely* rigid, as for $L = 10^6$, Σ^2 is only of the order of 3. This means that the typical fluctuation of the number of levels is 1 or 2 additional or missing levels over a range of one million level. In the Poisson model, the typical fluctuation would be $\sqrt{L} = 1000$ levels! This extraordinary large rigidity is due to the strong couplings existing between all the states in the model. If a fluctuation makes the level repulsion abnormally large between two states, they cannot repel too strongly because they are themselves strongly pushed by the other levels. From maximum disorder at the microscopic level, a globally rigid structure is born.

Finding universal properties in the local statistical properties of energy levels for chaotic systems is not a real surprise. As discussed in Section 2, this range of energy (mean level spacing Δ) corresponds to a long time behaviour ($\hbar/\Delta = T_H \gg T_{\text{Min}}$), where chaos is classically fully developed with its universal properties. Universality is also observed in the corresponding quantum dynamics. On the other hand, at shorter times, of the order of T_{Min} , non-universal properties exist in the classical behaviour. This implies also a deviation from the predictions of Random Matrix Theory on a large energy scale, as has been numerically and experimentally observed [27, 34].

3.5 Usefulness of Random Matrix Theory

Random Matrix Theory can also predict the behaviour of quantities beyond the energy levels. For example, it can predict the distribution of the wave-function amplitude [1], the lifetimes of resonances in open systems [37] or

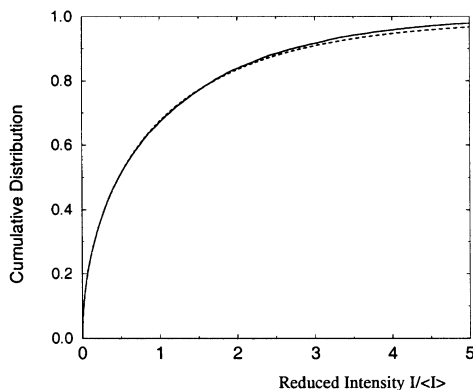


Fig. 14. Cumulative distribution of the intensities of the optical absorption lines from a low excited state for the hydrogen atom in a magnetic field (in the chaotic regime). The solid line is the result of the numerical calculation while the dashed line is the Porter-Thomas distribution, equation (3.15), the prediction of Random Matrix Theory. The agreement is clearly excellent, with a very large number of small intensities. This is a manifestation of random destructive interferences in a chaotic quantum system.

the distribution of excitation probability. Let us consider for example the optical excitation of a chaotic state of the hydrogen atom in a magnetic field from a low-lying state. From the Fermi golden rule, the intensity of the absorption line is proportional to the square of the matrix element of the dipole operator between the initial and final states. In the GOE, this matrix element has a Gaussian distribution. The intensity is proportional to its square and thus distributed according to the so-called Porter-Thomas distribution [37]:

$$P(I) = \frac{1}{\sqrt{2\pi\bar{I}}} \exp\left(-\frac{I}{2\bar{I}}\right), \quad (3.15)$$

where $\bar{I}$ is the mean value.

This distribution diverges near $I = 0$ which means that vanishingly small intensities are by far the most probable. This can be interpreted as due to mainly destructive interferences between the various (chaotic) excitation paths. In order to make a comparison with some numerical experiments, it is thus easier to consider the cumulative intensity distribution $\int P(I) dI$ which is plotted in Figure 14 together with the theoretical prediction, equation (3.15). The agreement is obviously excellent, which proves the usefulness of Random Matrix Theory.

Actually, Random Matrix Theory is used to predict properties of a wide variety of complex quantum systems [3, 19]. For example, the universal conductance fluctuations observed in mesoscopic samples can be quantitatively interpreted using Random Matrix Theory [20, 38].

3.6 Other statistical ensembles

If time-reversal symmetry (or more generally any anti-unitary symmetry) is broken, the Hamiltonian cannot be written as a real symmetric matrix, but rather as a complex Hermitean matrix. One has to change the ensemble of random matrices to use and define the Gaussian Unitary Ensemble (GUE). The natural (unnormalized) measure is now:

$$dH = \prod_{1 \leq i \leq N} dH_{ii} \prod_{1 \leq i < j \leq N} d\text{Re}H_{ij} d\text{Im}H_{ij} \quad (3.16)$$

which is invariant by any unitary transformation and thus puts again all the orthonormal basis on the same footing. The probability distribution for H is found again to be given by equation (3.10): both $\text{Re}H_{ij}$ and $\text{Im}H_{ij}$ are Gaussian distributed. This adds *more* level repulsion because two arbitrary states have two chances to be coupled and to repel. Not surprisingly, this is visible in the joint probability distribution which takes the form:

$$P(E_1, \dots, E_N) \propto \left(\prod_{1 \leq i < j \leq N} |E_i - E_j|^2 \right) \exp \left(-\frac{\sum_{i=1}^N E_i^2}{4\sigma^2} \right). \quad (3.17)$$

For large N , one finds quadratic level repulsion and the spacing distribution is very close to:

$$P(s) = \frac{32}{\pi^2} s^2 \exp \left(-\frac{4}{\pi} s^2 \right). \quad (3.18)$$

This agrees extremely well with numerical results obtained on model systems [29, 41]. In Figure 15, I show the numerical results obtained for an hydrogen atom in a combination of microwave external field and static electric field, in conditions where the dynamics is essentially chaotic and all anti-unitary symmetry is broken (for details, see [39]). The agreement with the prediction of the GUE is obviously excellent.

As far as I know, there is no convincing experimental result obtained in this regime on quantum systems. On the other hand, there have been several studies of the electromagnetic eigenmodes of microwave cavities which clearly show the transition from GOE to GUE when time-reversal is broken [40].

One also has to consider the special case of half-integer spin systems with time-reversal invariance: there, all levels are doubly degenerate (Kramers

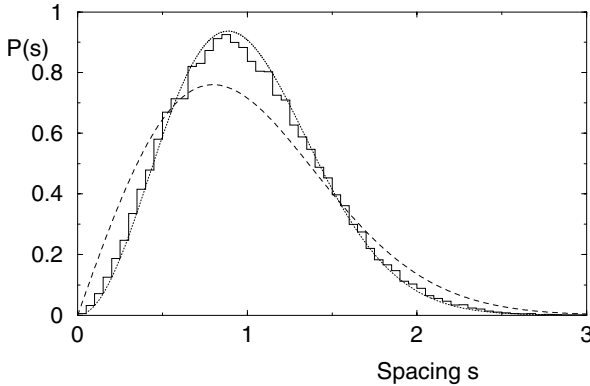


Fig. 15. Nearest neighbor spacing distribution for the energy levels of an hydrogen atom in a combination of a resonant microwave field and a static electric field, in conditions where the dynamics is essentially chaotic and time reversal invariance is broken. The histogram is the numerical result; the dotted line is the prediction of the Gaussian Unitary Ensemble of random matrices and agrees excellently with the numerical result. The prediction of the Gaussian Orthogonal Ensemble of random matrices, shown as a dashed line, is obviously incorrect.

degeneracy). If some rotational invariance exists, this degeneracy is hidden and the GOE should be used in each rotational series. If the rotational invariance is broken, every level will be exactly doubly degenerate and the Gaussian Symplectic Ensemble (GSE) of random matrices has to be used [12, 29, 41].

It is important to notice the role of symmetries for level statistics. If a good quantum number survives in a system (for example a discrete two-fold symmetry), the states with the same good quantum numbers interact, but ignore the other states. Thus, even if each series obeys the GOE statistics, the total spectrum will appear as the superposition of several uncorrelated GOE spectra, which has completely different statistical properties. It is very important to be sure that one has a pure sequence of levels before analyzing it. This may be difficult in a real experiment because of stray mixing between series, usually much easier in numerical experiments.

Finally, intermediate regimes have been studied, for example between the regular Poisson and the chaotic GOE regimes. In general, this transition is not universal [29].

4 Semiclassical approximation

The previous section has shown the existence of universal fluctuation properties associated with chaos. These properties take place at short energy range, of the order of the mean level spacing, that is for times of the order of the Heisenberg time, much longer than the period of the shortest periodic orbit. This also implies that a detailed analysis of all energy levels and eigenstates does not make sense: no interesting information can be brought to the physics of the chaotic phenomenon, beyond the statistical aspects. On the other hand, this does *not* mean that these energy levels do not carry any information; it is just that this information has to be extracted in a different way. More precisely, as the specificities of a chaotic system express at relatively short times, before universal chaotic features dominate, it has to be found in the long energy range characteristics of the quantum spectrum.

For such a short time scale, a semiclassical approximation might be used. It is the goal of this section to show how this can be implemented and eventually used to make some quantitative predictions on quantum chaotic systems which go beyond simple statistical statements.

4.1 Regular systems – EBK/WKB quantization

The simplest systems are the completely integrable ones, where the number of independent constants of motion equals the number of degree of freedoms. For such systems, there is a standard semiclassical theory which is a simple extension of the well known WKB theory for time-independent one-dimensional systems [42].

We assume the complete integrability of the system [7]: a single trajectory lives on a d -dimensional manifold (defined by the d constants of motion) embedded in the $2d$ dimensional phase space. A rather non-intuitive result is that – for a bound system – this manifold is a torus. Indeed, the Liouville-Arnold theorem ensures the existence of d pairs of canonically conjugate action-angle variables (I_i, θ_i) for $1 \leq i \leq d$ such that the Hamiltonian depends only on the actions:

$$H = H(I_1..I_d). \quad (4.1)$$

The canonical equations of motion, equation (1.2), can thus be solved straightforwardly:

$$I_i = \text{Constant} \quad (4.2)$$

$$\theta_i = \omega_i t + \theta_i^0 \quad (4.3)$$

where the ω_i are the frequencies along the various angle variables (defined

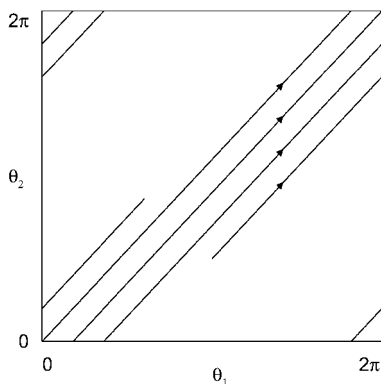


Fig. 16. Trajectory at the surface of an invariant torus (here shown for a two-dimensional system). While the actions are constant, both angles θ_1 and θ_2 evolve linearly in time. In the 2π -periodic angle coordinates, the trajectory is a straight line. In the original phase space coordinates, the trajectory winds on the invariant torus, see Figure 17.

modulo 2π) and given by:

$$\omega_i = \frac{\partial H}{\partial I_i}. \quad (4.4)$$

Generically, the ω_i are not rationally related and a trajectory densely and uniformly fills the invariant torus, see Figure 16. This implies that invariant tori are stationary structures during the time evolution. Hence, they are the relevant structures for building semiclassical approximations of the eigenstates.

Let us now turn to the technicalities. One writes the wavefunction as:

$$\psi(\mathbf{q}) = A(\mathbf{q}) \exp\left(i \frac{S(\mathbf{q})}{\hbar}\right) \quad (4.5)$$

where $A(\mathbf{q})$ and $S(\mathbf{q})$ are real functions. We also assume that the Hamiltonian is of the form:

$$H = \frac{\mathbf{p}^2}{2m} + V(\mathbf{q}). \quad (4.6)$$

An elementary manipulation of the time-independent Schrödinger equation shows that it is equivalent to the following real equations:

$$\nabla(A^2(\mathbf{q})\nabla S(\mathbf{q})) = 0 \quad (4.7)$$

$$\frac{(\nabla S(\mathbf{q}))^2}{2m} + V(\mathbf{q}) - E = -\frac{\hbar^2}{2m} \frac{\Delta A(\mathbf{q})}{A(\mathbf{q})}. \quad (4.8)$$

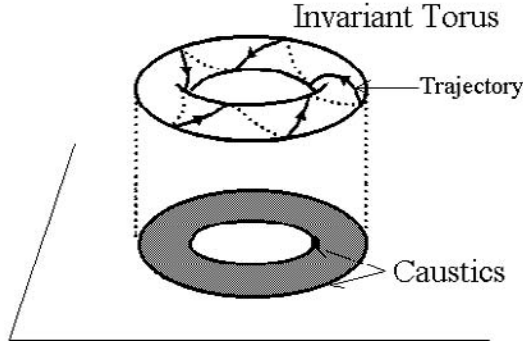


Fig. 17. For a classically integrable system, a typical trajectory in phase space winds on an invariant torus, filling it densely and uniformly. The projection of the torus onto configuration space is a finite region (gray region in the figure) limited by caustics. The EBK semiclassical approximation breaks down in the vicinity of these caustics (courtesy of Elise Cribier-Delande).

The EBK approximation amounts to neglect the right-hand side term in the second equation, because it is multiplied by $\hbar^2$ and thus likely to be small in the semiclassical limit. With this approximation, the equation becomes the classical Hamilton-Jacobi equation for the action [6]:

$$H(\mathbf{q}, \nabla S(\mathbf{q})) - E = 0. \quad (4.9)$$

Hence, its solutions are known and can be written, at least locally:

$$S(\mathbf{q}) = \int \mathbf{p} \cdot d\mathbf{q} \quad (4.10)$$

where the integral is calculated along a trajectory⁷.

As equation (4.9) is purely classical, we can perform a canonical change of coordinates to action-angle variables in order to solve it. As the actions are constant, we get the trivial solutions:

$$S(\theta_1 \dots \theta_d) = \sum_{i=1 \dots d} I_i \theta_i. \quad (4.11)$$

This is a locally uniquely defined function of the coordinates, *i.e.* a single-valued solution of the Hamilton-Jacobi equation, and provides us with an

⁷The first equation (4.7) is nothing but a continuity equation which allows to compute the amplitude A once the phase S is known. For a one-dimensional system, the calculation is straightforward and one finds $A = 1/\sqrt{p}$, which gives the standard form of the WKB wavefunction [42].

approximate solution of the Schrödinger equation. However, this solution is not defined everywhere in configuration space, because the projection of the invariant torus over configuration space is only a finite region of it. At the boundary of this region, there are *caustics* (see Fig. 16). There, $\nabla S(\mathbf{q})$ vanishes which produces a divergence of the amplitude $A(\mathbf{q})$. This in turn makes the rhs of equation (4.8) tend to infinity and invalidates the semiclassical approximation. Each caustic requires a careful specific treatment – which goes beyond the scope of these lectures – in order to overcome this problem [2, 42]. The solution, equation (4.11), can be continued through the caustics, provided a $-\pi/2$ phase factor is added to the wavefunction for each caustic crossed.

When the angle θ_i is smoothly increased by 2π (with other angles fixed), one follows a closed loop on the invariant torus and comes back to the initial point. In order for the wavefunction to be single-valued, the total phase accumulated on such a closed loop must be an integer multiple of 2π . There are two contributions to this phase: the first one $2\pi I_i/\hbar$ comes from the change in the action, the second one is $-\pi/2$ multiplied by the Maslov index α_i counting the number of caustics crossed. The single-valued character of the wavefunction thus implies:

$$I_i = \left(n_i + \frac{\alpha_i}{4}\right) \hbar \quad (4.12)$$

where n_i is a non-negative integer number.

Alternatively, this quantization condition can be rewritten with the original coordinates as:

$$\frac{1}{2\pi} \oint \mathbf{p} \cdot d\mathbf{q} = \left(n_i + \frac{\alpha_i}{4}\right) \hbar \quad (4.13)$$

where the integral is evaluated along a closed loop at the surface of the invariant torus.

As there are d independent irreducible closed loops at the surface of the invariant torus (or equivalently d actions I_i), this provides us with a set of d quantization conditions and d quantum numbers. These quantization rules are known as the EBK (Einstein, Brillouin, Keller) quantization conditions or invariant torus quantization [43].

The important point is that they do *not* use the classical trajectories, but the classical invariant tori. For a one-dimensional system, the trajectories coincide with the tori and one rediscovers the standard WKB quantization.

The EBK quantization rules can be used in a practical calculation. For example, for the hydrogen atom in a weak magnetic field, the classical dynamics is mainly regular. The semiclassical EBK prediction for the energy levels is very accurate and practically indistinguishable from the exact quantum result in Figure 9a.

Another consequence of the EBK semiclassical quantization is that the eigenstates are localized on the invariant tori and that d good quantum numbers exist. As discussed in Section 3.1, this implies that energy levels cross and that the statistical properties of the energy spectrum are well described by a Poisson law. In other words, the EBK quantization rules correctly predict the observed statistical properties of energy levels, see Section 3.3.

Of course, integrable systems are exceptional. However, it turns out that most invariant tori are structurally stable when an integrable system is perturbed⁸. In other words, a small perturbation generically makes the system non integrable but most tori survive (although of course slightly deformed). Thus, the EBK quantization rules can be used unchanged for all these tori which survive. This is for example the case for the hydrogen atom in a weak magnetic field. The only effect of the non integrability is that energy levels do not exactly cross but instead display tiny avoided crossings, much smaller than the mean level spacing. This is for example the case in Figure 9a where the avoided crossings are 20 orders of magnitude smaller than the mean level spacing, and EBK rules can be safely used.

4.2 Semiclassical propagator

For a chaotic system, the invariant tori do not exist and the preceding analysis breaks down. There is no longer any structure which can be used to build global solutions of the Hamilton-Jacobi equation with a single-valued wavefunction. A completely different approach has to be used. As a direct solution of the time-independent Schrödinger equation seems out of reach, one tries to calculate a semiclassical approximation of the evolution operator. The propagator is defined as a matrix element of the evolution operator in the configuration space representation:

$$K(\mathbf{q}', t'; \mathbf{q}, t) = \langle \mathbf{q}' | U(t', t) | \mathbf{q} \rangle. \quad (4.14)$$

The semiclassical approximation for the propagator is very similar to the one already discussed for the time-independent Schrödinger equation in Section 4.1. It relies on a separation of phase and amplitude and neglect of higher order terms in $\hbar$. One then finds the time-dependent

⁸This property is far from obvious and even somewhat counterintuitive. It is a consequence of the celebrated KAM theorem [7]. It also implies that chaos can be observed only in a non perturbative regime when two degrees of freedom are strongly coupled and any perturbative/adiabatic approach fails.

Hamilton-Jacobi equation for the action [6], which can be locally solved along trajectories. The result is known as the Van Vleck propagator [2, 44, 45]:

$$K(\mathbf{q}', t'; \mathbf{q}, t) = \sum_{\text{Clas. Traj.}} \left(\frac{1}{2i\pi\hbar} \right)^{d/2} \left| \text{Det} \frac{\partial^2 R(\mathbf{q}', t'; \mathbf{q}, t)}{\partial \mathbf{q}' \partial \mathbf{q}} \right|^{1/2} \times \exp \left(i \frac{R(\mathbf{q}', t'; \mathbf{q}, t)}{\hbar} - i \frac{\pi\nu}{2} \right) \quad (4.15)$$

where the sum is over all the classical trajectories going from $(\mathbf{q}, t)$ to $(\mathbf{q}', t')$. The function $R(\mathbf{q}', t'; \mathbf{q}, t)$ is called the classical action, although it is different from the action previously used which, according to [6], should be called *reduced action*. The difference is that R is relevant when the time interval (t, t') is fixed while S is used at fixed energy. Altogether, the two functions differ by $E(t' - t)$.

R is just the integral of the Lagrangian along the trajectory:

$$R(\mathbf{q}', t'; \mathbf{q}, t) = \int_t^{t'} L(\mathbf{q}, \dot{\mathbf{q}}, \tau) d\tau. \quad (4.16)$$

The non-negative integer ν counts the number of caustics encountered along the trajectory and is called a Morse index⁹.

Few remarks should be made on this formula:

- Its structure is completely analogous to the one used in the energy domain, with a phase expressed as a purely classical quantity evaluated along a trajectory, divided by $\hbar$, and a slowly varying amplitude;
- The fact that the same quantity R appears both in the phase and in the amplitude is not surprising. It ensures the unitarity of the time evolution. It is the counterpart – in time domain – of the continuity equation in the energy domain, equation (4.7). In fact, the prefactor $\sqrt{\text{Det}}$ is of purely classical origin. It just represents how a classical phase space density initially localized in $\mathbf{q}$ and uniformly spread in $\mathbf{p}$ evolves according to the Liouville equation, equation (1.6);
- At the caustics, the amplitude diverges and the semiclassical approximation breaks down. However, beyond the caustics, the semiclassical approximation recovers its validity, provided the convenient $-\pi/2$ phase factor is added (through the Morse index), in complete analogy with the EBK approximation;

⁹The Maslov and Morse indices are not necessarily equal as the first one deals with trajectories at fixed energy and the second one at fixed $t' - t$.

- At short time difference $t' - t$, there is only one classical trajectory connecting $(\mathbf{q}, t)$ to $(\mathbf{q}', t')$ (a straight line). The existence of multiple trajectories connecting the starting and ending points is analog to the existence of multiple paths at the surface of an invariant torus (see Sect. 4.1). For a chaotic system, at long times, the trajectories become very complicated and their number grows exponentially, which renders the use of the semiclassical propagator more and more difficult [46].

A completely different derivation of the Van Vleck propagator is possible using the Feynman path integral [47,48] formulation of quantum mechanics. The propagator can be *exactly* written as a superposition of contributions of all paths – *not* the classical trajectories – connecting the starting and ending points. The phase of each contribution is the integral of the Lagrangian along the path divided by $\hbar$ while all amplitudes are equal:

$$K(\mathbf{q}', t'; \mathbf{q}, t) = \int [dq(t)] \exp \left(\frac{i}{\hbar} \int_t^{t'} L(\mathbf{q}, \dot{\mathbf{q}}, \tau) d\tau \right) \quad (4.17)$$

where $[dq(t)]$ is a suitable measure over the paths.

There are some mathematical subtleties hidden in this formula, but the calculations can be carried out completely. In the semiclassical limit, the sum over paths can be calculated by stationary phase approximation. The paths with stationary phase are precisely the classical trajectories, and the prefactor in the stationary phase integration exactly gives the Van Vleck amplitude. This approach explains why the contributions of the different classical trajectories have to be added coherently in the propagator. It also explains why the semiclassical propagator can cross the caustics safely.

4.3 Green's function

The next step is to go from the time domain to the energy domain. The Green's function is:

$$G(E) \equiv \frac{1}{E - H} = \frac{1}{i\hbar} \int_0^\infty U(\tau, 0) \exp \left(i \frac{E\tau}{\hbar} \right) d\tau \quad (4.18)$$

where the last equality is valid for E in the upper half complex plane.

In configuration space, this gives:

$$G(\mathbf{q}', \mathbf{q}, E) \equiv \langle \mathbf{q}' | G(E) | \mathbf{q} \rangle = \frac{1}{i\hbar} \int_0^\infty K(\mathbf{q}', \tau; \mathbf{q}, 0) \exp \left(i \frac{E\tau}{\hbar} \right) d\tau. \quad (4.19)$$

In order to get a semiclassical approximation for the Green's function, one plugs the Van Vleck propagator, equation (4.15), into equation (4.19).

The integral over τ can be performed by stationary phase approximation. The stationary phase condition writes:

$$\frac{\partial R(\mathbf{q}', \tau; \mathbf{q}, 0)}{\partial \tau} + E = 0. \quad (4.20)$$

From the Lagrange-Hamilton equation [6, 45], the partial derivative is minus the Hamilton function. Hence, stationary phase selects trajectories going from $\mathbf{q}$ to $\mathbf{q}'$ with precisely energy E . This allows to write the semiclassical Green's function at energy E as a sum over classical trajectories with energy E , a physically satisfactory result. The phase of each contribution is the sum of R (calculated along the orbit) and $E\tau$, which gives the reduced action S . The detailed calculation of the various prefactors is not very difficult, but rather tedious; see [45] for details. It is convenient to distinguish the coordinate $q_{\parallel}$ chosen along the trajectory and the coordinates $\mathbf{q}_{\perp}$ transverse to the orbit. One finally obtains the semiclassical Green's function [44, 45, 49]:

$$G(\mathbf{q}', \mathbf{q}, E) = \frac{1}{i\hbar} \sum_{\text{Clas. Traj.}} \frac{\left| \text{Det} \frac{\partial^2 S(\mathbf{q}, \mathbf{q}', E)}{\partial \mathbf{q}_{\perp} \partial \mathbf{q}'_{\perp}} \right|^{1/2}}{(2i\pi\hbar)^{\frac{d-1}{2}} \sqrt{|\dot{q}_{\parallel} \dot{q}'_{\parallel}|}} \exp \left(\frac{iS(\mathbf{q}, \mathbf{q}', E)}{\hbar} - i\frac{\pi\nu}{2} \right) \quad (4.21)$$

with

$$S(\mathbf{q}, \mathbf{q}', E) = \int_{\mathbf{q}}^{\mathbf{q}'} \mathbf{p} \cdot d\mathbf{q}. \quad (4.22)$$

Again, the prefactor simply represents the classical evolution of a phase space density with fixed energy. This semiclassical approximation breaks down for very short trajectories. Indeed, the integral over τ cannot be performed by stationary phase in such a case. A specific short time expansion is possible for short action. It basically consists in ignoring the effect of the potential and using the free Green's function [44]. The result is:

$$G(\mathbf{q}', \mathbf{q}, E) = -\frac{im}{2\hbar^2} \left(\frac{\sqrt{2m(E - V(\mathbf{q}))}}{2\pi\hbar|\mathbf{q} - \mathbf{q}'|} \right)^{\frac{d-2}{2}} H_{\frac{d-2}{2}}^+ \left(\frac{S(\mathbf{q}, \mathbf{q}', E)}{\hbar} \right) \quad (4.23)$$

where H denotes the Hankel function [50]. At large actions, the asymptotic form of the Hankel function allows a smooth connection with equation (4.21).

The Green's function by itself is not very illuminating. In order to obtain some information on the energy spectrum and eigenstates, one needs a more global quantity.

4.4 Trace formula

The Green's function, equation (4.18), has a singularity at each energy level, like the density of states, equation (3.1). They are actually related by the simple equation:

$$d(E) = -\frac{1}{\pi} \text{Im Tr} G(E) = -\frac{1}{\pi} \text{Im} \int d\mathbf{q} G(\mathbf{q}, \mathbf{q}, E). \quad (4.24)$$

If one uses the semiclassical Green's function, equation (4.21), the density of states is obtained as a sum over *closed* trajectories, starting and ending at position $\mathbf{q}$. The last integral over position $\mathbf{q}$ can again be performed by stationary phase. The Lagrange equations tell us that the partial derivative of $S(\mathbf{q}, \mathbf{q}', E)$ with respect to $\mathbf{q}'$ is the final momentum $\mathbf{p}'$ while its partial derivative with respect to $\mathbf{q}$ is minus the initial momentum $\mathbf{p}$. Stationary phase thus selects closed orbits where the initial and final momenta are equal, that is **periodic orbits**.

Putting everything together gives the celebrated trace formula (also known as the Gutzwiller trace formula from one of its authors), written here for a two-dimensional system [2, 44, 45, 49]:

$$d(E) = \bar{d}(E) + \sum_{\text{p.p.o. } k, \text{ repetitions } r} \frac{T_k \cos \left[r \left(\frac{S_k}{\hbar} - \nu_k \frac{\pi}{2} \right) \right]}{\pi \hbar \sqrt{|\det(1 - M_k^r)|}} \quad (4.25)$$

where the sum is performed over all primitive periodic orbits (*i.e.* periodic orbits which do not retrace the same path several times) and all their repetitions $r > 0$. T_k is the period of the orbit, S_k its action, ν_k its Maslov index and M_k the 2 by 2 monodromy matrix describing the linear change of the transverse coordinates after one period; for details, see [44, 45].

The term $\bar{d}(E)$ whose expression is given in equation (3.3) comes from the “zero-length” trajectories. Indeed, for such trajectories, the semiclassical approximation for the Green's function breaks down and equation (4.23) has to be used. Using the asymptotic form of the Hankel function near the origin [50], it is easy to show that it produces this smooth term.

The trace formula deserves several comments:

- The trace formula is a central result in the area of quantum chaos, as it expresses a purely quantum quantity (the density of states) as a function of classical quantities (related to periodic orbits) and the constant $\hbar$;
- It uses only periodic orbits, which proves that they are the skeleton of the chaotic phase space. In that sense, they replace the invariant tori used for regular systems;

- Each periodic orbit contributes to the density of states with an oscillatory contribution. The period of these modulations correspond to a change of the argument of the cosine function $S_k/\hbar$ by 2π . As the derivative of the action with respect to energy is the period T_k of the orbit, the corresponding characteristic energy scale is $2\pi\hbar/T_k$. In the semiclassical regime, this is much larger than the mean level spacing $\Delta = 2\pi\hbar/T_H$. Hence, the trace formula describes the long range correlations in the energy spectrum;
- The trace formula breaks the simple connection between a given energy level and a simple structure in phase space. An energy level is a δ singularity in the density of states while each orbit contributes to a modulation of the density of states with finite amplitude. Thus, to build a δ peak requires a coherent conspiracy of an infinite number of periodic orbits;
- The present formula is restricted to isolated periodic orbits such that the phase space distance to the closest periodic orbit is larger than $\hbar$. For non isolated periodic orbits, the simple stationary phase treatment fails. A specific treatment is required and various similar formula can be written. Especially, for integrable systems, the sum over periodic orbits can be performed analytically using a Poisson sum formula [43]: the result is exactly equivalent to the EBK quantization scheme exposed in Section 4.1;
- The formula is valid only at lowest order in the Planck's constant $\hbar$. Including higher orders in the various stationary phase approximations is tedious, but feasible [51];
- At the very beginning, the trace formula relies on the semiclassical Green's function. This requires that the de Broglie wavelength of the quantum particle is smaller than any relevant spatial scale of the classical system. This is wrong in the presence of small scatterers. In some specific cases, the breakdown of the semiclassical approximation can be repaired and the trace formula can also be adapted [52];
- If one is not interested in the density of states, but in some other physical quantity, it is often possible to get similar expressions. The general strategy is to express the quantity of interest using the Green's function of the system, then to use the semiclassical Green's function. For example, the photo-ionization cross-section of an hydrogen atom in a magnetic field has been calculated in [53] as a sum over closed orbits starting and ending at the nucleus.

4.5 “Backward” application of the trace formula

As the convergence of the trace formula is uncertain (see below), it is not easy to use for quantitative predictions on the quantum properties of a chaotic system. On the other hand, it is very useful in the backward direction, that is from quantum to classical mechanics. The idea is to extract the classical properties of the system from the quantum calculated or observed properties. The simplest way to proceed is to measure a signal $f(E)$ depending on the energy and to Fourier transform it:

$$F(t) = \int f(E) \exp\left(-i\frac{Et}{\hbar}\right) dE. \quad (4.26)$$

This is known as a *vibrogram*. A non-intuitive result is that, although the signal itself is usually awfully complicated, see for example Figure 6, its vibrogram may have simple properties. If the signal $f(E)$ is the density of states, it is easy to plug the trace formula into the Fourier transform and to predict that the Fourier transform will be peaked at the periods of the (unstable) periodic orbits. This is indeed what is observed [2]. In the last ten years, there has been a successful “periodic orbit industry”, where the game is to find the fingerprints of periodic orbits in all kind of signals in a wide variety of atomic [54], molecular, solid state, acoustic, microwave [1] and mesoscopic systems.

This is especially simple in scaling systems. Indeed, the Planck’s constant $\hbar$ essentially enters the trace formula through the phase of the oscillatory terms. Hence, a vibrogram built as a Fourier transform *versus* $1/\hbar$ should display peaks at the actions of the periodic orbits. The advantage compared to the standard vibrogram is that the oscillations are perfectly periodic functions of $1/\hbar$ which is not true for the standard vibrogram where the period slowly changes with energy (because the classical dynamics changes) which limits the resolution.

An example of such a Fourier transform with respect to $1/\hbar$ is shown in Figure 18 for the hydrogen atom in a magnetic field (numerical results). What is used is not the density of states, but the photoionization cross-section. The weights of the various orbits are then slightly different from the weights in the trace formula, but the physical ideas are similar [53]. The comparison with the semiclassical prediction *à la Gutzwiller* is impressive. The positions and intensities of several hundred peaks are perfectly predicted by the semiclassical approximation [55]. Similar results have been obtained on experimental observations [25].

4.6 “Forward” application of the trace formula

Calculating quantum properties using only classical ingredients is much more difficult. Indeed, extracting individual energy levels by adding

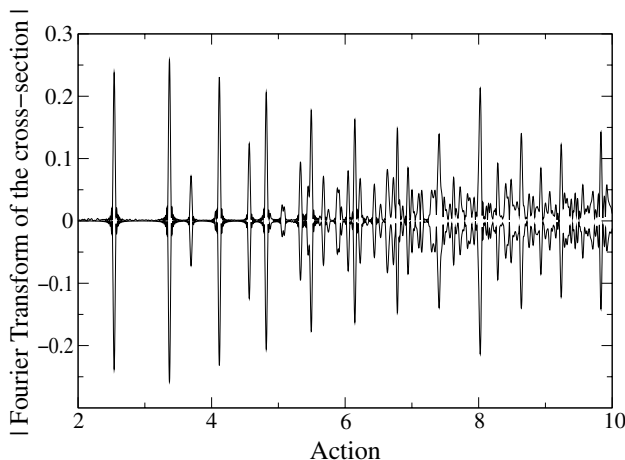


Fig. 18. Fourier transform (with respect to $1/\hbar$) of the photoionization cross-section for the hydrogen atom in a magnetic field in the chaotic regime (scaled energy $+0.5$), showing peaks at the actions of the closed orbits. The upper curve is the result of the numerical calculation. The lower curve, shown in a mirror, is the purely semiclassical prediction. The excellent agreement shows the power of semiclassical methods for chaotic systems.

oscillatory contributions requires in principle an infinite number of periodic orbits. In practice, it may be argued that it is enough to sum up all orbits with periods up to the Heisenberg time. Indeed, longer orbits will produce modulations on an energy scale smaller than the mean level spacing, and are thus expected to cancel out and to be irrelevant. In the semiclassical limit, T_H is so much longer than T_{Min} that the proliferation of long orbits makes the procedure impractical. However, for relatively low excited states, T_H is not much larger than T_{Min} and the trace formula has been successfully used to compute several states [45, 56].

Another possibility is to use an open system with resonances instead of bound states. There, the density of states has only bumps related to the resonances and the use of a relatively small number of periodic orbits may correctly reproduce the quantum properties. This is shown in Figure 19 for the hydrogen atom in a magnetic field at scaled energy $\epsilon = 0.5$. With few hundred periodic orbits, we are able to reproduce the finest details in the apparently random fluctuations of the photo-ionization cross-section [55]. This is a striking illustration of the strength of semiclassical methods.

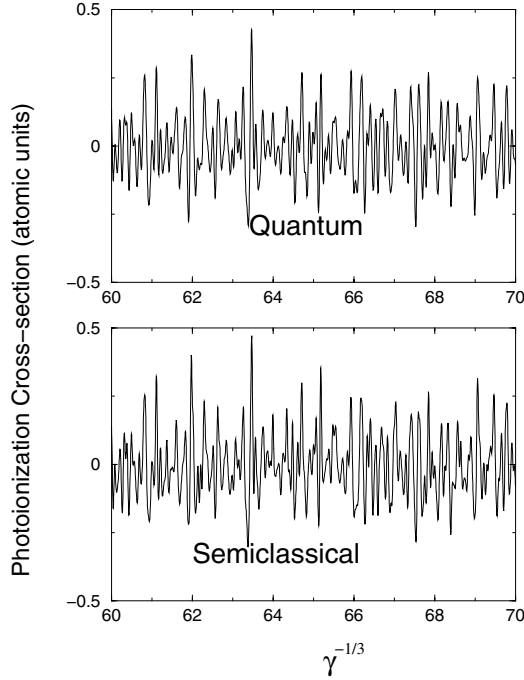


Fig. 19. The photo-ionization cross-section of the hydrogen atom in a magnetic field at constant scaled energy $\epsilon = 0.5$ (in the chaotic regime) plotted *versus* $\gamma^{-1/3}$. The smooth part of the cross-section is removed, in order to emphasize the apparently erratic fluctuations. Upper panel: the “exact” quantum cross-section calculated numerically. Lower panel: the semiclassical approximation of the cross-section, as calculated using periodic orbit theory. All the fine details – which look like random fluctuations – are well reproduced by periodic orbit theory.

4.7 Scarring

An important manifestation of the importance of periodic orbits is “scarring”. It has been observed numerically that wavefunctions of chaotic states often look like random waves without any clear pattern or localization. This is what is expected from Random Matrix Theory. However, some states present scars of unstable periodic orbits, that is a partial localization in the vicinity of periodic orbits [57]. In order to understand qualitatively the origin of this phenomenon, consider a wave-packet initially localized on an unstable periodic orbit. At least for short time, it propagates more or less classically along the orbit. Thus, the associated autocorrelation function, equation (2.7), will display peaks at integer multiples of the period T .

In turn, the Fourier transform of the autocorrelation must present modulations at the corresponding energy range $2\pi\hbar/T$. As, from equation (2.8), this is nothing but the weighted energy spectrum, this implies that the states near the maxima of the modulations have an increased overlap with the initial wavepacket, that is a residual localization in the vicinity of the orbit. These simple arguments can be made quantitative using the semiclassical Green's function and provide a full explanation of scarring [58].

4.8 Convergence properties of the trace formula

Because of the proliferation of long periodic orbits, it is not clear whether the sum in the trace formula converges or not. There is a competition between the exponential proliferation of periodic orbits and the decrease of the individual amplitudes (long orbits tend to be very unstable hence creating large denominators in the trace formula). On the average, long orbits explore more or less uniformly the whole phase space so that their instability depends only on the period. For example, for a bound 2-dimensional system, one has:

$$A_k = \frac{T_k}{\sqrt{|\det(1 - M_k)|}} \simeq T_k e^{-\frac{1}{2}\lambda T_k} \quad (4.27)$$

where λ is the average Lyapounov exponent per unit of time. Similarly, it is known that the number $N(T)$ of orbits with period less than T typically behaves as [35]:

$$N(T) \simeq \frac{e^{\lambda T}}{\lambda T} . \quad (4.28)$$

Thus the proliferation of orbits gives an increasing factor of the order of $\exp(\lambda T)$ in the trace formula which overcomes the decrease of the amplitude which scales as $\exp(-\lambda T/2)$ and the sum does not converge [44]. This means that, depending on the order in which the various periodic orbit contributions are added, the result can be anything! However, it is rather clear that the periodic orbits are not independent from each other and that the information that they contain is somewhat structured: most of the information contained in the very long orbits can be extracted from shorter periodic orbits.

The idea is thus to use this structure to improve convergence. The first step is to pass from the density of states to the so-called spectral determinant defined by:

$$f(E) = \prod_i (E - E_i) \quad (4.29)$$

which has a zero at each energy level. It can be rewritten as:

$$f(E) = \exp \left(-\frac{1}{\pi} \int^E \text{Im Tr} G(\epsilon) d\epsilon \right). \quad (4.30)$$

This quantity is of course highly divergent but can be regularized through multiplication by a smooth quantity having no zero [44]. This corresponds to removing in the Green's function the smooth contribution of the zero length trajectories.

One can thus define a “dynamical Zeta function” by:

$$Z(E) = \exp \left(-\frac{1}{\pi} \int^E \text{Im Tr} G_{\text{reg}}(\epsilon) d\epsilon \right) \quad (4.31)$$

where G_{reg} is the part of the Green's function which contains only the periodic orbit contributions. By inserting the semiclassical Green's function in equation (4.31), a rather simple manipulation allows to sum over the repetitions and to obtain the infinite product [44]:

$$Z(E) = \prod_{m=0}^{\infty} \prod_{\text{p.p.o.}} \left(1 - \frac{\exp \left(i \frac{S_k}{\hbar} - i \nu_k \frac{\pi}{2} \right)}{|\lambda_k|^{1/2} \lambda_k^m} \right) \quad (4.32)$$

where λ_k is the eigenvalue (larger than 1 in magnitude) of the monodromy matrix M_k .

The transformation from an infinite sum to an infinite product does not cure the lack of convergence¹⁰. Of course, the zeros of the infinite product are not the zeros of its individual terms (which do not have any for real energy, because $|\lambda_k|$ is always larger than 1). However, the larger m , the larger the denominator and the more convergent the infinite product over primitive periodic orbits. Hence, the most important zeros will come from the $m = 0$ term only.

Different approaches have been proposed for a practical calculation of the infinite product. For a bound system, the energy spectrum is known to lie on the real axis, which is not obvious from equation (4.32). This requires some subtle compensations between the various terms. By imposing this property, it is possible to show that periodic orbits with long periods do not carry any significant information to the infinite product which can be cut at half the Heisenberg time [59]. This makes it possible to calculate

¹⁰For a one-dimensional system, the denominator in equation (4.32) is equal to one (there is no transverse motion) and there is a single periodic orbit so that $Z(E) = 1 - \exp \left(i \frac{S}{\hbar} - i \nu \frac{\pi}{2} \right)$. The zeros are trivial to calculate and one rediscovers the WKB quantization condition.

semiclassically the energy levels of chaotic systems with a fair accuracy. It is however limited to bound systems.

Another approach is possible. When expanding the infinite product, there are some crossed terms between orbits which might approximately cancel with terms from more complicated orbits. The idea of the cycle expansion is to group such terms so that maximum cancellation takes place. Suppose that I have two simple orbits labelled 0 and 1 and a more complicated orbit labelled 01 which is roughly orbit 0 followed by orbit 1. If the action (resp. Maslov index) of orbit 01 were exactly the sum of the actions (resp. Maslov indices) of orbits 0 and 1 and its unstability eigenvalue λ the product of the unstability eigenvalues of orbits 0 and 1, complete cancellation would occur. As these properties are not exact, only partial cancellation takes place. For longer and longer orbits, the cancellation is better and better and the cycle expansion might be convergent (although there is no proof). This simple idea can be generalized to take into account all the orbits if there exist a efficient coding scheme – also known as a good symbolic dynamics – for the periodic orbits. Then, there are some cases like the 3-disks scattering problem [44], where the cycle expansion can be made convergent and can be used to efficiently calculate the quantum properties of the system. An even simpler case is the 2-disks problem where there is a single periodic orbit bouncing between the two disks: the semiclassical calculation is then entirely feasible, giving accurate predictions for the resonances of the system [44].

4.9 An example: The helium atom

The idea of the cycle expansion has been successfully used by Wintgen and coworkers [60] to calculate some energy levels of the helium atom. Although the system is not fully chaotic, most of the dynamics is [61]. Of special interest is the eZe configuration where the electrons and the nucleus lie on a straight line, with the electrons on opposite sides of the nucleus. In such a configuration, one can find a symbolic dynamics for the periodic orbits: any periodic orbit can be uniquely labelled by the sequence in which the electrons hit the nucleus. The motion transverse to the eZe configuration is stable and can be taken into account. By calculating the zeros of the infinite product, Wintgen *et al.* have been able to perform a fully semiclassical calculation of several energy levels of the helium atom. Some results are displayed in Table 1. For the ground state, it differs by only 0.7% from the exact quantum result. For excited states, it is even better. Thus, these authors have been able to solve a problem open since the beginning of the century, when pioneers of quantum mechanics tried to quantize helium after having successfully quantized the hydrogen atom. However, these pionners had no idea of the classically chaotic nature of phase space, they were not even thinking of a trace formula – not to speak of cycle expansion.

Table 1. Some energy levels (in atomic units) of the $1S^e$ series of the helium atom, compared with the semiclassical quantization using only the simplest periodic orbit and the more refined “cycle expansion” which includes a set of unstable periodic orbits. The agreement is remarkable, which proves the efficiency of semiclassical methods for this chaotic system (courtesy of D. Wintgen).

State	Periodic Orbit	Cycle Expansion	Exact quantum
1s1s	−3.0984	−2.9248	−2.9037
2s2s	−0.8044	−0.7727	−0.7779
2s3s		−0.5902	−0.5899
4s7s		−0.1426	−0.1426
5s5s	−0.131	−0.129	−0.129

They could not have the key idea that the correspondence between a classical orbit and an energy level is not one-to-one but that an infinite number of periodic orbits is needed to build a chaotic quantum eigenstate. It is only after 70 years of work on classical and semiclassical dynamics that their goal could be met.

4.10 Link with Random Matrix Theory

Although it is clear that the semiclassical approach gives a not-too-bad description of the global properties of highly excited states, it is not clear whether it can describe individual states. In other words, the question is to know whether the semiclassical approximation may be used up to and beyond the Heisenberg time. The answer is not presently very clear. Especially, there are some strong indications that results of the Random Matrix Theory can be obtained using a semiclassical approach, but we are still lacking a global understanding of the connection [4].

I now illustrate this point using the so-called form factor. It is related to the autocorrelation function, equation (2.7), averaged over the initial state. The idea is to use for the form factor something like:

$$K(t) \approx \frac{1}{\mathcal{N}} \left| \sum_i \exp \left(-i \frac{E_i t}{\hbar} \right) \right|^2 \quad (4.33)$$

where the sum extends over all states in an interval of energy centered around E and width $\Delta E \ll E$. The width has to be chosen sufficiently large to contain many states (so that individual fluctuations are washed out) but also sufficiently small such that the classical dynamics does not significantly change across the energy interval. The prefactor is, for convenience, chosen

as:

$$\mathcal{N} = \frac{\Delta E}{\Delta} = \bar{d}(E)\Delta E. \quad (4.34)$$

It represents the number of levels in the energy interval. At long time, the various oscillating terms in $K(t)$ are out of phase and add incoherently. This happens when the contributions between two consecutive energy levels are typically dephased by 2π , thus for times longer than the Heisenberg time. We then obtain:

$$K(t \gg T_H) = 1. \quad (4.35)$$

To make the connection with the trace formula, it is useful to reexpress $K(t)$ as a function of the density of states. From equation (4.33), $K(t)$ appears as the square modulus of the Fourier transform of the density of states. This quantity is however very singular at time $t = 0$ where all oscillatory terms add coherently, producing a huge δ -peak. In order to remove this uninteresting behaviour, we define the form factor using the fluctuating part only of the density of states:

$$K(t) = \frac{1}{\mathcal{N}} \left| \int_{E-\Delta E/2}^{E+\Delta E/2} [d(E) - \bar{d}(E)] \exp\left(-i\frac{Et}{\hbar}\right) dE \right|^2 \quad (4.36)$$

or

$$K(t) = \frac{1}{\Delta} \int \left\langle \left[(d - \bar{d}) \left(\mathcal{E} + \frac{x}{2} \right) \right] \left[(d - \bar{d}) \left(\mathcal{E} - \frac{x}{2} \right) \right] \right\rangle \exp\left(-i\frac{xt}{\hbar}\right) dx \quad (4.37)$$

where $\langle \rangle$ denotes the local average over the energy $\mathcal{E}$. Thus, $K(t)$ is nothing but the Fourier transform of the autocorrelation function of the spectrum, the latter being – up to a constant factor – the two-point correlation function R_2 introduced above in Section 3.2.4. More precisely, one has:

$$K(t) = 1 + \int (R_2(u) - 1) \exp\left(-2i\pi u \frac{t}{T_H}\right) du. \quad (4.38)$$

At this stage, $K(t)$ can be obtained exactly from Random Matrix Theory, by substituting the well known form of R_2 [12]. To make the connection with semiclassics, it can also be calculated using the semiclassical approximation (trace formula) for the density of states. One substitutes equation (4.25) in equation (4.37), and expands the classical quantities (such as the action) in the vicinity of the energy E of interest, and finally obtains [35]:

$$K(t) = \frac{\Delta}{2\pi\hbar} \sum_{i,j} A_i A_j \exp\left(\frac{i(S_i - S_j)}{\hbar}\right) \delta\left(t - \frac{T_i + T_j}{2}\right). \quad (4.39)$$

For very short times – of the order of T_{Min} – $K(t)$ displays a series of δ -peaks located at the combinations of the various periods. Because of the proliferation of orbits, these peaks rapidly overlap and $K(t)$ becomes a smooth function above the Ehrenfest time. It is not straightforward to calculate it, but a simple guess is to assume that, because the actions S_i change with energy, the non-diagonal terms in the double sum will be washed out. With this *diagonal* approximation, the sum can be calculated. Indeed, the asymptotic exponential divergence of the density of periodic orbits, equation (4.28), exactly cancels out the exponential decrease of the amplitudes, equation (4.27), and one gets:

$$K(t) = \frac{\Delta t}{2\pi\hbar} = \frac{t}{T_H} . \quad (4.40)$$

As this expression diverges at long times – which is clearly unphysical – it cannot be valid for arbitrarily long times. Indeed, around the Heisenberg time, the density of periodic orbits is so large that the diagonal approximation breaks down. The non-diagonal terms conspire to cancel the divergence of the diagonal terms and to finally obtain a constant value, equation (4.35), at long time.

We are thus left with two asymptotic forms of the form factor, equations (4.40) and (4.35) for short and long time (compared with the Heisenberg time) respectively. The simplest form for $K(t)$ is to assume that it grows linearly up to T_H and is then constant and equal to one. It turns out that this is **exactly** the result predicted by Random Matrix Theory for the Gaussian Unitary Ensemble. Thus, the semiclassical approximation certainly partly contains Random Matrix Theory. However, it is not clear whether it contains all of it. Indeed, we have shown that, for a specific quantity, the two approaches lead to same prediction, but we are not able to derive Random Matrix Theory from semiclassics. Also, our semiclassical calculation is limited to the short-time limit (the long-time limit requires some quantum ingredient) and we do not know how to interpolate between the two limits. The fact that the simplest form is the exact result must be considered as a piece of luck.

5 Transport properties – Localization

As discussed in Section 2, a key property of chaotic quantum systems is the existence of the Heisenberg time, beyond which the quantum dynamics feels the discrete character of the energy spectrum and is thus very different from the classical one. After the Heisenberg time, the quantum dynamics is more or less frozen, repeating forever the same behaviour, which inhibits transport. For a time-independent system, this is responsible for scarring, see Section 4.7.

For a time-dependent system, energy is no longer a constant of motion and the classical dynamics – if chaotic – may progressively invade a large part of phase space. Typically, because of the complexity of the trajectories, the global evolution (averaged over a large number of trajectories) often leads to a diffusive-like behaviour. This is of course a perfectly deterministic behaviour – known as chaotic diffusion – which has statistical properties similar to a true random diffusion. For such a system, there is no longer a discrete energy spectrum, so that the Heisenberg time does not exist and the quantum dynamics may mimic the classical one for very long time. However, there is an exception: for time-periodic system, it is possible – as shown in Section 5.2 – to define a quasi-energy spectrum and to associate with it an Heisenberg time. Localization is there expected to have a very dramatic effect: after the Heisenberg time, the quantum dynamics should stop invading phase space, in sharp contrast with the classical diffusive motion. This phenomenon is known as **dynamical localization** and is discussed in this section. It may affect very strongly the transport properties of the quantum system.

In a semiclassical picture, the quantum transport follows the same diffusive paths than classical transport, but each path has its amplitude and phase. If the various paths are uncorrelated, they statistically do not interfere, reproducing the classical chaotic diffusion. However, for a low-dimensional system and very long paths, there is not enough space for the various paths which proliferate and their phases have to be correlated after some time. This results statistically in a destructive interference which localizes the particle. This physical picture is very close to the one used for describing Anderson localization, that is localization in a disordered system because of destructive interferences [62]. The difference is that the randomness of the disordered medium is replaced by the complexity of the classical chaotic paths.

Although dynamical localization is probably a very general effect, I will use a simple example to demonstrate it: the kicked rotor, for which analytical, numerical and experimental results are available.

5.1 The classical kicked rotor

We consider a one-dimensional rotor whose position can be described by the angle θ (defined modulo 2π) and the associated momentum p , and apply on it periodic kicks whose amplitude depends on the position. In properly scaled units, the Hamiltonian can be written as:

$$H = \frac{p^2}{2} - k \cos \theta \sum_{n=-\infty}^{+\infty} \delta(t - nT) \quad (5.1)$$

where T and k are the period and strength of the kicks, respectively.

Because of the time-dependence, energy is not conserved. Because of time-periodicity, we can make a stroboscopic analysis of the motion and build a Poincaré map describing the evolution over one period. This map relates the phase space coordinates at kick $n + 1$ to the coordinates at kick n and writes:

$$\begin{cases} p_{n+1} = p_n + k \sin \theta_n \\ \theta_{n+1} = \theta_n + T p_{n+1}. \end{cases} \quad (5.2)$$

Using $I_n = T p_n$, it is nothing but the celebrated standard map [7] (also known as the Chirikov map):

$$\begin{cases} I_{n+1} = I_n + K \sin \theta_n \\ \theta_{n+1} = \theta_n + I_{n+1} \end{cases} \quad (5.3)$$

with

$$K = kT. \quad (5.4)$$

The dynamics of this map has been widely studied [7, 63]: it is almost fully chaotic and ergodic around $K = 10$ and above.

When K is very large, each kick is so strong that the positions of the consecutive kicks are statistically almost uncorrelated. After averaging, one thus gets:

$$\langle p_{n+1}^2 \rangle \simeq \langle p_n^2 \rangle + k^2 \langle \sin^2 \theta_n \rangle \simeq \langle p_n^2 \rangle + \frac{k^2}{2}. \quad (5.5)$$

It follows that the motion in momentum space is diffusive ($\langle p^2 \rangle$ increases linearly with time) with the diffusion constant:

$$D = \frac{k^2}{2T}. \quad (5.6)$$

Numerical experiments [7] show that this expression works well for $K \geq 10$.

5.2 The quantum kicked rotor

The quantum Hamiltonian is obtained from the classical one, equation (5.1), through replacement of p by $\frac{\hbar}{i} \frac{\partial}{\partial \theta}$. The Bloch theorem exploits the spatial periodicity of the potential. For simplicity, we will assume periodic boundary condition (similar results are obtained in the general case). The evolution operator over one period is the product of the free evolution operator and the kick operator:

$$U = U(T, 0) = \exp \left(-\frac{i}{\hbar} \frac{p^2 T}{2} \right) \exp \left(\frac{i}{\hbar} k \cos \theta \right). \quad (5.7)$$

The long-time dynamics is generated by successive iterations of U . Thus, one can use the eigenstates of U as a basis set. U being unitary, its eigenvalues are complex numbers with unit modulus which can be written as:

$$U|\phi_i\rangle = \exp\left(-\frac{iE_iT}{\hbar}\right) |\phi_i\rangle \quad (5.8)$$

with $0 < E_i \leq 2\pi\hbar/T$.

The E_i are defined modulo $2\pi\hbar/T$: they are not exactly the energy levels of the system – the $|\phi_i\rangle$ are not stationary states of the time evolution, but are only periodic – and are called quasi-energy levels, the $|\phi_i\rangle$ being the Floquet eigenstates. Indeed, their existence is guaranteed for any time-periodic system (not only the kicked ones) by the Floquet theorem [64] which is the temporal version of the Bloch theorem.

If an initial state is expanded over the Floquet eigenstates:

$$|\psi_0\rangle = \sum_i c_i |\phi_i\rangle, \quad (5.9)$$

its evolution after n kicks is:

$$U^n|\psi_0\rangle = \sum_i c_i \exp\left(-\frac{iE_inT}{\hbar}\right) |\phi_i\rangle, \quad (5.10)$$

which is completely similar to the time-evolution of a time-independent system, see Section 1.3.

5.3 Dynamical localization

Much of the long-time dynamics depends on the spectrum of U . At this point, there is a significant difference between time-independent and time-periodic systems. The former have a discrete pure point spectrum if the classical dynamics is bound; the latter usually have at least a dense spectrum. Indeed, the quasi-energy spectrum is defined modulo $2\pi\hbar/T$. Hence, there is an infinite number of energy levels in a finite energy range and the mean level spacing is not well defined. In fact, the quantity of interest is rather the local density of states, that is the density of states weighted by the overlap with the initial state, something like $\sum_i |c_i|^2 \delta(E - E_i)$. Most of the Floquet eigenstates are so weakly overlapping with the initial state that it may happen that the effective density of states contributing to equation (5.10) is finite. In such a case, the Heisenberg time is just $2\pi\hbar$ times this effective density of states.

This is what happens for the kicked rotor. We can derive a rough estimate of the Heisenberg time. Suppose that the initial state is effectively

coupled to ℓ Floquet states. Then, the mean level spacing is $2\pi\hbar/\ell T$ and the Heisenberg time is, according to equation (2.10):

$$T_H = \ell T. \quad (5.11)$$

After T_H , the system has undergone a chaotic diffusion and thus reached a typical value (assuming $p \simeq 0$ initially):

$$\langle p^2 \rangle \simeq DT_H = \frac{k^2}{2} \ell. \quad (5.12)$$

Because of the spatial periodicity, the natural basis states are the eigenstates $|m\rangle$ of the p operator labelled with the integer quantum number m :

$$\langle \theta | m \rangle = \frac{\exp(im\theta)}{\sqrt{2\pi}}. \quad (5.13)$$

They are eigenstates of p^2 with the eigenvalues $m^2\hbar^2$. Only states with sufficiently low m – such that $m^2\hbar^2 \leq \langle p^2 \rangle$ – will significantly contribute to the dynamics. The number of such states is, by definition, ℓ . This implies that:

$$\ell^2\hbar^2 \simeq \frac{k^2}{2} \ell. \quad (5.14)$$

This determines the “localization length”:

$$\ell \simeq \frac{k^2}{2\hbar^2} \quad (5.15)$$

and the localization time:

$$T_H \simeq \frac{k^2}{2\hbar^2} T. \quad (5.16)$$

In the semiclassical limit, both the localization length (actually in the momentum space) and the localization time diverge, which means that dynamical localization disappears.

Dynamical localization can be seen as the result of a competition between the classical diffusive transport which tends to increase the volume of phase space visited as time flows and the quantum freezing of the dynamics after some time (the Heisenberg time), which increases with the size of the phase space visited. If the classical transport is too slow, the quantum freezing wins after some time. This is the case in the example discussed. If the classical transport is faster (for example ballistic instead of diffusive), it may overcome the quantum freezing. Clearly, the number of degrees of freedom has to play a role, as it may increase the volume of phase space

which can be explored. Similar effects can be expected if additional “time dimensions” are used, for example with a quasi-periodic Hamiltonian [65].

An important property of dynamical localization is that it is rather robust. It relies strongly on the time-periodicity, but the details of the Hamiltonian are unimportant. As basically, all initial states localize after some time, a statistical mixture of initial states can be used. The only crucial constraint is to preserve the delicate destructive interferences at least up to the Heisenberg time. The effect of a loss of phase coherence is discussed below in Section 5.6.

Finally, it is worth mentioning that the Ehrenfest time, equation (2.3), does not play any role here. Indeed, after the Ehrenfest time, the detailed classical and quantum dynamics may differ (and probably do), but this has no effect on global quantities like the diffusion constant.

5.4 Link with Anderson localization

Dynamical localization is clearly similar to the Anderson localization of a quantum particle in a disordered medium. We now show the analogy of the two phenomena, following [66]. Consider the evolution operator, equation (5.7), and the associated eigenstate $|\phi\rangle$ with quasi-energy E . The part of the evolution operator associated with the kick can be written as:

$$\exp\left(\frac{i}{\hbar} k \cos \theta\right) = \frac{1 + iW(\theta)}{1 - iW(\theta)} \quad (5.17)$$

where $W(\theta)$ is a periodic Hermitean operator which can be expanded in a Fourier series:

$$W(\theta) = \sum_{r=-\infty}^{\infty} W_r \exp ir\theta. \quad (5.18)$$

Similarly, the kinetic part can be written as:

$$\exp\left[-\frac{i}{\hbar} \left(\frac{p^2}{2} - E\right) T\right] = \frac{1 + iV}{1 - iV}. \quad (5.19)$$

The operator V is diagonal in the eigenbasis of p , equation (5.13). If one performs the following expansion in this basis set:

$$\frac{1}{1 - iW(\theta)} |\phi\rangle = \sum_m \chi_m |m\rangle, \quad (5.20)$$

it is straightforward to show that the eigen-equation (5.8) can be rewritten as:

$$\epsilon_m \chi_m + \sum_{r \neq 0} W_r \chi_{m-r} = -W_0 \chi_m \quad (5.21)$$

where

$$\epsilon_m = \tan \left[\frac{\left(E - \frac{m^2 \hbar^2}{2} \right) T}{2\hbar} \right]. \quad (5.22)$$

This equation can be interpreted as the time-independent Schrödinger equation for a one-dimensional tight-binding model where m describes the site, ϵ_m its diagonal energy, W_r the coupling to the nearest sites and W_0 the total energy. In the case where there is only a constant coupling to the nearest neighbor and the ϵ_m are randomly distributed, this is the well known Anderson model. It has been proved that all the eigenstates are localized in this model: the random destructive interferences inhibit the quantum transport [62]. For the quantum kicked rotor, there are two main differences: firstly, there are additional hopping integrals to other neighbors. As they decrease sufficiently fast at large distance, they are not expected to play a major role. Secondly, the ϵ_m values are not random variables, but at best pseudo-random ones with a Lorentzian distribution. That localization is also expected in this case is plausible but not proved. A simple counterexample are the “quantum resonances” where the product $\hbar T/4$ is chosen as an integer multiple of 2π . Then, all the ϵ_m are equal and localization is lost. For a generic value of the product, dynamical localization is expected. It should be emphasized that space and time play different roles in the Anderson model and in dynamical localization. What plays the role of the sites of the Anderson model are the momentum states. Hence, dynamical localization is not expected in configuration space, but in momentum space.

5.5 *Experimental observation of dynamical localization*

The preceding theoretical discussion explained the plausibility of dynamical localization, but it suffers from several assumptions which cannot be firmly proved. Hence, numerical and real experiments are needed in order to confirm or modify the theoretical view. Several numerical experiments, mainly on the kicked rotor [63, 67] proved the existence and robustness of dynamical localization.

In a real experiment, we need a time-periodic one-dimensional system where phase coherence is well preserved beyond the localization time. The latter being often tens or hundreds periods, this rules out system not well isolated from the environment. A first possible choice is the dynamics of a Rydberg electron. The phase coherence is preserved during about 1 million periods and it is relatively easy to apply a time-periodic perturbation using an external microwave field. The drawback is the difficulty to measure the quantum state of the atom. The only quantity which is easy to measure is the ionization probability, that is the transport from the initially localized

Rydberg electron towards infinity. In other words, one can measure the diffusive growth of the total energy by measuring the ionization yield. Several experiments [68–70] have successfully measured a quantum ionization threshold higher than the corresponding classical one, that is a quantum inhibition of transport. This has been interpreted as a manifestation of dynamical localization. The amount of experimental and theoretical data is sufficiently large to support this interpretation. However, there is a lack of direct proof of localization.

The external dynamics of cold atoms can provide us with such a proof. Indeed, the time and length scales are favorable: the typical quantum time scale for cold atoms is the inverse of the recoil energy, that is around 100 microseconds. The typical length scale is the wavelength of the laser light used to manipulate the cold atoms, that is a fraction of a micro-meter. The associated velocity is of the order of 1 cm/s. All these orders of magnitude are rather easily reached with standard experimental techniques. I will not go into the details on the manipulation of cold atoms with laser light and external fields, the reader may refer to several excellent contributions in this book.

It is enough to say that, in the experiment, the cold atoms (either sodium or caesium) are prepared in a standard magneto-optical trap with a typical velocity spread of few recoil velocities [14, 65, 71]. After the trap is switched off, a periodic train of laser pulses is sent on the atoms. Each pulse is composed of two far detuned counter-propagating laser beams producing a spatially modulated optical potential. Each laser pulse thus produces a kick on the atom velocity, whose amplitude is proportional to the gradient of the optical potential.

If the kicks are infinitely short, we recover exactly the kicked rotor, equation (5.1), where the position of the atom in the standing wave plays the role of the θ variable and its velocity is the p variable. The kick strength k is proportional to the laser intensity divided by the detuning. The spatial dimensions perpendicular to the laser beams do not play any role in the problem, so that we have an effectively one-dimensional time-dependent problem¹¹. The effective Planck's constant of the problem is controlled via the frequency of the pulses.

After the series of pulses is applied, one expects a diffuse growth of the velocity distribution. The latter is measured by a time of flight technique (for details, see [14]). Figure 20 shows the average value $\langle p^2 \rangle$ as a function of time (number of kicks). One clearly sees a linear growth at short time followed by a saturation, that is a freezing of the diffusive growth when dynamical localization takes place. Figure 21 shows the full velocity

¹¹Another possibility is to keep the laser intensity constant and move the standing wave periodically [72]. The map is different but the physics is essentially the same.

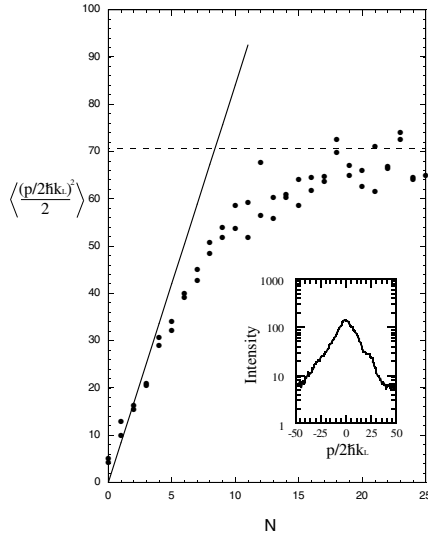


Fig. 20. Average value $\langle p^2 \rangle$ for a collection of cold atoms exposed to a series of kicks, as a function of time (the number of kicks). The solid line shows the linear growth predicted by theory at short time (classical chaotic diffusion). The dashed line is the saturation value predicted by dynamical localization and the dots are the experimental observation. The inset shows the final momentum distribution on a logarithmic scale, see also Figure 21 (courtesy of M. Raizen).

distribution as a function of time. While, at short time, the distribution looks Gaussian – as expected for a chaotic diffusion – its shape changes at the localization time and evolves to an exponential shape $\exp(-|p|/p_0)$ at long time. This is precisely the shape predicted by localization theory [62]. Thus, it is an unambiguous proof that what is observed is really dynamical localization.

5.6 The effect of noise and decoherence

Dynamical localization is built on destructive quantum interferences. Hence, any process which affects these interferences is expected to destroy dynamical localization and restore the classical transport properties [67]. If the inelastic time T_{Inel} (over which phase coherence is lost, see Sect. 2) is longer than the localization time T_H (which is the Heisenberg time), dynamical localization should take place and inelastic processes may kill it over long times, but some inhibition of transport should be visible. On the contrary, if T_{Inel} is shorter than T_H , phase coherence is lost before localization is established and the system should behave classically.

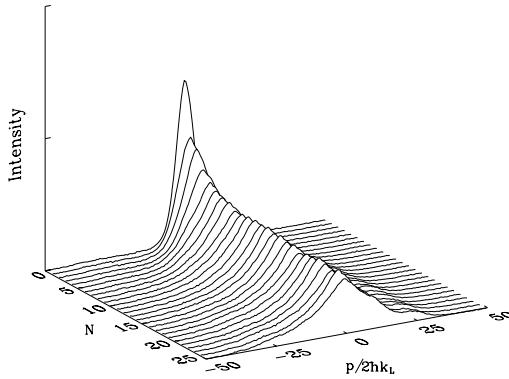


Fig. 21. Experimental time evolution of the momentum distribution from the initial Gaussian distribution until the exponentially localized distribution; N is the number of kicks (courtesy of M. Raizen).

For the external dynamics of cold atoms, spontaneous emission is the dominant inelastic process whose importance can be adjusted through the detuning from resonance [73]. Figure 22 shows the long time behaviour of p^2 for different T_{Inel} . It is clearly seen that when T_{Inel} is decreased towards the localization time, the quantum behaviour is less and less localized and tends to the classical one. The results obtained in another group [71] fully confirm this behaviour. Similarly, deviation from exact periodicity destroys dynamical localization. In the experiment, the amplitudes of the kicks are randomly chosen. The larger the dispersion in the kick amplitudes, the more localization is killed as shown in Figure 22. This again confirms that dynamical localization relies on delicate destructive quantum interferences which are very fragile *versus* any perturbation. Very recently, a similar experiment has been realized using a quasi-periodic series of pulses and, again, destruction of dynamical localization is observed when the two quasi-periods are not rationally related [65].

6 Conclusion

In these lectures, I hope I could give some partial answers to the questions raised in the introduction. Chaos manifests itself in the quantum properties of the systems like the energy levels and the eigenstates, in at least two ways:

- On a narrow energy interval - roughly at the level of individual eigenstates - the quantum structures display strong, apparently random,

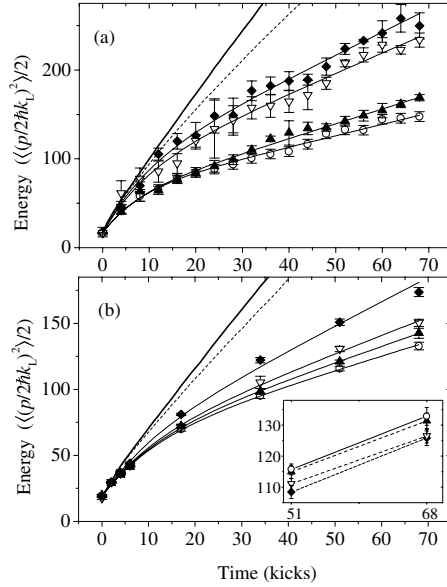


Fig. 22. Average value $\langle p^2 \rangle$ as a function of time (the number of kicks), in the presence of amplitude noise for the kicks (a) or spontaneous scattering of photons (b). Both effects destroy dynamical localization and partly restore the classical diffusive behaviour. The various curves correspond to various levels of noise or inelastic process. In each figure, the upper thick line is the classical behaviour (courtesy of M. Raizen).

fluctuations and a high sensitivity on any small change of an external parameter. This is the quantum counterpart of the classical sensitivity on initial conditions;

- On a large energy scale, where spectral properties are averaged over several states, the specific features of the studied system become manifest and are mainly related to the periodic orbits of the classical system;
- In a time-periodic system, quantum interferences can inhibit the classical transport and localize the system, in sharp contrast with the unbounded classical dynamics. However, this localization effect relies on delicate quantum interferences and can be destroyed when the quantum system is coupled to the external world.

For regular systems, efficient semiclassical methods exist. For chaotic systems, we understand the role of periodic orbits. Yet, we are not often able to compute individual highly excited states of a chaotic system from the knowledge of its classical dynamics. Using periodic orbits, we can compute low resolution spectra. Whether periodic orbit formulas are the end of the game or just an intermediate step towards a more global understanding is unknown.

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COURSE 7

**PHOTONIC BAND GAP MATERIALS: A NEW
FRONTIER IN QUANTUM AND NONLINEAR OPTICS**

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PHOTONIC BAND GAP MATERIALS: A NEW FRONTIER IN QUANTUM AND NONLINEAR OPTICS

S. John

1 Introduction

Photonic band gap materials represent a new paradigm in quantum and nonlinear optics. These materials were predicted theoretically as a means to realize two fundamentally new optical principles, namely (i) the localization and trapping of light in a bulk material [1, 2] and (ii) the complete inhibition of spontaneous emission [3, 4] over a broad frequency range. The novel consequences of PBG materials flow directly from the realization and implementation of these two underlying principles. Unlike optical confinement of a single resonance mode in a high quality (Q) optical cavity, localized electromagnetic modes in a bulk PBG material are completely decoupled from the vacuum modes of free space and the spatial extent of the localized modes can be engineered to be an arbitrary number of optical wavelengths. Unlike Fabry-Perot resonators or distributed feedback laser cavities which confine light in one spatial dimension, the PBG material facilitates coherent localization of light in all spatial directions. Unlike microdisk or microsphere cavity resonators which perturb the local density of states (LDOS) of the electromagnetic vacuum, the PBG material completely suppresses the total photon density of states (DOS). Accordingly, the trapping of light in localized modes of a PBG material is far more robust than the resonance trapping of light in conventional microcavity modes. Moreover, it is possible to engineer an arbitrary number of individual localized states which may interact weakly with each other inside a large scale PBG material, but which maintain their immunity from vacuum modes outside the PBG material. This facilitates the development of large scale integrated optical circuits within a PBG in which the nature of radiative dynamics is controlled by the LDOS of photons within the photonic crystal rather than the free space DOS outside the photonic crystal. This unique combination of light localization and the complete control of radiative dynamics distinguishes PBG materials from any previously studied optical system.

Although the band structure of classical scalar waves readily yields complete three-dimensional gaps for simple structures such as a face-centered

cubic lattice of spherical scatterers [5], the vector nature of the electromagnetic wave equation leads to much more restrictive conditions on the dielectric microstructure for the formation of a PBG. Initial concerns in designing structures that exhibit a complete Photonic Band Gap, were overcome by the discovery that the diamond lattice of dielectric spheres exhibits such a frequency range for which (linear) wave propagation is forbidden [6]. In the microwave regime, other diamond-like structures obtained by drilling cylindrical holes in a bulk dielectric material (with refractive index of 3.5) have been demonstrated to exhibit band-gap to center frequency ratios $\Delta\omega/\omega_0$ as large as 20% [7]. Since then, numerous structures amenable to layer by layer fabrication and drilling, that possess complete Photonic Band Gaps have been suggested [8–11]. A number of structures have already been fabricated with PBG's in the range of millimeter waves [12–14]. However it is very cumbersome and expensive to extend this micro-engineering method to produce large scale 3-d structures with periodicity on the scale of the wavelength of visible light.

The second approach involves self organizing systems such as colloidal crystals [15–17] and artificial opals [18–20] as templates for PBG micro-fabrication. These artificial templates can be produced with larger length scales than well-known organic materials which self-assemble into macroporous 3-d periodic structures. These structures may be used as templates for infiltration of inorganic semiconductor materials. However, in most of these systems [21, 22] the pore sizes are considerably smaller than the 0.2 – 1.0 micron pore size required for photonic band gap formation in the near infra-red or visible wavelength regime. On the other hand monodisperse colloidal suspensions of latex microspheres and SiO_2 spheres (opals) can sediment into crystalline structures with excellent long range periodicity at optical length scales [17]. Colloidal crystal growth produces inherently 3-dimensional structures, a significant advantage over lithographic techniques which primarily produce 2-dimensional patterns. However neither colloids nor opals (close-packed fcc lattice of SiO_2 spheres) achieve the high refractive index ratios and interconnectedness necessary for photonic band gap formation. Therefore, it is necessary to invert the structure by infiltrating the template with a high refractive index semiconductor such as GaP, Si or Ge. The original template may be finally removed by chemical or heat treatment. It has been demonstrated theoretically [23] that such structures exhibit near visible photonic band gaps on the scale of 10% of the gap frequency. This type of “inverted” opal structure has been experimentally realized in reference [24] where a closed-packed fcc lattice of air spheres in TiO_2 (refractive index $n = 2.8$) is reported. A similar structure made of carbon has been reported [25] using an artificial opal template. Recently, an inverse opal consisting of CdSe has been realized [26]. Such macroporous crystals suggest the feasibility of producing a new class of 3-d photonic

crystals for the optical spectrum. Structures of this type made out of GaP or Si would be relevant to quantum optical experiments in which atoms, dye molecules or other active materials are inserted into specific locations within the photonic crystal.

It is for visible and near-infrared frequencies where PBG materials are likely to have their most important impact. For example, applications in telecommunications may require the fabrication of large scale three-dimensional PBG materials with a gap centered around $1.5\text{ }\mu\text{m}$. These applications may include the design of zero-threshold micro-lasers, light emitting diodes which exhibit coherence properties at the single photon level, fast optical switches, and ultra-low threshold all-optical transistors. Most recently, the large scale synthesis of a pure silicon inverse opal structure with a complete three-dimensional PBG centered near 1.5 microns has been reported [27].

In addition, PBG materials represent a new frontier in photon-atom interaction phenomena and nonlinear optics. While linear wave propagation is absent in the gap of a PBG material, nonlinear propagation effects in the form of ultrashort solitary wave pulses can still occur. Recent studies indicate that as a result of their large group velocity dispersion near a photonic band edge and complex symmetries, PBG materials exhibit a much richer variety of nonlinear wave propagation phenomena than conventional waveguides or optical fibers [28–30]. In addition, PBG materials exhibit novel quantum optical features, related to the drastic alteration of the photon DOS. A vanishing DOS leads to bound photon-atom states, [31, 32] suppressed spontaneous emission [3, 4, 33, 34] and strong localization of photons [2, 31, 32, 35]. Unlike conventional microcavities and other confined optical systems, PBG materials support propagation effects on the scale of the localization length for photons leading to new types of cooperative behavior involving photons and atoms. In a PBG material, photon localization effects render the master equation approach of standard quantum optics problematic since localization implies highly non-Markovian memory effects in radiative dynamics. Among the novel phenomena predicted in this new frontier of quantum optics are: (i) collective switching of two-level atoms from ground to excited state with low intensity applied laser fields leading to all-optical transistor action [36] (ii) anomalous superradiant emission rates and low-threshold band-edge lasers [35], (iii) low threshold nonlinear optical response [37], and (iv) highly non-classical states of light within the PBG in the form of multiphoton localization and propagating quantum gap solitons [38].

2 The existence of photon localization

In the case of electron localization, nature provides a variety of readily available materials. Localization is more often the rule than the exception. This is easily seen from the Schrödinger equation for an electron with effective mass m^* :

$$\left[\frac{-\hbar^2}{2m^*} \nabla^2 + V(x) \right] \psi(x) = E\psi(x) . \quad (2.1)$$

A random potential $V(x)$ can trap electrons in deep local potential fluctuations when the energy E is sufficiently negative. As the energy increases, however, the probability of finding another nearby potential fluctuation into which the trapped electron can tunnel increases. To quantify these ideas, consider $V(x)$ to have a root mean square amplitude V_{rms} and a length scale a on which random fluctuations take place. The correlation length to the disorder a defines an energy scale $\epsilon_a \equiv \hbar^2/(2m^*a^2)$. For example in an amorphous semiconductor a is the interatomic spacing, ϵ_a plays a role analogous to the conduction band width of the semiconductor, and the zero of energy corresponds to the conduction band edge of the corresponding crystal. In the weak disorder limit ($V_{\text{rms}} \ll \epsilon_a$), a transition takes place as the electron energy is increased to about $-V_{\text{rms}}^2/\epsilon_a$ in which successive tunnelling events allow the electron to traverse the entire solid by a slow diffusive process and thereby conduct electricity. This transition energy has been termed a mobility edge by Mott. At higher and higher energies the scale on which multiple scattering takes place grows larger and larger than the electron's de Broglie wavelength and the electron traverses the solid with relative ease. If, on the other hand, the disorder is made strong $V_{\text{rms}} \gg \epsilon_a$, the mobility edge moves into the conduction band continuum ($E > 0$) and eventually the entire band succumbs to localization. This effect is referred to as the Anderson transition. Since disorder is a nearly universal feature of real materials, electron localization is an important ingredient in determining electrical, optical and other properties of solids.

In the case of monochromatic electromagnetic waves of frequency ω propagating in an inhomogeneous but nondissipative dielectric medium, the classical wave equation for the electric field amplitude $\vec{E}$ may be written in a form resembling the Schrödinger equation:

$$-\nabla^2 \vec{E} + \vec{\nabla}(\vec{\nabla} \cdot \vec{E}) - \frac{\omega^2}{c^2} \epsilon_{\text{fluct}}(x) \vec{E} = \epsilon_0 \frac{\omega^2}{c^2} \vec{E}. \quad (2.2)$$

This follows directly from Maxwell's equations. Here, I have separated the total dielectric constant $\epsilon(x) = \epsilon_0 + \epsilon_{\text{fluct}}(x)$ into its average value ϵ_0 and a spatially fluctuating part $\epsilon_{\text{fluct}}(x)$. The latter plays a role analogous to the random potential $V(x)$ in the Schrödinger equation, and scatters the electromagnetic wave. For the case of a lossless material in which the dielectric

constant $\epsilon(x)$ is everywhere real and positive, several important comments concerning the Schrödinger equation-Maxwell equation analogy are in order. First of all, the quantity $\epsilon_0\omega^2/c^2$ which plays a role analogous to an energy eigenvalue is always positive. This precludes the possibility of elementary bound states of light in deep negative potential wells. It must also be noted that the laser frequency ω multiplies the scattering potential $\epsilon_{\text{fluct}}(x)$. Unlike an electronic system, where localization was enhanced by lowering the electron energy, lowering the photon energy instead leads to a complete disappearance of the scattering mechanism itself! In the opposite, high frequency limit, geometric ray optics becomes valid and interference corrections to optical transport become less and less effective. In both limits the normal modes of the electromagnetic field are extended, not localized. Finally the condition that $\epsilon_0 + \epsilon_{\text{fluct}} > 0$ everywhere, translates into the requirement that the energy eigenvalue is always greater than the effective potential $|\frac{\omega^2}{c^2}\epsilon_{\text{fluct}}(x)|$. Unlike the familiar picture of electronic localization what we seek in the case of light is an *intermediate frequency window of localization* within the positive energy continuum and *which lies at an energy higher than the highest of the potential barriers!* It is for this simple reason that ordinary dielectrics appearing in nature do not easily exhibit photon localization. It should be pointed out here, that in the above analogy we have emphasized similarities more than actual differences. The vector nature of the electromagnetic wave equation (2.2) makes it even *more* difficult to localize light than the above analogy would suggest.

2.1 Independent scatterers and microscopic resonances

In the case of photons, the underlying physics of the high and low frequency limits can be made more precise by considering scattering from a single dielectric sphere. Consider a plane wave of wavelength λ impinging on a small dielectric sphere of radius $a \ll \lambda$ of dielectric constant ϵ_a embedded in a uniform background dielectric ϵ_b in $d = 3$ spatial dimensions. The scattered intensity I_{scatt} at a distance R from the sphere can be a function of only the incident intensity I_0 , the dielectric constants ϵ_a and ϵ_b and the lengths R , λ and a . In particular I_{scatt} must be proportional to the square of the induced dipole moment of the sphere which scales as the square of its volume $\sim (a^d)^2$ and by conservation of energy must fall off as $1/R^{d-1}$ with distance from the scattering center:

$$I_{\text{scatt}} = f_1(\lambda, \epsilon_a, \epsilon_b) \frac{a^{2d}}{R^{d-1}} I_0. \quad (2.3)$$

Here f_1 is some yet to be determined function. Since the ratio I_{scatt}/I_0 is dimensionless, it follows that $f_1(\lambda, \epsilon_a, \epsilon_b) = f_2(\epsilon_a, \epsilon_b)/\lambda^{d+1}$ where f_2 is another dimensionless function of the dielectric constants. The vanishing

of the scattering cross section for long wavelengths as $\lambda^{-(d+1)}$ is a fundamental result. It is the same reasoning which explains why the sky is blue. This weak scattering is the primary reason that electromagnetic modes are extended in most naturally occurring three dimensional systems. Although I have derived this result for single scattering, it remains true for a dense random collection of scatterers. This behavior is evident in the elastic, photon, mean free path ℓ^* which is proportional to λ^{d+1} for long wavelengths. This generalization of Rayleigh scattering to d spatial dimensions is particularly useful when describing anisotropic dielectric scattering systems. For example a layered random medium in which scattering is confined to directions perpendicular to the layers would be described by setting $d = 1$. Alternatively, a collection of randomly spaced uniaxial rods in which scattering is confined to the plane perpendicular to the axis of the rods would be described by setting $d = 2$. A consequence of the scaling theory of localization (which applies to electrons in disordered solids as well as electromagnetic waves in disordered dielectrics) is that in one and two dimensions, all states are localized but with localization lengths ξ_{loc} , which diverge due to Rayleigh scattering in the low frequency limit. In particular $\xi_{\text{loc}} \sim \ell^*$ in one dimension and $\xi_{\text{loc}} \sim \ell^* \exp(\frac{\omega}{c} \ell^*)$ in two dimensions [39, 40]. The divergence is apparent when we substitute the Rayleigh behaviour $\ell^* \sim \lambda^{d+1}$ into these formulae.

It is likewise instructive to consider the opposite limit in which the wavelength of light is *small* compared to the scale of the scattering structures. For scattering from a single sphere it is well known [41] that for $\lambda \ll a$ the cross section saturates at a value $2\pi a^2$. The factor of two includes the rays which are weakly diffracted out of the forward direction near the surface of the sphere. This is the result of geometric optics. For a dense random collection of scatterers it is useful to introduce the notion of a *correlation length* a . On scales shorter than a , the dielectric constant does not vary appreciably except for the occasional interface where the physics of refraction and diffraction apply. The essential point is that the elastic mean free path never becomes smaller than the correlation length. This classical elastic mean free path ℓ^* plays a central role in the physics of localization. Wave interference effects lead to large spatial fluctuations in the light intensity within the disordered medium. However, if $\ell^* \gg \lambda$, these fluctuations tend to average out to give a physical picture of essentially noninterfering, multiple scattering paths for electromagnetic transport. When $\ell^* \rightarrow \lambda/2\pi$ interference of multiple scattering paths drastically modifies the average transport properties and a transition from extended to localized

normal modes takes place. If one adopts the most naïve version of the Ioffe-Regel condition $2\pi\ell^*/\lambda \simeq 1$ for localization [42], with λ being the vacuum wavelength, it follows that extended states are expected at both high and low frequencies. However, for strong scattering, there arises the

distinct possibility of localization within a narrow frequency window when the quantity $\lambda/2\pi \simeq a$. It is this intermediate frequency regime which we wish to analyze in greater detail.

2.2 A new criterion for light localization

The existence or near existence of a gap in the photon density of states is of paramount importance in determining transport properties and especially localization [38]. Such a possibility was completely overlooked in the derivation of the free-photon Ioffe-Regel condition which assumed an essentially free-photon density of states. In the vicinity of a band edge the character of propagating states is modified. To a good approximation the electric field amplitude of the propagating wave is a linear superposition of the free photon with wavevector $\vec{k}$ and its Bragg reflected partner at $\vec{k}-\vec{G}$. As ω moves into the allowed band, this standing wave is modulated by an envelope function whose wavelength is given by $2\pi/q$ where q is the magnitude of the deviation of $\vec{k}$ from the Bragg plane. Under these circumstances the wavelength which must enter the localization criterion is that of the envelope. In the presence of even very weak disorder, the criterion $2\pi\ell^*/\lambda_{\text{envelope}} \sim 1$ is automatically satisfied as the photon frequency approaches the band edge frequency. In fact near a bandedge ω_c , $\lambda_{\text{envelope}} \sim |\omega - \omega_c|^{-\frac{1}{2}}$.

In the presence of a complete photonic band gap, the phase space available for photon propagation is restricted to a set of narrow symmetry related cones in $\vec{k}$ -space analogous to the pockets of electrons near a conduction band edge well known in semiconductor physics [43]. The perturbative introduction of randomness in the position of the dielectric scatterers leads to a mixing of all nearly degenerate photon branches. In complete analogy with semiconductors, the band gap is replaced by a pseudogap consisting of localized states. Localization is caused here by the severe restriction of the phase space available for propagation. Photon localization arises here not because of a high degree of uncontrolled disorder, but rather as a result of a subtle interplay between order and disorder. The true criterion for localization in fact depends strongly on the underlying static structure factor of the medium. What we have discussed in detail are the two extreme limits of a structureless random medium for which the criterion $2\pi\ell/\lambda \simeq 1$ applies, and of a medium with nearly sharp Bragg peaks and a band gap for which $2\pi\ell/\lambda_{\text{envelope}} \simeq 1$ yields localization. It follows that a continuous crossover occurs between these conditions as the structure factor of a high dielectric material evolves from one limit to the other.

Another way of expressing the same physics is by generalizing the Ioffe-Regel criterion as follows: Light localization in a disordered dielectric medium is expected [1, 2, 5] when

$$\pi^2 c \rho(\omega) (\ell^*)^2 \simeq 1. \quad (2.4)$$

Here, c is the speed of light in vacuum, $\rho(\omega)$ is the photon density of states at frequency ω , and ℓ^* is the transport mean free path for photons, determined by the extent of disorder in the medium. For photons in ordinary vacuum ($\omega = ck$), $\rho(\omega) = \omega^2/(\pi^2 c^3)$ and this condition reduces to the Ioffe-Regel condition, $\ell^*(\omega/c) \simeq 1$. The very low photon density of states near a photonic band gap, provides a very favorable scenario for the photon localization according to criterion (2.4) even when $\ell^*(\omega/c) \gg 1$.

2.3 Photonic band gap formation

The formation of a true photonic band gap is the result of a synergetic interplay between *microscopic* and *macroscopic* resonance mechanisms. This is distinct from the case of electronic bandstructure. In a semiconductor, a band of propagating electronic states arises from the overlap of localized atomic orbitals on individual lattice sites. The starting point consists of localized states and the end-product is the band of extended states. In the case of light in a periodic dielectric material, there are no localized states for individual, microscopic scatterers. Photons cannot be bound in any true sense to a single dielectric sphere or any other dielectric microcavity. Instead of bound states, scattering resonances occur when the wavelength of light becomes comparable to the size of the scatterer. Extended states are clearly the starting point and the end-product is localization. The creation of this end-product is guided by the formation of a photonic band gap. In three dimensions, this calls for highly restrictive conditions on the dielectric microstructure. One of these conditions is that the density of scatterers be chosen such that the microscopic scattering resonance of a single unit cell of the structure occur at the same frequency as the macroscopic (Bragg) resonance of the periodic array. This principle may be illustrated by a simple example of one-dimensional wave propagation through a periodic array of square wells of width a and spaced by a distance L . Suppose the refractive index is n inside each well and is unity outside. Then the Bragg scattering condition is given by $\lambda = 2L$ where λ is the vacuum wavelength of light. The analog of a Mie resonance in one dimension is a maximum in the reflection coefficient from a single well and this occurs when a quarter wavelength fits into the well: $\lambda/(4n) = a$. Combining these two conditions yields the optimum volume filling fraction $f \equiv a/L = 1/(2n)$. In analogy to the formation of an electronic band, the photonic band gap is the direct result of the coalescence of scattering resonances of individual microcavities. The generic form of the magnitude of the photonic bandgap with volume filling fraction f of dielectric material exhibits a peak at a specific volume filling fractions. For 3-d inverse opal PBG materials made out of a high index material such as silicon ($n \gtrsim 3.4$) the optimum filling fraction of solid material $f \simeq .25$. This is slightly higher than $1/(2n)$ since the lowest order Mie resonances in this case fail to open any complete PBG whatsoever. This is a complication

due to the vector nature of the electromagnetic field that is not captured in the simple argument given above. Nevertheless, it is clear that most of the PBG material (75 percent) consists of empty space. Ideally these void regions (consisting of an fcc lattice of slightly overlapping air spheres) form a connected network. This facilitates infiltration of active materials into the PBG backbone. It also opens the possibility of trapping and cooling atoms within the extensive void network of the PBG material.

To summarize this section, we have demonstrated that *the localization of light can occur within the positive energy continuum as the result of an interplay between order and disorder in the dielectric microstructure*. The photonic band gap provides a very useful guide for the choice of material parameters for the realization of this effect. The formation of a photonic band gap involves three basic considerations (i) the *vector nature* of the electromagnetic field, (ii) the synergy between *microscopic* and *macroscopic* resonances and finally (iii) the *network topology* of the dielectric microstructure. Given a periodic, photonic band gap material, localized states of light may be engineered within the photonic band gap. These states may act as ultra-high Q optical cavities with important device applications.

3 Quantum electrodynamics in a photonic band gap

3.1 Theory of the photon-atom bound state

Localization of light leads fundamentally to a novel strong coupling between radiation and matter. To describe this we utilize a quantum description of the radiation field Hamiltonian:

$$H_{\text{rad}} = \sum_{\lambda} \hbar \omega_{\lambda} a_{\lambda}^{\dagger} a_{\lambda} \quad (3.1)$$

where λ is a composite index describing both polarization and wavevector. The vector potential has an expansion in terms of the photon creation $a_{\lambda}^{\dagger}$ and annihilation operators a_{λ} of the form

$$\vec{A}(\vec{r}) = \sum_{\lambda} \sqrt{\frac{\hbar}{2\epsilon_0\omega_{\lambda}}} [a_{\lambda} \vec{u}_{\lambda}(\vec{r}) + a_{\lambda}^{\dagger} \vec{u}_{\lambda}^*(\vec{r})] \quad (3.2)$$

where $\vec{u}_{\lambda}(\vec{r})$ is mode function and the Coulomb constant $\epsilon_0 = 8.85 \times 10^{-12} \text{ Coul}^2 - m^2/N$. The strong coupling effects of interest are most transparent in the case of a periodic dielectric structure with a complete photonic bandgap. A simple model for the photon dispersion relation ω_{λ} follows from considering a periodic one dimensional system of square wells of refractive index n , width a and lattice constant L . Writing the total dielectric constant as $\epsilon(x) = \epsilon_{\text{avg}} + \epsilon_{\text{fluct}}(x)$, the classical scalar wave equation for this

system is

$$\left[-\nabla^2 - \frac{\omega^2}{c^2} \epsilon_{\text{fluct}}(x) \right] \phi(x) = \frac{\omega^2}{c^2} \epsilon_{\text{avg}} \phi(x) \quad (3.3)$$

where $\epsilon_{\text{avg}} = 1$,

$$\epsilon_{\text{fluct}}(x) = \sum_{m=-\infty}^{\infty} V(x - mL) \quad (3.4)$$

and

$$V(x) = \begin{cases} n^2 - 1 & |x| < a \\ 0 & \text{otherwise.} \end{cases}$$

The potential wells in this model correspond in the actual material to high dielectric spheres or cylinders in vacuum or alternatively pore regions in a high dielectric background. The detailed derivation of the dispersion ω_k may be found elsewhere [45]. The definition of the three dimensional model Hamiltonian is completed by symmetrizing the dispersion relation ω_k over all directions in $\vec{k}$ space and adopting a mode expansion (3.2) consisting of transverse plane waves outside the gap region:

$$\vec{u}_{\vec{k}\sigma}(\vec{r}) = \frac{1}{\sqrt{\Omega}} e^{i\vec{k} \cdot \vec{r}} \hat{e}_{\vec{k},\sigma}; \quad \hat{e}_{\vec{k}\sigma} \cdot \vec{k} = 0 \quad \sigma = 1, 2.$$

Here Ω is the sample volume and $\hat{e}_{\vec{k}\sigma}$ are the two transverse unit vectors. The resulting density of states is depicted in Figure 1.

The total Hamiltonian for an impurity atom interacting with the electromagnetic modes of the dielectric may be written as $H = H_{\text{atom}} + H_{\text{int}} + H_{\text{rad}} + H_{\text{ct}}$, where

$$H_{\text{atom}} = \frac{\vec{p}^2}{2m} + v(\vec{r}) ; \quad v(r) = \frac{e^2}{4\pi\epsilon_0 r} \quad (3.5)$$

$$H_{\text{int}} = \frac{e}{m} \vec{p} \cdot \vec{A}(\vec{r}) + \frac{e^2}{2m} A^2 \quad (3.6)$$

and

$$H_{\text{ct}} = \frac{\delta m}{m} \frac{p^2}{2m}. \quad (3.7)$$

Here $\vec{p}$ is the momentum of an electron of charge e and observable mass m in a hydrogenic atom. As in standard discussions of quantum electrodynamics [46], the renormalized, observable mass is given by $m = m_0 + \delta m$. Here m_0 is the bare electron mass and δm is a correction due to radiative coupling which we will consider to leading order in the fine structure constant $\alpha \equiv \frac{e^2}{4\pi\epsilon_0\hbar c} = 1/137$. The mass renormalization counterterm H_{ct} is accordingly introduced to accommodate the use of m rather than m_0 in H_{atom} . When the atomic $2p \rightarrow 1s$ transition lies in the photonic bandgap, ordinary spontaneous emission of light from the atom is absent. However, the photon can tunnel

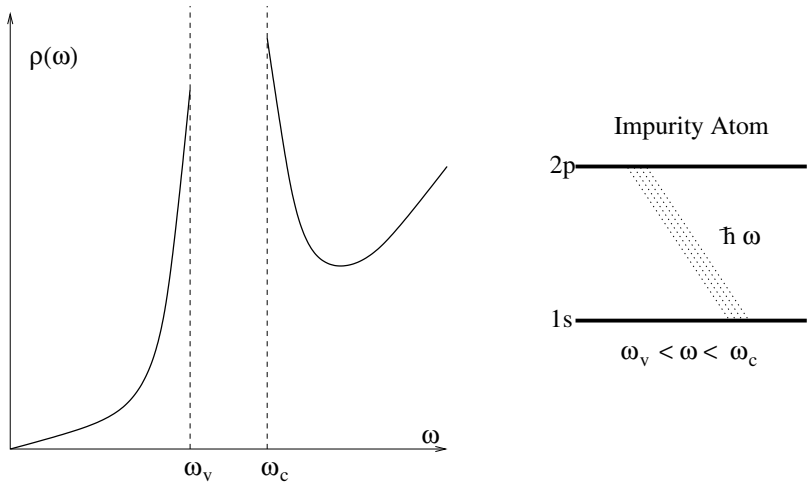


Fig. 1. Photon density of states for the isotropic model of the dispersion relation ω_k . Band edges occur at ω_v and ω_c . An impurity atom with transition frequency ω in the gap region will exhibit a photon-atom bound state.

into the classically forbidden gap. This suggests the occurrence of a photon-atom bound state in analogy to a deep level localized electronic state in the gap of a semiconductor.

A mathematical description of this effect is obtained by introducing a variational trial wavefunction which spans the single photon sector of atom plus electromagnetic Hilbert space:

$$|\psi\rangle = \sum_{n=1}^{\infty} \phi_n |n\rangle + \sum_{n=0}^{\infty} \sum_{\lambda} \psi_{\lambda}^{(n)} |\lambda; n\rangle. \quad (3.8)$$

Here, the state vector $|n\rangle$ describes the atom in its n^{th} excited state with energy E_n and no photons present, whereas the state vector $|\lambda; n\rangle$ describes an atom excited to its n^{th} level and a single photon in mode λ . The variational amplitudes ϕ_n and $\psi_{\lambda}^{(n)}$ are chosen to minimize the quantity $\frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle}$. In evaluating the matrix elements, the term $\frac{e^2}{2m} A^2$ merely causes a change in the zero of energy and may be neglected. The nontrivial matrix elements are:

$$\langle \lambda; n | H_{\text{int}} | \psi \rangle = \frac{e}{m} \sum_{n'} \sqrt{\frac{\hbar}{2\epsilon_0 \omega_k}} \vec{u}_{\lambda}^*(\vec{r}) \cdot \vec{p}_{nn'} \phi_{n'}$$

where

$$\vec{p}_{n,n'} \equiv \langle n | \vec{p} | n' \rangle$$

and

$$\langle n|H_{\text{int}}|\phi\rangle = \frac{e}{m} \sum_{n'} \sqrt{\frac{\hbar}{2\epsilon_0\omega_k}} \vec{u}_\lambda(\vec{r}) \cdot \vec{p}_{nn'} \psi_\lambda^{n'}.$$

Also for the mass renormalization counterterm

$$\langle \lambda; n|H_{\text{ct}}|\psi\rangle = \frac{\delta m}{m} \sum_{n'} k_{nn'} \psi_\lambda^{n'}$$

and

$$\langle n|H_{\text{ct}}|\psi\rangle = \frac{\delta m}{m} \sum_{n'} k_{nn'} \phi_n$$

where

$$k_{nn'} \equiv \langle n|p^2/2m|n'\rangle.$$

The variational procedure leads to projected Schrodinger equation $H|\psi\rangle = E|\psi\rangle$ which in turn leads to a set of coupled linear equations for the amplitudes ϕ_n and $\psi_\lambda^{(n)}$:

$$E_n \phi_n + \frac{e}{m} \sum_{\lambda, n'} \sqrt{\frac{\hbar}{2\epsilon_0\omega_k}} \vec{u}_\lambda(\vec{r}) \cdot \vec{p}_{nn'} \psi_\lambda^{(n')} + \frac{\delta m}{m} \sum_{n'} k_{nn'} \phi_{n'} = E \phi_n \quad (3.9)$$

$$(E_n + \hbar\omega_k) \psi_\lambda^{(n)} + \frac{e}{m} \sum_{n'} \sqrt{\frac{\hbar}{2\epsilon_0\omega_k}} \vec{u}_\lambda^* \cdot \vec{p}_{nn'} \phi_{n'} + \frac{\delta m}{m} \sum_n k_{nn'} \psi_\lambda^{(n)} = E \Psi_\lambda^{(n)}. \quad (3.10)$$

This procedure is completely equivalent to the Brillouin-Wigner perturbation theory commonly used in solid state physics [46]. Before proceeding further it is instructive to physically interpret the nature of the expected solutions to equations (3.9) and (3.10). For an atom in vacuum the dispersion relation is simple $\omega = ck$ where c is the vacuum speed of light. The solutions are depicted in Figure 2. In the complex energy E -plane there is a positive continuum of real energy solutions corresponding to the scattering states of the photon from the atom. This is depicted as a branch cut. In addition there is a single complex solution which appears on the second Riemann sheet of the complex energy plane at $E = E_1 + \Delta E - i\hbar/2\tau$ associated with the phenomenon of resonance fluorescence. Here ΔE describes the Lamb shift of the bare atomic level E_1 and $1/\tau$ is the rate of the spontaneous emission of light from this level. When the same calculation is performed for the atom in a photonic band gap the complex solution migrates to the real energy axis and describes a photon-atom bound state.

The projected Schrodinger equations (3.9) and (3.10) is solved by keeping only the dominant amplitudes $\psi_\lambda^{(0)}$ and ϕ_1 . All other amplitudes are perturbatively small in the interaction strength $\alpha \equiv e^2/(4\pi\epsilon_0\hbar c) = 1/137$.

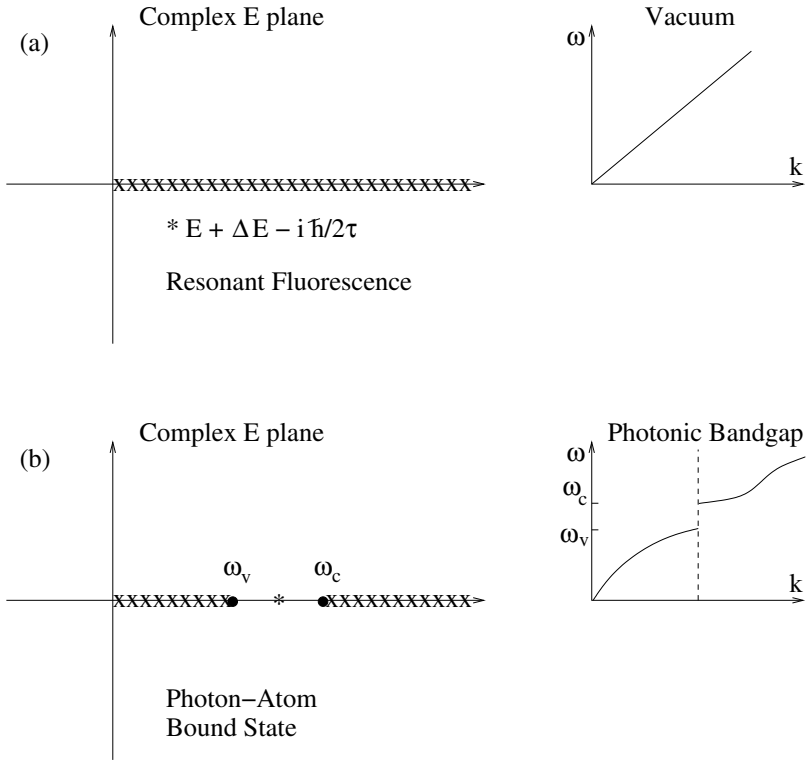


Fig. 2. Energy eigenvalue solutions of the projected Schrödinger equations (3.9) and (3.10). (a) For photons in vacuum ($\omega_k = ck$), there is a continuum of positive energy scattering states (crossed line) and a single complex solution on the second Riemann sheet describing resonance scattering. E_1 is the bare atomic level, ΔE is the Lamb shift and $1/\tau$ is the rate of spontaneous emission. (b) In a dielectric with photonic band gap the complex solution in (a) migrates to real axis and describes photon-atom bound state.

Actually, $|\psi_\lambda^{(0)}|^2$ is also of order α , but it can nevertheless become comparable to $|\phi_1|^2$ when the atomic transition frequency ω is near a band edge such as ω_c or ω_v . By substituting, $\psi_\lambda^{(n)}$, in equation (3.10) into (3.9) and then neglecting all ϕ_n other than ϕ_1 we arrive at the following eigenvalue equation for the complex energy E :

$$E - E_1 \simeq \frac{\hbar e^2}{2\epsilon_0 m^2} \sum_{\lambda, n} \frac{p_{1n}^i p_{n1}^j}{E - E_n - \hbar\omega_\lambda} \frac{1}{\omega_\lambda} u_\lambda^i(r) u_\lambda^{j*}(r) + \frac{\delta m}{m} k_{11}. \quad (3.11)$$

Here we have consistently kept only the leading order contribution in α to mass renormalization.

As in ordinary vacuum quantum electrodynamics, it is apparent that the electromagnetic mode summation over λ in equation (3.11) is linearly divergent in the ultraviolet $\omega_\lambda \rightarrow \infty$ limit. This linearly divergent piece may be separated out by means of the identity:

$$\frac{1}{E - E_n - \hbar\omega_\lambda} = -\frac{1}{\hbar\omega_\lambda} + \frac{E - E_n}{\hbar\omega_\lambda(E - E_n - \hbar\omega_\lambda)}.$$

The linearly divergent piece then precisely cancels the mass renormalization counterterm (see Chap. 7 of Ref. [47]). We regulate the remaining logarithmically divergent term using the cutoff prescription introduced by Bethe [48]. In this prescription all divergent photon wavevector integrals are cutoff at the Compton wavevector k_c defined by $\hbar ck_c = mc^2$. Photons of energy greater than the electron rest mass probe the relativistic nature of the electron wavepacket and the Schrodinger description of the electron must be replaced by the Dirac model. Since the wavevector integrals are multiplied by the coupling constant e^2 , this cutoff procedure is equivalent to associating a wavevector dependence to the observable electronic charge: at wavevectors larger than the Compton wavevector the physical vacuum acts as a polarizable dielectric of virtual electron-position pairs which screen out the effective electron charge. The eigenvalue equation after these cancellations becomes

$$z \equiv \frac{E - E_1}{E_1} \simeq \frac{2\alpha}{3\pi} \sum_n \frac{|\vec{p}_{1n}|^2/m}{mc^2} g(E - E_n) \quad (3.12)$$

where

$$g(E) \equiv \int_0^{mc^2} \frac{d(\hbar ck)k^2}{(\omega_k/c)^2} \frac{E/E_1}{E - \hbar\omega_k}. \quad (3.13)$$

Here we have converted the mode sum over transverse plane waves into an integral, made use of the completeness relation

$$\sum_{\sigma=1}^2 e_{k\sigma}^i e_{k\sigma}^j = (\delta_{ij} - \hat{k}_i \hat{k}_j)$$

and performed the angular integral

$$\int d\Omega_k (\delta_{ij} - \hat{k}_i \hat{k}_j) = \frac{8\pi}{3} \delta_{ij}.$$

As discussed earlier, the real and imaginary parts of the eigensolution E describe the Lamb shift and lifetime due to single photon spontaneous emission respectively. The magnitude of these effects is made transparent from the

dimensionless form of equation (3.12). For a hydrogen atom the strength of the relative electromagnetic perturbation on the bare atomic level E_1 is given by $z_0 \equiv \frac{2\alpha}{3\pi} \frac{|\vec{p}_{10}|^2/m}{mc^2} \sim 10^{-7} - 10^{-8}$. Anomalies, however, can occur if the wavevector integral in (3.12) has a singularity. This can occur if the atomic level is near a photonic bandedge. As we will see shortly this gives rise to anomalous Lamb shifts and atomic level splittings.

The standard perturbative results for the Lamb shift and radiative lifetime of an atom in vacuum ($\omega = ck$) may be reproduced from equation (3.12) by setting $E = E_1$ everywhere on the right hand side. After some elementary manipulation this gives $\Delta E = \frac{4\alpha^2 \hbar^3}{3m^2 c} |\psi_1(0)|^2 \ln |\frac{mc^2}{E - E_1}|$ where $\psi_1(\vec{r})$ is the electronic wavefunction and for the $2S_{1/2}$ hydrogen level $|\bar{E} - E_{2s}| = 16.64$ Rydbergs. Also $1/\tau = \frac{1}{3\pi\epsilon_0\hbar} (\frac{\omega}{c})^3 |\vec{\mu}_{10}|^2$ where $\vec{\mu}_{10} \equiv \langle 1|e\vec{r}|0\rangle$ is the dipole moment matrix element. In the photonic bandgap a graphical solution of equation (3.12) is depicted in Figure 3. Near a photonic bandedge, the dominant contribution to the sum over atomic levels comes from the $n = 0$ term. The singular part of the function $g(E)$ can be isolated by expanding the photon dispersion relation near ω_c : $\hbar\omega_k \simeq \hbar\omega_c + A(k - k_0)^2 + \dots$

In this case, for $E \simeq E_1 \simeq \hbar\omega_c$

$$g(E) \simeq \int_0^{mc^2} \frac{d(\hbar ck)}{E - \hbar\omega_c - A(k - k_0)^2} \simeq -\frac{\hbar\pi c}{\sqrt{A(\hbar\omega_c - E)}}. \quad (3.14)$$

Analytically continuing this expression to the complex E -plane places a branch cut in the multivalued function $g(E)$ for $E > \hbar\omega_c$. A similar analysis near $\hbar\omega_v$ gives a squareroot singularity with opposite sign in the real part of the photon Green's function as $E \rightarrow \hbar\omega_v$ from above. A simple dimensional analysis suggests that the coefficient $A \sim \hbar\omega_c/k_0^2$, the constant of proportionality being determined refractive index of the scatterers. Using this fact, and setting $E_1 = \hbar\omega_c$ yields the approximate form $g(E) = -i\pi/\sqrt{z}$, where $z \equiv (E - E_1)/E_1$. The eigenvalue equation then simplifies to

$$z \simeq -\frac{i\pi z_0}{\sqrt{z}}. \quad (3.15)$$

On the first Riemann sheet we may write $z = |z_0|^{2/3} e^{i\theta}$ where $0 < \theta < 2\pi$. The second Riemann sheet corresponds to solutions for which $\theta < 0$. Clearly equation (3.15) has two solutions (i) $z = -|z_0|^{2/3}$ which corresponds to a photon-atom bound state in the photonic bandgap and (ii) $z = |z_0|^{2/3} e^{-i\pi/3}$ which is a complex solution on the second Riemann sheet. The existence of two solutions associated with a single atomic level E_1 placed near the band edge suggests that the resonant coupling of the atom to photons of vanishing group velocity is sufficiently strong to split the atomic level into a doublet. This corresponds an atom strongly dressed by its own radiation

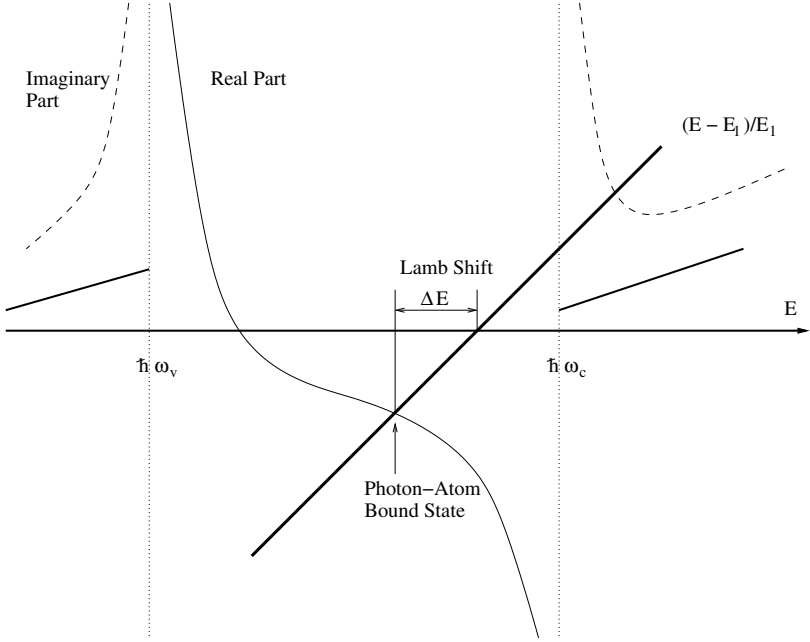


Fig. 3. Graphical solution of eigenvalue equation (3.12). The energy eigenvalue solution corresponds to a intersection of the straight line $(E - E_1)/E_1$ with the curved solid line representing the real part of the right hand side of equation (3.12). Also depicted (dashed curve line) is the imaginary part of the right hand side of equation (3.12).

field and is analogous to vacuum Rabi splitting in cavity quantum electrodynamics. The vacuum Rabi line splitting caused by the dielectric cavity in our model Hamiltonian approach has a magnitude $|z_0|^{2/3} \sim 10^{-5}$ times the transition frequency ω . This anomalously large value is an artifact of the strong band edge singularity in the photon density of states caused by our isotropic dispersion relation ω_k . In a more realistic anisotropic model [45], this splitting is approximately 10^{-7} times the transition frequency. This is comparable to the ordinary Lamb splitting of the $2s_{1/2}$ and $2p_{1/2}$ levels of hydrogen.

3.2 Lifetime of the photon-atom bound state

In the previous discussion, the interaction of atoms with single photons was considered. However, the electromagnetic coupling allows the possibility of multi-photon processes. In addition, the impurity atom may interact with

other atoms in the dielectric host materials. This gives rise to *phonon* absorption and emission effects. All of these additional interactions determine the lifetime of the photon-atom bound state, which in their absence would be infinite. As it turns out, the dominant factor that limits the lifetime of the photon-atom bound state are non-electromagnetic relaxation events caused either by multiple phonon sidebands and/or collisions of the impurity atoms with surfaces of the solid dielectric. This latter effect may be very deleterious to the *single* impurity atom, and very special experimental conditions may be required to preserve the integrity of the bound state. For example, an impurity atom may be laser-cooled in the void regions of a photonic bandgap material with a network topology. Dipolar optical potential traps are readily created in a 3-d inverse opal PBG material simply by illuminating the crystal with a single laser beam whose frequency corresponds to the upper edge of the photonic band gap. The majority of the field energy is then concentrated in the void regions where field intensity maxima arise. These act as dipolar optical traps for atoms. This single mode near the photonic band edge is essentially a standing wave consisting of the incident laser beam and its Bragg scattered partners. As such it provides an optical molasses for Doppler cooling to the sub-milli Kelvin temperature scale. Furthermore, interesting optical polarization gradients occur within the void regions (even for a single Bloch model!) leading to the possibility of cooling to the sub-micro Kelvin temperature scale.

In the absence of interatomic collisions and non-radiative relaxation, the electromagnetic decay rate of the excited atom due to two-photon spontaneous emission is on the scale of several days [45]. Consider for instance two-photon decay of the excited $2p_{1/2}$ level. A dipole emission from this odd parity state will create a virtual state of even parity which must then decay by a quadrupole transition to the ground state. Unlike the two photon decay of the even parity $2s_{1/2}$ level which proceeds by a pair of dipole emissions and occurs in $1/7$ s, the lifetime of the odd parity state is considerably longer. Real dielectrics on the other hand have a finite absorption length l_{abs} for the orbiting photon. In present day fiber optic quality materials $l_{\text{abs}} \gg 1$ kilometer. The lifetime of the bound state is then given by $\tau = \frac{l_{\text{abs}}}{c_{\text{eff}} f_p}$ where $c_{\text{eff}} \equiv c/n \sim 10^8$ m s $^{-1}$ is the effective speed of light in the dielectric and f_p is the fraction of time which the eigenstate is likely to be found as an orbiting photon as opposed to an excited atom. From equations (3.9) and (3.10)

$$f_p \simeq \sum_{\lambda} |\psi_{\lambda}^{(0)}|^2 / |\phi_1|^2 \simeq z_0 \int_0^{mc^2} \frac{d(\hbar ck) \hbar ck}{(E - \hbar \omega_k)^2} \left(\frac{ck}{\omega_k} \right). \quad (3.16)$$

The order of magnitude of f_p for a midgap state is given by the dimensionless parameter $z_0 \sim 10^{-7}$. This yields $\tau \sim 1$ minute per km of absorption length in the dielectric. For a bandgap to center frequency ratio $\Delta\omega/\omega_0 \simeq .05$, the

photon tunnelling distance is on the scale of ten optical wavelengths. As the impurity level approaches the bandedge, the photon localization length ξ_{loc} grows larger and eventually diverges near ω_c : $\xi_{\text{loc}} \sim c/\sqrt{\omega_c|\omega_c - \omega|}$. In this case the fraction f_p can be of order unity and the lifetime is made accordingly shorter [45].

4 Non-Markovian spontaneous emission dynamics near a photonic band edge

4.1 Single atom radiative dynamics

It is instructive to consider the properties of photon-atom bound state as revealed in the dynamical behaviour a single excited atom near a photonic band edge. This is facilitated by retaining only the $n = 0$ and $n = 1$ terms in equation (3.8). That is to say, we treat the atoms as a quantum two-level system.

We begin by investigating a two-level atom coupled to the radiation field in a three-dimensional periodic dielectric. The atom has excited state $|2\rangle$, ground state $|1\rangle$, and resonant transition frequency ω_{21} . The Hamiltonian of the system in the interaction picture takes the form

$$H = \sum_{\lambda} \hbar \Delta_{\lambda} a_{\lambda}^{\dagger} a_{\lambda} + i \hbar \sum_{\lambda} g_{\lambda} (a_{\lambda}^{\dagger} \sigma_{12} - \sigma_{21} a_{\lambda}), \quad (4.1)$$

where $\sigma_{ij} = |i\rangle\langle j|$ ($i, j = 1, 2$) are the atomic operators; a_{λ} and $a_{\lambda}^{\dagger}$ are the radiation field annihilation and creation operators; $\Delta_{\lambda} = \omega_{\lambda} - \omega_{21}$ is a detuning of the radiation mode frequency ω_{λ} from the atomic resonant frequency ω_{21} and g_{λ} is the atomic field coupling constant

$$g_{\lambda} = \frac{\omega_{21} d_{21}}{\hbar} \left(\frac{\hbar}{2\epsilon_0 \omega_{\lambda} V} \right)^{\frac{1}{2}} \vec{e}_{\lambda} \cdot \vec{u}_d. \quad (4.2)$$

Here d_{21} and $\vec{u}_d$ are the absolute value and unit vector of the atomic dipole moment, V is the sample volume, $\vec{e}_{\lambda} \equiv \vec{e}_{\vec{k}, \sigma}$ are the two transverse (polarization) unit vectors, and ϵ_0 is the Coulomb constant.

Assume the atom is initially on the excited state $|2\rangle$ and the field is in the vacuum state. The wave function of the system then has the form

$$|\psi(t)\rangle = b_2(t)|2, \{0\}\rangle + \sum_{\lambda} b_{1,\lambda}(t)|1, \{\lambda\}\rangle e^{-i\Delta_{\lambda}t}. \quad (4.3)$$

The state vector $|2, \{0\}\rangle$ describes the atom in its excited state $|2\rangle$ and no photons present, whereas the state vector $|1, \{\lambda\}\rangle$ describes the atom in its ground state $|1\rangle$ and a single photon in mode $\{\lambda\}$. The time-dependent

Schrödinger equation projected on the one-photon sector of the Hilbert space takes the form:

$$\frac{d}{dt}b_2(t) = - \sum_{\lambda} g_{\lambda} b_{1,\lambda}(t) e^{-i\Delta_{\lambda}t}, \quad (4.4)$$

$$\frac{d}{dt}b_{1,\lambda}(t) = g_{\lambda} b_2(t) e^{i\Delta_{\lambda}t}. \quad (4.5)$$

The formal solution of equation (4.5) is

$$b_{1,\lambda}(t) = g_{\lambda} \int_0^t b_2(t') e^{i\Delta_{\lambda}t'} dt'. \quad (4.6)$$

Substituting equation (4.6) into equation (4.5) we have

$$\frac{d}{dt}b_2(t) = - \sum_{\lambda} g_{\lambda}^2 \int_0^t b_2(t') e^{-i\Delta_{\lambda}(t-t')} dt'. \quad (4.7)$$

The Laplace transform

$$\tilde{b}_2(s) = \int_0^{\infty} e^{-st} b_2(t) dt,$$

can be found from equation (4.7) as

$$\tilde{b}_2(s) = \left[s + \sum_{\lambda} g_{\lambda}^2 \cdot \frac{1}{s + i(\omega_{\lambda} - \omega_a)} \right]^{-1}. \quad (4.8)$$

Converting the mode sum over transverse plane waves into an integral and performing the angular integral we obtain

$$\tilde{b}_2(s) = \left(s + \frac{\omega_{21}^2 d_{21}^2}{6\pi^2 \epsilon_0 \hbar} \int_0^{\Lambda} \frac{k^2 dk}{\omega_k [s + i(\omega_k - \omega_{21})]} \right)^{-1} \quad (4.9)$$

and Λ is the Compton cutoff in the photon wave vector since photons of energy higher than the electron rest mass mc^2 probe the relativistic structure of the electron wave packet.

For a broad band of the density of states, such as in vacuum, one can use the Wigner-Weisskopf approximation. That is, only the pole contribution of $s (s \rightarrow 0^+)$ in the integral of equation (4.9) is retained:

$$\lim_{s \rightarrow 0^+} \frac{1}{s + i(\omega_k - \omega_a)} = -iP \frac{1}{\omega - \omega_a} + \pi \delta(\omega_k - \omega_a). \quad (4.10)$$

Substituting equation (4.10) into equation (4.9) yields

$$\tilde{b}_2(s) = \left[s + i\delta_{21} + \frac{1}{2}\gamma_{21} \right]^{-1},$$

where δ_{21} and γ_{21} are the usual Lamb shift and spontaneous emission rate respectively. Clearly, the spontaneous emission decay is purely exponential.

The Wigner-Weisskopf perturbation theory, however, is inadequate when the density of electromagnetic modes changes rapidly in the vicinity of the atomic transition frequency ω_{21} . In this case we must perform an exact integration in equation (4.9). For the purpose of discussion we consider a simple model Hamiltonian for electromagnetic waves in a three-dimensional periodic dielectric described by equation (3.3) and equation (3.4).

By symmetrizing ω_k , given in by this model, to all directions in $\vec{k}$ space, we produce photonic bandgaps at the spheres $|\vec{k}| = m\pi/L$ with $m = 1, 2, 3, \dots$. Near the band gap edges the density of states becomes singular, the atom-field interaction becomes strong and we can expect new dynamical features of spontaneous emission decay. For $k \cong k_0 \equiv \frac{\pi}{L}$ the dispersion relation near the bandedge ω_c can be approximated by

$$\omega_k = \omega_c + A(k - k_0)^2, \quad (4.11)$$

where $A \cong \omega_c/k_0^2$.

Using equation (4.11), we evaluate equation (4.9) as

$$\tilde{b}_2(s) = \frac{(s - i\delta)^{\frac{1}{2}}}{s(s - i\delta)^{\frac{1}{2}} - (i\beta)^{\frac{3}{2}}}. \quad (4.12)$$

Here

$$\beta^{\frac{3}{2}} = \frac{\omega_{21}^{\frac{7}{2}} d^2}{6\pi\epsilon_0 \hbar c^3},$$

and $\delta = \omega_{21} - \omega_c$. The amplitude $b_2(t)$ is given by the inverse Laplace transform

$$b_2(t) = \frac{1}{2\pi i} \int_{\epsilon - i\infty}^{\epsilon + i\infty} e^{st} \tilde{b}_2(s) ds,$$

where the real number ϵ is chosen so that $s = \epsilon$ lies to the right of all the singularities (poles and branch point) of function $\tilde{b}_2(s)$. The probability that the atom remains excited is given by $P(t) \equiv |b_2(t)|^2$. The results is plotted if Figure 4 for various choices of the atomic detuning frequency δ .

A photon which is emitted by the atom exhibits tunneling on a length scale given by the localization length before being Bragg reflected back to the emitting atom. The photon-atom bound state *inside* the band gap has been predicted in reference [44]. We emphasize here that the photon-atom bound dressed state is present even when the resonant atomic frequency ω_{21} lies *outside* the band gap. This bound dressed state leads to

the novel fractionalized steady-state atomic population in the excited state $P_s = \lim_{t \rightarrow \infty} |b_2(t)|^2$ (Fig. 4b). Clearly, the non-zero steady-state atomic population in the excited state is present even when the resonant atomic frequency ω_{21} lies *outside* the bandgap, where the density of states is not equal zero. The atomic level splitting, oscillatory behavior and fractionalized steady-state atomic population in the excited state are all direct consequences of strong interaction between the atom and its own localized radiation when the atomic resonant frequency lies near the edge of a perfect photonic bandgap. These properties are strongly dependent on the detuning of the resonant atomic frequency ω_{21} from the bandedge frequency ω_c . Physically, the atom exchanges energy back and forth with its own radiation, backscattered after tunnelling a localized distance. This in turn is a result of the vacuum Rabi splitting of the atomic level by the photonic band edge. One level of the doublet is a localized state within the photonic bandgap, whereas the other level is a resonance in the extended state continuum. The frequency of oscillations is directly determined by the magnitude of the atomic level splitting. It is distinct from the well known Jaynes-Cummings oscillations which arise from the interaction of the atom with an isolated cavity or dielectric mode [49, 50]. In our model, no defect mode is present.

The excited-state population density can be measured *via* absorption of a probe beam at different decay times [51]. Alternatively, the nature of the fractionalized excited state can be probed by spontaneous emission from the excited state into the third level $|3\rangle$ of a λ -configuration (Fig. 5). Assume that the transition frequency ω_{23} lies far from the gap, so that we can use the Wigner-Weisskopf approximation equation (4.10) for spontaneous emission $|2\rangle \rightarrow |3\rangle$. The Laplace transform $\tilde{b}_2(s)$, can be found in this case as

$$\tilde{b}_2(s) = \frac{(s - i\delta)^{\frac{1}{2}}}{s(s - i\delta)^{\frac{1}{2}} + (i\delta_{23} + \frac{1}{2}\gamma_{23})(s - i\delta)^{\frac{1}{2}} - (i\beta)^{\frac{3}{2}}}, \quad (4.13)$$

where δ_{23} and γ_{23} are the Lamb shift and spontaneous emission decay of the transition $|2\rangle \rightarrow |3\rangle$.

The spectrum of spontaneous emission $|2\rangle \rightarrow |3\rangle$ also exhibits interesting properties. This spectrum is given by

$$S(\omega_\lambda) \sim |\tilde{b}_2(-i(\omega_\lambda - \omega_{23}))|^2, \quad (4.14)$$

where $\tilde{b}_2(s)$ is given in equation (4.13). In Figure 6 we plot spectrum $S(\omega_\lambda)$ for different values of $\delta = \omega_{21} - \omega_c$. Clearly, the spectrum $S(\omega_\lambda)$ splits into a doublet. This splitting is analogous to the Autler-Townes splitting [52]. In our case, however, there is no external field and splitting is caused entirely by strong interaction between the atom and its own radiation field. The linewidth of the left sideband can be much smaller than γ_{21} (solid curve in Fig. 6), the natural linewidth of the spontaneous transition $|2\rangle \rightarrow |3\rangle$.

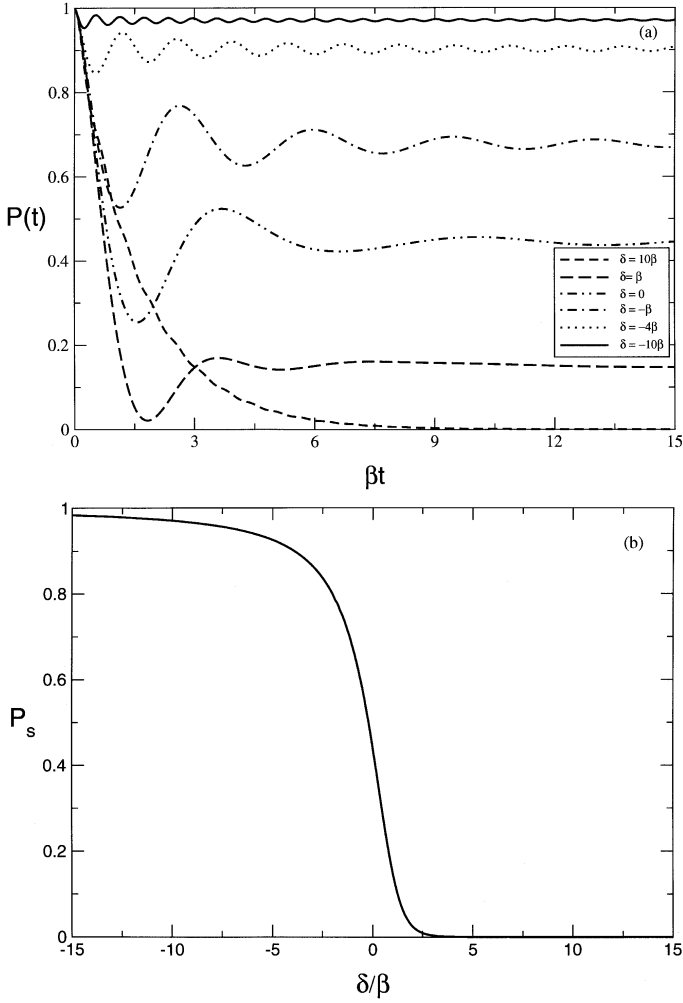


Fig. 4. (a) Atomic population on the excited state, $P(t) = |b_2(t)|^2$ as a function of βt and for various values of detuning from photonic band edge $\delta = -10\beta$ (solid curve), $\delta = -4\beta$ (dotted curve), $\delta = -\beta$ (long-short-dashed curve), $\delta = 0$ (long-short-short-dashed curve), $\delta = \beta$ (long-dashed curve), and $\delta = 10\beta$ (short-dashed curve). (b) Steady-state atomic population $P_s = \lim_{t \rightarrow \infty} |b_2(t)|^2$ as a function of δ/β .

4.2 Collective time scale factors

We now generalize the previous discussion to spontaneous emission of an excited two-level atom in a presence of $N - 1$ unexcited atoms in a PBG.

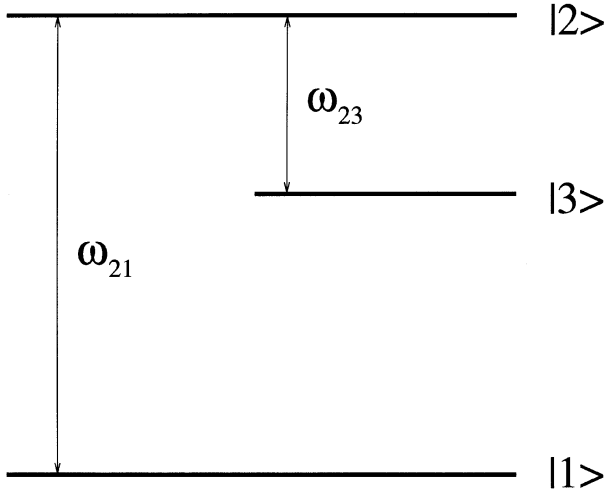


Fig. 5. Three-level atom of a λ configuration. The transition frequency ω_{21} lies near the band edge while ω_{23} is assumed to be far from the gap.

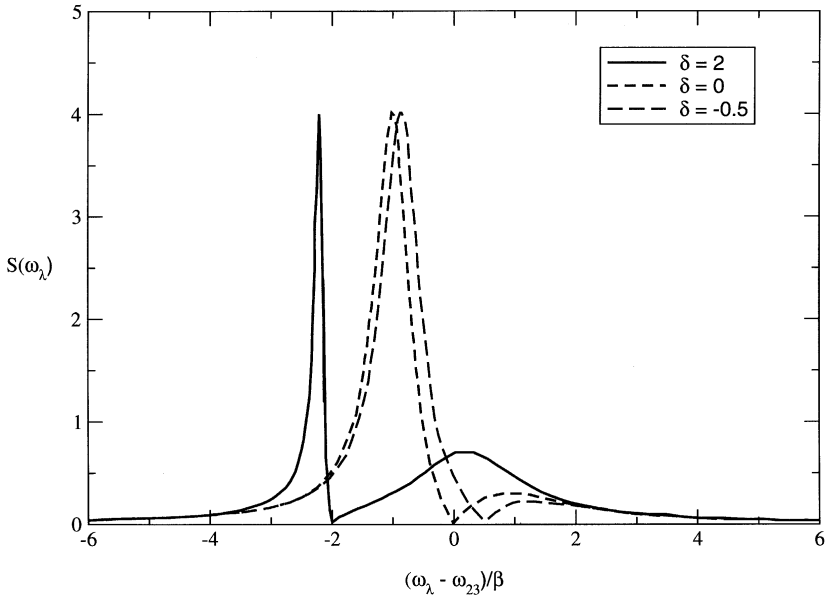


Fig. 6. Autler-Townes spectrum $S(\omega_\lambda)$ of spontaneous emission $|2\rangle \rightarrow |3\rangle$ (in a system of the resonant frequency splitting $\beta = 1$) for $\delta_{23} = 0$, $\gamma_{23} = 1$, and for various values of detuning from the band edge $\delta = -0.5$ (long-dashed curve), $\delta = 0$ (short-dashed curve) and $\delta = 2$ (solid curve).

We limit our studies to the Dicke model in a perfect photonic bandgap. The Hamiltonian (4.1) for the multi-atom case is given by

$$H = \sum_{\lambda} \hbar \Delta_{\lambda} a_{\lambda}^{\dagger} a_{\lambda} + i \hbar \sum_{\lambda} g_{\lambda} (a_{\lambda}^{\dagger} J_{12} - J_{21} a_{\lambda}), \quad (4.15)$$

where

$$J_{ij} = \sum_{k=1}^N \sigma_{ij}^{(k)}, \quad (i, j = 1, 2) \quad (4.16)$$

and the superscript k refers to the k^{th} atom.

Assume that the atomic system is initially in the symmetrical superradiant state [51] $|J, M = 1 - J\rangle$ with only one atom being in the excited state and the field is in the vacuum state. Here $|J, M\rangle$ states are the normalized eigenstates of operators $J_3 = \frac{1}{2}(J_{22} - J_{11})$ and $J^2 = \frac{1}{2}(J_{21}J_{12} + J_{12}J_{21}) + J_3^2$. The wave function of the system then has the form

$$|\psi(t)\rangle_N = b_{2N}|J, M = 1 - J, \{0\}\rangle + \sum_{\lambda} b_{1N,\lambda}(t)|J, M = -J, \{\lambda\}\rangle e^{-i\Delta_{\lambda}t}. \quad (4.17)$$

The state vector $|J, M = 1 - J, 0\rangle$ describes the atomic system in the state $|J, M = 1 - J\rangle$ and no photons present, whereas the state vector $|J, M = -J, \lambda\rangle$ describes the all atoms are in their ground state and a single photon in mode $\{\lambda\}$. It is straightforward to verify that the time-dependent Schrodinger equation yields a solution analogous to (4.9) except that d_{12}^2 is replaced by Nd_{12}^2 . In free space with a continuous broad band density of states we can again use the Wigner-Weisskopf approximation (4.10). The atomic population in the excited state is given by:

$$|b_{2N}(t)|^2 = e^{-N\gamma_{21}t}.$$

That is, the collective time scale factor is proportional to N .

In the case when the atomic resonant frequency lies near the edge of a PBG, we used the dispersion relation (4.11) and the Laplace transform $\tilde{b}_{2N}(s)$ is found as

$$\tilde{b}_{2N}(s) = \frac{(s - i\delta)^{\frac{1}{2}}}{s(s - i\delta)^{\frac{1}{2}} - (i\beta_N)^{\frac{3}{2}}}, \quad (4.18)$$

where

$$\beta_N^{\frac{3}{2}} = N\beta^{\frac{3}{2}}.$$

Clearly $b_{2N}(t)$ has the same form as $b_2(t)$ except with the factor β of a single atom case replaced by $N^{2/3}\beta$. This means that in the presence of $N - 1$ unexcited atoms, the resonant frequency splitting increases by the factor of

$N^{2/3}$. Clearly the rate of spontaneous emission is also increased by a factor of $N^{2/3}$.

The collective time scale factor $N^{2/3}$ found above made use of the isotropic model of a PBG described by equation (4.11). The exponent of N , however depends sensitively on the dimension of the phase space occupied by band-edge photons of vanishing group velocity and the resulting bandedge singularity in the overall photon density of states. In an isotropic bandedge, we have overestimated this phase space using the entire sphere $|\vec{k}| = \pi/L$. For a real dielectric crystal in three dimensions with an allowed point-group symmetry, the band edge is associated with a specific point $\vec{k} = \vec{k}_0$ rather than the entire sphere $|\vec{k}| = |\vec{k}_0|$

$$\omega_{\vec{k}} \cong \omega_c + A(\vec{k} - \vec{k}_0)^2. \quad (4.19)$$

The dispersion relation (4.19) leads to a photonic density of states $\rho(\omega)$ at a bandedge ω_c which behaves as $(\omega - \omega_c)^{\frac{d}{2}-1}$ for $\omega \geq \omega_c$. Here d is the dimensionality of space. We discuss, finally the influence of the anisotropic dispersion relation on the collective scale factor. The Laplace transform $\tilde{b}_{2N}(s)$ in this case can be found as

$$\tilde{b}_{2N}(s) = \left[s + \frac{N\alpha}{(2\pi)^d} \int \frac{d^d \vec{k}}{\omega_{\vec{k}}[s + i(\omega_{\vec{k}} - \omega_{21})]} \right]^{-1}, \quad (4.20)$$

where

$$\alpha \cong \frac{\omega_{21}^2 d_{21}^2}{2\epsilon_0 \hbar},$$

and $d = 1, 2, 3$ is the band-edge dimension. Using the dispersion relation (4.19) and changing variables of integration to $\vec{q} = \vec{k} - \vec{k}_0$ we can write equation (4.20) in the form

$$\tilde{b}_{2N}(s) = \left[s - \frac{iN\alpha}{(2\pi)^d} \int \frac{d^d \vec{q}}{(\omega_c + Aq^2)[Aq^2 - is]} \right]^{-1}. \quad (4.21)$$

For a simplicity we assume $\omega_c = \omega_{21}$, *i.e.* the atomic resonance frequency lies at the edge of a PBG. The integral in equation (4.21) can be evaluated by contour integration and $\tilde{b}_{2N}(s)$ is given by

$$\tilde{b}_{2N}(s) = \begin{cases} \left[s - i^{3/2} \frac{N\alpha_1}{\sqrt{s}} \right]^{-1}, & \text{if } d = 1; \\ \left[s - iN\alpha_2 \ln\left(\frac{i\omega_c}{s}\right) \right]^{-1}, & \text{if } d = 2; \\ \left[s - iN\alpha_3 + \sqrt{i}N\alpha_4\sqrt{s} \right]^{-1}, & \text{if } d = 3, \end{cases} \quad (4.22)$$

where $\alpha_1 \dots \alpha_4$ are constants.

Dynamical properties of spontaneous emission can be studied in detail from the inverse Laplace transform of $\tilde{b}_{2N}(s)$ given in equation (4.22).

The most important distinction of anisotropic band edges from isotropic band gaps is in the collective scale factor, which we can evaluate directly from equation (4.22). For 1-d band edges, $\tilde{b}_{2N}(s)$ has a pole when $s^{\frac{2}{3}} \sim N$, that is the collective scale factor is equal $N^{\frac{3}{2}}$, the same as for the isotropic bandgap. For 2-d band-edges, $\tilde{b}_{2N}(s)$ has a pole $s \sim N$ with a weak logarithmic correction, *i.e.* the collective scale factor is approximately equal to N as for free space. In the 3-d bandedge case, $\tilde{b}_{2N}(s)$ has a pole $s \sim N^2$. As a result the collective scale factor becomes N^2 . The last case may lead to the intensity of superradiance being proportional to N^3 , that is much more intense than Dicke superradiance. We now proceed to discuss the interesting consequences of the PBG on collective spontaneous emission.

4.3 Superradiance near a photonic band edge

Although photonic bandgaps are analogous to electronic bandgaps in semiconductors, there are many intriguing aspects of photons which are not shared by electronic systems. Among these are laser action and superradiance. These are related to the bosonic nature of light through which many photons can occupy the same mode. In this section we derive theoretically the nature of collective spontaneous emission of N two-level atoms whose resonance frequency lies at the edge of an isotropic or anisotropic 3-d photonic bandgap. The collective decay rate turns out to be proportional to $N^{2/3}$ and N^2 for isotropic and anisotropic 3-d bandgaps, respectively. The corresponding peak intensity is proportional to $N^{5/3}$ and N^3 , respectively. Furthermore, if atomic population inversion exists at the outset, then a fraction of the superradiant emission remains localized in the vicinity of the atoms leading to a steady state in which the atomic system acquires a macroscopic polarization. A nonzero atomic population in the excited state remains in the long time, steady state limit. This novel form of spontaneous symmetry breaking is the analog of lasing without a cavity mode! The collective emission near the photonic bandedge is accompanied by self-induced oscillations, a simple illustration of the “ringing” regime in superradiance. In addition to being a fundamental phenomenon, localization of superradiance may play an important role in low threshold microlasers based on photonic bandgap engineering. It suggests that a light emitting diode operating near a photonic band edge will exhibit very high modulation speed and coherence properties without recourse to external mirrors or even a true cavity mode.

We consider a Dicke model of N identical two-level atoms coupled to the radiation field in a three-dimensional periodic dielectric. The atoms have excited state $|2\rangle$, ground state $|1\rangle$, and resonant transition frequency ω_{21} . The Hamiltonian of the system is precisely that of equations (4.15) and (4.16).

Assume that the radiation field is initially in the vacuum state. When many atoms are initially excited, the wavefunction approach of Sections 4.1 and 4.2 is no longer useful. Instead, we must consider the Heisenberg equations of motion for the atomic operators. The equations of motion for $\langle J_{12}(t) \rangle$ and $\langle J_3(t) \rangle = \langle J_{22}(t) \rangle - \langle J_{11}(t) \rangle$ are:

$$\frac{d}{dt} \langle J_{12}(t) \rangle = \int_0^t G(t-t') \langle J_3(t') J_{12}(t') \rangle dt', \quad (4.23)$$

$$\frac{d}{dt} \langle J_3(t) \rangle = -2 \int_0^t G(t-t') \langle J_{21}(t') J_{12}(t') \rangle dt' + c.c. \quad (4.24)$$

Here $G(t-t') = \sum_{\lambda} g_{\lambda}^2 e^{-i\Delta_{\lambda}(t-t')}$ is the delay Green's function, and $\langle A \rangle$ indicates the expectation value of the system operator A . The Green's function $G(t-t')$ depends strongly on the dispersion relation and density of states of the medium.

To discuss the possibility of spontaneous symmetry breaking during the process of superradiant emission, we introduce a very small external perturbation which endows the atomic system with an infinitesimal polarization. This is analogous to the addition of a small magnetic field, h , in describing the thermodynamic phases of a collection of N magnetic moments. A ferromagnetic phase transition at zero field is described by taking the limit $h \rightarrow 0$ only after the thermodynamic limit $N \rightarrow \infty$. Accordingly, we find that an infinitesimal initial polarization of the atomic dipoles gives rise to a macroscopic polarization in the steady state limit $t \rightarrow \infty$. Assume that initially the atomic system is in the state

$$|\psi_N\rangle = \prod_{k=1}^N (\sqrt{r}|1\rangle + \sqrt{1-r}|2\rangle)_k, \quad (4.25)$$

where $r \ll 1$, *i.e.* atoms are mostly populated in the excited state $|2\rangle$ and the atomic coherence is infinitesimal. Such a state can be created by interaction of atoms with an external pulse. Qualitatively similar results to the ones we present occur for various values of the initial atomic inversion per atom $\langle J_3(0) \rangle / N$ and for an infinitesimal initial polarization $\langle J_{12}(0) \rangle / N$. The system can be considered semiclassical and equations of motion for $x(t) \equiv \langle J_{12}(t) \rangle / N$ and $y(t) \equiv \langle J_3(t) \rangle / N$ may be obtained from (4.23) and (4.24) by factorizing the quantum expectation value of the operator products:

$$\frac{dx}{dt} = Ny(t) \int_0^t G(t-t') x(t') dt', \quad (4.26)$$

$$\frac{dy}{dt} = -2Nx^*(t) \int_0^t G(t-t') x(t') dt' + c.c. \quad (4.27)$$

It is easy to verify, using the isotropic, effective mass solution to the Green's function $G(t - t')$, that x and y are functions of the dimensionless, scaled, time variable $\beta N^{2/3}t$. The factor $\beta N^{2/3}$ is analogous to a bandwidth parameter in solid state physics. As a result of the band edge mediated interaction between atoms, the effective Rabi splitting is enhanced and the spectrum is broadened by a factor of $N^{2/3}$.

We have solved system of equations (4.26) and (4.27) exactly using numerical methods. In Figure 7 we plot the atomic population inversion $\langle J_3(t) \rangle / N$ (solid curve) and atomic dipole moment $D(t)/N = |\langle J_{12}(t) \rangle| / N$ (dashed curve) as a function of $\beta N^{2/3}t$. In Figure 8, we plot the phase $\mu(t)$ of the atomic polarization $\langle J_{12}(t) \rangle$ for the same initial condition (4.25). Clearly, the collective spontaneous emission at the edge of a PBG displays striking distinctions from the free space case: (i) in the steady-state limit the population inversion $\langle J_3(t) \rangle / N$ is not equal -1 . This follows from the fact that the single atomic population inversion in the excited state $|2\rangle$ remains nonzero. This signifies localization of superradiant emission in the vicinity of the atoms. (ii) The atomic polarization evolves from its infinitesimal initial value to a steady-state macroscopic value. This is distinct from the free space superradiance where the atomic steady-state polarization is equal to zero. This spontaneous symmetry breaking in the atomic polarization field is analogous to lasing without a cavity mode. It suggests the possibility of observing macroscopic quantum coherent superpositions of states. (iii) The evolution of $\langle J_3(t) \rangle$, $D(t)$ and $\mu(t)$ displays collective self-induced oscillation instead of a simple decay as it is in free space. These oscillations are analogous to the collective Rabi oscillations of N Rydberg's atoms in a resonant high-Q cavity [52,53]. In addition to amplitude oscillations, the phase of the macroscopic polarization rotates in the steady-state limit with a frequency proportional to the magnitude of vacuum Rabi splitting. (iv) The collective time scale factor for the isotropic PBG is proportional to $N^{2/3}$ rather than N as it is in free space. That is, the collective decay rate of superradiance is proportional to $N^{2/3}$ and the peak superradiance intensity, which is proportional to $-\frac{d}{dt}\langle J_3(t) \rangle$, is proportional to $N^{5/3}$ rather than N^2 .

Our numerical results reveal qualitatively similar behavior for different initial conditions. In particular, macroscopic polarization emerges for *any* initial state for which $\langle J_3(0) \rangle / N > 0$ and the steady state limit $\langle J_{12}(\infty) \rangle / N$ is independent of the initial (infinitesimal) value $\langle J_{12}(0) \rangle / N$. The delay time required for superradiant emission, however decreases noticeably as $\langle J_{12}(0) \rangle / N$ was varied from 10^{-4} to 10^{-3} . The magnitude of the macroscopic steady state polarization $\langle J_{12}(\infty) \rangle / N$ decreases monotonically from 0.42 to 0.15 as the initial inversion $\langle J_3(0) \rangle / N$ was decreased from 0.95 to 0.3. In the absence of population inversion ($\langle J_3(0) \rangle / N < 0$), we find that macroscopic polarization (in the long time limit) occurs only if the initial state itself has a macroscopic polarization.

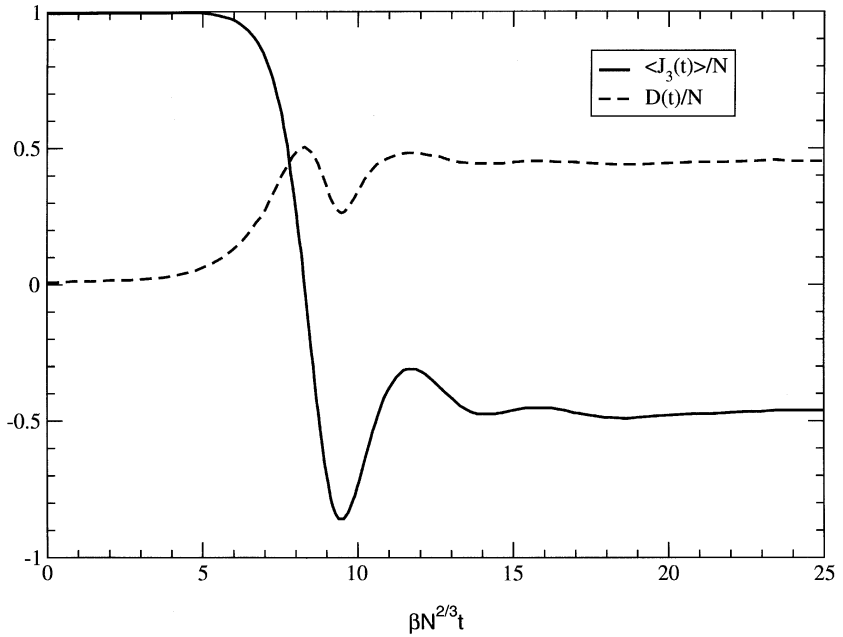


Fig. 7. Atomic inversion $\langle J_3(t) \rangle / N$ (solid curve) and amplitude of the atomic polarization $D(t)/N = |\langle J_{12}(t) \rangle| / N$ (dashed curve) in an isotropic PBG as a function of the scale time $\beta N^{2/3} t$ for initial condition (10) with $r = 10^{-6}$.

5 Quantum and nonlinear optics in a three-dimensional PBG material

5.1 Low-threshold nonlinear optics

Photonic band gap materials represent a fundamentally new paradigm for low threshold nonlinear optical phenomena. The ability to achieve ultrafast nonlinear optical response in a nonabsorbing material is crucial in applications such as all-optical switching and all-optical transistors for integrated optical circuits. In a conventional Fabry-Perot device containing a weakly nonlinear layer, transistor-like response requires relatively high intensity laser fields. The situation may be dramatically different in the context of a three-dimensional PBG material where the inhibition of spontaneous emission from atoms and molecules is essentially complete.

Consider the interaction of a classical monochromatic electromagnetic wave of frequency ω with a two-level atom which has a radiative transition at a near visible frequency ω_0 . We suppose that the detuning $\Delta = \omega - \omega_0 \ll \omega_0$. For weak fields, the response of the two-level atom is that of a simple harmonic oscillator since the atom spends the majority of time in its ground

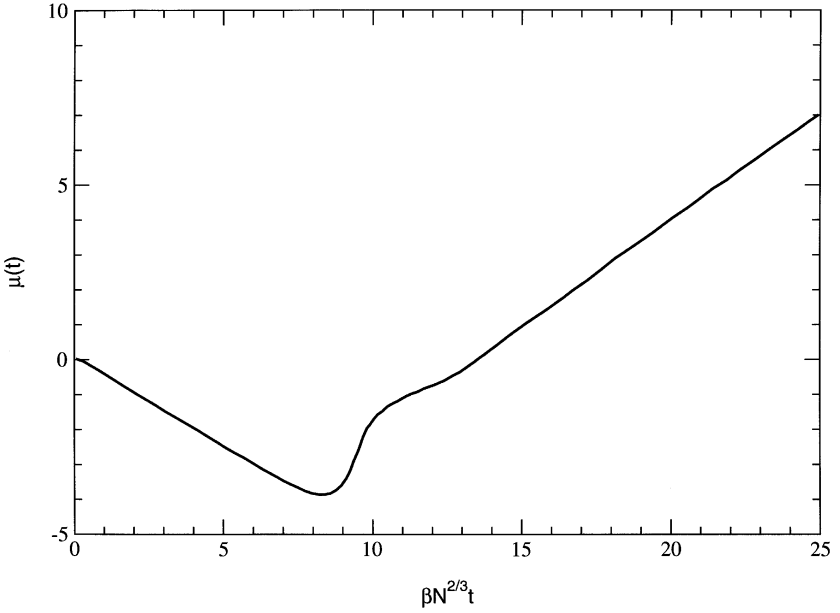


Fig. 8. Phase angle of the atomic polarization as a function of $\beta N^{2/3}t$ for the same parameters as in Figure 7.

state. Whenever the external field excites the atom, it quickly returns to its ground state due to the rapid rate of spontaneous emission. As the external field intensity is increased, the upper state population increases and eventually saturates. This is associated with nonlinear response. The appropriate mechanical analogy for the quantum two-level system is no longer a classical harmonic oscillator, but rather a simple pendulum (atomic Bloch vector) whose coordinates are given by the different components of the 2×2 atomic density matrix. Small angle oscillation of the atomic Bloch vector describes linear response whereas large angle oscillations probe the nonlinear susceptibility of the atom. The threshold external field required to probe nonlinear response is called the line center saturation field strength E_s^0 which is related to the rate of spontaneous emission $1/T_1$ by the formula [54]:

$$|E_s^0|^2 = \frac{\hbar^2}{4\mu_{ba}T_1T_2}. \quad (5.1)$$

Here, $1/T_2$ is the rate of dipolar dephasing and μ_{ba} is the electric dipole transition matrix element for the atom. In ordinary vacuum, the textbook

formula [54] for the nonlinear susceptibility is:

$$\chi = \chi_0 \frac{\Delta T_2 - i}{1 + \Delta^2 T_2^2 + |E|^2/|E_s^0|^2}. \quad (5.2)$$

Here, χ_0 is a frequency independent constant, $\Delta = \omega - \omega_0$ is the detuning of the external field of amplitude E and frequency ω . Clearly, the susceptibility, χ , is independent of E for $E \ll E_s^0$ whereas it has a highly nonlinear dependence on E for $E \gtrsim E_s^0$. This widely accepted picture of nonlinear optical response in ordinary materials is no longer applicable in a three-dimensional PBG material in which two-level atoms have a radiative transition at frequency ω_0 that lies within the PBG.

Inside a PBG, the rate $1/T_1$ and accordingly the threshold intensity $|E_s^0|^2$ formally vanish. While this is suggestive of low threshold nonlinear optical response, it is in fact an indication that the entire derivation of the conventional susceptibility, equation (5.2), must be carefully re-examined in the context of the PBG. In particular, equation (5.2) is based on retaining only the leading order photon-atom interaction, namely spontaneous emission. In the PBG, this leading process is almost absent. Therefore, it is necessary to consider the next process, namely resonance dipole-dipole interaction (RDDI) between a pair of two-level atoms. A straightforward derivation [37] of the nonlinear susceptibility in this context leads to some remarkable effects. For example, it is possible (at relatively low field intensities) to completely saturate the imaginary (absorptive) part of χ while retaining a large real part for χ . This arises in a situation where a collection of atoms inside a PBG interact randomly by RDDI and an external field enters the material through a small number of defect (waveguide) modes. Due to the inhibition of spontaneous emission, the single atom absorptive transition is saturated at nearly the one-photon level. However, due to the random nature of RDDI, the induced atomic dipoles are randomly oriented and remain highly susceptible to alignment (macroscopic polarization) by the external field.

5.2 Collective switching and transistor effects

A second illustration of novel radiation-matter interaction in a PBG material arises if a collection of two-level atoms is selected such that their radiative transition lies very close to a photonic band edge. Near the photonic band edge, the electromagnetic density of states varies rapidly with frequency and the spontaneous emission processes cannot be adequately described using Fermi's Golden Rule. We refer to the case in which $\rho(\omega)$ exhibits singularities or abrupt variation as a "colored vacuum". In the colored vacuum of a photonic band edge it is possible to achieve population inversion for a collection of two-level atoms driven by a weak coherent pump

laser field. As the number of atoms in a cubic wavelength increases, this switching from a passive medium (most atoms in ground state) to an active medium (population inverted) occurs as an abrupt jump as a function of external pump laser field intensity. In the region of this collective jump in atomic population, there is a large differential optical gain. If the pump laser intensity is chosen slightly below threshold for population inversion, a second control laser field can be introduced to act as a gate which determines whether the pump laser field is either attenuated or amplified by the medium. Since all of these processes involve coherent radiation-atom interactions, this system may form the basis of a low threshold optical switch or all-optical transistor [36].

When a coherent laser field with average incident energy density W and frequency ω interacts with a collection of N two-level atoms in ordinary vacuum, the steady state behavior of the system is governed by the well-known Einstein rate equations. These equations implicitly make use of the smooth nature of the vacuum density of states $\rho(\omega) = \omega^2/(\pi^2 c^3)$ in the vicinity of the atomic transition frequency $\omega \simeq \omega_0$. In steady state equilibrium, the ratio of the number of excited atoms, N_2 , to the total number of atoms is given by [55]:

$$\frac{N_2}{N} = \frac{W}{\hbar\omega_0\rho(\omega_0) + 2W}. \quad (5.3)$$

Clearly, as W increases, the maximum value of N_2/N is less than $1/2$. In other words, it is not possible to invert a collection of two-level atoms with a coherent laser field.

From a more quantum mechanical point of view, the external laser field may be regarded as consisting of a large collection of n photons. The atom-radiation field interaction Hamiltonian, H_{int} , breaks the degeneracy between a state consisting of a given atom in its excited and $(n-1)$ -photons in the radiation field (which we denote by the ket $|2, n-1\rangle$) and a state consisting of the given atom in its ground state and n -photons in the radiation field (which we denote by the ket $|1, n\rangle$). The matrix element $\langle 2, n-1 | H_{\text{int}} | 1, n \rangle$ is nonzero and the true eigenstates of the system are called dressed atomic states. These “dressed states” are linear combinations of the “bare” kets listed above. Accordingly, the eigenenergies of the dressed states are shifted from their bare values by an amount $\Delta \sim \mu_{ba}|E|/\hbar$ (Rabi frequency) where μ_{ba} is the atomic dipole matrix element and $|E|$ is the laser field amplitude. This leads to the well-known Mollow fluorescence spectrum in ordinary vacuum [55]. Rather than a single peak in the atomic spectrum centered at the bare atomic transition frequency ω_0 , the fluorescence spectrum exhibits three peaks centered at ω_0 , $\omega_0 + 2\Delta$, and $\omega_0 - 2\Delta$.

The Einstein rate equation picture of the steady state atomic inversion, equation (5.3), relies on the fact that the vacuum density of electromagnetic modes $N(\omega)$ is relatively smooth on the scale of Δ . That is to say,

the Einstein picture assumes that the rate of spontaneous emission in the Mollow sidebands at $\omega_0 + 2\Delta$ and $\omega_0 - 2\Delta$ is roughly the same. In ordinary vacuum ($\rho(\omega) = \omega^2/(\pi^2 c^3)$) this assumption is easily satisfied. Moreover, in ordinary vacuum, very high intensity fields are required to observe any Mollow splitting whatsoever. The situation is dramatically different in a PBG material where the density of states itself exhibits rapid variation from frequency $\omega_0 - 2\Delta$ to $\omega_0 + 2\Delta$. Another striking property of the photonic band edge is that atomic line splitting may be achieved with very low intensity fields. In particular, vacuum Rabi splitting of an atomic transition placed directly at the band edge has been predicted [30–32]. In other words, at a band edge, significant splitting can be expected in an atomic line even in the presence of a few photons! This leads to a dramatic modification of the Einstein picture.

In a weak applied laser field, atoms with a bare transition frequency ω_0 which coincides with a photonic band edge will exhibit a pair of dressed states that straddle the band edge [30–32]. These two spectral sidebands will experience vastly different rates of spontaneous emission. The spectral component that is pulled into the gap will exhibit negligible decay. This component corresponds to a photon-atom bound state [30]. The spectral component that is pushed away from the gap can exhibit emission into the allowed modes of the photonic band. Population inversion for a collection of such atoms can readily be achieved by an external laser field due to trapping of excitation energy in the photon-atom bound state component [36]. This transition becomes increasingly sharp as the number of atoms increases and defines a region of large differential a very low applied field and that the switching effect is robust with respect to variety of dephasing effects due to lattice vibrations in the host PBG material.

Two-level atoms are an idealization which illustrate the fundamentally new principles of electromagnetic interaction in a PBG material. Experimental realization of these new phenomena in quantum and nonlinear optics could take one of several forms. One of these is direct implantation doping of ions into a PBG material. For example Erbium ions implanted in silicon have recently been shown to exhibit sharp atom-like electroluminescence spectra [56]. A related possibility is the engineering of quantum dots or “artificial atoms” into the PBG backbone. These also exhibit sharp spectral lines [57] and coherent optical control of the exciton wavefunction in quantum dots has been demonstrated [58]. Finally there is the possibility of laser cooling of atoms and atom trapping within the void regions of a PBG. For example, laser illumination of an inverse opal PBG at a laser frequency corresponding to the upper band edge leads to an optical trapping potential for atoms in the spherical void regions [59]. This could be used to trap and cool Rubidium atoms in a GaP inverse opal or other PBG material for quantum optical experiments.

When an atomic transition lies deep inside the gap, the spontaneous emission is strongly suppressed whereas coherent dipole-dipole interaction between identical atoms persists on a length scale given by the localization length of the dielectric microstructure [60, 61]. On length scales short compared to the optical wavelength, the resonance dipole-dipole interaction (RDDI) is mediated by the exchange of high energy virtual photons between the atoms. This leads to new coherent processes such as photon hopping conduction [62] and the formation of a quantum-optical spin glass state [63].

6 Resonant nonlinear dielectric response in a doped photonic band gap material

We now describe the response of two-level atoms placed within an imperfect PBG from an applied laser field. This laser field may be injected into the PBG material by a single mode waveguide channel whose frequency lies within the 3-d PBG. When the average interatomic spacing is less than an optical wavelength the dominant contribution to RDDI comes the traceless matrix interaction between the dipole vectors on each atom. The absence of ordinary, vacuum, spontaneous emission is manifest in the cutoff the transverse (propagating) part of the the RDDI on the scale of the localization length. We consider a simplified scalar model using two-level atoms in which the random atomic positions are modeled by means of a Gaussian distribution of RDDI's.

Localized states appear within the PBG by means of dielectric defects within the otherwise periodic microstructure. Alternatively, a small density of propagating states may occur within an incomplete PBG [64]. In either case, spontaneous emission occurs selectively into such a PBG cavity mode. Strong coupling occurs when the energy scale of RDDI, J , is large compared to both the rate of atomic population decay $1/T_1$ and the rate of dipole dephasing $1/T_2$. In addition, J is larger than the extent of inhomogeneous broadening of the atomic line due to the random crystal field in the PBG microstructure. In this case, novel nonlinear effects occur: when the Rabi interaction energy scale $\hbar\Omega$ of the applied laser field exceeds the RDDI energy scale J , the absorptive part of the dielectric susceptibility saturates whereas the real part of the nonlinear response remains large. This suggests that PBG system may act as nearly lossless, nonlinear materials. As we show below, this is a direct consequence of a novel spin-glass type polarization of the atomic dipoles by the external classical field.

We study the response to an applied field of N two-level atoms placed within a PBG material in which a small number of waveguide channels and localized states of light have been engineered. The coherent part of the model Hamiltonian can be written, in the interaction picture, in the form

(choosing units in which $\hbar = 1$)

$$H = -\frac{\delta}{2} \sum_i^N \sigma_i^z - \Omega \sum_i^N (\sigma_i^\dagger + \sigma_i) + \sum_{i \neq j}^N J_{ij} \sigma_i^\dagger \sigma_j. \quad (6.1)$$

Here, $\sigma_i^\dagger$ and σ_i describe atomic excitation and de-excitation of i^{th} atom, respectively; σ^z describes the atomic inversion; $\Omega = \mu E$ is the resonant Rabi frequency where μ is the atomic dipole moment and E is the amplitude of the applied field; $\delta = \omega - \omega_a$ is the detuning of laser frequency ω from the atomic resonant frequency ω_a ; and $J_{ij} = J_{ji}$ denotes the RDDI between atoms i and j . The detailed, microscopic evaluation of J_{ij} as a function of atomic distance r_{ij} and atomic configurations may be found in [65] for free space and [60,61] for a PBG. In a realistic description, the RDDI term in (1) would be replaced by a traceless tensor interaction for atomic excitation transfer between two sets of triply degenerate atomic orbitals. We simulate this interaction in the simpler two-level atom system by the Gaussian random scalar variable, J_{ij} , with zero mean value and variance J .

In the semi-classical (mean field) approximation, the optical Bloch equations for the operator expectation values are [66,67]

$$\frac{d}{dt} \langle \sigma_j^- \rangle = (-1/T_2 + i\delta) \langle \sigma_j^- \rangle - i(\Omega - F_j) \langle \sigma_j^z \rangle, \quad (6.2)$$

$$\frac{d}{dt} \langle \sigma_j^z \rangle = -(\langle \sigma_j^z \rangle - \langle \sigma^z \rangle_0) / T_1 + 2i\Omega(\langle \sigma_j^\dagger \rangle - \langle \sigma_j^- \rangle) - 2i(\langle \sigma_j^\dagger \rangle F_j - \langle \sigma_j^- \rangle F_j^*). \quad (6.3)$$

Here, $F_j \equiv \sum_{i(\neq j)} J_{ji} \langle \sigma_i^- \rangle$; T_1 and T_2 are the relaxation times of $\langle \sigma^z \rangle$ and $\langle \sigma^- \rangle$, respectively; and $\langle \sigma^z \rangle_0$ is the atomic population inversion in the thermal equilibrium. We use the fact that in the optical domain $\langle \sigma^z \rangle_0 \cong -1$ even at the room temperature. In general, T_1 and T_2 describe spontaneous emission into extraneous modes as well as nonradiative broadening. The collective effects of the incoherent interaction are assumed to be small compared to RDDI's and are simply ignored. Steady-state solutions of (6.2) and (6.3) satisfy the conditions:

$$w_j^2 + w_j + 4(T_1/T_2)|p_j|^2 = 0, \quad (6.4)$$

$$-\Omega w_j + (\delta + i/T_2)p_j + w_j \sum_{i(\neq j)} J_{ji} p_i = 0. \quad (6.5)$$

Here, $p_j \equiv \langle \sigma_j^- \rangle_s$, $w_j \equiv \langle \sigma_j^z \rangle_s$ are steady state expectation values. It is clear from equation (6.4) that the population difference, w_j , is negative for all atoms and is not directly driven by random fluctuations of J_{ij} . On the other hand, random fluctuations in RDDI drive *phase* changes in the atomic dipoles, p_i . These phase fluctuations dominate the system behavior

in the long time limit. We have performed detailed numerical simulations of equations (6.4) and (6.5) for a small number of atoms which confirm this picture. Below, we present a simple mean-field solution of the steady state equations (6.4) and (6.5), compatible with the conclusions of our more general numerical studies.

Configuration averaging over the random atomic positions corresponds to performing a statistical average over the possible values of J_{ij} using the Gaussian distribution. It is denoted by the square brackets $[\dots]_c$. Using the mean-field approximation $[\langle \sigma_j^z \rangle^2]_c \cong [\langle \sigma_j^z \rangle]_c^2$ (verified numerically), equation (6.4) becomes: $w^2 + w + 4(T_1/T_2)q = 0$. Here, $q \equiv (1/N) \sum_j^N [|p_j|^2]_c$ is the Edwards-Anderson order parameter [68,69] and $w \equiv (1/N) \sum_j^N [w_j]_c$ is the average atomic population difference. Mean-field theory may also be applied to equation (6.5) by replacing w_j by its average value, w . It is convenient to decompose the symmetric matrix J_{ij} using the spectral representation [70] $J_{ij} = \sum_\lambda^N J_\lambda \langle i|\lambda \rangle \langle \lambda|j \rangle$. Here, J_λ and $\langle \lambda|i \rangle$ are the eigenvalues and orthonormal eigenvectors of J_{ij} , respectively. The polarization eigenmode, $p_\lambda \equiv \sum_j^N \langle \lambda|j \rangle p_j$, is then given by: $p_\lambda = \Omega w (\delta + i/T_2 + wJ_\lambda)^{-1} \sum_j^N \langle \lambda|j \rangle$. In the limit of large N , the eigenvalue density $\rho(J_\lambda)$ obeys a semicircular law [71]: $\rho(J_\lambda) = (2\pi\tilde{J}^2)^{-1} (4\tilde{J}^2 - J_\lambda^2)^{\frac{1}{2}}$, where $\tilde{J} = J\sqrt{N}$. Using the semicircular distribution of the eigenvalue J_λ we can easily find average atomic polarization $p = (1/N) \sum_j^N [p_j]_c = \chi\Omega$. Here,

$$\chi \equiv w \int dJ_\lambda \rho(J_\lambda) (\delta + i/T_2 + wJ_\lambda)^{-1} \quad (6.6)$$

is the susceptibility per atom [66]. The scaled spin-glass order parameter $q_\Omega \equiv q/\Omega^2$ is then given by $q_\Omega = -wT_2\chi''$, where $\chi'' \equiv \text{Im}\chi$. The atomic population difference w is found then as: $w = I\chi'' - 1$, where $I \equiv 4T_1\Omega^2$ is a scaled intensity parameter. Using the semicircular eigenvalue density, the susceptibility (6.6) can be expressed implicitly in the form

$$\chi = (1/2\tilde{J}^2 w) \{ \delta + i/T_2 - [(\delta + i/T_2)^2 - 4w^2\tilde{J}^2]^{1/2} \}. \quad (6.7)$$

In the weak coupling case of $\tilde{J} \ll 1/T_2$, χ and q_Ω reduce to

$$\chi = -(\delta - i/T_2) / [\delta^2 + 1/T_2^2 + 4T_1\Omega^2/T_2] \quad (6.8)$$

and $q_\Omega = |\chi|^2$. Equation (6.8) is the conventional nonlinear susceptibility for ordinary materials [66] and exhibits conventional saturation in both the real and imaginary parts. A second limiting case may be recaptured for weak applied field $I \ll 1$. Here, $w \cong -1$ and χ becomes independent of Ω (linear susceptibility χ_L):

$$\chi_L = -(1/2\tilde{J}^2) \{ (\delta + i/T_2) - [(\delta + i/T_2)^2 - 4\tilde{J}^2]^{1/2} \}. \quad (6.9)$$

In this linear regime, it is instructive to consider the relative importance of glassy configurations which are measured by the ratio of the ferro-electric to ferro-glass order parameters. At exact resonance $\delta = 0$, $|\chi|^2/q_\Omega = [(1 + 4\tilde{J}^2 T_2^2)^{1/2} - 1]/2\tilde{J}^2 T_2^2$. Clearly $|\chi|^2/q_\Omega \ll 1$ for $\tilde{J} \gg 1/T_2$. That is, the glassy behavior of the atomic dipoles becomes dominant relative to any macroscopic ferro-electric response. As we will see shortly, the glass-order parameter and atomic polarization change dramatically with nonzero detuning and increased intensity of the applied field. This suggests that the quantum spin-glass state may be created and controllably altered by means of an external laser field. This also leads to nearly lossless, resonant nonlinearity at high fields.

In Figure 9 we plot the real (χ') (solid curve), imaginary (χ'') (dashed curve) parts of the *linear* susceptibility and associated the glass-order parameter q_Ω (dotted curve) as a function of $\delta = \omega - \omega_a$ for the case of $\tilde{J} \gg 1/T_2$. As a result of photon hopping conduction, the excited levels of the impurity atoms broaden into a photonic impurity band [61]. The imaginary part of the linear susceptibility describes the density of states of this impurity band. Outside the impurity band, $|\delta| > 2\tilde{J}$, the index of refraction $(\chi')^{1/2}$ remains large while the absorption coefficient (χ'') becomes negligible. Important applications of a linear, transparent, high-index optical material have been suggested in [72]. In contrast to [72], the absorptionless index of refraction is present over a large frequency interval. A second feature of the linear susceptibility is that, near resonance, the glass-order parameter is much larger than atomic polarization while far from resonance they are of the same order. We emphasize that in the PBG, the linear absorption in the frequency interval $|\delta| \leq 2\tilde{J}$ (dashed curve in Fig. 9) is the result of collectively enhanced photon hopping conduction between impurity atoms rather than single atom relaxation. This kind of absorption within the photonic impurity band, as we now show, can be greatly suppressed by a strong applied field.

For $\tilde{J} \gg 1/T_2$, and in the frequency interval $1/T_2 \ll |\delta| \leq 2\tilde{J}$, $1/T_2$ in equation (6.7) can be ignored. The atomic population difference is then found for the case of strong applied field as $w \cong -|\delta|/2\tilde{J}$. It yields $\chi' \cong -\text{sign}(\delta)/\tilde{J}$ and $\chi'' \cong (1 - |\delta|/2\tilde{J})/I$. Clearly, in the frequency interval $|\delta| \leq 2\tilde{J}$, χ'' is strongly suppressed ($\sim 1/I$) as intensity of the applied field increases, whereas χ' remains large.

In Figure 10 we plot the nonlinear susceptibility and the glass-order parameter numerically evaluated from equation (6.7) for the case of $\tilde{J} \gg 1/T_2$. The strong nonlinear suppression of absorption accompanied by large real refractive is particularly evident in Figure 10b where $T_2 \gg I/\tilde{J} \gg 1$. Such a photonic material may have important applications in high-refractive nonlinear devices. It may lead to nonlinear transparency in the form of gap soliton propagation. On the other hand, when dipole dephasing and

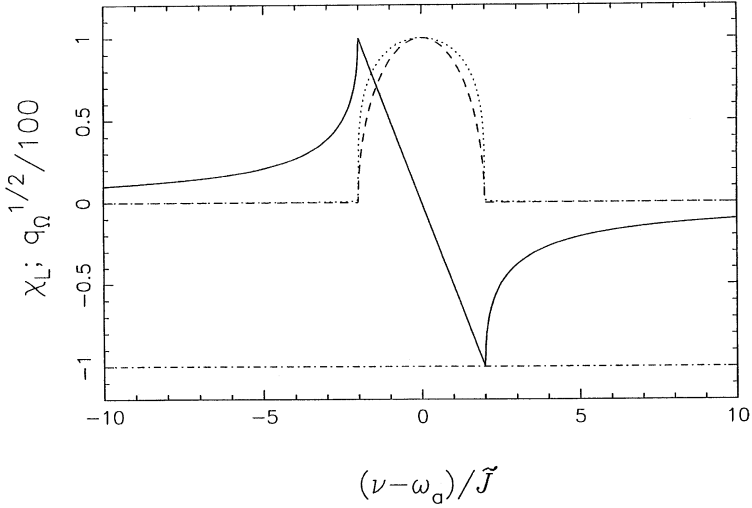


Fig. 9. Real (χ' , solid curve) and imaginary (χ'' , dashed curve) parts of the linear susceptibility χ_L , associated glass-order parameter $q_\Omega^{1/2}$ (dotted curve) (in units of $\tilde{J} = 1$) and atomic population difference w (dash-dotted curve) as a function of detuning $(\omega - \omega_a)/\tilde{J}$ and for $1/\tilde{J}T_2 = 10^{-4}$.

nonradiative relaxation rates exceed the rate of RDDI hopping conduction both the real and imaginary parts of nonlinear susceptibility exhibit conventional power broadening with increasing intensity of the applied field. In ordinary vacuum, where rapid spontaneous emission also occurs, T_1 and T_2 are many orders of magnitude smaller than in a PBG. This leads to the requirement of high atomic density and very strong applied field Ω in ordinary vacuum for realization of the condition $I = 4T_1\Omega^2 \gg \tilde{J} \gg 1/T_2$ to see the nonlinear effects described in Figure 10.

7 Collective switching and inversion without fluctuation in a colored vacuum

Quantum optics in confined photonic systems [73] such as microcavities, optical fibers, optical wires, and photonic band gap (PBG) materials exhibits novel features arising from our ability to tailor the photon density of states (DOS) in a prescribed manner. The distinguishing common feature of the confined photonic systems is that the photonic mode density exhibits rapid variation with frequency at certain edge or cutoff frequencies. In the optical fibers, the mode density vanishes abruptly below a waveguide cutoff frequency ω_0 . For $\omega \geq \omega_0$, the mode density of the fiber diverges as

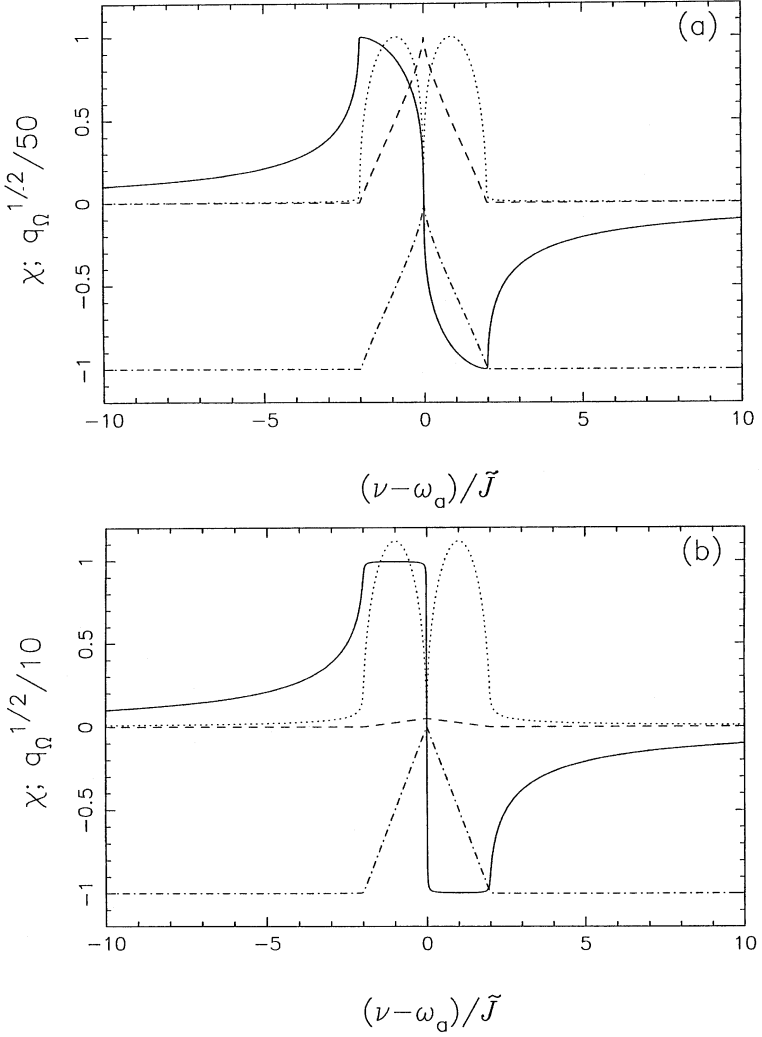


Fig. 10. Real (χ' , solid curve) and imaginary (χ'' , dashed curve) parts of the nonlinear susceptibility χ_L , associated glass-order parameter $q_\Omega^{1/2}$ (dotted curve) (in units of $\tilde{J} = 1$) and atomic population difference w (dash-dotted curve) as a function of detuning $(\omega - \omega_a)/\tilde{J}$ for $1/\tilde{J}T_2 = 10^{-4}$ and for (a) $I/\tilde{J} = 1$ and (b) $I/\tilde{J} = 20$.

$(\omega - \omega_0)^{-1/2}$ [74]. A similar situation appears in the optical wires [75]. In photonic band gap materials, the DOS exhibits band edge and other van-Hove singularities. At the band edge frequency ω_{edge} , this can take the form

of a step discontinuity (two-dimensional PBG) or a singularity of the form $|\omega - \omega_{\text{edge}}|^{1/2}$ in a true three-dimensional PBG.

In this section, we study collective atomic population inversion and statistics of atoms driven by a laser field in confined photonic systems. When the deviation of the photonic mode density between the two Mollow sidebands is large, strong atomic population inversion occurs. We show that when the number of atoms, N , is large, collective switching from the ground state into excited state occurs at a sharp threshold value of the applied field intensity. We show that, under certain conditions, the statistics of the atoms in the excited state can be strongly sub-Poissonian. This suggests a new mechanism of sub-Poissonian pumping for lasers, fast optical switching, and large differential optical gain relevant to an all-optical transistor.

Consider a system of N identical two-level atoms driven by a strong external laser field and coupled to the radiation field reservoir of the confined photonic material. The atoms have excited state $|2\rangle$, ground state $|1\rangle$, resonant transition frequency ω_{21} , and may interact with lattice vibrations of the host photonic material. The Hamiltonian of the system in the interaction picture takes the form: $H = H_0 + H_1 + H_{\text{dephase}}$ where

$$H_0 = \frac{1}{2}\hbar\Delta J_3 + \hbar\varepsilon(J_{12} + J_{21}) + \sum_{\lambda} \hbar\delta_{\lambda} a_{\lambda}^{\dagger} a_{\lambda}, \quad (7.1)$$

$$H_1 = i\hbar \sum_{\lambda} g_{\lambda} (a_{\lambda}^{\dagger} J_{12} - J_{21} a_{\lambda}). \quad (7.2)$$

Here $J_{ij} = \sum_{k=1}^N |i\rangle_k \langle j|_k$ ($i, j = 1, 2$) are the collective atomic operators; $J_3 = J_{22} - J_{11}$ describes the atomic population inversion; a_{λ} and $a_{\lambda}^{\dagger}$ are the radiation field annihilation and creation operators; $\Delta = \omega_a - \omega_L$ and $\delta_{\lambda} = \omega_{\lambda} - \omega_L$. ω_a , ω_L and ω_{λ} are the atomic resonant frequency, the applied field frequency and the frequency of a mode λ , respectively. ε is the resonant Rabi frequency of the applied field and g_{λ} is the atom-radiation field coupling constant. The Hamiltonian H_{dephase} describes additional dephasing interactions which may arise from atomic collisions and the scattering of phonons from the impurity atoms if the atoms are embedded in the solid part of a dielectric material. We assume for simplicity that the *phonon* DOS is broad and displays no sharp features. In this case, the dephasing part of the master equation for the atomic density operator can then be written as [77]

$$\left(\frac{\partial \rho}{\partial t} \right)_{\text{dephase}} = (\gamma_p/2)(2J_3 \rho J_3 - J_3^2 \rho - \rho J_3^2), \quad (7.3)$$

where γ_p is a phenomenological dephasing decay rate.

It is convenient to express the atomic operator J_{ij} in the Schwinger (boson) representation [78, 79]. We write $J_{ij} = a_i^{\dagger} a_j$ ($i, j = 1, 2$), where

$a_i^\dagger$ and a_i satisfy bosonic commutation relations and describe creation and annihilation of atoms in the state $|i\rangle$ with the additional constraint that $a_1^\dagger a_1 + a_2^\dagger a_2 = N$. The atom-applied field part of the Hamiltonian H_0 can be diagonalized using the following canonical transformation [78]: $a_1 = \cos \phi q_1 + \sin \phi q_2$, $a_2 = -\sin \phi q_1 + \cos \phi q_2$. This leads to the dressed state Hamiltonian,

$$H_0 = \hbar \Omega R_3 + \sum_{\lambda} \hbar \delta_{\lambda} a_{\lambda}^{\dagger} a_{\lambda}, \quad (7.4)$$

where $\sin^2 \phi = \frac{1}{2}[1 - \text{sign}(\Delta)/(4\varepsilon^2/\Delta^2 + 1)^{1/2}]$, $\Omega = (\varepsilon^2 + \Delta^2/4)^{1/2}$, $R_{ij} = q_i^\dagger q_j$ ($i, j = 1, 2$) are the dressed atomic operators, and $R_3 = R_{22} - R_{11}$. Clearly, $q_i^\dagger$ and q_i satisfy the bosonic commutation relations and represent creation and annihilation of atoms in the dressed state $|\tilde{i}\rangle$.

In dressed state basis $|\tilde{i}\rangle$, J_{21} and J_3 in the interaction Hamiltonian H_1 and $((\partial\rho/\partial t)_{\text{dephase}})$ must be replaced by $J_{21} = \sin \phi \cos \phi R_3 + \cos^2 \phi R_{21} - \sin^2 \phi R_{12}$ and $J_3 = \cos(2\phi)R_3 - \sin(2\phi)(R_{21} + R_{12})$. We define the time-dependent interaction picture Hamiltonian $\tilde{H}_1(t) = U^\dagger(t)H_1U(t)$ where $U(t) = \exp(-iH_0t/\hbar)$. The dressed state collective atomic operators in this interaction picture exhibit the time dependence $\tilde{R}_{21}(t) = \tilde{R}_{21}(0)\exp(2i\Omega t)$, $\tilde{R}_{12}(t) = \tilde{R}_{12}(0)\exp(-2i\Omega t)$, and $\tilde{R}_3(t) = \tilde{R}_3(0)$. Hereafter we drop the tilde on the interaction picture operators. Clearly R_3 , R_{12} , and R_{21} can be considered as the source operators for the central component, left and right sidebands of the Mollow triplet at frequencies ω_L , $\omega_L - 2\Omega$ and $\omega_L + 2\Omega$, respectively. In this interaction picture, the interaction Hamiltonian H_1 takes the form

$$\begin{aligned} H_1 = & i\hbar \sum_{\lambda} g_{\lambda} \left(\sin \phi \cos \phi a_{\lambda}^{\dagger} R_3 e^{i\delta_{\lambda} t} + \cos^2 \phi a_{\lambda}^{\dagger} R_{12} e^{i(\delta_{\lambda} - 2\Omega)t} \right. \\ & \left. - \sin^2 \phi a_{\lambda}^{\dagger} R_{21} e^{i(\delta_{\lambda} + 2\Omega)t} \right) + h.c. \end{aligned} \quad (7.5)$$

The dephasing part of the master equation remains in the same form (7.3) except with

$$J_3 = \cos(2\phi)R_3 - \sin(2\phi)(R_{21}e^{2i\Omega t} + R_{12}e^{-2i\Omega t}). \quad (7.6)$$

The collective spectral and statistical properties of these spectral components in free space (where the photonic DOS is smooth and featureless) can be found in [79, 80]. In this paper we consider the case when the DOS at the atomic transition frequency exhibits a step discontinuity or some other singularity so that the resulting Mollow spectral components experience strongly different mode densities. We also assume for simplicity that the photonic mode density, while singular at one frequency, is constant over the immediate spectral regions surrounding the dressed-state resonant frequencies ω_L , $\omega_L - 2\Omega$ and $\omega_L + 2\Omega$. In this case, the radiative part [77] of the

master equation for the reduced atomic density operator, ρ , takes the form:

$$\left(\frac{\partial \rho}{\partial t}\right)_{\text{rad}} = -\frac{1}{\hbar^2} \int_0^t dt' \text{Tr}_R \{ [H_1(t), [H_1(t'), \chi(t')]] \}. \quad (7.7)$$

Here χ is the density operator of the full atomic system plus electromagnetic reservoir, $\rho = \text{Tr}_R \{ \chi \}$, and Tr_R denotes a trace over the reservoir variables. In the Born approximation [77, 79–81] we replace $\chi(t')$ in equation (7.7) by $\rho(t') R_0$, where R_0 is an initial reservoir density operator. This corresponds to the second order perturbation theory in the interaction between atoms and reservoir. It assumes that changes in reservoir as a result of atom-reservoir interaction are negligible. Our second major simplification is the Markovian approximation which replaces $\rho(t')$ by $\rho(t)$. That is to say, we ignore the memory effects such as those arising from photon localization [76]. The dressed-state master equation for the density operator ρ in the *Born-Markoff approximation* for the case of a strong external field, takes the form:

$$\begin{aligned} 2\frac{\partial \rho}{\partial t} = & A_0 [R_3 \rho R_3 - R_3^2 \rho] + A_- [R_{21} \rho R_{12} - R_{12} R_{21} \rho] \\ & + A_+ [R_{12} \rho R_{21} - R_{21} R_{12} \rho] + h.c. \end{aligned} \quad (7.8)$$

Here, $A_0 = \gamma_0 \sin^2 \phi \cos^2 \phi + \gamma_p \cos^2(2\phi)$, $A_- = \gamma_- \sin^4 \phi + \gamma_p \sin^2(2\phi)$, and $A_+ = \gamma_+ \cos^4 \phi + \gamma_p \sin^2(2\phi)$. The spontaneous emission decay rates $\gamma_0 = 2\pi \sum_{\lambda} g_{\lambda}^2 \delta(\omega_{\lambda} - \omega_L)$, $\gamma_- = 2\pi \sum_{\lambda} g_{\lambda}^2 \delta(\omega_{\lambda} - \omega_L + 2\Omega)$ and $\gamma_+ = 2\pi \sum_{\lambda} g_{\lambda}^2 \delta(\omega_{\lambda} - \omega_L - 2\Omega)$ are proportional to the density of modes at the dressed-state transition frequencies. In deriving (7.8), we have also used the secular approximation [79–81] strong applied laser field with $\Omega \gg N\gamma_0$, $\Omega \gg N\gamma_-$, $\Omega \gg N\gamma_+$. That is, the fast oscillating terms with frequencies 2Ω and 4Ω in the master equation were ignored. Physically, it means the three Mollow spectral components are well separated and the overlap between them is negligible. We note, finally, that the master equation (7.8) reduces to the free space case [79, 80] when $\gamma_0 \cong \gamma_- \cong \gamma_+$.

It is convenient to introduce the dressed state ket vector $|n\rangle \equiv |N-n, n\rangle$ which denotes a symmetrized N -atom state in which $N-n$ atoms are in the lower dressed state $|\tilde{1}\rangle$ and n atoms are excited to the upper dressed state $|\tilde{2}\rangle$. Using the harmonic oscillator property of the Schwinger bosons, it follows that $R_{12}|n\rangle = \sqrt{n(N-n+1)}|n-1\rangle$, $R_{21}|n\rangle = \sqrt{(N-n)(n+1)}|n+1\rangle$, and $R_3|n\rangle = (2n-N)|n\rangle$. Using these rules and the master equation (7.8), it is straightforward to verify that diagonal matrix elements of the density operator $P_n \equiv \langle n|\rho|n\rangle$ satisfy the equation

$$\frac{\partial P_n}{\partial t} = n(N-n+1)[A_- P_{n-1} - A_+ P_n] - (n \rightarrow n+1). \quad (7.9)$$

In the steady state limit, $\partial \rho / \partial t = 0$, the off-diagonal elements of the density matrix vanish and the diagonal elements can be found by the detailed balance from equation (7.9) as $P_n = P_0 \xi^n$, where $\xi = A_- / A_+$ and

$P_0 = (\xi - 1)/(\xi^{N+1} - 1)$. Using atomic distribution function P_n , we derive $\langle n \rangle$ and $\langle n^2 \rangle$ in the form

$$\langle n \rangle = P_0 [N\xi^{N+2} - (N+1)\xi^{N+1} + \xi]/(\xi - 1)^2, \quad (7.10)$$

$$\langle n^2 \rangle = P_0 [N^2\xi^{N+3} - (2N^2 + 2N - 1)\xi^{N+2} + (N+1)^2\xi^{N+1} - \xi^2 - \xi]/(\xi - 1)^3, \quad (7.11)$$

where $\langle \dots \rangle$ stands for a steady-state expectation value. The atomic population per atom on the upper dressed state and bare state can be found for the case of $N \gg 1$ as

$$\langle R_{22} \rangle / N \cong \begin{cases} 1, & \text{if } \xi > 1 \\ 1/2, & \text{if } \xi = 1 \\ 0, & \text{if } \xi < 1 \end{cases} \quad (7.12)$$

$$\langle J_{22} \rangle / N \cong \begin{cases} \cos^2 \phi, & \text{if } \xi > 1 \\ 1/2, & \text{if } \xi = 1 \\ \sin^2 \phi, & \text{if } \xi < 1. \end{cases} \quad (7.13)$$

Clearly, the atomic population displays a sharp collective jump in which the active region of the photonic material switches from an absorptive medium to a gain medium as a function of the control laser field (change in the angle ϕ). A probe laser beam will experience a substantial differential gain when the control laser amplitude is in the vicinity of $\xi = 1$. In this sense, the system acts as a quantum optical transistor. For a *single* atom case, equation (7.12) is replaced by $\langle R_{22} \rangle / N = \xi/(\xi + 1)$. That is, there is no jump in a single atom case. It is apparent from the above analysis that phonon mediated dephasing processes have a tendency to destroy the collective switching. However, the influence of dephasing can be reduced or eliminated by increasing the number of atoms N or by detuning the control laser field frequency so that $\sin^2(2\phi)$ is small. In Figure 11 we plot $\langle J_{22} \rangle / N$ as functions of resonance Rabi frequency ε for the case of $\gamma_-/\gamma_+ = 10^{-3}$ and $\gamma_p/\gamma_+ = 0.5$. A large jump in the DOS, of this nature, may arise in a 3-d PBG material [82,83]. In other confined photonic systems such as wires and fibers, the jump in the DOS may be much weaker. In Figure 12, we show the collective jump for $0.3 < \gamma_-/\gamma_+ < 0.5$ for $N = 5000$. It is clear that a sizable switching behavior can be achieved even for small DOS variations and substantial phonon dephasing ($\gamma_p/\gamma_+ = 0.5$) when a large number of atoms responds collectively. This is possible when the left sideband lies in the gap of a PBG or in the cutoff region of the optical fibers and wires while the right sideband lies outside of the gap or of the cutoff region. It is apparent from Figures 11 and 12 that in the case of $N \gg 1$ ($N = 5 \cdot 10^3$ for Fig. 12 and the solid curve in Fig. 11) the atomic system switches very sharply from the ground state to the excited states at the critical value of ε .

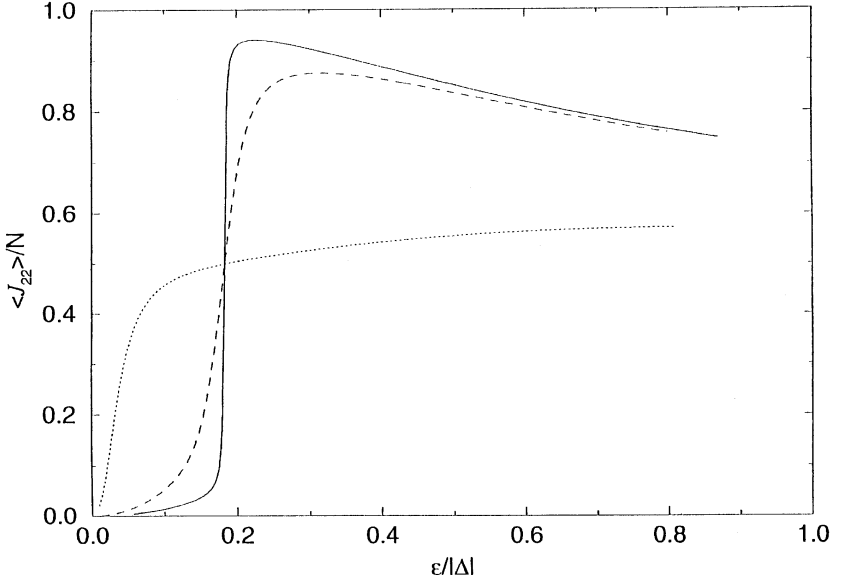


Fig. 11. Atomic population per atom on the bare excited states $\langle J_{22} \rangle / N$ as a function of $\epsilon / |\Delta|$ for $\gamma_- / \gamma_+ = 10^{-3}$, $\gamma_p / \gamma_+ = 0.5$, $\Delta = -1$, and for $N = 10$ (dotted curve), 500 (dashed curve), and 5000 (solid curve).

We note finally that the collective time scale for this switching is proportional to N^{-1} . As a result, this effect may be relevant for a very fast optical switching devices [84].

To characterize atomic fluctuations in the excited dressed and bare states, we introduce the Mandel q -parameters $Q_d = (\langle R_{22}^2 \rangle - \langle R_{22} \rangle^2) / \langle R_{22} \rangle$ and $Q_b = (\langle J_{22}^2 \rangle - \langle J_{22} \rangle^2) / \langle J_{22} \rangle$. The detailed analytical expression for Q_d and Q_b can be easily found using equations (7.10, 7.11). In particular, when $N \gg 1$, Q_d and Q_b are found as

$$Q_d \cong \begin{cases} 1/N, & \text{if } \xi > 1 \\ N/12, & \text{if } \xi = 1 \\ 1/(1 - \xi), & \text{if } \xi < 1 \end{cases} \quad (7.14)$$

$$Q_b \cong \begin{cases} \sin^2 \phi(\xi + 1)/(\xi - 1), & \text{if } \xi > 1 \\ (N + 2)/6, & \text{if } \xi = 1 \\ \cos^2 \phi(\xi + 1)/(1 - \xi), & \text{if } \xi < 1. \end{cases} \quad (7.15)$$

It is apparent from equation (7.14) that for $N \gg 1$ and $\xi > 1$, the q -Mandel parameter $Q_d \cong 0$. That is, the dressed-state atomic population inversion with strong sub-Poissonian atomic statistics occurs. Clearly, the

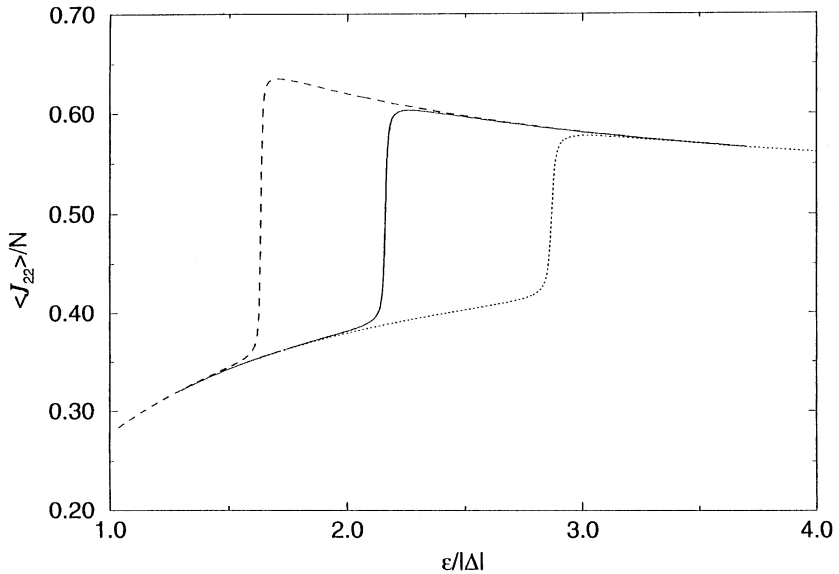


Fig. 12. Atomic population per atom on the bare excited states $\langle J_{22} \rangle / N$ as a function of $\epsilon / |\Delta|$ for $\gamma_p / \gamma_+ = 0.5$, $\Delta = -1$, $N = 5000$, and for $\gamma_- / \gamma_+ = 0.3$ (dashed curve), 0.4 (solid curve), and 0.5 (dotted curve).

dipole dephasing due to phonons has only a limited influence on the sub-Poissonian distribution of atoms on the upper dressed state. In contrast, the atom statistics on the excited bare state $|2\rangle$ depends quite strongly on the dephasing decay rate γ_p . For example, in the case of $\gamma_- / \gamma_+ \ll 1$, equation (7.15) reduces to: $Q_b \cong \cos^2 \phi + 8(\gamma_p / \gamma_+) \sin^2 \phi$. That is, Q_b tends to zero only if $\cos^2 \phi \ll 1$ and $\gamma_p / \gamma_+ \ll 1$. It is useful to note here that in free space no population inversion is available in this system [79, 80] and that the distribution of atoms on the excited state $|2\rangle$ is super-Poissonian rather than sub-Poissonian.

In Figure 13 plot Q_b as functions of resonance Rabi frequency ϵ for the case of $N = 5.10^3$, $\gamma_- / \gamma_+ = 10^{-3}$ and for different values of γ_p / γ_+ . At the switching threshold there is a large (proportional to the number of atoms N) increase in fluctuations, characteristic of a phase transition. It is apparent from Figure 13 that the Mandel parameter Q_b for atoms on the bare excited state can be small for the case when the dephasing decay rate caused by atomic collisions or phonons is small compared to the radiative decay rate outside the gap ($Q_b \cong 0.19$ for $\gamma_p / \gamma_+ = 0.01$). It suggests that the above considered system may be relevant for a new mechanism of sub-Poissonian pumping for lasers [85, 86] and dressed-state lasers [87]. Lasers exhibiting

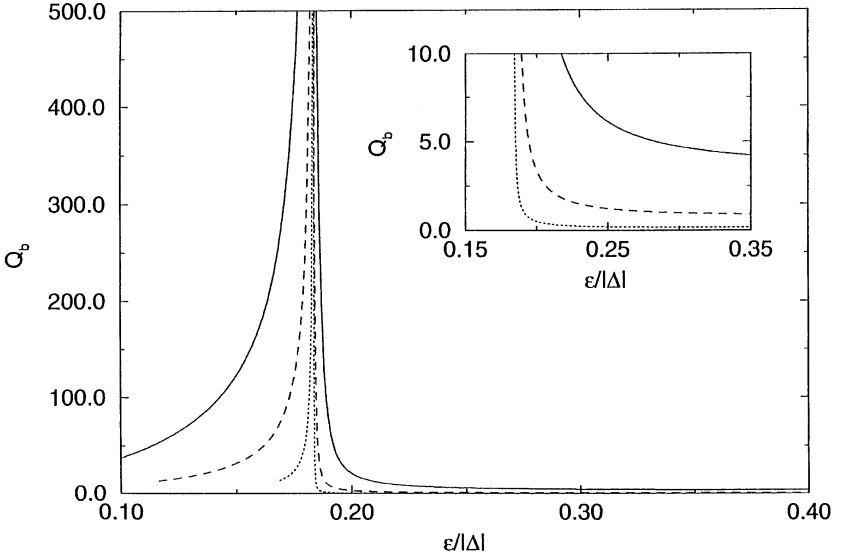


Fig. 13. q -Mandel's parameter Q_b as a function of $\epsilon/|\Delta|$. $\gamma_-/\gamma_+ = 10^{-3}$, $\Delta = -1$, $N = 5000$, and for $\gamma_p/\gamma_+ = 0.5$ (solid curve), 0.1 (dashed curve), and 0.01 (dotted curve). Inset shows an expanded view of the same curves in the regime of sub-Poissonian statistics of excited atoms.

sub-Poissonian photon statistics may have applications in noiseless optical data transfer.

The analysis we have presented in this paper provides a qualitative picture of collective switching, sub-Poissonian statistics, and optical amplification in the regime of strong external laser fields. By using a strong laser field, it is possible to drive the Mollow spectral components away from the photon DOS singularity so that over the width of the individual sidebands, the DOS is smooth. For weaker fields, the singularity in the DOS can lead to important non-Markovian effects. A more detailed calculation for a specific van Hove singularity may lead to the lower threshold and much faster switching. In particular, the collective time scale factor near a three-dimensional photonic band edge has been shown to be proportional to N^2 [32]. That is, the switching speed may be proportional to N^2 when photon localization and other non-Markovian effects are included.

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COURSE 8

ENVIRONMENT-INDUCED DECOHERENCE AND THE TRANSITION FROM QUANTUM TO CLASSICAL

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ENVIRONMENT-INDUCED DECOHERENCE AND THE TRANSITION FROM QUANTUM TO CLASSICAL

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Abstract

We study dynamics of quantum open systems, paying special attention to these aspects of their evolution which are relevant to the transition from quantum to classical. We begin with a discussion of the conditional dynamics of simple systems. The resulting models are straightforward but suffice to illustrate basic physical ideas behind quantum measurements and decoherence. To discuss decoherence and *environment-induced superselection* (*einselection*) in a more general setting, we sketch perturbative as well as exact derivations of several master equations valid for various systems. Using these equations we study einselection employing the general strategy of the predictability sieve. Assumptions that are usually made in the discussion of decoherence are critically reexamined along with the “standard lore” to which they lead. Restoration of quantum-classical correspondence in systems that are classically chaotic is discussed. The dynamical second law – it is shown – can be traced to the same phenomena that allow for the restoration of the correspondence principle in decohering chaotic systems (where it is otherwise lost on a very short time-scale). Quantum error correction is discussed as an example of an anti-decoherence strategy. Implications of decoherence and einselection for the interpretation of quantum theory are briefly pointed out.

1 Introduction and overview

The quantum origin of the classical world was so difficult to imagine for the forefathers of quantum theory that they were often willing to either postulate its independent existence (Bohr), or even to give up quantum theory and look for something with more fundamental classical underpinnings

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(de Broglie, and, to a lesser extent, also Einstein). The source of the problem is the quantum principle of superposition, which, in effect, exponentially expands the set of available states to all of the conceivable superpositions. Thus, coherent superpositions of dead and alive cats have – in the light of the quantum theory – the same right to exist as either of the two classical alternatives. Within the Hilbert space describing a given system “classically legal” states are exceptional. The set of all states in the Hilbert space is enormous as compared with the size of the set of states where one finds classical systems. Yet, it is a fact of life that classical objects are only found in a very small subset of all possible (and in principle, allowed) states. So, one has to explain the origin of this apparent “super-selection” rule that prevents the existence of most states in the Hilbert space of some physical systems. Decoherence and its principal consequence – environment-induced super-selection or *einselection* – account for this experimental fact of life.

Decoherence is caused by the interaction between the system and its environment. Under a variety of conditions, which are particularly easy to satisfy for macroscopic objects, it leads to the *einselection* of a small subset of quasi-classical states from within the enormous Hilbert space. The classicality is then an emergent property, induced in the system by its interaction with the environment. Arbitrary superpositions are dismissed, and a preferred set of “pointer states” emerges. These preferred states are the candidate classical states. They correspond to the definite readings of the apparatus pointer in quantum measurements, as well as to the points in the phase space of a classical dynamical system.

The role of the process of decoherence in inducing classicality has become clear only relatively recently – within the past two decades. The key idea is relatively simple: an environment of a quantum system can, in effect, monitor its states through continuous interaction. The imprint of the system left on the environment will contain information about selected states of the system. The states that leave the imprint without getting perturbed in the process are the preferred states. Thus, the key property of quasi-classical pointer states is their insensitivity to monitoring by – and consequently their resistance to the entanglement caused by – interaction with the environment: states that entangle least are most stable. They are also, almost by definition, the only states that remain an accurate description of the system alone: All other states evolve into joint system-environment states, preserving their purity (and, consequently, the information the observer has about them) only when both the system and the environment are included in a larger “super system”.

The fact that the interaction between quantum systems produces entanglement was well known almost since the beginning of quantum theory. Indeed, because the ideas of decoherence and *einselection* rely on quantum theory, and on quantum theory alone, it may be useful to ask why it took

so long to arrive at a natural explanation of the quantum origins of classicality. There are several possible explanations for this delay. We shall return to them later in the paper. But, for the moment, it is useful to note that the ability of environment-induced decoherence to result in the same set of preferred states, essentially independently of the initial state of the system and the environment, is crucial. This was not appreciated until relatively recently [1, 2]. It is precisely this stability of the set of preferred states that allows them to be regarded as good candidates for the quantum counterparts of classical reality. Indeed, only still more recent research on the predictability sieve has allowed for more fundamental and general understanding of the emergent classicality (see [3, 4] and also [5]).

The prejudice that seems to have delayed serious study of the role of the “openness” of a quantum system in the emergence of classicality is itself rooted in the classical way of thinking about the Universe. Within the context of classical physics, all fundamental questions were always settled in the context of closed systems. The standard strategy to ensure isolation involved enlarging a system – *i.e.*, by including the immediate environment. The expectation was that in this manner one can always reduce any open system to a larger closed system. This strategy does indeed work in classical physics, where the enlargement can help in satisfying conservation laws for quantities such as energy or momentum. It fails in the quantum case under discussion, because now it is the information (about the state of the system) that must be prevented from spreading. Information is much harder to contain when the system in question becomes larger. Thus, in the end, the only truly isolated macroscopic system is the Universe as a whole. And we, the observers, are certainly not in a position to study it from the outside.

In what sense is the preferred set of states preferred? It is clear that generic superposition of the members of this preferred set will decay into mixtures. On the other hand, if the initial state is just one of the members of the preferred set, the temporal evolution will minimally affect the state, which will resist becoming entangled with the environment. Einselection can thus be thought of as a process by which a “record” of the state of the system is created dynamically (through interaction) in the state of the environment. It is this ongoing process by which the system is being continuously monitored by the environment that leads to the emergence of a natural set of preferred states that are the least affected by the interaction.

As sketched above, the physical principles of decoherence and einselection appear, in retrospect, rather straightforward. How much can be accomplished by exploring their consequences? There are several interesting and important questions that naturally arise in this context and that have been asked (and answered, in most cases) over the last two decades. First, one naturally asks how much can we explain with these ideas (*i.e.*, is it consistent to think that all objects that are known to behave classically

are doing so because of decoherence?). A closely related question is the one concerning natural time-scales associated with decoherence. How fast does decoherence take place? This is a very important question because a first look at the decoherence process may leave us wondering if decoherence may be consistent with the existence of a “reversible” classical world. Thus, if one believes that classicality is really an emergent property of quantum open systems one may be tempted to conclude that the existence of emergent classicality will always be accompanied by other manifestations of openness such as dissipation of energy into the environment (this would be a problem because, as we know, there are many systems that behave classically while conserving energy). Second, one also wonders how, in detail, is the preferred set of states dynamically selected through the interaction with the environment. In particular, it is interesting to know how this pointer basis is determined by the structure of the interaction Hamiltonian between system and environment and/or to the other details of the physics involved. Third, a related question arises in this context: are there observable manifestations of decoherence other than einselection?

A remarkable characteristic of the current debates on the nature of the quantum to classical transition and on the problem of quantum measurement is that for the first time in history there have been actual experiments probing the boundary between the quantum and the classical domains in a controlled way [6–10]. Controlled decoherence experiments (which are very difficult because nature provides us with classical or quantum systems but not with objects whose interaction with the environment can be controlled at will) were recently carried on for the first time and help us in understanding the nature of this process. Some of the most notable experiments in this area were performed at the École Normale Supérieure in Paris and are be part of Brune’s lectures.

Our lectures start with an introduction to quantum conditional dynamics using two-state systems. Conditional dynamics is responsible both for setting up the problem of measurement, and for the decoherence and einselection that solve it. The resulting models are straightforward and can serve in the idealized studies of the measurement process. However, they are clearly too simple to be realistic – classicality is, after all, a property of essentially every sufficiently macroscopic object. To discuss decoherence and einselection in this more general setting, we shall therefore study dynamics of quantum open systems. Section 3 is devoted to the derivation of the key tool – a master equation for the reduced density matrix. This basic tool is immediately used in Section 4, where environment-induced superselection is studied, including, in particular, the predictability sieve. Section 5 analyzes some “loose ends” – that is, essentially technical issues that are usually omitted in the derivations of the master equations. We show there that although the qualitative conclusions arrived at on the

basis of the “naive” master equation approach are essentially unaffected by the detailed examination of some of the idealized assumptions that go into its derivation, quantitative estimates can change quite significantly when a more realistic approach is adopted. Section 6 is devoted to the study of the effect of decoherence on the quantum-classical correspondence in systems that are classically chaotic. We show there that decoherence not only explains the origin of classical dynamics, but that it may be responsible for the loss of information that accounts for the second law of thermodynamics as well. Section 7 is devoted to quantum error correction – to the strategies which can be used to suppress decoherence. The summary and conclusions are briefly stated in Section 8.

2 Quantum measurements

In this section we shall introduce the measurement problem – the issue that has dominated the discussion of the relation between quantum and classical for a very long time. This will afford us the opportunity to study conditional dynamics that will be employed in one form or another throughout this review. Such interactions are necessary to achieve entanglement between quantum systems that set up the measurement problem. They are necessary for accomplishing decoherence, which leads to environment-induced superselection (or einselection), and thus resolves many of the problems arising on the border between quantum and classical. Last, but not least, quantum conditional dynamics and entanglement underlie quantum logic and will be of importance in the latter part of the paper devoted to quantum error correction.

Predictability is rightly regarded as one of the key attributes of classical dynamics. On the other hand, the defining feature of quantum mechanics is thought to be its probabilistic nature, which manifests itself in measurements. This discord between classical determinism and quantum randomness is often blamed for the difficulties with interpretation of quantum theory. Yet, the fundamental equations of either classical or quantum theory allow them – indeed, demand of them – to be perfectly predictable: it is just that what can be predicted with certainty, especially in the quantum case, cannot be often accessed by measurements. And, conversely, what can be measured in an evolving quantum system cannot usually be predicted, except in the probabilistic sense.

The Schrödinger equation allows one to predict the state of an isolated system at any subsequent moment of time. In an isolated quantum system, dynamical evolution is strictly deterministic. This perfect quantum predictability could be of use only if one were to measure observables that have the resulting evolving state as one of its eigenstates. These observables

are generally inaccessible to reasonable measuring devices, and therefore are of no interest.

Quantum determinism is of little use for an observer who is only a part of the whole system. The overall quantum determinism could have predictive power only for someone who is (i) monitoring quantum systems from the outside. Moreover, it would help if the observer was endowed with (ii) enough memory to measure and store data, and (iii) sufficient ability to compute and to model deterministic evolution of the system of interest. For an observer trapped inside of the quantum universe, this is obviously not the case.

The universe is all there is. Therefore, by definition, it is a closed quantum system. Given the deterministic nature of the Schrödinger evolution, one may be surprised that there is a problem with the interpretation of quantum theory. After all, the interpretational ideal often mentioned in such discussions is deterministic Newtonian dynamics. However, the interpretation problem stems from the fact that deterministic unitary evolution of quantum theory is incompatible with classical determinism. Indeed, as the studies of chaotic systems demonstrate, classical dynamics has more room for randomness than quantum physics.

States of the quantum systems are perturbed by the very act of monitoring them. The elemental unpredictability associated with the act of observation cannot be avoided unless the observer knows in advance which observables can be measured with impunity. This feature of quantum information is essential to guarantee the security of quantum cryptography (see lectures of Ekert; also [11]) – the state of a quantum system cannot be found out by the eavesdropper unless the observation is carried out on the same basis as the one used by the intended recipient of the message. The “no cloning theorem” [12, 13] prevents duplication of quantum information – amplification is associated with breaking the symmetry associated with the superposition principle.

Environment-induced superselection rules allow the observer to be a successful eavesdropper, and to extract useful information from the quantum systems without the environment getting in the way because (in contrast to the strategies employed in quantum cryptography) the measurements carried out by the environment are restricted to few observables. The state of the system is therefore of necessity “precollapsed” and commutes with these observables. Further measurements carried out by the observer will only reveal (rather than perturb) the pre-existing state of affairs. Thus, environment-induced decoherence supplies a justification for the persistent impression of “reality”. In contrast to the observables encountered in the microscopic realm, macroscopic quantum systems can appear only in one of the preselected (pointer basis) set of quantum states. The “collapse of the wavepacket” viewed in this way is just a familiar classical process of finding

out which of the possible outcomes has actually occurred. The danger of interference between the alternatives was eradicated by decoherence long before the observer became involved.

How can one ever hope for a resolution that would allow for the familiar combination of classical determinism and classical randomness to emerge? At the risk of anticipating results that will be justified in detail only later, we note that quantum determinism may be relevant only for an observer who knows the initial state of an isolated quantum system. For a quantum observer immersed in a quantum universe this is a very rare exception, attainable only in carefully controlled laboratory experiments, and only for rather small quantum systems. The information capacity, memory, and information processing abilities of an observer that is a (macroscopic, yet comparatively small) subsystem of the universe are miniscule compared to the task of simulating even a small quantum system, let alone the universe as a whole. And as soon as the idea of the observer knowing the entire state of the universe is recognized as not feasible, “environmental monitoring” of both the state of the observer and of the observables he recorded begins to matter. An observer with decohering memory can keep reliable records only in the einselected states of his/her memory bits [3, 14–17]. Records will have predictive power only when they correlate with the einselected observables in the rest of the universe.

2.1 Bit-by-bit measurement and quantum entanglement

This problem of transition from quantum determinism to classical definiteness is illustrated most vividly by the analysis of quantum measurements. An answer to a “generic” question about the state of a quantum system (and the outcome of a measurement of the corresponding observable) is *not* deterministic. In the usual textbook discussions, this random element is blamed on the “collapse of the wavepacket” that is invoked whenever a quantum system comes into contact with a classical apparatus. In a fully quantum discussion of the problem, this issue still arises, in spite (or rather because) of the overall deterministic quantum evolution of the state vector of the universe. Indeed, as carefully pointed out by von Neumann [18] in his quantum analysis of measurements, there seems to be no room for “real collapse” in purely unitary models of measurements.

To illustrate the ensuing difficulties, we consider with von Neumann a quantum system $\mathcal{S}$ initially in a state $|\psi\rangle$ interacting with a quantum apparatus $\mathcal{A}$ initially in a state $|A_0\rangle$. The interaction will generally result in an entangled final state,

$$|\Psi_0\rangle = |\psi\rangle|A_0\rangle = \left(\sum_i a_i |s_i\rangle \right) |A_0\rangle \longrightarrow \sum_i a_i |s_i\rangle |A_i\rangle = |\Psi_t\rangle. \quad (2.1)$$

Here $\{|A_i\rangle\}$ and $\{|s_i\rangle\}$ are states in the Hilbert spaces of the apparatus and of the system, respectively, and a_i are complex coefficients. This transition can be accomplished by means of a unitary Schrödinger evolution. It leads to an uncomfortable conclusion. All that an appropriate interaction between $\mathcal{A}$ and $\mathcal{S}$ can achieve is putting the measuring apparatus (or an observer) in an EPR-like *entangled state* of all the possible outcomes consistent with the initial state [1]. Operationally, this EPR-like nature of the state emerging from the pre-measurement (as the step achieved by Eq. (2.1) is often called) can be made more explicit by rewriting the sum in a different basis

$$|\Psi_t\rangle = \sum_i a_i |A_i\rangle |s_i\rangle = \sum_i b_i |B_i\rangle |r_i\rangle = |\Psi_t\rangle. \quad (2.2)$$

All we have done is use an alternative basis for both the apparatus and the system, exploiting the freedom of choice guaranteed by the quantum principle of superposition. Therefore, if one were to associate the state of the apparatus (observer) with a state in the decomposition of $|\Psi_t\rangle$, then even before one could start enquiring about the specific outcome of the measurement one would have to decide what decomposition of $|\Psi_t\rangle$ is to be used, because the change of the basis corresponds to a redefinition of the measured quantity.

One could make the clash between quantum and classical even more dramatic by making an additional measurement on the same quantum system after the premeasurement correlation is established. In accord with equation (2.2), such additional measurement would have a power to select an arbitrary observable of the system $\mathcal{S}$ and would single out the corresponding states of the apparatus $\mathcal{A}$. Yet, given the freedom to rewrite $|\Psi_t\rangle$ in an infinite number of ways, this state of $\mathcal{A}$ would be for almost any choice of the decomposition of the sum of equation (2.2) completely “nonclassical” in any reasonable sense, and it would depend on the initial state of the quantum system.

In a quantum domain, such an entanglement must be commonplace, along with its disturbing consequences. Indeed, a “Schrödinger kitten” state recently implemented by means of an atomic physics experiment ([19] is an excellent illustration of the distinction between the quantum entanglement and the classical correlation in the context of quantum measurements). The NIST group in Boulder has managed – manipulating a single ion inside a trap with lasers – to establish a correlation between its internal state (designated here by $\{|\uparrow\rangle, |\downarrow\rangle\}$, respectively, for “excited” and “ground”) and its location ($|L\rangle$ or $|R\rangle$ for “left” or “right”). The final correlated wavefunction has a premeasurement, EPR-like form,

$$|\Psi_A\rangle = (|+\rangle|L\rangle + |-\rangle|R\rangle)/\sqrt{2}, \quad (2.3)$$

where

$$|\pm\rangle = (|\uparrow\rangle \pm |\downarrow\rangle)/\sqrt{2} \ , \quad (2.4)$$

are superpositions of the ground and excited states. This very same $|\Psi_A\rangle$ can be written therefore as

$$|\Psi_A\rangle = \{|\uparrow\rangle(|L\rangle + |R\rangle) + |\downarrow\rangle(|L\rangle - |R\rangle)\}/\sqrt{2} \ . \quad (2.5)$$

Thus, the same correlated state of the “atom cat” can be expressed in two very different-looking ways, implying the potential for still more kinds of ambiguous correlations. Expressed in the first way (see Eq. (2.3)), the atom can be in one of the two alternative locations, depending on its internal state that is defined as a superposition of ground and excited states. In the second way (given by Eq. (2.5)) the natural internal states of the atom are correlated with a very nonclassical state – a superposition of an atom in two locations. Monroe *et al.* [19] measure the internal state of the atom in the basis corresponding to the decomposition of equation (2.5) and verify that it is indeed in a superposition of $|L\rangle$ and $|R\rangle$ with either a positive or a negative sign (an “even” or an “odd” Schrödinger cat).

Given the atomic size of this “kitten”, its ability to appear in a superposition of two different widely separated locations may or may not be a surprise. But the point this recent experiment allows us to make is at the heart of the interpretation problem. If the quantum laws are universally valid, very nonclassical Schrödinger cat-like states should be commonplace for an apparatus that measures a quantum system and, indeed, for run-of-the-mill macroscopic systems in general. One should be able to prepare such nonclassical states at will, by entangling arbitrarily large objects with quantum states of microscopic systems and then measuring these quantum objects in some arbitrary basis. If such sequences of events were common, classical objects would almost always be in very nonlocal superposition states.

Quantum theory mandates this pandemonium. Yet, we never seem to encounter it, least of all in the course of measurements. The task of the interpretation of quantum theory is to understand why. In the Copenhagen interpretation, this problem never arises, because the apparatus is by definition classical. However, if one insists on the universality of quantum theory, the difficulty described above is inevitable. It arises, for instance, in Everett’s Many Worlds Interpretation, which was in fact originally called “the Relative State Interpretation” [20]. Everett and other followers of the MWI philosophy tried to occasionally bypass this question by insisting that one should only discuss correlations. Correlations are indeed at the heart of the problem, but it is not enough to explain how to compute them; for that, quantum formalism is straightforward enough. What is needed instead is an explanation of why some states retain correlations, but most of them do not, in spite of the arbitrariness in basis selection that is implied

by equation (2.2). Or, equivalently, what is needed is an explanation of the loss of general quantum entanglement, but a selective retention of classical correlations – correlations that are also quantum in their origin, but which consistently single out the same basis of the quantum states violating the spirit of the superposition principle.

2.2 Interactions and the information transfer in quantum measurements

The interaction required to accomplish the correlation between the measured system and the apparatus, equation (2.1), can be regarded as a generalization of the basic logical operation known as a “controlled not” or a **c-not**. Classically, **c-not** changes the state of the target bit when the control bit is in a state 1, and does nothing otherwise:

$$\begin{array}{ccc} 0_c & \begin{array}{c} 0_t \\ 1_t \end{array} & \longrightarrow & 0_c & \begin{array}{c} 0_t \\ 1_t \end{array} \\ 1_c & \begin{array}{c} 0_t \\ 1_t \end{array} & \longrightarrow & 1_c & \begin{array}{c} 1_t \\ 0_t \end{array} \end{array} \quad (2.6)$$

Quantum **c-not** is a straightforward quantum version of equation (2.6). It differs from the classical case only because arbitrary superpositions of the control bit and of the target bit are allowed

$$(\alpha|0_c\rangle + \beta|1_c\rangle)|a_t\rangle \longrightarrow \alpha|0_c\rangle|a_t\rangle + \beta|1_c\rangle|\neg a_t\rangle. \quad (2.7)$$

Above a “negation” of a state $|\neg a_t\rangle$ is a basis-dependent operation defined by

$$\neg(\gamma|0_t\rangle + \delta|1_t\rangle) = \gamma|1_t\rangle + \delta|0_t\rangle. \quad (2.8)$$

It suffices to identify $|A_0\rangle = |0_t\rangle$, and $|A_1\rangle = |1_t\rangle$ to have an obvious correspondence between the **c-not** and a premeasurement.

In the classical **c-not** the direction of the information transfer is always consistent with the designations of the two participating bits. The state of the control bit remains unchanged while it controls the state of the target bit, equation (2.6). Written in terms of the logical $\{|0\rangle, |1\rangle\}$ basis, the truth table of the quantum **c-not** is essentially – that is, save for the possibility of superpositions – the same as equation (2.6). One might therefore anticipate that the direction of information transfer and the designations (“control/system” and “target/apparatus”) of the two qubits will also be unambiguous, as they are in the classical case. This expectation however is incorrect, as can be readily demonstrated by expressing the process in the conjugate basis $\{|+\rangle, |-\rangle\}$ that, for either control or target bit, is obtained through the Hadamard transform:

$$|\pm\rangle = (|0\rangle \pm |1\rangle)/\sqrt{2}. \quad (2.9)$$

The truth table of equation (2.6) in conjunction with the principle of superposition (which allows one to write down Eq. (2.9)) leads to a new complementary truth table

$$\begin{aligned} |\pm\rangle|+\rangle &\longrightarrow |\pm\rangle|+\rangle \\ |\pm\rangle|-\rangle &\longrightarrow |\mp\rangle|-\rangle. \end{aligned} \quad (2.10)$$

That is, in the complementary basis $\{|+\rangle, |-\rangle\}$ the roles of the control and the target bit are reversed. The state of the former target – represented by the second ket in equation (2.10) – remains unaffected in the new basis, and the state of the former control is conditionally “flipped”.

In the above **c-not** (or bit-by-bit measurement), the appropriate interaction Hamiltonian is

$$\begin{aligned} H_{\text{int}} &= g|1\rangle\langle 1|_S|-\rangle\langle -|_{\mathcal{A}} = \frac{g}{2}|1\rangle\langle 1|_S(\mathbf{1} - (|0\rangle\langle 1| + |1\rangle\langle 0|))_{\mathcal{A}} \\ &= g\left(\frac{1}{2} - \sigma_z\right)_{\mathcal{A}}\left(\frac{1}{2} - \sigma_x\right)_S. \end{aligned} \quad (2.11)$$

Above, g is a coupling constant, σ_i are Pauli matrices, and the two operators refer to the system (*i.e.*, to the former control), and to the apparatus pointer (the former target), respectively. It is easy to see that the states $\{|0\rangle, |1\rangle\}_S$ of the system are unaffected by H_{int} , because

$$[H_{\text{int}}, e_0|0\rangle\langle 0| + e_1|1\rangle\langle 1|] = 0. \quad (2.12)$$

Thus, the measured (control) observable $\hat{e} = e_0|0\rangle\langle 0| + e_1|1\rangle\langle 1|$ is a constant of motion under the evolution generated by H_{int} .

The states $\{|+\rangle, |-\rangle\}_{\mathcal{A}}$ of the apparatus (which encode the information about the phase between the logical states) have exactly the same “immunity”

$$[H_{\text{int}}, f_+|+\rangle\langle +| + f_-|-\rangle\langle -|] = 0. \quad (2.13)$$

Hence, when the apparatus is prepared in a definite phase state (rather than in a definite pointer/logical state), it will pass its phase onto the system, as the truth table, equation (2.10), shows. Indeed, H_{int} can be rewritten in the Hadamard transformed basis

$$\begin{aligned} H_{\text{int}} &= g|1\rangle\langle 1|_S|-\rangle\langle -|_{\mathcal{A}} \\ &= \frac{g}{2}(\mathbf{1} - (|-\rangle\langle +| + |+\rangle\langle -|))_S|-\rangle\langle -|_{\mathcal{A}}, \end{aligned} \quad (2.14)$$

which, in comparison with equation (2.11), makes this “immunity” obvious.

This basis-dependent direction of the information flow in a quantum **c-not** (or in a premeasurement) is a direct consequence of complementarity. It can be summed up by stating that although the information about the

observable with the eigenstates $\{|0\rangle, |1\rangle\}$ travels from the measured system to the apparatus, in the complementary $\{|+\rangle, |-\rangle\}$ basis it seems to be the apparatus that is being measured by the system. This observation also clarifies the sense in which phases are inevitably “disturbed” in measurements. They are not really destroyed, but, rather, as the apparatus measures a certain observable of the system, the system “measures” the phases between the possible outcome states of the apparatus. These phases in a macroscopic apparatus coupled to the environment are fluctuating rapidly and uncontrollably, thus leading to the destruction of phase coherence. However, even if this consequence of decoherence were somehow prevented (*i.e.*, by perfectly isolating the apparatus pointer from the environment), preexisting phases between the outcome states of the apparatus would have to be known while, simultaneously, $\mathcal{A}$ is in $|A_0\rangle$, the “ready-to-measure-state”. This would require a simultaneous knowledge of the two non-commuting observables, and is therefore impossible because of Heisenberg indeterminacy.

It appears that even the question “which of the two interacting systems is a measuring device?” (which should be decided by the direction of the flow of information) depends on the initial states. In “classical practice” this ambiguity does not arise because the initial state of the apparatus can never be selected at the whim of the observer. Einselection limits the set of possible states of the apparatus to a small subset of all the states available in Hilbert space.

2.3 *Monitoring by the environment and decoherence*

In this section, we shall see how the quantum-classical correspondence can be reestablished by decoherence and einselection, caused by the monitoring of the to-be-classical observables by the environment. The environment is defined as any set of degrees of freedom that are coupled to the system of interest, and which can therefore “monitor” – become entangled with – its states. Environments can be external (such as particles of air or photons that scatter off, say, the apparatus pointer) or internal (*e.g.*, collections of phonons or other excitations in the materials from which an apparatus is constructed). Often, environmental degrees of freedom emerge from the split of the original set of degrees of freedom into the “system of interest” that is some collective observable (order parameter in a phase transition), and the “microscopic remainder”.

The superposition principle applies only when the quantum system is closed. When the system is open, interaction with the environment will inevitably result in an incessant “monitoring” of some of the observables by the environmental degrees of freedom. This will result in the degradation of the pure states into mixtures. These mixtures will often – remarkably often – turn out to be diagonal in the same set of “preferred states” that are nearly independent of the initial state of the system and of the environment,

but which are selected with the crucial help of the interaction Hamiltonian. This decoherence process determines the relative “fitness” of all the possible superpositions that exist in the Hilbert space. The resulting “natural selection” is responsible for the emergence of classical reality. Its consequence is known as environment-induced superselection [2], or einselection.

The set of habitually decohering states is often called “the pointer basis”, in recognition of its role in the measurement problem. The criterion for the selection of pointer states goes well beyond the often-repeated characterizations based solely on the instantaneous eigenstates of the density matrix. What is of the essence is the ability of the einselected states to survive monitoring by the external degrees of freedom. This heuristic criterion can be made rigorous by quantifying the predictability of the evolution of the candidate classical states or of the associated pointer observables. To put it succinctly, measurement of the pointer observables yields an optimal initial condition. In spite of the openness of the system, its results can be employed for the purpose of prediction better than the other Hilbert space alternatives.

The contrast between the resilience of the states associated with the preferred (pointer) observables and the fragility of their superpositions can be analyzed in terms of Heisenberg’s principle of indeterminacy. The environment monitors observables with the accuracy dictated by the interaction Hamiltonian. Thus, only a measurement that happens to commute with the observables monitored by the environment will result in a useful record that can be successfully employed for the purpose of prediction. In contrast, a system prepared by the measurement in an arbitrary superposition will also be monitored by the environment, which will tend to correlate with the pointer observable. When the initial superposition prepared by the observer does not commute with the observables monitored by the environment, Heisenberg’s indeterminacy implies that the records of the observer are of no use for the purpose of prediction. The monitoring continuously carried out by the environment on the pointer observables makes anything except for the pointer states a poor choice.

Three quantum systems – the measured system $\mathcal{S}$, the apparatus pointer or the memory of the observer $\mathcal{A}$, and the environment $\mathcal{E}$ – and the correlations between them will be the subject of the discussion below. In quantum measurements, $\mathcal{S}$ and $\mathcal{A}$ will be coupled. Their quantum entanglement will be converted into an effectively classical correlation as a result of the interaction between $\mathcal{A}$ and $\mathcal{E}$. In measurements of classical systems, both $\mathcal{S}$ and $\mathcal{A}$ will interact with $\mathcal{E}$ and decohere. In either case, states einselected by the environment will be the focus of attention. In $\mathcal{A}$, they will be the repository of information, serving as pointer states of the apparatus or memory states of the observer. The system $\mathcal{S}$ can also look effectively classical when it is subject to einselection, and when $\mathcal{A}$ keeps records of its einselected states.

This $\mathcal{SAE}$ triangle (or a triangle much like it) is necessary for careful study of decoherence and its consequences. By keeping all three corners of this triangle in mind, one can avoid the confusion about the relation of the instantaneous eigenstates of the density matrix (see, for example, the discussion following [21]). This three-system context is necessary to keep track of the correlations between the memory of the observer and the state of the measured system. The evolution from a quantum entanglement to the classical correlation may be the easiest relevant theme to define operationally. In spite of this focus on the correlation, I shall often suppress one of the corners of the above triangle to simplify the equations. All three parts of the triangle will however play a role in formulation of the questions we shall pose and in motivating of the criteria for classicality that we shall devise.

2.4 One-bit environment for a bit-by-bit measurement

The simplest discussion of a single act of decoherence involves just three one-bit systems [1,22]. They are denoted by $\mathcal{S}$, $\mathcal{A}$, and $\mathcal{E}$ in an obvious reference to their designated roles. The measurement starts with the interaction of a measured system with the apparatus,

$$\begin{aligned} |\uparrow\rangle|A_0\rangle &\longrightarrow |\uparrow\rangle|A_1\rangle \\ |\downarrow\rangle|A_0\rangle &\longrightarrow |\downarrow\rangle|A_0\rangle, \end{aligned} \quad (2.15)$$

where $\langle A_0|A_1\rangle = 0$. For a general state,

$$(\alpha|\uparrow\rangle + \beta|\downarrow\rangle)|A_0\rangle \longrightarrow \alpha|\uparrow\rangle|A_1\rangle + \beta|\downarrow\rangle|A_0\rangle = |\Phi\rangle. \quad (2.16)$$

These formulae are an example of a **c-not**-like premeasurement that has already been discussed. As was noted previously, a correlated state of this form is not enough to claim that a measurement has taken place. The biggest problem with $|\Phi\rangle$ is the basis ambiguity. Equation (2.16) represents only an entanglement, the same as in Bohm's version of the EPR state [23]. The ambiguity of the basis selection in this simple example can be settled with the help of one additional system, $\mathcal{E}$, which performs a premeasurement on the apparatus. As a result,

$$\begin{aligned} |\Psi(0)\rangle_{\text{SAE}} &= (\alpha|\uparrow\rangle|A_1\rangle + \beta|\downarrow\rangle|A_0\rangle)|\varepsilon_0\rangle \longrightarrow \\ &\longrightarrow \alpha|\uparrow\rangle|A_1\rangle|\varepsilon_1\rangle + \beta|\downarrow\rangle|A_0\rangle|\varepsilon_0\rangle = |\Psi\rangle. \end{aligned} \quad (2.17)$$

It may seem that very little can be accomplished by repeating the step that has led to the $\mathcal{S} - \mathcal{A}$ correlation and the associated problems. But this is not the case. A collection of three correlated quantum systems is no longer subject to the basis ambiguity we have pointed out in connection with the EPR-like state $|\Phi\rangle$, equation (2.16). This is especially true when the states

of the environment are correlated with the simple products of the states of the apparatus–system combination [1]. In equation (2.17) above, this can be guaranteed (irrespective of the value of α and β) providing that:

$$\langle \varepsilon_0 | \varepsilon_1 \rangle = 0 . \quad (2.18)$$

When this condition is satisfied, the description of the $\mathcal{A} - \mathcal{S}$ pair can be readily obtained in terms of a reduced–density–matrix:

$$\begin{aligned} \rho_{\mathcal{AS}} &= \text{Tr}_{\mathcal{E}} |\Psi\rangle\langle\Psi| \\ &= |\alpha|^2 |\uparrow\rangle\langle\uparrow| |A_1\rangle\langle A_1| + |\beta|^2 |\downarrow\rangle\langle\downarrow| |A_0\rangle\langle A_0|. \end{aligned} \quad (2.19)$$

This reduced–density–matrix contains only terms corresponding to classical correlations.

If the condition of equation (2.18) did not hold – that is, if the orthogonal states of the environment were not correlated with the apparatus in the basis in which the original premeasurement was carried out – then the terms on the diagonal of the reduced density matrix $\rho_{\mathcal{AS}}$ would be the sum of products rather than simply products of states of $\mathcal{S}$ and $\mathcal{A}$. An extreme example of that situation is the pre-decoherence density matrix of the pure state:

$$\begin{aligned} |\Phi\rangle\langle\Phi| &= |\alpha|^2 |\uparrow\rangle\langle\uparrow| |A_1\rangle\langle A_1| + \alpha\beta^* |\uparrow\rangle\langle\downarrow| |A_1\rangle\langle A_0| + \\ &+ \alpha^*\beta |\downarrow\rangle\langle\uparrow| |A_0\rangle\langle A_1| + |\beta|^2 |\downarrow\rangle\langle\downarrow| |A_0\rangle\langle A_0|. \end{aligned} \quad (2.20)$$

Its eigenstate is simply $|\Phi\rangle$. When expanded, $|\Phi\rangle\langle\Phi|$ contains terms that are off–diagonal when expressed in the natural basis consisting of tensor products of states in the two subspaces. Their disappearance as a result of tracing over the environment signals the disappearance of the basis ambiguity. There is of course a conceptual difference with the classical case. In classical mechanics, it was in principle possible to imagine that the outcome was predetermined. In quantum mechanics this is usually impossible even in principle. However, that distinction can be made only with a more complete knowledge than the one typically available to the observer.

The pointer observable that emerges from this simple case is easy to characterize. The interaction Hamiltonian between the apparatus and the environment, $H_{\mathcal{AE}}$, should have the same structure as for the **c-not**. It should be a function of the pointer observable

$$\hat{A} = a_1 |A_1\rangle\langle A_1| + a_0 |A_0\rangle\langle A_0|, \quad (2.21)$$

of the apparatus. Consequently, the states of the environment will bear an imprint of the pointer states $\{|A_1\rangle, |A_0\rangle\}$. As was also noted in the discussion of **c-nots**, $[H_{\mathcal{AE}}, \hat{A}] = 0$ immediately implies that $\hat{A}$ is a control, and its eigenstates will be preserved.

Disappearance of quantum coherence because of a “one-bit” measurement has been verified experimentally in neutron and, more recently, in atomic interferometry [24–26]. A single act of quantum measurement we have discussed here should be regarded as an elementary discrete instance of continuous monitoring, which is required to bring about the appearance of classicality.

2.5 Decoherence of a single (qu)bit

Another example of decoherence is afforded by a two-state apparatus $\mathcal{A}$ interacting with an environment of N other spins [2]. We can think of it as just another two-state system, and, in that spirit, we shall identify in this section the two apparatus states as $\{|\uparrow\rangle, |\downarrow\rangle\}$. The process of decoherence is definitely not limited to states of the apparatus pointers, so these two generic candidate pointer states can belong to any system.

The simplest, yet already quite illustrative example of this situation occurs when the self-Hamiltonian of the apparatus disappears, $H_{\mathcal{A}} = 0$, and the interaction Hamiltonian has the form:

$$H_{\mathcal{AE}} = (|\uparrow\rangle\langle\uparrow| - |\downarrow\rangle\langle\downarrow|) \otimes \sum_k g_k (|\uparrow\rangle\langle\uparrow| - |\downarrow\rangle\langle\downarrow|)_k. \quad (2.22)$$

Under the influence of this Hamiltonian, the initial state

$$|\Phi(0)\rangle = (a|\uparrow\rangle + b|\downarrow\rangle) \prod_{k=1}^N (\alpha_k|\uparrow\rangle_k + \beta_k|\downarrow\rangle_k) \quad (2.23)$$

evolves into

$$|\Phi(t)\rangle = a|\uparrow\rangle \otimes |\mathcal{E}_{\uparrow}(t)\rangle + b|\downarrow\rangle \otimes |\mathcal{E}_{\downarrow}(t)\rangle. \quad (2.24)$$

Here:

$$|\mathcal{E}_{\uparrow}(t)\rangle = \prod_{k=1}^N (\alpha_k \exp(ig_k t) |\uparrow\rangle_k + \beta_k \exp(-ig_k t) |\downarrow\rangle_k) = |\mathcal{E}_{\downarrow}(-t)\rangle. \quad (2.25)$$

The reduced density matrix is then

$$\rho_{\mathcal{A}} = |a|^2 |\uparrow\rangle\langle\uparrow| + ab^* r(t) |\uparrow\rangle\langle\downarrow| + a^* b r^*(t) |\downarrow\rangle\langle\uparrow| + |b|^2 |\downarrow\rangle\langle\downarrow|. \quad (2.26)$$

The coefficient $r(t)$ determines the relative size of the off-diagonal terms. It is given by

$$r(t) = \langle\mathcal{E}_{\uparrow}|\mathcal{E}_{\downarrow}\rangle = \prod_{k=1}^N [\cos 2g_k t + i(|\alpha_k|^2 - |\beta_k|^2) \sin 2g_k t]. \quad (2.27)$$

Unless k 'th spin of the environment is initially in an eigenstate of the interaction Hamiltonian, its contribution to the product will be less than unity. Consequently, for large environments consisting of many (N) spins and at large times the off-diagonal terms are typically small,

$$|r(t)|^2 \simeq 2^{-N} \prod_{k=1}^N [1 + (|\alpha_k|^2 - |\beta_k|^2)^2]. \quad (2.28)$$

This effect can be illustrated with the help of the Bloch sphere. The density matrix of any two-state system can be represented by a point in the 3-D space. In terms of the coefficients a , b , and $r(t)$ that we have previously used, the coordinates of the point representing $\rho(t)$ are: $z = (|a|^2 - |b|^2)$, $x = \Re(ab^*r)$, and $y = \Im(ab^*r)$. When the state is pure, $x^2 + y^2 + z^2 = 1$ – pure states lie on the surface of the Bloch sphere (Fig. 1). When the state is mixed, the point representing it lies inside that sphere. Any conceivable (unitary or non-unitary) quantum evolution of the two-state system can be thought of as a transformation of the surface of the pure states into the ellipsoid contained inside the Bloch sphere. Deformation of the Bloch sphere caused by decoherence is a special case of such general evolutions. The decoherence process does not affect a or b . Hence, evolution caused by decoherence alone occurs in a constant- z plane. Such a “slice” through the Bloch sphere would show the point representing the state at a fraction $|r(t)|$ of its maximum distance. The complex number $r(t)$ can be expressed as the sum of the complex phase factors rotating with the frequencies given by differences $\Delta\omega_j$ between the energy eigenvalues of the interaction Hamiltonian, weighted with the probabilities of finding these energy eigenstates in the initial state,

$$r(t) = \sum_{j=1}^{2^N} p_j \exp(-i\Delta\omega_j t). \quad (2.29)$$

The index j now denotes partial energy eigenstates of the environment of the interaction Hamiltonian (tensor products of $\uparrow$ and $\downarrow$ states of the environmental spins). The corresponding eigenvalue differences between the two complete energy eigenstates $|\uparrow\rangle|j\rangle$ and $|\downarrow\rangle|j\rangle$ are

$$\Delta\omega_j = \langle\uparrow| \langle j| H_{\mathcal{AE}} |j\rangle | \downarrow\rangle. \quad (2.30)$$

There are 2^N distinct states $|j\rangle$, and, barring degeneracies, the same number of different $\Delta\omega_j$'s. The probabilities p_j are given by

$$p_j = |\langle j| \mathcal{E}(t=0) \rangle|^2, \quad (2.31)$$

which, in turn, is easily expressed in terms of the appropriate squares of the products of α_k and β_k .

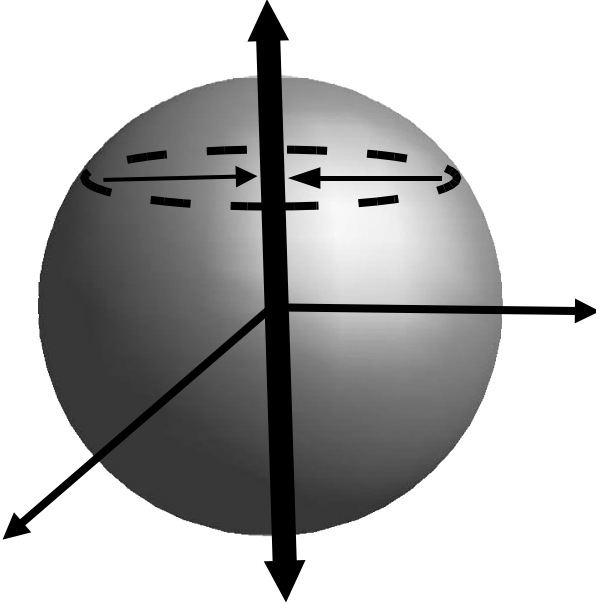


Fig. 1. Decoherence can be seen in the Bloch sphere as the process that induce the states to “move towards the vertical axis”, which is defined by the two pointer states on the poles. Classical domain consists of just two pointer states. The classical core is the set of all mixtures of pointer states.

The evolution of $r(t)$ given by equation (2.29) is a consequence of the rotations of the complex vectors $p_k \exp(-i\Delta\omega_j t)$ with different frequencies. The resultant $r(t)$ will then start with the amplitude 1 and quickly “crumble” to a value approximately equal to

$$\langle |r(t)|^2 \rangle = \sum_{j=1}^{2^N} p_j^2 \sim 2^{-N}. \quad (2.32)$$

In this sense, decoherence is exponentially effective – the expected magnitude of the off-diagonal terms decreases exponentially fast with the physical size N of the environment – with the number of systems (spins in our example). In effect, any initial state asymptotically approaches the z -axis as a result of decoherence.

We note that the effectiveness of einselection depends on the initial state of the environment: when $\mathcal{E}$ is in the k 'th eigenstate of $H_{\mathcal{A}\mathcal{E}}$, and $p_j = \delta_{jk}$, the coherence in the system will be retained because the environment is now in an eigenstate of the “control”. This situation is, however, unlikely in realistic circumstances because the self-Hamiltonian of the environment $H_{\mathcal{E}}$ will

not commute, in general, with $H_{\mathcal{AE}}$. Moreover, even when $H_{\mathcal{E}} = 0$, finding an environment in an energy eigenstate of the Hamiltonian seems extremely unlikely – the eigenvalues of such eigenstates are bound to be dense in large systems, and therefore they will be easily perturbed by the interaction with their environments. Furthermore, the 2^N partial eigenstates of the interaction Hamiltonian are exponentially rare among arbitrary superpositions.

The geometry of the flows induced by decoherence inside the Bloch sphere exhibits characteristics that are encountered in more general physical situations, involving decoherence in bigger Hilbert spaces as follows:

- (i) Domain of pure quasi-classical states consisting of all the einselected pointer states ($\{|\uparrow\rangle, |\downarrow\rangle\}$ in our case). Pointer states are the pure states least affected (here, unaffected) by decoherence;
- (ii) Classical core of probability distributions, *i.e.*, all the mixtures of pointer states. In Figure 1 it corresponds to the section $[-1, +1]$ of the z -axis;
- (iii) The rest of the space – the rest of the volume of the Bloch sphere – consists of more general density matrices. As a result of decoherence, that part of the Hilbert space is “ruled out” by einselection.

Visualization of this decoherence-induced decomposition of the Hilbert space is still possible in the simple two-dimensional case studied here, but the existence of the elements (i)–(iii) is a general feature. It characterizes the emergence of classicality under all circumstances. We shall therefore appeal to the intuitions developed in the course of this discussion later. However, it may be useful to anticipate a few of the phenomena that can take place when decoherence combines with the evolution induced by the self-Hamiltonian of the system or when it is caused by more complicated couplings to the environment.

- (a) Approach to equilibrium would affect elements diagonal in the pointer basis, so that the density matrix would asymptotically approach a time-independent distribution (such as $\rho \sim 1$ for a thermal equilibrium at infinite temperature or $\rho \sim |\downarrow\rangle\langle\downarrow|$ for decay). This corresponds to a flow towards some specific point (*i.e.*, the center or the “south pole” in the above two examples) within the Bloch sphere. However, when decoherence dominates, the flow would start somewhere within the Bloch sphere, and quickly (on the decoherence timescale) converge towards a point on the z -axis (the classical core). This would be followed by a much slower relaxation, a flow more or less along the z -axis (and therefore essentially within the classical core) on a *relaxation timescale*;

- (b) Approximately reversible classical dynamics can coexist with decoherence when the self-Hamiltonian of the system can generate motions within the surfaces of constant entropy inside the classical core. In the case considered here, the core is one-dimensional and the subspaces of constant entropy within it are zero-dimensional. Therefore, it is impossible to generate continuous isentropic motion within them. In multidimensional Hilbert spaces with richer dynamics that are nearly isentropic, approximately reversible evolution is often possible and allows for the idealization of trajectories in the classical limit;
- (c) A sharp distinction between the classical core and the rest of the Hilbert space is possible only in idealized situations (or in an even more idealized “mathematical classical limit”, in which $\hbar \rightarrow 0$, $\text{mass} \rightarrow \infty$, etc.). In realistic situations, all that will be required is a clear contrast between the rates of the entropy production between the inside and the outside of the classical core. We shall refine such criteria in the discussion of the *predictability sieve* – a criterion for the selection of the preferred pointer states, which in effect demands that the entropy production rate should be minimized for the einselected states. In the case discussed here, pointer states obviously satisfy this criterion, and the entropy production vanishes in the classical domain. In more general situations, we shall not be equally lucky. For instance, in the case of chaotic systems, entropy will also be produced in a classical core, but at a rate set by the classical dynamics (*i.e.*, by the self-hamiltonian rather than by the coupling with the environment) and much more slowly than outside of the classical core.

2.6 Decoherence, einselection, and controlled shifts

The above discussion of decoherence can be straightforwardly generalized to the situation where the system, the apparatus, and the environment have many states, and where the interactions between them are much more complicated. Here we assume that the system is isolated and that it interacts with the apparatus only briefly. As a result of that interaction, the state of the apparatus becomes entangled with the state of the system, $(\sum_i \alpha_i |s_i\rangle) |A_0\rangle \rightarrow \sum_i \alpha_i |s_i\rangle |A_i\rangle$. By analogy with a **c-not**, we shall refer to this conditional operation as a **c-shift**. This quantum correlation suffers from the basis ambiguity we have discussed previously: the $\mathcal{S} - \mathcal{A}$ entanglement implies that for any state of either of the two systems there exists a corresponding pure state of the other. Indeed, when the initial state of $\mathcal{S}$ is chosen to be one of the eigenstates of the conjugate basis, $|r_l\rangle = N^{-\frac{1}{2}} \sum_{k=0}^{N-1} \exp(2\pi i k l / N) |s_k\rangle$, this **c-shift** would equally well represent a measurement of the apparatus state (in the basis conjugate to $\{|A_k\rangle\}$) by the system [27]. Thus, it is not just the basis that is

ambiguous, but also the roles of the control (system) and of the target (apparatus) can be reversed when the conjugate basis is selected. These ambiguities that exist for the $\mathcal{SA}$ pair can be removed by recognizing the role of the environment.

Decoherence is represented schematically in Figure 2 by a sequence of **c-nots** (or **c-shifts**) which, in some fixed basis, “measure” the state of the apparatus and record the outcome of the measurement in the environment. The requirement for a good apparatus is to retain correlations between the measured observable of the system and some “pointer observable”. This will happen when the **c-shift** between $\mathcal{S}$ and $\mathcal{A}$ correlates the state of the system with the observable of the apparatus that is itself monitored (but not perturbed) by the environment. That is, in an idealized measurement, the measured observable of the system is playing the role of the control with respect to the $\mathcal{S} - \mathcal{A}$ **c-shift**. In a well-designed apparatus, the pointer observable is a target of the $\mathcal{S} - \mathcal{A}$ **c-shift**, but a control of the $\mathcal{A} - \mathcal{E}$ **c-shifts**. Eigenstates of the pointer observable of the apparatus play the role of an alphabet of a communication channel. They encode a state of the system and retain the correlation in spite of the interaction with the environment.

The graph in Figure 2 captures the essence of the idealized decoherence process, which yields – in spite of the interaction with the environment – a noiseless classical communication channel [28, 29]. This is possible because in the pointer basis, the $\mathcal{A} - \mathcal{E}$ **c-shifts** operate without disturbing the pointer observable, which is the constant of motion of the $\mathcal{A} - \mathcal{E}$ interaction Hamiltonian.

The advantage of the graphical representation of the decoherence process as a sequence of **c-shifts** lies in its simplicity and suggestiveness. However, the actual process of decoherence is usually caused by a continuous interaction (so that it can be only approximately broken up into discrete **c-shifts**). Moreover, in contrast to the **c-nots** used in quantum logic circuits, the record inscribed in the environment is more often than not distributed over many degrees of freedom. Last but not least, the observable of the apparatus (or any other open system) may be a subject to noise (and not just decoherence) or it may evolve in a manner that will rotate pointer states into their superpositions.

The basic physics of decoherence is a simple premeasurement-like process carried out by the environment $\mathcal{E}$ as a result of the interaction with the apparatus,

$$\begin{aligned}
 |\Psi_{\mathcal{SA}}\rangle|\varepsilon_0\rangle &= \left(\sum_j \alpha_j |s_j\rangle |A_j\rangle\right)|\varepsilon_0\rangle \longrightarrow \\
 &\longrightarrow \sum_j \alpha_j |s_j\rangle |A_j\rangle |\varepsilon_j\rangle = |\Phi_{\mathcal{SAE}}\rangle.
 \end{aligned} \tag{2.33}$$

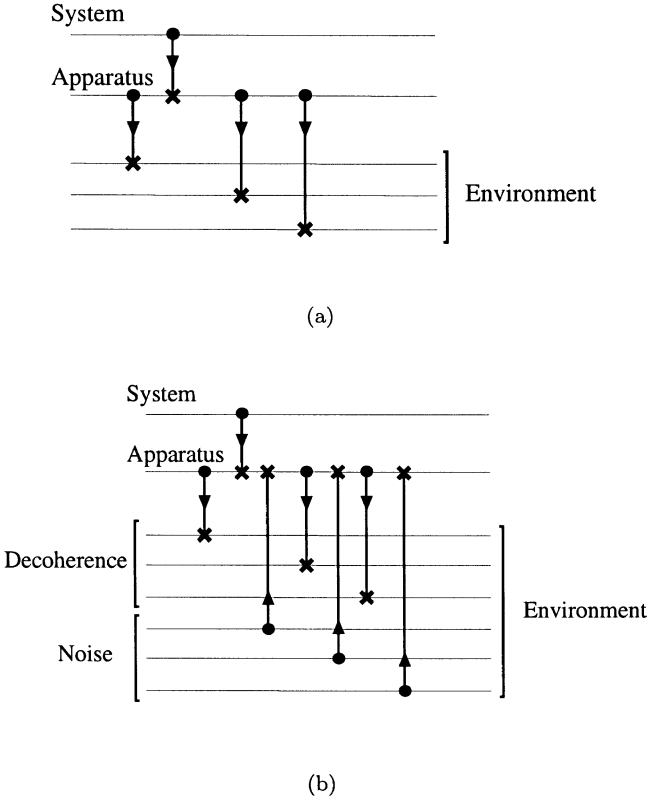


Fig. 2. (a) Decoherence can be viewed as the consequence of the monitoring of the state of the system by the environment. This is symbolically represented here by a sequence of c-not gates where the pointer states of the apparatus act as the control and the environment is the target. (b) The distinction between decoherence and noise depends on the direction of the information flow in the preferred basis. Preferred states minimize the number of c-nots directed from the environment.

Decoherence leads to the einselection when the states of the environment $|\varepsilon_j\rangle$ corresponding to different pointer states become orthogonal,

$$\langle \varepsilon_i | \varepsilon_j \rangle = \delta_{ij}. \quad (2.34)$$

When this orthogonality condition is satisfied, Schmidt decomposition of the state vector $|\Phi_{\mathcal{SA}\mathcal{E}}\rangle$ into a composite subsystem $\mathcal{SA}$ and $\mathcal{E}$ yields product states $|s_j\rangle|A_j\rangle$ as partners of the orthogonal environment states.

The density matrix describing the correlated but decohered $\mathcal{SA}$ pair is then:

$$\rho_{\mathcal{SA}}^D = \sum_j |\alpha_j|^2 |s_j\rangle\langle s_j| |A_j\rangle\langle A_j| = \text{Tr}_{\mathcal{E}} |\Phi_{\mathcal{SAE}}\rangle\langle\Phi_{\mathcal{SAE}}| . \quad (2.35)$$

The reduced density matrix of the $\mathcal{SA}$ pair is diagonal in the product states.

For notational simplicity, we shall often discard reference to the object that does not interact with the environment (here, the system $\mathcal{S}$). Nevertheless, it is useful to keep in mind that the preservation of the $\mathcal{SA}$ correlations is the criterion used to define the pointer basis. The density matrix of a single object evolving in contact with the environment will be always diagonal in the same (instantaneous) Schmidt basis. This instantaneous diagonality should not be used as a sole criterion for classicality (although see [31,32]; as well as [33,34]). Rather, the ability of certain sets of states to retain correlations in spite of the coupling to the environment is decisive in the emergence of “classical reality”. This is especially obvious in quantum measurements.

When the interaction with the apparatus has the form

$$H_{\mathcal{AE}} = \sum_{k,l,m} g_{klm}^{\mathcal{AE}} |A_k\rangle\langle A_k| |\varepsilon_l\rangle\langle\varepsilon_m| + h.c. , \quad (2.36)$$

the basis $\{|A_k\rangle\}$ is left unperturbed. Then, any correlation with the states $\{|A_k\rangle\}$ will be preserved. And, by definition, the states that preserve correlations will be the pointer states. Any observable A co-diagonal with the interaction Hamiltonian will be an effective pointer observable. For, when the Hamiltonian depends on A , it will commute with A ,

$$[H_{\mathcal{AE}}(A), A] = 0. \quad (2.37)$$

Moreover, the dependence of the interaction Hamiltonian on the observable is an obvious precondition for the monitoring of that observable by the environment.

3 Dynamics of quantum open systems: Master equations

One of the most practical tools for analyzing the dynamics of a quantum open system is the evolution equation for the reduced density matrix, known as the “master equation”. In this section we will review some of the most common techniques to obtain such an equation. As usual, we divide our universe into a system of interest $\mathcal{S}$ that interacts with an environment $\mathcal{E}$. The reduced density matrix of the system is the operator that allows us to answer all physical questions that concern the system $\mathcal{S}$ only. We will denote the reduced density matrix as ρ , which is obtained from the total density

matrix of the universe by tracing over the environment Hilbert space. Thus,

$$\rho = \text{Tr}_E \rho_T,$$

where the total density matrix is denoted as ρ_T .

In principle, the evolution equation for ρ could be obtained by solving Schrödinger (or von Neumann) equation for the total density matrix and then taking the trace. However, this task can be analytically completed in very few cases, and the study of the evolution of the reduced density matrix should be done by using some approximations.

This section is divided in two parts. First we review some of the standard techniques used to obtain approximate master equations. Our plan is not to give a complete review of master equation techniques but to present some useful tools to be applied later in studying decoherence. We do this not only to ensure that the paper is self-contained but also because we think it might be useful to present some simple and helpful results that are not so well known. We focus on the simplest approximation scheme, obtaining master equations valid to a second order in a perturbative expansion in the system–environment coupling strength. We first review the general perturbative scheme and apply it to two physically interesting examples: (1) the Brownian motion of a particle coupled to an environment of independent oscillators and (2) a quantum particle locally coupled to an environment formed by a quantum scalar field. As a further illustration of the way in which perturbative master equations can be obtained, we find the corresponding equations for a two–level system coupled to a bosonic bath in two physically relevant cases (the decay of a two–level atom and the spin boson model).

In the second part of this section we review the properties of an important model that is amenable to an exact solution. Thus, we concentrate on the linear quantum Brownian motion model analyzing the properties of its exact master equation. In particular, we stress the fact that in this simple but physically relevant model, the exact master equation has the same functional form as the one obtained using perturbation theory and can always be cast in terms of a local differential equation with time–dependent coefficients.

3.1 Master equation: Perturbative evaluation

Here we present the general procedure that can be used to derive the master equation, assuming that the system–environment coupling is small. Thus, we sketch a textbook derivation of the master equation using perturbation theory. We think it is convenient to present this derivation just to stress the fact that perturbative master equations can always be shown to be local in time. The calculation we follow is closely related to the one presented, for

example, in [35] and can be seen to be a variant of the time-convolutionless method discussed in [36].

Let us consider the total Hamiltonian to be

$$H = H_S + H_E + V,$$

where H_S and H_E are respectively the self-Hamiltonian of the system and the environment and V is the interaction term. The equation for the complete density matrix ρ_T , in the interaction picture, reads (we use a tilde to denote operators in the interaction picture),

$$i\hbar\dot{\tilde{\rho}}_T = [\tilde{V}(t), \tilde{\rho}_T], \quad (3.1)$$

where the interaction potential and density matrix are $\tilde{V}(t) = U_0^\dagger V U_0$ and $\tilde{\rho}_T = U_0^\dagger \rho_T U_0$, where $U_0 = \exp(-i(H_S + H_E)t/\hbar)$. Solving equation (3.1) perturbatively is rather straightforward and leads to the Dyson series,

$$\tilde{\rho}_T(t) = \sum_{n \geq 1} \int_0^t dt_1 \dots \int_0^{t_{n-1}} dt_n \left(\frac{1}{i\hbar} \right)^n \left[\tilde{V}(t_1), \dots, [\tilde{V}(t_n), \tilde{\rho}_T(0)] \right]. \quad (3.2)$$

We can use this to compute the reduced density matrix to second order. To obtain the master equation we compute the time derivative of the resulting expression and perform the trace over the environment. We get

$$\dot{\rho} = \frac{1}{i\hbar} \text{Tr}_E \left[\tilde{V}(t), \rho_T(0) \right] - \frac{1}{\hbar^2} \int_0^t dt_1 \text{Tr}_E \left[\tilde{V}(t), [\tilde{V}(t_1), \rho_T(0)] \right]. \quad (3.3)$$

So far, the only assumption we made was the validity of a perturbative expansion up to second order. Now we will assume that the initial state is not entangled, *i.e.*, that the total density matrix is a tensor product of the form $\rho_T(0) = \rho(0) \otimes \rho_E(0)$. Substituting this into (3.3) we find,

$$\begin{aligned} \dot{\rho} = & \frac{1}{i\hbar} \text{Tr}_E \left[\tilde{V}(t), \rho(0) \otimes \rho_E(0) \right] \\ & - \frac{1}{\hbar^2} \int_0^t dt_1 \text{Tr}_E \left[\tilde{V}(t), [\tilde{V}(t_1), \rho(0) \otimes \rho_E(0)] \right]. \end{aligned} \quad (3.4)$$

To finish the derivation, we make a rather trivial observation that enables us to rewrite the master equation in a very simple way: the initial state $\rho(0)$ that appears in the right-hand-side of equation (3.4) could again be expressed in terms of $\tilde{\rho}(t)$ using the same perturbative expansion that enabled us to obtain (3.4). By doing this we can rewrite the right-hand-side

of the master equation entirely in terms of the reduced density matrix evaluated at time t . The resulting equation is

$$\begin{aligned} \dot{\tilde{\rho}} = & \frac{1}{i\hbar} \text{Tr}_{\mathcal{E}} \left[\tilde{V}(t), \tilde{\rho} \otimes \rho_{\mathcal{E}}(0) \right] - \frac{1}{\hbar^2} \int_0^t dt_1 \text{Tr}_{\mathcal{E}} \left[\tilde{V}(t), \left[\tilde{V}(t_1), \tilde{\rho} \otimes \rho_{\mathcal{E}} \right] \right] \\ & + \frac{1}{\hbar^2} \int_0^t dt_1 \text{Tr}_{\mathcal{E}} \left(\left[\tilde{V}(t), \text{Tr}_{\mathcal{E}} \left(\left[\tilde{V}(t_1), \tilde{\rho} \otimes \rho_{\mathcal{E}} \right] \right) \otimes \rho_{\mathcal{E}} \right] \right). \end{aligned} \quad (3.5)$$

This, when rewritten in the Schrödinger picture, is the basic master equation we will use in this section. It is important to keep in mind that to derive it, we only made two important assumptions: (a) we used a perturbative expansion up to second order in the system–environment coupling constant and (b) we assumed uncorrelated initial conditions.

Below, we will apply this equation to study three interesting examples. Before doing that, let us stress that the master equation is local in time even though to obtain it, no Markovian assumption was made (see below). Moreover, this rather simple form can be simplified further by assuming that the system–environment coupling is of the form

$$V = \sum_n (S_n E_n + S_n^\dagger E_n^\dagger), \quad (3.6)$$

where S_n (E_n) are operators acting on the Hilbert space of the system (environment) only. In such case, the master equation in the Schrödinger picture can be written as

$$\begin{aligned} \dot{\rho} = & \frac{1}{i\hbar} [H_S, \rho] + \frac{1}{i\hbar} \sum_n [\langle E_n \rangle S_n + \langle E_n^\dagger \rangle S_n^\dagger, \rho] \\ & - \frac{1}{2\hbar^2} \sum_{nm} \int_0^t dt_1 \left(K_{nm}^{(1)}(t, t_1) [S_n, [S_m^\dagger(t_1 - t), \rho]] \right. \\ & + K_{nm}^{(2)}(t, t_1) [S_n, \{S_m^\dagger(t_1 - t), \rho\}] + K_{nm}^{(3)}(t, t_1) [S_n, [S_m(t_1 - t), \rho]] \\ & \left. + K_{nm}^{(4)}(t, t_1) [S_n, \{S_m(t_1 - t), \rho\}] + h.c. \right), \end{aligned} \quad (3.7)$$

where the bracket notation indicates the expectation value over the initial state of the environment and the kernels $K_{nm}^{(i)}$ are simply determined by the two time correlation functions of the environment as follows:

$$\begin{aligned} K_{nm}^{(1)}(t, t_1) &= \frac{1}{2} \langle \{E_n(t), E_m^\dagger(t_1)\} \rangle - \langle E_n \rangle \langle E_m^\dagger \rangle \\ K_{nm}^{(2)}(t, t_1) &= \frac{1}{2} \langle [E_n(t), E_m^\dagger(t_1)] \rangle \\ K_{nm}^{(3)}(t, t_1) &= \frac{1}{2} \langle \{E_n(t), E_m(t_1)\} \rangle - \langle E_n \rangle \langle E_m \rangle \\ K_{nm}^{(4)}(t, t_1) &= \frac{1}{2} \langle [E_n(t), E_m(t_1)] \rangle. \end{aligned} \quad (3.8)$$

At this point, it is interesting to consider another important approximation that is usually employed in this context, *i.e.*, the Markovian approximation that we have refrained from using so far. The Markovian approximation corresponds to considering cases for which the kernels $K^{(i)}$ are strongly peaked about $t = t_1$. When this is the case, *i.e.* when the environment has a very short correlation time, one can transform the temporal integrals into integrals over the variable $\tau = t - t_1$, which can then be extended over the entire interval $[0, \infty)$. As we mentioned above, so far, we have not used the Markovian assumption and therefore the above equations are valid even if the environment has a long correlation time and the kernels $K^{(i)}$ are not strongly peaked. In the examples below, we will mention some cases where this happens and use the above equation to study decoherence produced by a non Markovian environment.

It is also worth mentioning that to go one step beyond equation (3.7), one needs to know the temporal dependence of the free Heisenberg operators of the system (*i.e.*, $S_n(t)$) which obviously depend on the Hamiltonian H_S that we have not specified so far. We will do so in some concrete examples below.

3.2 Example 1: Perturbative master equation in quantum Brownian motion

The system of interest is a quantum particle, which moves in a one dimensional space (generalization to higher dimensions is immediate). The environment is an ensemble of harmonic oscillators interacting bilinearly through position with the system. Thus, the complete Hamiltonian is $H = H_S + H_E + V$ where

$$H_E = \sum_n \left(\frac{1}{2m_n} p_n^2 + \frac{1}{2} m_n \omega_n^2 q_n^2 \right) \quad (3.9)$$

and $V = \sum_n \lambda_n q_n x$. The Hamiltonian of the system will be left unspecified for the moment (we will concentrate later on the case of a harmonic oscillator). The initial state of the environment will be assumed to be a thermal equilibrium state at temperature $T = 1/k_B \beta$. Under these assumptions the first-order term in the master equation disappears because $\text{Tr}_E(\tilde{V}(t)\rho_E) = 0$. Therefore, the master equation in the Schrödinger picture is

$$\dot{\rho} = \frac{1}{i\hbar} [H_S, \rho] - \frac{1}{\hbar} \int_0^t dt_1 \left(\nu(t_1) [x, [x(-t_1), \rho]] - i\eta(t_1) [x, \{x(-t_1), \rho\}] \right). \quad (3.10)$$

The two kernels appearing here are respectively called the noise and the dissipation kernel and are defined as

$$\begin{aligned}\nu(t) &= \frac{1}{2\hbar} \sum_n \lambda_n^2 \langle \{q_n(t), q_n(0)\} \rangle = \int_0^\infty d\omega J(\omega) \cos \omega t (1 + 2N(\omega)) \\ \eta(t) &= \frac{i}{2\hbar} \sum_n \lambda_n^2 \langle [q_n(t), q_n(0)] \rangle = \int_0^\infty d\omega J(\omega) \sin \omega t,\end{aligned}\quad (3.11)$$

where $J(\omega) = \sum_n \lambda_n^2 \delta(\omega - \omega_n) / 2m_n \omega_n$ is the spectral density of the environment and $N(\omega)$ is the mean occupation number of the environmental oscillators (*i.e.*, $1 + 2N(\omega) = \coth(\beta \hbar \omega / 2)$).

Equation (3.10) is already very simple but it can be further simplified if one assumes that the system is a harmonic oscillator. Thus, if we consider the Hamiltonian of the system to be $H_S = p^2/2M + M\Omega^2 x^2/2$, we can explicitly solve the Heisenberg equations for the system and determine the operator $x(t)$ to be $x(t) = x \cos(\Omega t) + \frac{1}{M\Omega} p \sin(\Omega t)$. Inserting this into (3.10), we get the final expression for the master equation,

$$\begin{aligned}\dot{\rho} = & - \frac{i}{\hbar} \left[H_S + \frac{1}{2} M \tilde{\Omega}^2(t) x^2, \rho \right] - \frac{i}{\hbar} \gamma(t) [x, \{p, \rho\}] \\ & - D(t) [x, [x, \rho]] - \frac{1}{\hbar} f(t) [x, [p, \rho]].\end{aligned}\quad (3.12)$$

Here the time-dependent coefficients (the frequency renormalization $\tilde{\Omega}(t)$, the damping coefficient $\gamma(t)$, and the two diffusion coefficients $D(t)$ and $f(t)$) are

$$\begin{aligned}\tilde{\Omega}^2(t) &= -\frac{2}{M} \int_0^t dt' \cos(\Omega t') \eta(t'), \quad \gamma(t) = \frac{1}{M\Omega} \int_0^t dt' \sin(\Omega t') \eta(t') \\ D(t) &= \frac{1}{\hbar} \int_0^t dt' \cos(\Omega t') \nu(t'), \quad f(t) = -\frac{1}{M\Omega} \int_0^t dt' \sin(\Omega t') \nu(t').\end{aligned}\quad (3.13)$$

From this equation it is possible to have a qualitative idea of the effects the environment produces on the system. First we observe that there is a frequency renormalization. Thus, the “bare” frequency of the oscillator is renormalized by $\tilde{\Omega}^2$. This term does not affect the unitarity of the evolution. The terms proportional to $\gamma(t)$, $D(t)$ and $f(t)$ bring about non-unitary effects. Thus, one can easily see that the second term is responsible for producing friction ($\gamma(t)$ plays the role of a time-dependent relaxation rate). The last two are diffusion terms. The one proportional to $D(t)$ is the main cause for decoherence.

Of course, the explicit time dependence of the coefficients can only be computed once we specify the spectral density of the environment.

To illustrate their qualitative behavior, we will consider a typical ohmic environment characterized by a spectral density of the form

$$J(\omega) = 2M\gamma_0 \frac{\omega}{\pi} \frac{\Lambda^2}{\Lambda^2 + \omega^2}, \quad (3.14)$$

where Λ plays the role of a high-frequency cutoff and γ_0 is a constant characterizing the strength of the interaction. For this environment, it is rather straightforward to find the following exact expressions for the coefficients $\tilde{\Omega}(t)$ and $\gamma(t)$:

$$\gamma(t) = \gamma_0 \frac{\Lambda^2}{\Lambda^2 + \Omega^2} \left(1 - \left(\cos \Omega t + \frac{\Lambda}{\Omega} \sin \Omega t \right) \exp(-\Lambda t) \right) \quad (3.15)$$

$$\tilde{\Omega}^2(t) = -2\gamma_0 \Lambda \frac{\Lambda^2}{\Lambda^2 + \Omega^2} \left(1 - \left(\cos \Omega t - \frac{\Omega}{\Lambda} \sin \Omega t \right) \exp(-\Lambda t) \right). \quad (3.16)$$

From these equations we see that these coefficients are initially zero and grow to asymptotic values on a timescale that is fixed by the high-frequency cutoff Λ . Thus, we see the relation between this result and the one we would obtain by using a Markovian approximation simply corresponds to taking the limit $\Lambda \rightarrow \infty$. In such a case both coefficients are not continuous at $t = 0$ and jump into constant values (the frequency renormalization diverges as it is proportional to the product $\gamma_0 \Lambda$).

The time dependence of the diffusion coefficients can also be studied for the above environment. However, the form of the coefficients for arbitrary temperature is quite complicated. To analyze the qualitative behavior, it is convenient to evaluate them numerically. In Figure 3 one can see the dependence of the coefficients (for both the long and short timescales) for several temperatures (high and low). We observe that both coefficients have an initial transient where they exhibit a behavior that is essentially temperature independent (over periods of time comparable with the one fixed by the cutoff). The direct diffusion coefficient $D(t)$ after the initial transient rapidly settles into the asymptotic value given by $D_\infty = M\gamma_0 \Omega \coth(\beta \hbar \Omega / 2) \Lambda^2 / \hbar (\Lambda^2 + \Omega^2)$. The anomalous diffusion coefficient $f(t)$ also approaches an asymptotic value (which for high temperatures is suppressed with respect to D_∞ by a factor of Λ), but the approach is algebraic rather than exponential. More general environments can be studied using our equation. In fact, the behavior of the coefficients is rather different for environments with different spectral content. This has been analyzed in the literature, in particular in relation to decoherence [37].

It is interesting to mention that the master equation (3.12) (although it has been derived perturbatively) can be shown to be very similar to its exact counterpart whose derivation we will discuss later in this section.

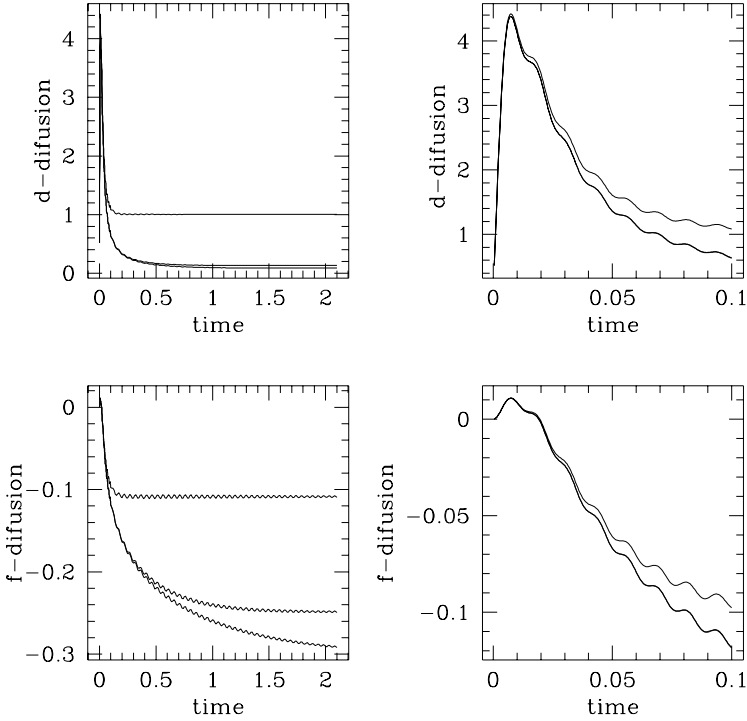


Fig. 3. Time dependence of the diffusion coefficients of the perturbative master equation for quantum Brownian motion. Plots on the right show that the initial transient is temperature independent (different curves correspond to different temperatures, higher temperatures produce higher final values of the coefficients). Plots on the left show that the final values of the coefficients are strongly dependent on the temperature of the environment. The parameters used in the plot (where time is measured in units of $1/\Omega$) are $\gamma/\Omega = 0.05$, $\Lambda/\Omega = 100$, $k_B T/\hbar\Omega = 10, 1, 0.1$.

3.3 Example 2: Perturbative master equation for a two-level system coupled to a bosonic heat bath

As a second example we obtain the perturbative master equation for a two-level system coupled to an oscillator environment. We consider two different models characterized by different interaction Hamiltonians. First, we discuss the model describing the physics of the decay of a two-level atom

(in the rotating wave approximation),

$$H = \frac{1}{2}\hbar\Delta\sigma_z + \sum_n \lambda_n (a_n\sigma_+ + a_n^\dagger\sigma_-) + \sum_n \hbar\omega_n a_n^\dagger a_n, \quad (3.17)$$

where a_n and $a_n^\dagger$ are annihilation and creation operators of the environment oscillators, and $\sigma_\pm$ are the raising and lowering operators of the two-level system. The perturbative master equation obtained following the procedure described above is

$$\begin{aligned} \dot{\rho} = & \frac{1}{i\hbar} [H_S, \rho] - \frac{1}{2\hbar^2} \int_0^t dt_1 k(t_1) ([\sigma_+, [\sigma_-(-t_1), \rho]] \\ & + [\sigma_+, \{\sigma_-(-t_1), \rho\}]) + h.c.), \end{aligned}$$

where the kernel $k(t)$ is defined as

$$k(t) = \sum_n \lambda_n^2 \langle [a_n(t), a_n^\dagger] \rangle = \sum_n \lambda_n^2 \exp(-i\omega_n t). \quad (3.18)$$

Using the solution of the free Heisenberg equations for the spin operator (*i.e.*, $\sigma_\pm(t) = \sigma_\pm \exp(\pm i\Delta t)$), we can deduce that the master equation is

$$\dot{\rho} = \frac{1}{i\hbar} [\hbar \left(\frac{\Delta}{2} - c(t) \right), \rho] + a(t) (\sigma_+ \sigma_- \rho + \rho \sigma_+ \sigma_- - 2\sigma_- \rho \sigma_+), \quad (3.19)$$

where the time-dependent coefficients are

$$a(t) = 2\text{Re}f(t), \quad c(t) = \text{Im}(f(t)), \quad (3.20)$$

with

$$f(t) = \frac{1}{2\hbar^2} \int_0^t ds k(s) \exp(i\Delta s). \quad (3.21)$$

We recognize in this equation similar features to those present in the one for quantum Brownian motion (QBM). The interaction with the environment on the one hand renormalizes the Hamiltonian of the particle through the term $c(t)$ (including thermal fluctuations, we could verify that $c(t)$ is generally temperature dependent, as opposed to the QBM case). The non-hermitian part has a zero temperature contribution that is responsible for the spontaneous decay of the two-level system. The decay rate is determined by $b(t)$ and has a time dependence that is essentially the same as the one found for the diffusion coefficient in the zero temperature QBM case analyzed above. The finite temperature contributions can be shown to be responsible not only for the changes in the value of the decay rate $b(t)$ (which in that case would account also for the induced decay) but also for

adding new terms to the master equation that take into account the induced absorption.

Finally we obtain the perturbative master equation for the spin boson Hamiltonian, which is also widely used in various condensed-matter physics problems (and was thoroughly studied in the nonperturbative regime in [38])

$$H = \frac{1}{2}\hbar\Delta\sigma_x + \sigma_z \sum_n \lambda_n q_n + \sum_n \hbar\omega_n a_n^\dagger a_n, \quad (3.22)$$

where q_n are the coordinates of the environmental oscillators. The master equation can be shown to be

$$\dot{\rho} = \frac{1}{i\hbar}[H_S, \rho] - \frac{1}{\hbar} \int_0^t dt_1 \left(\nu(t_1)[\sigma_z, [\sigma_z(-t_1), \rho]] - i\eta(t_1)[\sigma_z, \{\sigma_z(-t_1), \rho\}] \right), \quad (3.23)$$

where the two kernels are the same as defined above in the QBM case (3.11). Using the free Heisenberg operator $\sigma_z(t) = \sigma_z \cos \Delta t + \sigma_y \sin \Delta t$ we obtain the master equation,

$$\dot{\rho} = \frac{1}{i\hbar}[H_{\text{eff}}, \rho] - \tilde{D}(t)[\sigma_z, [\sigma_z, \rho]] + z(t)\sigma_z\rho\sigma_y + z^*(t)\sigma_y\rho\sigma_z, \quad (3.24)$$

where the effective Hamiltonian and the time-dependent coefficients are now given by

$$H_{\text{eff}} = \hbar \left(\frac{\Delta}{2} - z^*(t) \right) \sigma_x, \\ \tilde{D}(t) = \int_0^t ds \nu(s) \cos \Delta s, \quad z(t) = \int_0^t ds (\nu(s) - i\eta(s)) \sin \Delta s.$$

As before, the interpretation is quite straightforward. The effect of the environment is to renormalize the frequency as well as to introduce the decay of the system. This effect takes place only if the bare frequency Δ is nonzero (otherwise $z(t)$ vanishes). The other effect of the environment is to destroy the nondiagonal terms in the density matrix, a task that is carried out by the term proportional to $\tilde{D}$, which is present even when the bare driving vanishes. As before, the expression for the time-dependent coefficients is qualitatively similar to the one observed in the QBM model.

3.4 Example 3: Perturbative master equation for a particle interacting with a quantum field

We consider the following simple model: The system is a particle with position $\vec{x}$ (moving in a 3-dimensional space) and the environment is a quantum

scalar field ϕ . The interaction between them is local as described by the Hamiltonian $V = e\phi(\vec{x})$, where e is the coupling constant (the “charge” of the particle). Expanding the scalar field in normal modes, the Hamiltonian can be written as $V = \int d\vec{k} (h_{\vec{k}} \exp(i\vec{k}\vec{x}) + h.c.)$ where the Fourier components $h_{\vec{k}}$ are proportional to annihilation operators of the quantum field (*i.e.*, $h_{\vec{k}} = e a_{\vec{k}}/(2\pi)^{1/2}(2\omega_k)^{1/2}$). More generally, we could consider models in which the particle–field interaction is slightly nonlocal taking into account the finite extent of the particle (thus, a nonrelativistic treatment of the quantum particle would only give consistent results if we do not attempt to localize it beyond its Compton wavelength). In this case, the interaction Hamiltonian $\tilde{H}_{\text{int}} = e \int d\vec{y} W(\vec{x} - \vec{y}) \phi(\vec{y})$ depends upon the window function $W(\vec{r})$ whose support lies inside a sphere of radius R (the Compton radius of the particle) centered around the origin. This nonlocal interaction corresponds to a Hamiltonian whose Fourier components $h_{\vec{k}}$ are multiplied by $\hat{W}(\vec{k})$ (the Fourier transform of $W(\vec{r})$). As we can see, the net effect of taking into account the finite size of the particle is to introduce an ultraviolet cutoff in the scalar field (the particle does not interact with the field modes with frequencies higher than its rest mass).

It is interesting to note that for this class of models we can also derive a master equation for the reduced density matrix of the particle. Thus, using the perturbative approach described above, we simply obtain (assuming the initial state of the quantum field is thermal equilibrium) the master equation as follows:

$$\begin{aligned} \dot{\rho} = & -\frac{i}{\hbar}[H, \rho] - \frac{e^2}{\hbar^2} \int d\vec{k} \int_0^t dt_1 \left(G_{\text{H}}(\vec{k}, t_1) [e^{i\vec{k}\vec{x}}, [e^{-i\vec{k}\vec{x}(-t_1)}, \rho]] - \right. \\ & \left. - iG_{\text{R}}(\vec{k}, t_1) [e^{i\vec{k}\vec{x}}, \{e^{-i\vec{k}\vec{x}(-t_1)}, \rho\}] \right). \end{aligned} \quad (3.25)$$

Here, $\vec{x}(t)$ is the Heisenberg position operator for the particle (evolved with the free Hamiltonian H) and $G_{\text{R,H}}(\vec{k}, t)$ are the Fourier transforms of the retarded and symmetric two–point functions of the scalar field (multiplied by the appropriate window function if the interaction is nonlocal). When the environment is a free field, we have

$$\begin{aligned} G_{\text{R}}(\vec{k}, t) &= W(\vec{k}) \sin(\omega_{\vec{k}} t) / 2\omega_{\vec{k}}, \\ G_{\text{H}}(\vec{k}, t) &= W(\vec{k}) \cos(\omega_{\vec{k}} t) (1 + 2N_k) / 2\omega_{\vec{k}}, \end{aligned} \quad (3.26)$$

where N_k is the number density of particles in the initial state of the quantum field (the above result is valid if the field is not free, in which case the propagators are appropriately dressed). This master equation is extremely rich. Here, we will use it for two main purposes. On the one hand, we can see that the Quantum Brownian Motion case is a special limit of this particle–field model that arises in the so-called dipole approximation.

This is the most widely used approximation in this context and is valid whenever the dominant wavelengths in the environment are much larger than the lengthscale over which the position of the particle varies. If this is the case, we can expand the exponentials up to second order ($\vec{k}\vec{x} \ll 1$) and obtain:

$$\begin{aligned} \dot{\rho} = & -\frac{i}{\hbar}[H, \rho] - \frac{e^2}{\hbar^2} \int_0^t dt_1 \left(F_H(t_1) [\vec{x}, [\vec{x}(-t_1), \rho]] \right. \\ & \left. - iF_R(t_1) [\vec{x}, \{\vec{x}(-t_1), \rho\}] \right), \end{aligned}$$

where $F_{R,H}(t_1) = \int d\vec{k} k^2 G_{R,H}(\vec{k}, t_1) / N(2\pi)^{3/2}$. Thus, our first example of a linear Brownian particle coupled to an oscillator environment arises as the dipole approximation of the particle field model. With this in mind, we will use the particle field model as an example to show that some of the results obtained in the QBM case are just artifacts of the dipole approximation. In particular, this will be the case with the dependence of the decoherence rate on distance. Using the master equation of our particle-field model we will easily show that the decoherence rate does not indefinitely grow with distance but exhibits saturation.

3.5 Exact master equation for quantum Brownian motion

After presenting some simple perturbative master equations one may wonder under what circumstances are they a reasonable approximation. To partially address this issue, it is interesting to compare these equations with the ones that can be obtained for exactly solvable problems. In particular, we describe the master equation for a model that has been thoroughly studied in connection with decoherence, *i.e.*, the linear quantum Brownian motion. Thus, because the Hamiltonian is quadratic both in the coordinates of the system and the environment, it is not surprising that it can be exactly solved. In this subsection, we will describe a simple derivation of the exact master equation, discuss its main features, and show that its functional form is the same as the one obtained by using perturbation theory. Indeed, the exact master equation has the same functional form as (3.12), the only difference being that the time dependence of the coefficients is different in general, as expected.

It is interesting to note that the exact master equation for QBM has only been found recently in spite of the simplicity of the model (in particular, the fact that it can always be written as an equation that is local in time was not appreciated until very recently [37]). Unfortunately, the derivation of the exact master equation is not so simple and, to say the least, the original one presented in [37] is indeed rather complicated. Here we will present the simplest derivation of the exact master equation that we know of,

which is done following the method proposed first in [39]. Previous studies of the master equation for QBM, obtained under various approximations, include the celebrated paper by Caldeira and Legget [40] among others (see also [41, 42]).

The derivation will focus on properties of the evolution operator for the reduced density matrix. This operator will be denoted as J and is defined as the one that enables us to find the reduced density matrix at some arbitrary time from the initial one. Thus, by definition, this operator satisfies:

$$\rho(x, x', t) = \int dx_0 \int dx'_0 J(x, x', t; x_0, x'_0, t_0) \rho(x_0, x'_0, t_0) . \quad (3.27)$$

The derivation of the exact master equation has two essential steps. The first step is to find an explicit form for the evolution operator of the reduced density matrix. The second step is to use this explicit form to obtain the master equation satisfied by the reduced density matrix. To make our presentation simpler, we postpone the proof of the first step, which will be done below using path integral techniques. Here, we first want to demonstrate how to obtain the master equation once we know the explicit form of the evolution operator. So, let us show what the evolution operator for the reduced density matrix looks like. For linear QBM we will show later that it can always be written as

$$J(X, Y, t; X_0, Y_0, t_0) = \frac{b_3}{2\pi} \exp i (b_1 XY + b_2 X_0 Y - b_3 XY_0 - b_4 X_0 Y_0) \\ \times \exp (-a_{11} Y^2 - a_{12} Y Y_0 - a_{22} Y_0^2) , \quad (3.28)$$

where for notational convenience we are using sum and difference coordinates (*i.e.*, $X = x + x'$, $Y = x - x'$, etc.) and the coefficients b_i and a_{jl} are time-dependent functions whose explicit form will be given below (and depend on the properties of the environment). Thus, the evolution operator (3.28) is simply a Gaussian function of its arguments with time-dependent coefficients. This comes as no surprise because the problem is linear.

Knowing the propagator for the reduced density matrix, it is easy to obtain the master equation following the simple method described in [39]. This is the second step of the derivation of the master equation and is done as follows. We compute the temporal derivative of the propagator J noting that the only time dependence is through the coefficients b_i and a_{jl} . Thus, we obtain

$$\dot{J} = \left(\frac{\dot{b}_3}{b_3} + i \left(\dot{b}_1 XY + \dot{b}_2 X_0 Y + \dot{b}_3 XY_0 + \dot{b}_4 X_0 Y_0 \right) \right. \\ \left. - \dot{a}_{11} Y^2 - \dot{a}_{12} Y Y_0 - \dot{a}_{22} Y_0^2 \right) J . \quad (3.29)$$

Using this equation, we can try to find the master equation through multiplying by the initial density matrix and integrating this over the initial coordinates. The master equation would be trivially obtained in this way if, after multiplying by the initial density matrix, we could integrate over all the initial coordinates. This is straightforward, with some of the terms appearing in (3.29) but it is not so obvious how to handle terms that explicitly depend upon the initial coordinates X_0 and Y_0 . Fortunately, there is a simple trick that we can use: because we know that the propagator (3.28) is Gaussian, we can make use of this fact to obtain the following simple relations:

$$\begin{aligned} Y_0 J &= \left(\frac{b_1}{b_3} Y + \frac{i}{b_3} \partial_X \right) J, \text{ and} \\ X_0 J &= \left(-\frac{b_1}{b_2} X - \frac{i}{b_2} \partial_Y - i \left(\frac{2a_{11}}{b_2} + \frac{a_{12}b_1}{b_2b_3} Y \right) + \frac{a_{12}}{b_2b_3} \partial_X \right) J. \end{aligned}$$

These two equations can be used in (3.29) and in this way we can express the right hand side of this equation entirely in terms of the reduced density matrix. The resulting master equation is

$$\begin{aligned} \dot{\rho}(x, x') &= \frac{1}{i\hbar} \langle x | [H_R(t), \rho] | x' \rangle - \gamma(t)(x - x')(\partial_x - \partial'_x) \rho(x, x') \\ &\quad - D(t)(x - x')^2 \rho(x, x') + i f(t)(x - x')(\partial_x + \partial'_x) \rho(x, x'). \end{aligned} \quad (3.30)$$

The coefficients appearing in this equation are determined by b_i and a_{jl} as follows:

$$\begin{aligned} \Omega^2(t) &= 2(\dot{b}_2 b_1 / b_2 - \dot{b}_1) & \gamma(t) &= -\dot{b}_2 / 2b_2 - b_1 \\ D(t) &= \dot{a}_{11} - 4a_{11}b_1 + \dot{a}_{12}b_1 / b_2 - \dot{b}_2(2a_{11} + a_{12}b_1 / b_3) / b_2 \\ 2f(t) &= \dot{a}_{12} / b_3 - \dot{b}_2 a_{12} / b_2 b_3 - 4a_{11}. \end{aligned} \quad (3.31)$$

Thus, we showed that the exact master equation is a simple consequence of the Gaussian form of the evolution operator (3.28). To complete our derivation of this equation we need to explicitly show how to obtain equation (3.28) and also find the explicit form of the time-dependent coefficients (which is also required to simplify the expressions leading to the master equation (3.30)).

To obtain the explicit form of the evolution operator we will follow a derivation based on the use of path integral techniques (see [37, 39, 43–45]). To understand it, very little previous knowledge of path integrals is required. The main ingredient is the path integral expression for the evolution operator of the complete wave function. Thus, if the action of the combined system is $S_T[x, q]$, the matrix elements of the evolution operator U can be written as

$$U(x, q, t; x_0, q_0, t_0) = \int Dx Dq e^{iS_T[x, q]}, \quad (3.32)$$

where the integration is over all paths that satisfy the boundary conditions,

$$x(0) = x_0, \quad x(t) = x, \quad q(0) = q_0, \quad q(t) = q. \quad (3.33)$$

In the above and following equations, to avoid the proliferation of sub-indices we use q to collectively denote all the coordinates of the oscillators q_n (we will not write the subscript n that should be implicitly assumed). Using this equation, one can obtain a path integral representation of the evolution operator of the complete density matrix and, after taking the final trace over the environment, we find a path integral representation of the propagator for the reduced density matrix. It is clear that the resulting expression will involve a double path integral (one to evolve kets and another one to evolve bras). For a generic initial state $\rho_{\mathcal{T}}$, the propagator is a somewhat complicated-looking expression. To simplify our presentation, we will only consider here factorizable initial states (and refer the reader to [45] for the most general situation where initial correlations are included). Thus, if the initial state can be factored we can express the reduced density matrix at arbitrary times as a function of the reduced density matrix at initial time using a (state-independent) propagator that has the following path integral representation:

$$J(x, x', t; x_0, x'_0, t_0) = \int \mathrm{D}x \int \mathrm{D}x' \exp(iS[x] - iS[x']) F[x, x']. \quad (3.34)$$

where the integral is over paths satisfying the above boundary conditions, $S[x]$ is the action for the system only, and $F[x, x']$ is the so-called ‘‘Influence Functional’’ first introduced by Feynman and Vernon [46]. This functional is responsible for carrying all the physical effects produced by the environment on the evolution of the system. In fact, if there is no coupling between the system and the environment, the Influence Functional is equal to the identity, and the above expression reduces to the one corresponding to the free Schrödinger evolution for the isolated system. The Influence Functional is defined as

$$F[x, x'] = \int \mathrm{d}q \mathrm{d}q_0 \mathrm{d}q'_0 \rho_{\mathcal{E}}(q_0, q'_0) \int \mathrm{D}q \mathrm{D}q' \exp(i(S_{\mathcal{SE}}[x, q] - S_{\mathcal{SE}}[q', x'])), \quad (3.35)$$

where $\rho_{\mathcal{E}}$ is the initial state of the environment and $S_{\mathcal{SE}}[q, x]$ is the action of the environment (including the interaction term with the system). It is easy to see that if there is no interaction (or if the two systems trajectories are the same, *i.e.*, $x = x'$), then the influence functional is equal to one.

Calculating the Influence Functional for an environment formed by a set of independent oscillators coupled linearly to the system is a rather straightforward task (and, to our knowledge, was first done by Feynman and

Vernon in [46]). Assuming the initial state of the environment is thermal equilibrium at temperature $T = 1/k_B\beta$, the result is

$$F[x, x'] = \exp \left(-i \int_0^t dt_1 \int_0^{t_1} dt_2 Y(t_1) \eta(t_1 - t_2) X(t_2) - \int_0^t dt_1 \int_0^{t_1} dt_2 Y(t_1) \nu(t_1 - t_2) Y(t_2) \right), \quad (3.36)$$

where $X = x + x'$, $Y = x - x'$, and the two kernels $\nu(s)$ and $\eta(s)$ are the so-called noise and dissipation kernels that were defined above in (3.11). Thus, all the influence of the environment on the evolution of the system is encoded in the noise and dissipation kernels (two different environments that produce the same kernels would be equivalent as to the impact they have on the system). To obtain the above expression is a simple exercise in path integrals. However, the calculation can also be done by a more straightforward procedure that makes no reference to path integrals. Indeed, one can notice that the influence functional can always be expressed in operator language as

$$F[x, x'] = \text{Tr}_{\mathcal{E}} \left(T(e^{-i \int_0^t dt_1 V_{\text{int}}[x'(t_1), q(t_1)]}) \rho_{\mathcal{E}} \times \tilde{T}(e^{i \int_0^t dt_1 V_{\text{int}}[x(t_1), q(t_1)]}) \right),$$

where T ($\tilde{T}$) denotes the time ordered (antitime ordered) product of the corresponding Heisenberg operators, and V_{int} is the interaction term between the system and the environment. If the interaction is bilinear and the initial state of the environment is thermal, one can easily realize that the result should be a Gaussian functional of both x and x' . Therefore, one can just write down such most general Gaussian functionals in terms of unknown kernels. These kernels could be identified by using the above expression, taking functional derivatives with respect to x and x' and evaluating the result when $x = x'$. In this way, one realizes that the result is given by (3.36), where the noise and dissipation kernels are given by expectation of symmetric and antisymmetric two-time correlation functions of the environment oscillators, exactly as in (3.11).

Knowing the Influence Functional enables us to compute the exact expression for the evolution operator of the reduced density matrix. In fact, all we need is to perform the path integral in (3.34). If the system is linear we see that the integrand is Gaussian and, therefore, the integral can also be explicitly computed. To perform this integral is not so trivial because the integrand is not separable into a product of functions of x and x' . However, the integral can be calculated simply by changing variables. First we should integrate over sum and difference coordinates X and Y . Then, we should change variables writing $X = X_c + \tilde{X}$ and $Y = Y_c + \tilde{Y}$ where X_c

and Y_c satisfy the equations obtained by varying the phase of the integrand and imposing the corresponding boundary conditions. In this way, we show that the result of the path integral is simply the integrand evaluated in the trajectories X_c , Y_c , multiplied by a time-dependent function that can be determined by normalization. The only nontrivial part of this derivation is to realize that the trajectories X_c and Y_c can be chosen as the ones extremizing only the phase of the integrand, (and not the entire exponent that, as we saw, has a real part coming from the noise). For more details on this derivation the interested reader can look in [37, 44, 45]. Therefore, the final result is given in equation (3.28) where the coefficients b_i and a_{jl} are time-dependent functions that are determined in the following way. Let the functions u_1, u_2 be two solutions of the equation,

$$\ddot{u}(s) + \Omega^2 u(s) + 2 \int_0^s ds' \eta(s-s') u(s') = 0, \quad (3.37)$$

satisfying the boundary conditions $u_1(0) = u_2(t) = 1$ and $u_1(t) = u_2(0) = 0$. Then, the coefficients appearing in (3.28) are simply given by

$$\begin{aligned} b_1 &= \frac{1}{2} \dot{u}_2(t), & b_3 &= \frac{1}{2} \dot{u}_1(0) \\ a_{jl} &= (1 + \delta_{jl})^{-1} \int_0^t ds \int_0^t ds' u_j(s) u_k(s') \nu(s-s'). \end{aligned} \quad (3.38)$$

The time dependence of the coefficients of the master equation can be investigated after specifying the spectral density and the temperature of the environment. This has been done in great detail in a series of papers [37, 39, 43, 47]. We will not review these results in detail but would just like to mention that for the case that is most interesting for studying decoherence, which is the underdamped (*i.e.*, weakly coupled) harmonic oscillator, the time dependence of the exact coefficients is very similar to the one obtained by analyzing the coefficients appearing in the perturbative master equation. Indeed, the perturbative coefficients obtained above can be recovered by solving the equation for the functions u_1 perturbatively and replacing these equations inside (3.38) and (3.31). Thus, to get a qualitative idea about the behavior of the coefficients, we restrict ourselves to the analysis already made for the perturbative ones (see Fig. 3).

It will be useful to analyze decoherence not only using the reduced density matrix but also the Wigner function that is the phase space distribution function that can be obtained from the density matrix as [48]

$$W(x, p) = \int_{-\infty}^{+\infty} \frac{dz}{2\pi\hbar} e^{ipz/\hbar} \rho(x-z/2, x+z/2). \quad (3.39)$$

It is simple to show that for the case of the harmonic oscillator, the evolution equation for the Wigner function can be obtained from the master equation

and has the form of a Fokker Planck equation

$$\dot{W} = -\{H_{\text{ren}}(t), W\}_{\text{PB}} + \gamma(t)\partial_p(pW) + D(t)\partial_{pp}^2 W - f(t)\partial_{px}^2 W. \quad (3.40)$$

The form of the evolution equation for the Wigner function for more general (nonlinear) systems will be discussed in Section 6.

As a final remark, it is worth pointing out that the exact master equation does not have the so-called ‘‘Lindblad form’’. A master equation is of the Lindblad form [49] if it can be written as

$$\dot{\rho} = \frac{1}{i\hbar}[H, \rho] - \sum_n \gamma_n (L_n^\dagger L_n \rho + \rho L_n^\dagger L_n - 2L_n \rho L_n^\dagger), \quad (3.41)$$

for some operators L_n and some (positive) constants γ_n . As shown by Lindblad, this is the most general master equation with the property of being Markovian and preserving the positivity of the density matrix. The fact that the exact master equation does not have the Lindblad form may be puzzling but after some thinking becomes natural. Of course, the exact evolution also preserves positivity of the density matrix, but it does so in a more subtle way than through a Lindblad master equation. The true evolution is not Markovian (but in a very weak sense). The only memory effect relies on the fact that the system remembers the initial time when the (factorizable) initial conditions were imposed. This effect appears in the time dependence of the coefficients that is responsible also for enforcing positivity in an interesting way (see [45, 47] for some discussion on the way positivity follows from the exact master equation). As a final comment, we would like to mention the fact that exact master equations are rather rare, but the above equation for QBM is not the only interesting exact master equation known. For example, it is possible to derive an exact master equation that has strong similarities with the one for QBM (*i.e.*, an equation that is local in time and has time-dependent coefficients) for the model of a two-level system coupled to a bosonic bath through the Hamiltonian (3.17) (this equation was derived first in [50] and rediscovered by other means in [51]).

4 Einselection in quantum Brownian motion

4.1 Decoherence of a superposition of two coherent states

We will analyze here the decoherence process in a simple example: the linear quantum Brownian motion model whose exact master equation is given in (3.30). For this we will first set up an initial state that is delocalized in position (or momentum) space and examine its temporal evolution, paying special attention to the fate of interference effects. Thus, we will consider a

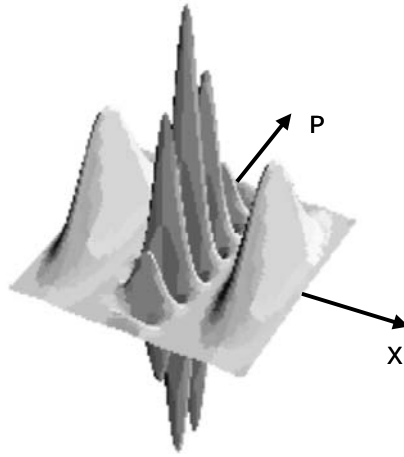


Fig. 4. Wigner function for a quantum state which is a superposition of two Gaussian wave-packets separated in position. The interference fringes are aligned along the p axes.

state of the form [47, 52]

$$\Psi(x, t = 0) = \Psi_1(x) + \Psi_2(x) , \quad (4.1)$$

where

$$\Psi_{1,2}(x) = N \exp \left(-\frac{(x \mp L_0)^2}{2\delta^2} \right) \exp(\pm i P_0 x) , \quad (4.2)$$

$$N^2 \equiv \frac{\bar{N}^2}{\pi\delta^2} = \frac{1}{2\pi^2\delta^2} \left[1 + \exp \left(-\frac{L_0^2}{\delta^2} - \delta^2 P_0^2 \right) \right]^{-1} . \quad (4.3)$$

Note that we assumed (just for simplicity) that the two wave packets are symmetrically located in phase space. The above expression allows us to study two extreme cases: the coherent states are separated in position or in momentum. In both cases, as a consequence of quantum interference, the Wigner function oscillates and becomes negative in some regions of phase space (and therefore cannot be interpreted as a probability distribution). When the coherent states are separated in position (momentum), the fringes are aligned along the p (x) axis.

To evolve this initial state, we should solve the master equation (3.30). Rather than doing this, one can use the explicit form of the evolution operator (3.28) and obtain the exact form of the reduced density matrix or the Wigner function at any time. We will adopt this strategy but will use the

master equation (3.30) and the equation for the Wigner function (3.40) as a guide to interpret our results and to obtain simple estimates for the most important effects that take place as a result of the interaction between the system and the environment. The exact evolution of the above initial state is such that the Wigner function can be written always as the sum of two Gaussian peaks and an interference term,

$$W(x, p, t) = W_1(x, p, t) + W_2(x, p, t) + W_{\text{int}}(x, p, t) , \quad (4.4)$$

where

$$\begin{aligned} W_{1,2}(x, p, t) &= \frac{\bar{N}^2}{\pi} \frac{\delta_2}{\delta_1} \exp \left(-\frac{(x \mp x_c)^2}{\delta_1^2} \right) \exp \left(-\delta_2^2 (p \mp p_c - \beta(x \mp x_c))^2 \right) , \\ W_{\text{int}}(x, p, t) &= 2 \frac{\bar{N}^2}{\pi} \frac{\delta_2}{\delta_1} \delta_2^2 (p - \beta x)^2 \\ &\quad \times \cos(2\kappa_p p + 2(\kappa_x - \beta\kappa_p)x) . \end{aligned} \quad (4.5)$$

All the coefficients appearing in these expressions are somewhat complicated functions of time that are determined by the coefficients that appear in the propagator (3.28) and the initial state (in the same way, they also depend on temperature and on the spectral density of the environment). Their explicit form can be found in [47]. The initial state is such that $\delta_1^2 = \delta_2^2 = \delta^2$, $\kappa_x = P_0 = p_c$, $\kappa_p = L_0 = x_c$ and $A_{\text{int}} = 0$.

From the form of the exact solution, it is clear what the qualitative behavior of the quantum state is. The two Gaussian peaks follow the two classical trajectories (which get distorted by the interaction with the environment) and change their width along their evolution. On top of this, the interference fringes change their wavelength and also rotate somewhat following the rotation of the two wavepackets. The effect of decoherence is clearly manifested in the damping of the interference fringes that, in the above formulae, is produced by the exponential term $\exp(-A_{\text{int}})$. Thus, we will look carefully at this term, which can be seen to be the “fringe visibility factor” defined as

$$\exp(-A_{\text{int}}) = \frac{1}{2} \frac{W_{\text{int}}(x, p)|_{\text{peak}}}{(W_1(x, p)|_{\text{peak}} W_2(x, p)|_{\text{peak}})^{1/2}} . \quad (4.6)$$

A close analysis of the definition of A_{int} shows that it vanishes initially and is always bounded from above, *i.e.*,

$$A_{\text{int}} \leq \frac{L_0^2}{\delta^2} + \delta^2 P_0^2 = A_{\text{int}}|_{\text{max}} . \quad (4.7)$$

The value of A_{int} cannot grow to infinity as a consequence of the fact that the two Gaussian initial states have a finite overlap that is proportional to $\exp(-A_{\text{int}}|_{\text{max}})$.

To understand qualitatively and quantitatively the time dependence of the fringe visibility factor, it is interesting to obtain an evolution equation for A_{int} . Using its definition, we know that

$$\dot{A}_{\text{int}} = \frac{\dot{W}_{\text{int}}}{W_{\text{int}}}|_{\text{peak}} - \frac{1}{2} \left(\frac{\dot{W}_1}{W_1} + \frac{\dot{W}_2}{W_2} \right) |_{\text{peak}} . \quad (4.8)$$

This, after using the form of the Wigner function together with the evolution equation, can be transformed into

$$\dot{A}_{\text{int}} = 4D(t)\kappa_p^2 - 4f(t)\kappa_p(\kappa_x - \beta\kappa_p) . \quad (4.9)$$

This equation enables us to obtain a clear picture of the time evolution of the fringe visibility function. Thus, we can see that the first term on the right-hand side is always positive and corresponds to the effect of normal diffusion. The normal diffusion will tend to wash out interference. The initial rate at which A_{int} grows is determined by the diffusion coefficient and by the initial wavelength of the fringes in the momentum direction (remember that initially we have $\kappa_p = L_0/\hbar$. As time goes by, we see that the effect of this term will be less important as the effective wavelength of the fringes grows (making κ_p decrease).

Various simple estimates of the temporal behavior of the fringe visibility factor can be obtained from this equation. The most naive one is to neglect the time dependence of the diffusion coefficient and assume that the fringes always stay more or less frozen, as in the initial state. In such a case, we have $A_{\text{int}} \approx 4L_0^2Dt/\hbar^2$. Thus, if we use the asymptotic expression of the diffusion coefficient, we obtain (at high temperatures) $A_{\text{int}} \approx \gamma t 4L_0^2/\lambda_{\text{DB}}^2$ where λ_{DB} is the thermal de Broglie wavelength. Consequently, we find that decoherence takes place at a rate

$$t_{\text{dec}} = \gamma_0^{-1}(\lambda_{\text{DB}}/L_0)^2 , \quad (4.10)$$

which is the relaxation rate multiplied by a factor that could be very large in the macroscopic domain (this is the result originally obtained by one of us, see [52] where it is shown that for typical macroscopic parameters, *i.e.*, room temperature, cm-scale distances and masses on the order of a gram, the factor $4L_0^2/\lambda_{\text{DB}}^2$ can be as large as 10^{40}).

By analyzing the temporal behavior of A_{int} obtained using the exact solution, we can check that this naive estimate is an excellent approximation in many important situations. However, it may fail in other important cases. Here, we want to stress a message that we believe is very important (see [55]): it may be rather dangerous to draw conclusions that are too general from the theoretical analysis of simple models of decoherence (like the one of linear QBM). The reason is that simple estimates like the one corresponding to the decoherence timescale (4.10) are just that: simple

estimates that apply to specific situations. They do not apply in other circumstances, some of which we will describe here (and in the next section). For example, the above simple estimate of the decoherence timescale fails in the simple case of “ultrafast” decoherence. For, in the high-temperature approximation of the master equation we neglected (among other things) initial transients occurring in the timescale fixed by the cutoff. Nothing (not even decoherence) can happen faster than the cutoff timescale since only after such timescale the diffusion coefficient reaches a sizable value. Thus, studying the initial time behavior of the normal diffusion coefficient one realizes that for very short times, A_{int} always grows quadratically (and not linearly). In fact, we have

$$A_{\text{int}} \simeq \frac{4M\gamma_0 k_B T L_0^2}{\hbar^2} \Lambda t^2. \quad (4.11)$$

From this expression one sees that in this case A_{int} is smaller than the one obtained under the assumption of a constant diffusion coefficient (at least for times $t \leq \Lambda^{-1}$). In this case, the decoherence timescale may be longer than the one corresponding to the high temperature approximation,

$$t'_{\text{dec}} = \frac{\hbar}{2L_0 \sqrt{M\gamma_0 \Lambda k_B T}}. \quad (4.12)$$

On the other hand, the above estimate for A_{int} also fails to take into account the fact that A_{int} does not grow forever because it finally saturates to the value fixed by equation (4.7). Saturation is achieved in a timescale that can be estimated to be $t_{\text{sat}} \approx \gamma_0^{-1}(\hbar\Omega/k_B T)$. At approximately this time the saturation of A_{int} takes place (it is clear that this is a very short time, much shorter than any dynamical timescale).

The high-temperature approximation to the behavior of A_{int} will clearly fail at very low temperatures (however, it is quite remarkable how robust an approximation this is; see [47] for a detailed analysis). We will comment in the next section about the effects arising at low temperatures giving more accurate estimates for A_{int} in such a domain.

4.2 Predictability sieve and preferred states for QBM

The most important consequence of the decoherence process is the dynamical selection of a set of stable, preferred states. These are, by definition, the least affected by the interaction with the environment in the sense that they are the ones that become less entangled with it. To obtain these states, a systematic (“predictability sieve”) criterion has been proposed [3, 53]. The basic idea is the following: to find the pointer states, one should consider all possible pure initial states for the system and compute the entropy associated with its reduced density matrix after some time t . The pointer states

are the ones that minimize the entropy production for a dynamic range of times.

The predictability sieve can be applied to the simplest models of a quantum measurement, for which the Hamiltonian of the system can be completely neglected. In such a case, the pointer states are directly associated with the eigenstates of the interaction Hamiltonian (actually, to its eigensubspaces that may be degenerate). In other more realistic situations where the self-Hamiltonian of the system is not negligible the pointer states are not going to be picked only by the interaction Hamiltonian but by the interplay between it and the evolution produced by the systems own Hamiltonian. The best example where we can explicitly compute these pointer states is the QBM model we have been studying in this section. To do this, the master equation is, as we will see, a very convenient tool.

To find pointer states, we should minimize the entropy production at some time (varying over times to find a stable answer). However, to make our task simpler, instead of using von Neumann entropy, we will simply study the evolution of the purity of the system as measured by $\varsigma = \text{Tr}\rho^2$. This quantity is equal to one for a pure state and decreases when the state of the system gets mixed because entanglement is generated by the evolution. The master equation directly enables us to write down an evolution equation for the purity ς . Thus, using the definition of ς and the equation (3.12) we obtain [3]:

$$\dot{\varsigma} = 2\gamma\varsigma - 4D\text{Tr}(\rho^2 x^2 - \rho x \rho x) - 2f\text{Tr}(\rho^2 (xp + px) - 2\rho x \rho p). \quad (4.13)$$

To simplify our treatment, we will once again use a perturbative approximation and substitute in the right hand side of this equation the expression for the free Heisenberg operators: $x(t) = x \cos \Omega t + p/M\Omega \sin \Omega t$ and $p(t) = p \cos \Omega t - M\Omega x \sin \Omega t$. Moreover, we will average over one period of the harmonic motion, assuming that the coefficients of the master equation do not vary during that time (clearly, this is a crude approximation, and we will comment later about what happens when we relax it). We also assume that the initial state is pure (and use the fact that in that case $\rho^2 = \rho$). Moreover, we neglect the effect of the friction term because, as we see, this term will always try to increase the purity in a way that is not sensitive to the state itself (thus, friction always tries to localize the state competing against diffusion that has the opposite effect). Doing this, we find out that the change in purity over one period is simply given by

$$\varsigma(T) - \varsigma(0) = -2D(\Delta x^2 + \Delta p^2/M^2\Omega^2). \quad (4.14)$$

where Δx and Δp are respectively the position and momentum dispersion of the initial state. The anomalous diffusion term does not produce any net entropy increase (or purity decrease) because its effect averages out over one oscillation. The term responsible for purity decrease is simply coming

from diffusion, and to minimize it, we should vary over all possible initial states. This can easily be implemented by varying over all values of the initial dispersion in position and momentum in such a way that the right-hand side of (4.14) is minimized. Because $\Delta x \Delta p \geq \hbar/2$ must always be satisfied, it is clear that the minimum is obtained when the state saturates uncertainty relations. From the resulting equation we obtain the pointer states as having $\Delta x^2 = \hbar/2M\Omega$ and $\Delta p^2 = \hbar M\Omega/2$. Therefore, the pointer states are simply given by coherent states with minimum uncertainty. This result is simple and satisfying. In fact, coherent states are the closest we can get to points in phase space. They are preferred states in QBM because they turn out to be the most robust and most effectively resist the combined effect of the system and the environment. They are also well localized in position and, therefore, are not significantly perturbed by the environment monitoring their position. Moreover, because of their symmetry, they are also not drastically altered by the evolution induced by the Hamiltonian of the system.

4.3 *Energy eigenstates can also be selected by the environment!*

So far, we have discussed two regimes in which the predictability sieve can be successfully applied. We first mentioned the case of a measurement (where the Hamiltonian of the system is negligible), and we just studied the case where both the system and the environment induce nontrivial evolution. There is a third regime that is interesting to study and is one in which the evolution of the environment is very slow as compared with the dynamic timescales of the system. If this is the case, it is possible to show [54] that the preferred states are simply the eigenstates of the Hamiltonian of the system. However, it is interesting to note that to find out this result, it is not possible to use a model like the linear QBM we described before. In fact, in such a model we can see that if we consider a very slow environment (with frequencies much smaller than the one belonging to the system) the master equation (3.12), which is still applicable, has time-dependent coefficients that are oscillatory functions of time with no well-defined sign. Therefore, the predictability sieve criterion does not give a robust set of states in this case.

However, the third regime of einselection can be examined using a simple argument based on an adiabatic solution of the full Schrödinger equation. The main ingredient we need is, as will be shown below, a slow environment that couples to the system through an interaction Hamiltonian that has a nonzero expectation value in the energy eigenstates of the system. To see this, we will solve the full Schrödinger equation treating the environment adiabatically. Suppose that the initial state of the universe given as $|\Psi(0)\rangle = \sum_n c_n |\phi_n\rangle |\epsilon_0\rangle$ where the states $|\phi_n\rangle$ are nondegenerate eigenstates of the Hamiltonian of the system (with distinct energies E_n), and $|\epsilon_0\rangle$ is a

state of the environment that, for simplicity, we will consider as a coherent state (the vacuum, for example). We can solve the full Schrödinger equation in the adiabatic approximation and show that this state evolves into $|\Psi(t)\rangle = \sum_n c_n \exp(-iE_n t/\hbar) |\phi_n\rangle |\epsilon_n(t)\rangle$ where the state $|\epsilon_n(t)\rangle$, that gets correlated with the n -th energy eigenstate of the system, obeys the following Schrödinger equation

$$i\hbar \frac{d}{dt} |\epsilon_n\rangle = \langle \phi_n | H_{\text{int}} | \phi_n \rangle |\epsilon_n\rangle. \quad (4.15)$$

Note that in this equation the operator $\langle \phi_n | H_{\text{int}} | \phi_n \rangle$ acts on the Hilbert space of the environment and depends parametrically on the energy eigenstates of the system. We will assume that the interaction is such that the Hamiltonian is of the form $H_{\text{int}} = S \otimes \Pi_{\mathcal{E}}$, where the operator S acts on the system Hilbert space, and the environment operator $\Pi_{\mathcal{E}}$ acts on the environment as a translation generator (it could be the momentum operator, for example, but from our discussion it will be clear that the choice of momentum here is not crucial).

The decoherence in energy eigenbasis can easily be established as follows. Because $\Pi_{\mathcal{E}}$ is a momentum operator and the initial state of the environment is a coherent state, the evolution turns out to be simply such that $|\epsilon_n(t)\rangle = |\epsilon_0 + S_{nn}t\rangle$, where $S_{nn} = \langle \phi_n | S | \phi_n \rangle$. Therefore, the overlap between the two states that correlate with different energy eigenstates can be estimated as $\langle \epsilon_n(t) | \epsilon_m(t) \rangle \approx \exp(-t^2(S_{nn} - S_{mm})^2 \hbar^2)$. Consequently, in this case, we see einselection of energy eigenstates (superpositions of energy eigenstates are degraded while pure energy eigenstates are not affected). For this reason, pointer states are energy eigenstates. This result has a rather natural interpretation. It just tells us that the environment is not able to react before the system has time to evolve and therefore only probes time-averaged quantities of the system. Energy, being the only observable that does not average out to zero is therefore the preferred observable. The conditions for energy eigenstates to become the pointer basis are the following: the environment must behave adiabatically (and be slow as compared with the dynamics of the system), and the interaction with the system must be through an observable with a nonvanishing expectation value in energy eigenstates.

5 Deconstructing decoherence: Landscape beyond the standard models

Simple models of decoherence, like the one we discussed so far (linear quantum Brownian motion) are important to illustrate the simplicity and high efficiency of the decoherence process (two characteristics that may be interpreted as indicating its generality). However, it is important to keep in mind

that no generic conclusions should be drawn from simple estimates. This is especially important in view of the possibility of carrying out experiments to test decoherence in a controlled manner. In such cases, it is essential to study specific models of the decoherence process in the correct context. Estimates of the decoherence timescale, nature of pointer states, and other characteristics of decoherence obtained in models like QBM should be taken as indications rather than as strong predictions.

In this section, we would like to stress the fact that some of the simple features that have become identified as “standard lore” in the decoherence process for the simplest case of linear QBM are not generic by showing explicitly how they fail in two specific examples. We will address basically two issues. First we will consider the status of one of the simplest predictions arising from studying decoherence in linear QBM: the “decoherence rate grows quadratically with distance”. We will show that this is not the case for more realistic models where local interactions between particles and fields (rather than oscillators) are taken into account. Second, we will consider the status of predictions of the decoherence timescale like the ones in equation (4.10) at low temperature. In this case, by analyzing the same linear QBM at low temperatures, we will show that the decoherence process may be more complicated, allowing even for nonmonotonic behavior.

5.1 *Saturation of the decoherence rate at large distances*

One of the results obtained studying the decoherence process in linear QBM models is that the decoherence rate grows quadratically with the separation between different pieces of the system wavefunction. This result is natural (delocalized wavepackets decohere faster) but would certainly not be physical if it held for arbitrarily large separations. Apart from any arguments involving cutoff (see discussion following Eq. (4.10)), it is clear that the environment should have a coherence length so that separations that are bigger than this natural lengthscale should be equivalent and therefore induce the saturation of the decoherence rate.

However, saturation is not present in the linear QBM model, as is clear from the discussion above. One therefore asks what kinds of models predict saturation. We will describe here the simplest of such models. The environment is formed by a quantum scalar field; the system is a quantum particle, and the interaction between them is local. This is the model whose perturbative master equation we derived in Section 3.4. It is important to stress once more that the linear QBM model is obtained from the particle-field model by means of the dipole approximation. Thus, saturation in this context arises only if we do not make the dipole approximation (which is certainly not well justified for large separations). The issue of the saturation of the decoherence rate was analyzed first in [56] and also discussed in [55]. In this review we present a simpler discussion than the one of [55] that

captures the main ingredients necessary for saturation and enables us to obtain the principal results without complicated calculations (some experimental results related to these issues were reported in [7]).

As we discussed in 3.4, the reduced density matrix of the particle obeys the perturbative master equation (3.25). In this equation, the Heisenberg operator of the particle $x(t_1)$ appears. To simplify our argument, we will consider the system that is a free and very massive particle and therefore replace $x(t) = x(0)$ in (3.25) (corrections to this approximation can be computed also). In the simplest example, we will consider as environment a massless scalar field (and replace the corresponding expressions for the Fourier transform of the two point functions; see Eq. (3.7)). In this case, we can express the master equation in the position representation as

$$\dot{\rho}(x, x') = -\Gamma(x - x')\rho(x, x') + \dots, \quad (5.1)$$

where only the term producing decoherence has been written out, and the function $\Gamma(x, x')$ is defined as

$$\Gamma(x, x') = -8\pi \frac{e^2}{\hbar^2} \int_0^\infty dk W(k) \sin kt \coth(\beta k/2) \left(1 - \frac{\sin kr}{kr}\right), \quad (5.2)$$

where $r = |x - x'|$ (and, as before, $W(k)$ is the Fourier transform of the window function that introduces a natural high-frequency cutoff). It is simplest to analyze the high-frequency limit of the above expression. In that case, the integral can be exactly computed and turns out to be

$$\begin{aligned} \Gamma(r) &= 8\pi^2 \frac{e^2}{\beta \hbar^2} \left(\frac{\sinh \Lambda r}{\Lambda r} - 1 \right) \exp(-\Lambda t) \quad \text{if } r \leq t \\ &= 8\pi^2 \frac{e^2}{\beta \hbar^2} \left(1 - \frac{t}{r} - \exp(-\Lambda t) + \frac{\sinh \Lambda t}{\Lambda r} \exp(-\Lambda r) \right), \text{ if } r \geq t. \end{aligned} \quad (5.3)$$

From this expression we clearly see the saturation. Thus, the solution of the master equation in the “decoherence-dominated” approximation (neglecting all terms except the one producing decoherence) is simply $\rho(x, x') \approx \exp(-\int_0^t dt_1 \Gamma(x - x', t_1)) \rho(x, x')$. The dependence of $\Gamma(r)$ for long distances is given by the second instance in equation (5.3) that approaches a constant as r grows larger than $1/\Lambda$ and t . On the other hand, the quadratic dependence of the decoherence rate is recovered for small distances: by expanding the function $\Gamma(r)$ around $r \approx 0$, we obtain a quadratic behavior.

5.2 Decoherence at zero temperature

A simple estimate for the low temperature behavior of the fringe visibility function can be obtained as follows. Use the asymptotic form of the diffusion coefficient for low temperatures given by perturbation theory and

integrate the equation for A_{int} , neglecting both its time dependence as well as the temporal evolution of the wavelength of the fringes. In this way, we obtain $A_{\text{int}} \approx \gamma_0 t (4L_0^2/\Delta x^2) \coth \beta\Omega/2$. However, this is not always a good approximation. On the one hand, if this behavior were correct, we could estimate the saturation time (the time for which A_{int} would approach its maximum value) to be on the order of $t_{\text{sat}} \approx \gamma_0^{-1} \tanh \beta\Omega/2$, which for very low temperatures can be very close to, or even larger than, a dynamical timescale. Note that this does not imply that decoherence occurs in a dynamical timescale: for that, the important fact is the actual value of A_{int} and not how close to the maximum value we are. The decoherence timescale at low temperatures is on the order of $t_{\text{dec}} \approx \gamma_0^{-1} (\Delta x/2L_0)^2$, which is still much shorter than γ_0^{-1} for macroscopic parameters). The fact that the naive estimate for the saturation timescale becomes larger than typical dynamical times means that A_{int} does not have a monotonic behavior in time. In fact, it turns out that at very low temperatures, the role of the anomalous diffusion term in the master equation starts to be relevant (its value is of the same order of magnitude as the normal diffusion coefficient). The contribution of this term to the evolution of A_{int} is clearly seen in equation (4.9) where we see that the second term (associated with anomalous diffusion) does not have a well-defined sign (its sign changes as the interference fringes rotate in phase space). From this observation, one expects that if at low temperatures the fringe visibility factor does not saturate, its time dependence should exhibit some oscillatory behavior (modulating an overall increase dictated by normal diffusion). The periods of slower decoherence coincide with the moments when fringes get oriented along the position axis (this coincides with the instant when the two wavepackets are most separated in momentum). This qualitative prediction concerning the behavior of A_{int} is confirmed by the exact numerical calculations shown in Figure 5. In this figure, the oscillations are clearly seen.

A very simple and interesting expression for A_{int} can be obtained for the QBM model. Thus, in [45] it has been shown that the fringe visibility factor can always be written as follows:

$$A_{\text{int}} = \frac{1}{2} \left(\frac{2L_0}{\Delta x} \right)^2 \coth^2(\beta\Omega/2) \left(1 - \left(\ddot{S}/\Omega^4 + \dot{S}^2/\Omega^2 \right) \right), \quad (5.4)$$

where Δx^2 is the position dispersion in thermal equilibrium (*i.e.*, $\Delta x^2 = \hbar \coth(\beta\Omega/2)/M\Omega$) and S is the normalized position autocorrelation function defined as

$$\Delta x^2 S(t) = \frac{1}{2} \langle \{x(t), x\} \rangle - \langle x(t) \rangle \langle x \rangle. \quad (5.5)$$

This equation enables us to obtain very simple qualitative estimates of the efficiency of decoherence. More interestingly, it clearly shows that decoherence has the same physical origin as other dissipative effects (and is closely

related to the decay of the autocorrelation function through Eq. (5.4)). However, in spite of their common origin, the decay of correlations and the decoherence process have very different timescales. In fact, from the above equation we can estimate how much the correlation functions have to decay in order for the system to decohere. Thus, at the time for which A_{int} approaches unity, the spatial correlations in the system should have decayed by a factor $S(t_{\text{dec}})/S(0) = \sqrt{1 - \Delta x^2/4L_0^2}$, which is indeed very small (note that Δx approaches the thermal de Broglie wavelength at high temperatures and the spread of the ground state at zero temperature).

On the other hand, the above formula (5.4) can also allow us to estimate correctly A_{int} both at high and low temperatures for the underdamped Brownian motion model. In fact, we just need to obtain a reasonable approximation for the position correlation function. For example, assuming a simple exponential decay would lead us to conclude that

$$A_{\text{int}} = \frac{1}{2} \frac{4L_0^2}{\Delta x^2} \coth^2(\beta\Omega/2)(1 - \exp(-\gamma_0 t)).$$

This is a crude but very reasonable approximation that is, for example, not only very good at high temperatures and very early times but also exhibits the correct saturation behavior for long times. It can be further improved by better approximating the position correlation function. For example, computing $S(t)$ in the highly underdamped regime we obtain

$$A_{\text{int}} = \frac{1}{2} \frac{4L_0^2}{\Delta x^2} \coth^2(\beta\Omega/2) \left(1 - \exp(-\gamma_0 t) \times (1 + \gamma_0^2 \sin^2 \Omega t / 2\Omega_0^2 - \gamma_0 \sin 2\Omega_0 t / 2\Omega_0) \right), \quad (5.6)$$

which is a very good approximation for the low-temperature (low-damping) behavior exhibited in Figure 5.

5.3 Preexisting correlations between the system and the environment

Almost all papers concerning decoherence assume that the initial state has no correlations between the system and the environment (*i.e.*, that the state can be factored). In this section we will analyze what happens if we consider more general initial conditions. In particular, we are interested in analyzing initial conditions that are closer to what we encounter experimentally. Thus, we consider a situation in which the system and the environment are initially in a thermal equilibrium state at some temperature (which could be zero) and at the initial time we perform a measurement on the system to prepare an initial state. This measurement could be imperfect (*i.e.*, may be characterized not by a projection operator, but by a POVM). After this measurement, we consider the evolution of the system coupled to the environment in the usual way. Under these circumstances, the initial state of the

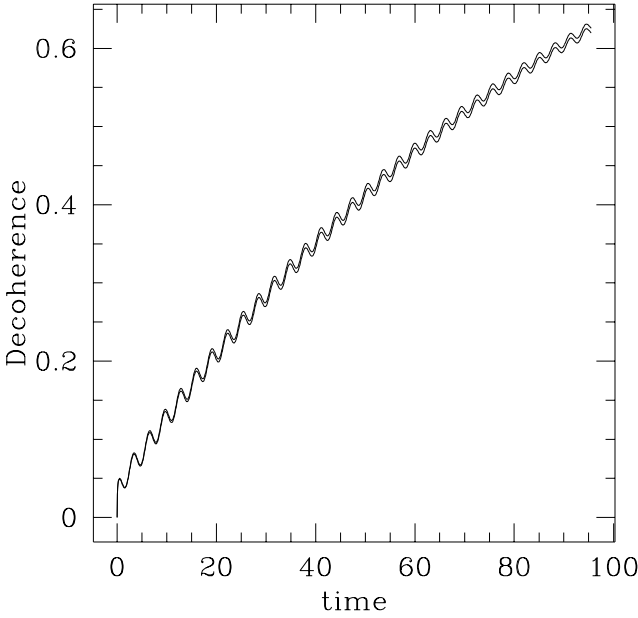


Fig. 5. Decoherence at zero temperature proceeds nonmonotonically. Here, the time dependence of A_{int} for a harmonic oscillator interacting with a zero temperature environment is displayed. Oscillations correspond to the change in orientation of the interference fringes.

universe is generally not a product. Moreover, in the case when the initial state is a product (*i.e.*, when the measurement performed on the system is perfect), the state of the environment depends functionally on the state of the system. This type of initial states can generally be written as

$$\rho_o = \sum_j A_j \rho_\beta A'_j , \quad (5.7)$$

where A_j and A'_j are Krauss operators (not necessarily projectors) acting on the Hilbert space of the system (see [29] for a good review).

We are not going to present any details of the calculations leading to the (exact) solution of this model. Our presentation follows closely the one in [45] where the influence of initial correlations on decoherence was examined. Here we present a summary of the results obtained in that paper.

First, it is worth stressing the fact that it is still possible to find a relatively simple master equation for the reduced density matrix of the system. However, the existence of initial correlations prevents us from expressing this equation entirely in terms of the reduced density matrix. Thus, the evolution of ρ not only depends on ρ itself but also on initial correlations

between the system and the environment. Interestingly enough, for the case of the linear QBM model, an exact master equation that is very similar to (3.12) can be obtained. It reads as follows:

$$\begin{aligned}
 \dot{\rho}(q, q', t) = & i \left(\frac{1}{2} (\partial_q^2 - \partial_{q'}^2) - \frac{1}{2} \Omega^2(t) (q^2 - q'^2) \right) \rho(q, q', t) \\
 & - \gamma(t) (q - q') (\partial_q - \partial_{q'}) \rho(q, q', t) \\
 & - D_1(t) (q - q')^2 \rho(q, q', t) \\
 & - i D_2(t) (q - q') (\partial_q + \partial_{q'}) \rho(q, q', t) \\
 & + i \tilde{C}_1(t) (q - q') \rho_{11}(q, q', t) \\
 & - i \tilde{C}_2(t) (q - q') \rho_{12}(q, q', t) .
 \end{aligned} \tag{5.8}$$

It is important to stress that this equation is exact and valid for all spectral densities and initial temperatures. The time-dependent coefficients appearing in (5.8) are functions of time and temperature (and of the spectral density of the environment, of course). Explicit formulae are given in [45]. The interpretation of the first three lines of this equation is identical to the ordinary case where no correlations are present. The initial correlations appear in the time dependence of the coefficients but, for realistic environments, this dependence is very weak (thus, these coefficients are qualitatively the same as before). The last two lines make this equation nonhomogeneous. In fact, these terms are present because of the correlated nature of the initial state. Thus, in that case, the master equation cannot be entirely written in terms of the reduced density matrix. It can be shown that the two density matrices ρ_{11} and ρ_{12} are obtained by propagating two different initial states given by the “density matrices” $\rho_{11} = \{q, \rho\}$ and $\rho_{12} = i[q, \rho]$. The evolution of ρ_{1i} can also be studied with this formalism because (apart from not being normalized) they belong to the class of initial conditions defined by (5.7). Therefore, the evolution equation obeyed by these operators is also (5.8), with new inhomogeneous terms. Thus, a hierarchy of equations, which are coupled because of the initial correlations, can be derived in this way (see [45] for more details).

The time dependence of all the coefficients has been studied in detail in [45] and the conclusion is that, for an ohmic environment at arbitrary temperatures, the coefficients $\tilde{C}_1$ and $\tilde{C}_2$, entering in the inhomogeneous terms of the master equation are exceedingly small and become negligible after a time that is on the order of the cutoff timescale. After this short initial transient, the impact of the initial correlations on the future evolution of the system can be entirely neglected. Of course, in less-realistic situations, it is possible to show that these coefficients have an important effect. For example, the formalism we described could be applied to the case of two coupled oscillators in which one considers one of them as the system and the other one as the environment. In this case, when the size

of the system and environment are comparable, initial correlations play an important role. The time dependence of the other coefficients of the master equation is also affected by the correlations but they all behave qualitatively in a similar way as in the absence of such initial correlations (see [45] for a detailed study of these coefficients).

It is interesting to analyze the evolution of a delocalized initial state to see how decoherence takes place in this model, which includes the effect of initial correlations. For this, we consider the initial condition (5.7 with the operators associated to a projection onto a Schrödinger cat state (say, a superposition of two coherent states separated in position). Thus, we take

$$\rho = \frac{\hat{P}\rho_\beta\hat{P}}{\text{Tr}(\rho_\beta\hat{P})}, \quad (5.9)$$

where $\hat{P}$ is a projector onto a pure state of the system $\hat{P} = |\Psi\rangle\langle\Psi|$ and the state $|\Psi\rangle$ is itself a Schrödinger's cat state (*i.e.*, a superposition of two Gaussian packets),

$$|\Psi\rangle = |\Psi_+\rangle + |\Psi_-\rangle, \quad (5.10)$$

where $|\Psi_\pm\rangle$ are such that

$$\langle x|\Psi_\pm\rangle = N \exp\left[-\frac{(q \mp L_o)^2}{2\delta^2} \pm iP_o q\right]. \quad (5.11)$$

The decoherence process for this initial state has been analyzed in the previous section in the absence of initial correlations. The fate of this state is not very different from the behavior we described before but there are some subtle differences. Thus, initial correlations distort the Gaussian peaks in the initial Wigner function as well as the intermediate interference fringes. An exact solution of the problem is possible (see [45]) and it turns out that it is no longer true that the Wigner function can be written as the sum of two Gaussian peaks plus interference fringes. In fact, it turns out that each Gaussian peak is distorted in such a way that it can be written as the sum of two nearby Gaussians with a term between them. The same is true for the interference fringes, which get distorted and split into several (actually ten) terms. However, for realistic (ohmic) environments, this effect is very small (as discussed in [45]), and the decoherence process goes qualitatively in the same way as described in the previous section (in fact, in Fig. 5, the two curves for the decoherence factor are almost indistinguishable from each other: one corresponds to an initially uncorrelated state while the other to the case described in this section).

6 Decoherence and chaos

Here we investigate environment induced superselection in the context of quantum chaos (*i.e.*, quantum dynamics of systems that are classically chaotic). We first argue [60] that the evolution of a chaotic macroscopic (but, ultimately, quantum) system is not just difficult to predict (requiring accuracy exponentially increasing with time) but quickly ceases to be deterministic in principle as a result of the Heisenberg indeterminacy (which limits the resolution available in the initial conditions). This happens after a time $t_{\hbar}$, which is only logarithmic in the Planck constant. A definitely macroscopic (if somewhat outrageous) example [61] is afforded by various components of the solar system that are chaotic, with the Lyapunov timescales ranging from a bit more than a month (Hyperion, a prolate moon of Saturn [57]) to millions of years (planetary system as a whole [58,59]). On the timescale $t_{\hbar}$ the initial minimum uncertainty wavepackets corresponding to celestial bodies would be smeared over distances of the order of the radii of their orbits into “Schrödinger cat-like” states, and the concept of a trajectory would cease to apply. In reality, such paradoxical states are eliminated by decoherence that helps restore quantum-classical correspondence. We shall also see that the price for the recovery of classicality is the loss of predictability. In the classical limit (associated with effective decoherence, and not just with the smallness of $\hbar$) the rate of increase of the von Neumann entropy of the decohering system is independent of the strength of the coupling to the environment and equal to the sum of the positive Lyapunov exponents.

6.1 Quantum predictability horizon: How the correspondence is lost

As a result of chaotic evolution, a patch in the phase space that corresponds to some regular (and classically “reasonable”) initial condition becomes drastically deformed. Classical chaotic dynamics is characterized by the exponential divergence of trajectories. Moreover, conservation of the volume in the phase space in the course of Hamiltonian evolution (which is initially a good approximation for sufficiently regular initial conditions, even in cases that are ultimately quantum) implies that the exponential divergence in some of the directions must be balanced by the exponential squeezing – convergence of trajectories – in other directions. It is that squeezing that forces a chaotic system to explore the quantum regime. As the wavepacket becomes narrow in the direction corresponding to momentum,

$$\Delta p(t) = \Delta p_0 \exp(-\lambda t) , \quad (6.1)$$

(where Δp_0 is its initial extent in momentum, and λ is the relevant Lyapunov exponent) the position becomes delocalized: the wavepacket

becomes coherent over the distance $\ell(t)$ that can be inferred from Heisenberg's principle,

$$\ell(t) \geq (\hbar/\Delta p_0) \exp(\lambda t) . \quad (6.2)$$

Coherent spreading of the wavepacket over large domains of space is disturbing in its own right. Moreover, it may lead to a breakdown of the correspondence principle at an even more serious level. Predictions of the classical and quantum dynamics concerning some of the expectation values no longer coincide after a time t_h when the wave-packet coherence length $\ell(t)$ reaches the scale on which the potential is nonlinear.

Such a scale χ can usually be defined by comparing the classical force (given by the gradient of the potential $\partial_x V$) with the leading order nonlinear contribution $\sim \partial_x^3 V$,

$$\chi \simeq \sqrt{\frac{\partial_x V}{\partial_x^3 V}} . \quad (6.3)$$

For instance, for the gravitational potential $\chi \simeq R/\sqrt{2}$, where R is a size of the system (*i.e.*, a size of the orbit of the planet). The reason for the breakdown of the correspondence is that when the coherence length of the wavepacket reaches the scale of nonlinearity,

$$\ell(t) \simeq \chi , \quad (6.4)$$

the effect of the potential energy on the motion can no longer be represented by the classical expression for the force [60], $F(x) = \partial_x V(x)$, because it is not even clear where the gradient is to be evaluated for a delocalized wavepacket. As a consequence, after a time given by

$$t_h = \lambda^{-1} \ln \frac{\Delta p_0 \chi}{\hbar} , \quad (6.5)$$

the expectation value of some of the observables of the system may even begin to exhibit noticeable deviations from the classical evolution [64].

This is also close to the time beyond which the combination of classical chaos and Heisenberg's indeterminacy makes it impossible *in principle* to employ the concept of a trajectory. Over the time $\sim t_h$ a chaotic system will spread from a regular Planck-sized volume in the phase space into a (possibly quite complicated) wavepacket with the dimensions of its envelope comparable to the range of the system. This timescale defines the quantum predictability horizon – a time beyond which the combination of classical chaos and quantum indeterminacy makes predictions not just exponentially difficult, but impossible in principle. The shift of the origin of the loss of predictability from classical deterministic chaos to quantum indeterminacy

amplified by exponential instabilities is just one of the symptoms of the inability of classical evolution to track the underlying quantum dynamics.

This breakdown of correspondence can be investigated more rigorously by following the evolution of the Wigner function (defined in (3.39)) for the possibly macroscopic, yet ultimately quantum system. Dynamics of the Wigner function is generated by the *Moyal bracket* (that is simply the Wigner transform of the right-hand side of von Neumann equation for the density matrix). This Moyal bracket can be expressed through the familiar classical Poisson bracket:

$$\dot{W} = \{H, W\}_{\text{MB}} = -i \sin(i\hbar\{H, W\}_{\text{PB}})/\hbar. \quad (6.6)$$

Above, H is the Hamiltonian of the system, and W is the Wigner transform of the density matrix.

When the potential V in H is analytic, the Moyal bracket can be expanded in powers of the Planck constant. Consequently, the evolution of the Wigner function is given by

$$\dot{W} = \{H, W\}_{\text{PB}} + \sum_{n \geq 1} \frac{\hbar(-)^n}{2^{2n}(2n+1)!} \partial_x^{2n+1} V(x) \partial_p^{2n+1} W(x, p). \quad (6.7)$$

Correction terms above will be negligible when $W(x, p)$ is a reasonably smooth function of p , that is, when the higher derivatives of W with respect to momentum are small. However, the Poisson bracket alone predicts that, in the chaotic system, they will increase exponentially quickly as a result of the “squeezing” of W in momentum, equation (6.1). Hence, after $t_\hbar$, quantum “corrections” will become comparable to the first classical term on the right-hand side of equation (6.7). At that point, the Poisson bracket will no longer suffice as an approximate generator of evolution. The phase space distribution will be coherently extended over macroscopic distances, and interference between the fragments of W will play a crucial role.

The timescale on which the quantum-classical correspondence is lost in a chaotic system can also be estimated (or rather, bounded from above) by the formula [62, 63]

$$t_r = \lambda^{-1} \ln(I/\hbar), \quad (6.8)$$

where I is the action.

6.2 Exponential instability vs. decoherence

In a quantum chaotic system weakly coupled to the environment, the process of decoherence briefly sketched above will compete with the tendency for coherent delocalization, which occurs on the characteristic timescale given by

the Lyapunov exponent λ . Exponential instability would spread the wavepacket to the “paradoxical” size, but monitoring by the environment will attempt to limit its coherent extent by smoothing out interference fringes. The two processes shall reach *status quo* when their rates are comparable,

$$\tau_D(\delta x) \lambda \simeq 1. \quad (6.9)$$

Because the decoherence rate depends on δx , this equation can be solved for the critical, steady state coherence length, which yields $\ell_c \sim \Lambda_{\text{dB}}(T) \times \sqrt{\lambda/\gamma}$.

A more careful analysis can be based on the combination of the Moyal bracket and the master equation approach to decoherence we have just sketched. In many cases, (including the situation of large bodies immersed in the typical environment of photons, rarefied gases, etc.) an effective approximate equation can be derived and translated into the phase space by performing a Wigner transform of the master equation. Then:

$$\begin{aligned} \dot{W} = \{H, W\}_{\text{PB}} &+ \sum_{n \geq 1} \frac{\hbar^{2n} (-1)^n}{2^{2n} (2n+1)!} \partial_x^{2n+1} V(x) \partial_p^{2n+1} W(x, p) \\ &+ 2\gamma \partial_p p W + D \partial_p^2 W. \end{aligned} \quad (6.10)$$

As before, we are interested in the regime where we can neglect the term that causes relaxation, which, in the macroscopic limit, can be made very small without decreasing the effect of decoherence caused by the last, diffusive term. As we saw in the previous section, the role of this decoherence term is to destroy the quantum coherence of the fragments of the wavefunction between spatially separated regions. Thus, in effect, this *decoherence term* can ensure that the Poisson bracket is always reasonably accurate. Diffusion prevents the wavepacket from becoming too finely structured in momentum, which would have caused the failure of the correspondence principle. In the case of the thermal environment, the diffusion coefficient $D = \eta k_B T$, where η is viscosity. The competition between the squeezing resulting from the chaotic instability and spreading resulting from diffusion leads to a standoff when the Wigner function becomes coherently spread over

$$\ell_c = \hbar \sqrt{\frac{\lambda}{2D}} = \Lambda_{\text{dB}}(T) \sqrt{\lambda/2\gamma}. \quad (6.11)$$

This translates into the critical (spatial) momentum scale of

$$\sigma_c = \sqrt{\frac{2D}{\lambda}}, \quad (6.12)$$

which nearly coincides with the quick estimate given by equation (6.9).

Returning to an outrageous example of the solar system, for a planet of the size of Jupiter a chaotic instability on the four-million-year timescale and the consequent delocalization would be easily halted even by a very rarefied medium (0.1 atoms/cm^3 , comparable to the density of interplanetary gas in the vicinity of massive outer planets) at a temperature of 100 K (comparable to the surface temperature of major planets): The resulting ℓ_c is on the order of 10^{-29} cm ! Thus, decoherence is exceedingly effective in preventing the packet from spreading; $\ell_c \ll \chi$, by an enormous margin. Hence, the paradox we have described in the first part of the paper has no chance of materializing.

The example of quantum chaos in the solar system is a dramatic illustration of the effectiveness of decoherence, but its consequences are, obviously, not restricted to celestial bodies: Schrödinger cats, Wigners friends, and, generally, all of the systems that are in principle quantum but sufficiently macroscopic will be forced to behave in accordance with classical mechanics as a result of the environment-induced superselection [1, 2]. This will be the case whenever

$$\ell_c \ll \chi, \quad (6.13)$$

because ℓ_c is a measure of the resolution of “measurements” carried out by the environment.

This incredible efficiency of the environment in monitoring (and, therefore, localizing) states of quantum objects is actually not all that surprising. We know (through direct experience) that photons are capable of maintaining an excellent record of the location of Jupiter (or any other macroscopic body). This must be the case, because we obtain our visual information about the universe by intercepting a minute fraction of the reflected (or emitted) radiation with our eyes.

Our discussion extends and complements developments that go back more than a decade [65]. We have established a simple criterion for the recovery of the correspondence, equation (6.13), which is generously met in the macroscopic examples discussed above. And, above all, we have demonstrated that the *very same* process of decoherence that delivers “pointer basis” in the measuring apparatus can guard against violation of the quantum-classical correspondence in dynamics.

6.3 The arrow of time: A price of classicality?

Decoherence is caused by the continuous measurement-like interactions between the system and the environment. Measurements involve the transfer of information, and decoherence is no exception: the state of the environment acquires information about the system. For an observer who has measured the state of the system at some initial instant the information

he will still have at some later time will be influenced (and, in general, diminished) by the subsequent interaction between the system and the environment. When the observer and the environment monitor the same set of observables, information losses will be minimized. This is in fact the idea behind the *predictability sieve* [3, 4] – an information-based tool which allows one to look for the einselected, effectively classical states under quite general circumstances. When, however, the state implied by the information acquired by the observer either differs right away from the preferred basis selected by the environment, or – as will be the case here – evolves dynamically into such a “discordant” state, the environment will proceed to measure it in the preferred basis, and, from the observer’s point of view, information loss will ensue.

This information loss can be analyzed in several ways. The simplest is to compute the (von Neumann) entropy increase in the system. This will be our objective in this section. However, it is enlightening to complement this “external” view by looking at the consequences of decoherence from the point of view of the observer, who is repeatedly monitoring the system and updating his records. [66] The loss of information can be quantified by the increase of the von Neumann entropy,

$$\mathcal{H} = -\text{Tr } \rho \ln \rho , \quad (6.14)$$

where ρ is the reduced density matrix of the system. We shall now focus on the rate of increase of the von Neumann entropy in a dynamically evolving system subject to decoherence. As we have seen before, decoherence restricts the spatial extent of the quantum-coherent patches to the critical coherence length ℓ_c , equation (6.11). A coherent wavepacket that overlaps a region larger than ℓ_c will decohere rapidly, on a time-scale τ_D shorter than the one associated with the classical predictability loss rate given by the Lyapunov exponent λ . Such a wavepacket will deteriorate into a mixture of states, each of which is coherent over a scale of dimension ℓ_c by $\sigma_c = \hbar/\ell_c$. Consequently, the density matrix can be approximated by an incoherent sum of reasonably localized and approximately pure states. When N such states contribute more or less equally to the density matrix, the resulting entropy is $\mathcal{H} \simeq \ln N$.

The coherence length ℓ_c determines the resolution with which the environment is monitoring the position of the state of a chaotic quantum system. That is, by making an appropriate measurement on the environment, one could in principle localize the system to within ℓ_c . As time goes on, the initial phase space patch characterizing the observer’s information about the state of the system will be smeared over an exponentially increasing range of the coordinate, equation (6.2). When the evolution is reversible, such stretching does not matter, at least in principle: it is matched by the squeezing of the probability density in the complementary directions

(corresponding to negative Lyapunov exponents). Moreover, in the quantum case folding will result in the interference fringes – telltale signature of the long range quantum coherence, best visible in the structure of the Wigner functions.

Narrow wavepackets, and, especially, small-scale interference fringes are exceedingly susceptible to monitoring by the environment. Thus, the situation changes dramatically as a result of decoherence. In a chaotic quantum system, the number of independent eigenstates of the density matrix will increase as

$$N \simeq \ell(t)/\ell_c \simeq \frac{\hbar}{\Delta p_0 \ell_c} \exp(\lambda t) . \quad (6.15)$$

Consequently, the von Neumann entropy will grow at the rate:

$$\dot{\mathcal{H}} \simeq \frac{d}{dt} \ln(\ell(t)/\ell_c) \simeq \lambda . \quad (6.16)$$

This equation emerged as a “corollary” of our discussion, but perhaps it is even its key result: decoherence will help restore the quantum-classical correspondence. But we have now seen that this will happen at a price. Loss of information is an inevitable consequence of the eradication of the “Schrödinger cat” states that were otherwise induced by the chaotic dynamics. They disappear because the environment is “keeping an eye” on the phase space, monitoring the location of the system with an accuracy set by ℓ_c .

Throughout this section we have “saved” on notation, using “ λ ” to denote (somewhat vaguely) the rate of divergence of the trajectories of the hypothetical chaotic system. It is now useful to become a bit more precise. A Hamiltonian system with $\mathcal{D}$ degrees of freedom will have in general many ($\mathcal{D}$) pairs of Lyapunov exponents with the same absolute value but with opposite signs. These global Lyapunov exponents are obtained by averaging local Lyapunov exponents, which are the eigenvalues of the Jacobian of the local transformation, and which describe the rates at which a small patch centered on a trajectory passing through a certain location in the phase space is being deformed.

The evolution of the Wigner function in the phase space is governed by the local dynamics. However, over the long haul, and in the macroscopic case, the patch that supports the probability density of the system will be exponentially stretched. This stretching and folding will produce a phase-space structure that differs from the classical probability distribution because of the presence of the interference fringes, with the fine structure whose typical scale is on the order of $\hbar/\ell^{(i)}(t)$. In an isolated system, this fine structure will saturate only when the envelope of the Wigner function fills in the available phase space volume. Monitoring by the environment destroys these small-scale interference fringes and keeps W from

becoming narrower than σ_c in momentum. As a result – and in accord with equation (6.16) above – the entropy production will asymptotically approach the rate given by the sum of the positive Lyapunov exponents,

$$\dot{\mathcal{H}} = \sum_{i=1}^{\mathcal{D}} \lambda_+^{(i)}. \quad (6.17)$$

This result [60] is at the same time familiar and quite surprising. It is familiar because it coincides with the Kolmogorov-Sinai formula for the entropy production rate for a *classical* chaotic system. Here we have seen underpinnings of its more fundamental quantum counterpart. All the same, it is surprising because it is independent of the strength of the coupling between the system and the environment, even though the process of decoherence (caused by the coupling to the environment) is the ultimate source of entropy increase. Over the last few years, the argument we presented above has been investigated and confirmed, using numerical simulations (see [67–71]). Figure 6 presents clear evidence showing that in the chaotic regime the entropy production rate approaches the value set by the Lyapunov exponent (data correspond to studies of a quantum particle moving in a harmonically driven double well potential [71]).

This independence is indeed remarkable, and leads one to suspect that the cause of the arrow of time may be traced to the same phenomena that are responsible for the emergence of classicality in chaotic dynamics, and elsewhere (*i.e.*, in quantum measurements). In a sense, this is of course not a complete surprise: Von Neumann knew that the measurements are irreversible [18]. And Zeh [32] emphasized the close kinship between the irreversibility of the “collapse” in quantum measurements and in the second law, cautioning against circularity of using one to solve the other. However, what is surprising is that both the classical-looking result ultimately has quantum roots, and that these roots are so well hidden from view that the entropy production rate depends solely on the classical Lyapunov exponents.

Environment may not enter explicitly into the entropy production rate, equation (6.17), but it will help determine when this asymptotic formula becomes valid. The Lyapunov exponents will “kick in” as the dimensions of the patch begin to exceed the critical sizes in the corresponding directions, $\ell^{(i)}(t)/\ell_c^{(i)} \gg 1$. The instant when that happens will be set by the strength of the interaction with the environment, which determines ℓ_c . This “border territory” may be ultimately the best place to test the transition from quantum to classical. One may, for example, imagine a situation where the above inequality is comfortably satisfied in some directions in the phase space, but not in the others. In that case, the rate of the entropy production will be lowered to include only these Lyapunov exponents for which decoherence is effective.

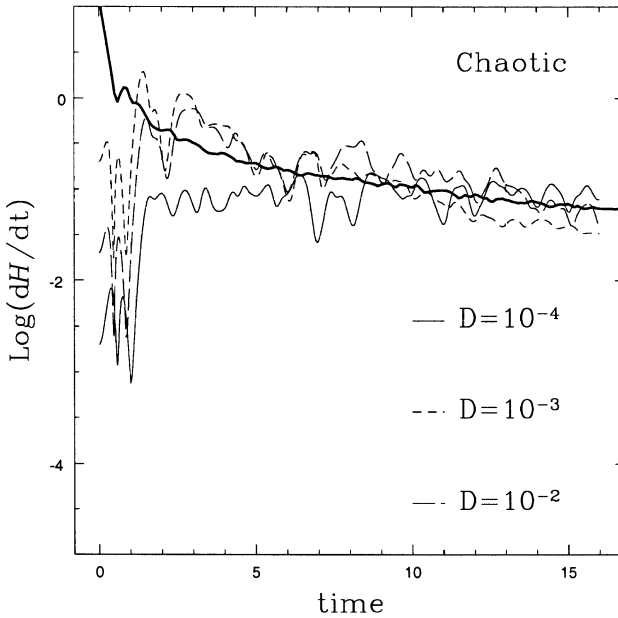


Fig. 6. Entropy production resulting from decoherence for a classically chaotic system becomes, after an initial transient, independent of the value of the diffusion constant and set by the Lyapunov exponent, see [71].

6.4 Decoherence, einselection, and the entropy production.

The significance of the efficiency of decoherence goes beyond the example of the solar system or the task of reconciling quantum and classical predictions for classically chaotic systems. Every degree of freedom coupled to the environment will suffer loss of quantum coherence. Objects that are more macroscopic are generally more susceptible. In particular, the “hardware” responsible for our perceptions of the external universe and for keeping records of the information acquired in the course of our observations is obviously very susceptible to decoherence. Neurons are strongly coupled to the environment and are definitely macroscopic enough to behave in an effectively classical fashion. That is, they have a decoherence timescale many orders of magnitude smaller than the relatively sluggish timescale on which they can exchange and process information. As a result, in spite of the undeniably quantum nature of the fundamental physics involved, perception and memory have to rely on the information stored in the decohered (and, therefore, effectively classical) degrees of freedom.

An excellent illustration of the constraint imposed on information processing by decoherence comes from the recent discussions of the possibility

of implementing real quantum computers. Decoherence is viewed as perhaps the most serious threat to the ability of a quantum information processing system to carry out a superposition of computations [11,30]. Yet, precisely such an ability to “compute” in an arbitrary superposition would be necessary for an observer to be able to “perceive” an arbitrary quantum state. Moreover, in the external universe only those observables that are resistant to decoherence and which correspond to “pointer states” are worth recording. Records are valuable because they allow for predictions, and resistance to decoherence is a precondition to predictability [3,14].

It is too early to claim that all the issues arising in the context of the transition from quantum to classical have been settled with the help of decoherence. Decoherence and einselection are, however, rapidly becoming a part of a standard lore [72,73]. Where expected, they deliver classical states, and – as we have seen above – guard against violations of the correspondence principle. The answers that emerge may not be to everyone’s liking, and do not really discriminate between the Copenhagen Interpretation and the Many Worlds approach. Rather, they fit within either mold, effectively providing the missing elements – delineating the quantum-classical border postulated by Bohr (decoherence time fast or slow compared to the dynamical timescales on the two sides of the “border”), and supplying the scheme for defining distinct branches required by Everett (overlap of the branches is eliminated by decoherence).

7 How to fight against decoherence: Quantum error correcting codes

It is clear that decoherence is a process that has a crucial role in the quantum-to-classical transition. But in many cases, physicists are interested in understanding the specific causes of decoherence just because we want to get rid of it. Thus, decoherence is responsible for washing out the quantum interference effects we would very much like to see as a signal in some experiments. This is the type of situation one is clearly facing in quantum computation (and in the physics of quantum information in general). A quantum computer is a gigantic interferometer whose wave function explores an exponential number of classical computations simultaneously. Coherence between branches of the computer wave function should be maintained because the existence of quantum interference between these branches is the basic reason why these computers can outperform their classical counterparts. Thus, decoherence in this context is a major problem.

An obvious way of try to prevent decoherence from damaging quantum states is to reduce the strength of the coupling between the system and its environment. However, it is never possible to reduce this coupling to zero and eliminate decoherence in this way. Remarkably, in recent years new techniques that enable the active protection of the information stored in

quantum states from the degrading effect of the interaction with the environment have emerged. They come under the name of “Quantum Error Correcting Codes” (QECC) and were invented by people working on quantum computation [74, 75]. They are based on remarkably simple and beautiful ideas and could be found to be useful in other areas of physics. For this reason, we believe it could be interesting to include this final main theme to give a simple-minded presentation of the methods that could enable us in principle to “fight against decoherence” preserving quantum states.

7.1 *How to protect a classical bit*

To introduce the basic idea of Quantum Error Correcting Codes it is better to start with a short discussion of the simplest ways in which one can protect classical information. Suppose that we have a single qubit b that lives in a noisy environment. Because of the effect of the noise we will assume that the bit has a probability p to flip after some time. Therefore, if we look at the bit after this time, the probability of the bit being unaltered by the noise is $1 - p$ and therefore, the information is degraded. Can we protect this classical bit? The answer is “yes” and the way to do it is by using an error correcting code. The simplest such procedure is based on the brute force use of redundancy as follows. We can “encode” this one bit of information using more carriers, mapping the state of the bit into many identical copies (*i.e.* $b \rightarrow (b, b, \dots, b)$). If we do this, we can recover the initial information after the noise occurred by voting on and adopting as our result the one that gets the majority of votes. In this way we also discover which carriers were altered by the noise (*i.e.*, the minority) and recuperate the information. Of course, this works if the error probability is small enough. To be precise, let us assume that we encode the information in three carrier bits (this is the simplest repetition code). The probability that no flip occurs is $P(\text{no flip}) = (1 - p)^3$, and the others are simply $P(\text{one flip}) = 3p(1 - p)^2$, $P(\text{two flips}) = 3p^2(1 - p)$, and $P(\text{three flips}) = p^3$. Thus, the above error-correcting strategy (encoding one into three bits and voting at the end) increases the probability of keeping the information intact from $1 - p$ to $1 - 3p^2 + 2p^3 = 1 - O(p^2)$, which is close to unity, provided p is small enough. This example illustrates the simplest classical error correction code. Of course, much more sophisticated codes exist, and we are probably not doing justice to the beautiful theory of classical error-correcting codes (see [76]) by using this naive code as an example. However, we think it is enough for the purpose of our discussion.

7.2 *How to protect a quantum bit*

The basic question then becomes if it is possible to generalize this simple procedure to quantum mechanics. One may be tempted to guess that this

task is impossible because a quantum version of the naive repetition code described above could never work as a consequence of the nonclonability of quantum states. Also, the fact that measurements drastically affect the state of quantum systems [12, 13] is somehow suggestive of the difficulties of implementing an error-correcting quantum strategy naively translating the classical error-correcting ideas. However, these expectations were proven to be incorrect when in 1995 Peter Shor created the first quantum error-correcting code [75]. His work, once again triggered a lot of activity and over the last four years the theory of Quantum Error Correcting Codes was fully developed. So far, there have been some experimental demonstrations showing the workings of these codes (only in NMR experiments) but in our view, the interesting ideas of QECC still are waiting for physicists to give a definite answer to whether or not they will be useful for other purposes than the ones that originally motivated them. For this reason, we find it interesting to bring these issues to this review.

Let us now describe how it is possible to create QECC. For this, we consider a quantum bit prepared in an arbitrary quantum state $\Psi = \alpha|0\rangle + \beta|1\rangle$. To be precise, we will first describe how noise affects the state of the qubit whose state we want to protect. We will first consider the simplest case of a noise that just produces “dephasing”. We assume that the noise introduces a random phase with a probability p or leaves the state intact with a probability $1 - p$. Although this is not the most general kind of operation that a noisy environment can produce on a quantum system, we will later show that this is not a restrictive assumption and that the treatment we present here can be generalized to include all of the effects that the noise can produce. So, for the moment we will just consider this “dephasing” noise. The dephasing can be simply described by the action of a σ_z operator on the state of the system. In this chapter, we will adopt the following notation. The Pauli matrices $\sigma_{x,y,z}$ are simply denoted as X, Y, Z . Thus, if the initial state of the system is $\Psi_0 = \alpha|0\rangle + \beta|1\rangle$ the final state (after the noise has occurred) is described by a density matrix as,

$$\rho_{\text{out}} = (1 - p)\rho_{\text{in}} + pZ\rho_{\text{in}}Z, \quad (7.1)$$

where $\rho_{\text{in}} = |\Psi_0\rangle\langle\Psi_0|$. It is easy to see that the interaction with the noise degrades the quantum state, causing the loss of quantum coherence. As a measure of this degradation, we can compute the “fidelity” of the process that is simply given by the overlap between the ideal state and the actual state. Using the above form for the density matrix, we find out that fidelity is reduced to $F = \text{Tr}(\rho_{\text{out}}\rho_{\text{in}}) = 1 - 4p|\alpha\beta|^2$. Thus, fidelity is reduced by an amount that is linear in the error probability p . Another measure of the degradation is given by the loss of purity of the final state that can be measured, for example, by $\text{Tr}\left(\rho_{\text{out}}^2\right) = 1 - 8p(1 - p)|\alpha\beta|^2$. In what follows, we will present a method that enables us to protect the quantum

state in such a way that the fidelity (or the loss of purity) does not decay linearly with the error probability but it does so quadratically.

So, let us present a way to protect the state of our qubit from the effect of a dephasing environment. As in the classical case, we will use many carriers to protect one qubit of information (in our example, we use three qubits to protect one). But the use of redundancy has to be more subtle in the quantum case. The key idea is to encode the logical states into entangled states of the three qubits in such a way that when an error occurs, the logical states are mapped into other orthogonal subspaces (one subspace for each error we want to correct). If this is the case, we can learn about the error by measuring an observable that just tells us in what two-dimensional subspace the state is in. In this way, we learn what the error was without getting any information about the state itself. Once we know the error, we can correct it and start the process all over again. This idea is illustrated clearly (we hope!) by the three-qubit example. In this case, we can use the following encoding for the logical states:

$$\begin{aligned} |0\rangle_L &= \frac{1}{2}(|000\rangle + |110\rangle + |101\rangle + |011\rangle) \\ |1\rangle_L &= \frac{1}{2}(|111\rangle + |001\rangle + |010\rangle + |100\rangle), \end{aligned} \quad (7.2)$$

(the subscript L is used to denote the logical states). The “encoding” process is simply the mapping of the physical states of the three independent carriers onto the above entangled logical states. This task is the first one that one has to do to protect the information and is represented by a unitary operator (the encoding operator E). One takes the qubit whose quantum state is to be protected and applies an operation to it together with the other two carriers we use. This operation maps the initial state into the encoded state, *i.e.*, $E|\alpha|0\rangle + \beta|1\rangle|00\rangle = \alpha||0\rangle_L + \beta|1\rangle_L$. Later in this section we will describe ways in which the encoding operation can be implemented.

The reason why (7.2) is a good encoding can be seen as follows. It is a simple exercise to show that when we apply an error operator to any of the two logical states (*i.e.*, when we act with a Z operator on any one of the qubits) we obtain mutually orthogonal states. Thus, one can show that $|0\rangle_L \perp Z_i|0\rangle_L \perp |1\rangle_L \perp Z_i|1\rangle_L$ for $i = 1, 2, 3$, *i.e.*, that the two logical states and their “erroneous descendants” are a set of eight mutually orthogonal states that constitute a basis of the complete Hilbert space of the three qubits. Therefore, the total Hilbert space can be decomposed in the direct sum of four two-dimensional subspaces. The “logical subspace” H_L , which is generated by the two vectors $\{|0\rangle_L, |1\rangle_L\}$, has three “erroneous descendants” which are simply $Z_i H_L$, and the total Hilbert space is the direct sum of H_L and $Z_i H_L$ ($i = 1, 2, 3$). As a consequence, there is an observable that we could measure to determine in which one of the four subspaces the state is in. In so doing, we discover the error and can correct it trivially.

To complete our description, we just have to exhibit what this observable whose measurement reveals the error is. To do this, it is interesting to look at the symmetries of the logical states (7.2). It is clear that these states are eigenstates of the operators $M_1 = X_1X_2$ and $M_2 = X_2X_3$ with eigenvalue ± 1 (thus, $|0\rangle_L$ is an homogeneous superposition of all states with an even number of ones and $|1\rangle_L$ contains all states with an odd number of ones; therefore these states are invariant when we flip any two states, which is precisely what the X_iX_j operators do). Moreover, it is easy to show that M_1 and M_2 are two commuting hermitian operators whose eigenvalues are ± 1 (this follows from the fact that these operators square to the identity, *i.e.*, $M_i^2 = 1$). Moreover, it is simple to show that all the “erroneous descendents” of the logical subspace are also eigenspaces of M_i . For example, the subspace Z_1H_L is formed by linear superpositions of the vectors $\{z_1|0\rangle_L, |1\rangle_L\}$ that are eigenstates of M_1 and M_2 with eigenvalues equal to -1 . This follows from the fact that as the error-operator Z_1 anticommutes with M_1 and M_2 , it transforms eigenstates of these operators into eigenstates with a different eigenvalue (*i.e.*, if $M_i|\phi\rangle = |\phi\rangle$, then $M_iZ_1|\phi\rangle = -Z_1|\phi\rangle$). Therefore, if our goal is to find out in which of the four two-dimensional subspaces the state is in, we just have to measure the two operators M_1 and M_2 . The result of this measurement is always represented by a set of two numbers that are ± 1 (the two eigenvalues of M_i) and each of the four possible alternatives (that are known as the error syndromes) identify uniquely one of the four subspaces (H_L corresponds to the syndrome $(+1, +1)$, Z_1H_L to $(-1, -1)$, Z_2H_L to $(-1, +1)$ and Z_3H_L to $(+1, -1)$).

It is also interesting to think about what kind of physical procedure we should follow to perform this kind of measurement. As discussed, we need to measure the operators M_i that are constructed as tensor products of Pauli matrices. However, it is very important to realize that we must do this **without** measuring individually the factors appearing in these products! Thus, in our case, we need to measure only $M_1 = X_1X_2$ and $M_2 = X_1X_3$, but we cannot do this by measuring the three operators X_i individually. If we were to do this, we would be measuring a complete set of commuting observables and causing the system to collapse into a particular state. Instead, quantum error correction needs measuring, not a complete set of observables but only enough observables to gain information about the error without destroying the coherence in the state of the system (thus, we want our measurement to project the state into a two-dimensional subspace and not to collapse it into one ray).

It is not hard to find a systematic way to devise a strategy that will enable us to measure any operator that is the tensor product of Pauli matrices without measuring the individual factors. To do this, it is clear that because the observables we measure are collective, we should induce an interaction

between the qbits in such a way that after the interaction, the result of the measurement is “written” on only one particle. For example, suppose that we have two particles and we want to measure the operator $M = X_1 X_2$. Suppose also that we find a unitary operator D satisfying the condition $Z_2 D = D M$. This condition implies that the operator D will transform an eigenstate of M with eigenvalue m (that can only be ± 1) into an eigenstate of Z with eigenvalue m . Therefore, if we want to measure M , we can first apply the unitary operation D and then measure Z_2 (in other words, D is the operator that changes basis from M to Z_2 eigenstates). Thus, now we just need to construct this operator. This can be done by using a simple quantum circuit. In fact, the quantum circuit for the operator D is shown in Figure 7. We just have to apply a Hadamard rotation to each qubit and then do a **c-not** using the first qubit as the control and the second one as the target. To show that this is the correct circuit for D , we just have to show that the relation $Z_2 D = D M$ is satisfied. For this purpose, we apply $M = X_1 X_2$ to the left of the circuit and start moving the X_i operators to the right. As these operators satisfy that $RX = ZR$, they transform into Z operators when they pass through the Hadamard rotations. Then, the Z operator in the control goes through the end of the circuit but the one acting on the target generates an extra Z in the control qubit that cancels the first one. Therefore, this implies that the circuit satisfies the required identity. Using this simple idea, is possible to design simple quantum circuits that can be used to measure any collective observables built as tensor products of Pauli matrices. Moreover, this can be generalized to any number of qubits. For example, the circuit to measure $M_1 = X_1 X_2$ and $M_2 = X_1 X_3$ is given in Figure 6 and consists of three Hadamard rotations (one in each qubit) followed by two **c-not** gates with the first qubit acting as the control. It is easy to see that if we measure the second and third qubits after the circuit, we learn about the syndrome and therefore find out what the error was.

To recover from the error, we just have to apply a simple operation to the remaining qubit that we do not measure (the first one in our example). This qubit contains the quantum state up to some unitary transformation that we can undo. To find out how to recover from the error, the idea is simply to see what the circuit does to the errors themselves. In fact, it is easy to show that the operator D associated with the decoding circuit appearing in Figure 7 satisfies that $Z_1 D = D X_1 X_2 X_3$, and that $Z_2 D = D X_2$, $Z_3 D = D X_3$. Therefore, this means that if the encoded state is affected by a Z_1 -type error, the resulting state after decoding will have the last two qubits set to one (we already knew that this was the syndrome corresponding to this error), and the first qubit will be affected by an X rotation that we should undo. On the contrary, the other two errors (Z_2 and Z_3) do not require any corrective action.

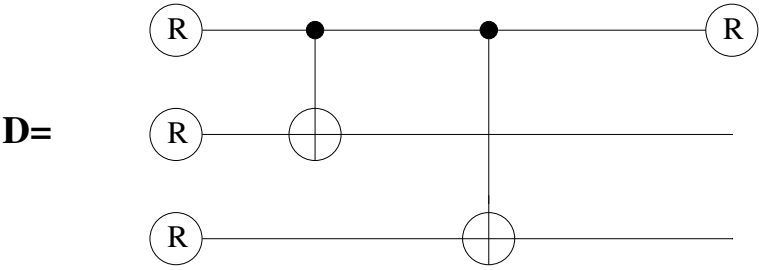


Fig. 7. Decoding circuit for the three qubit quantum error-correcting code.

So, to summarize, the error-correcting procedure is the following: (1) We encode the qubit in three carriers applying the encoding circuit shown in Figure 7. (2) After the errors act on the system, we decode the state, detect the syndromes, and apply corrective operations. (3) We refresh the syndrome qubits (resetting them to the zero state) and encoding again. It is clear that measurement of the syndrome is not really necessary because it can always be replaced by a corrective operation performed by means of a quantum circuit (in our case a **c-c-not** that is controlled by the second and third qubits). The essential part of this method is the refreshing of the syndrome qubits that is the part responsible for taking away the “entropy” generated by errors.

Two final comments are worth making before giving a more formal presentation. First, we should remark that our discussion so far assumed that errors were applied by some agent that acted on a single (unknown) qubit. However, we can extend this method to consider a situation in which there is a probability p for any one qubit to be affected by a Z -type error. In this case, the state of the three qubits before the decoding and corrective circuit is applied is given by the following density matrix:

$$\begin{aligned} \rho_{\text{out}} = & (1 - p)^3 \rho_{\text{in}} + p(1 - p)^2 \sum_i Z_i \rho_{\text{in}} Z_i \\ & + p^2(1 - p) \sum_{i \neq j} Z_i Z_j \rho_{\text{in}} Z_i Z_j + p^3 Z_1 Z_2 Z_3 \rho_{\text{in}} Z_1 Z_2 Z_3. \end{aligned} \quad (7.3)$$

After we apply the decoding and corrective procedure to this density matrix, it is clear that the first two terms will now be simply proportional to ρ_{in} . Thus, in this way we have completely eliminated the term that is linear in the error probability p . The final state differs from the ideal one only through terms that are quadratic in the error probability. Therefore, the fidelity of the whole process will be given by $F = 1 - O(p^2)$. On this linear-to-quadratic change in the dependence of F on p relies the whole power of

quantum error correction (which clearly only has a good chance of working at this level, without concatenation, if p is small enough).

Finally, we could worry about not having considered more general classes of errors. However, it should be clear by now that the general idea described so far could be generalized to include more general operations. It is important to realize that to take into account all possible effects the environment could cause on a qubit, we should protect not only against phase errors (associated with Z operators) but also against bit flips (associated with X operators) and on a combination of both (associated with Y operators). It is clear that if we are able to protect against three types of independent errors, we could also fight efficiently against arbitrary unitary (or nonunitary) errors that can always be written in terms of operators that are linear combinations of these three elements and of the identity. So, the question is how to invent codes that protect against arbitrary errors affecting any one of the carrier qubits. A code like this was first presented by Peter Shor [75] and can be constructed using our previous three qubit QECC as a building block. In fact, Shor encodes one qubit using nine carriers organized in three blocks of three qubits each. The logical states are a product of three factors like the ones shown in (7.2). This code has the following eight symmetry operations (the previous one had the two symmetries, M_1 and M_2): first, we easily find six symmetry operators that generalize the previous M_1 and M_2 in the three blocks of three qubits. Second, we find two other independent symmetries corresponding to the fact that the three blocks are repeated: $M_7 = Z_1 Z_2 Z_3 Z_4 Z_5 Z_6$ and $M_8 = Z_1 Z_2 Z_3 Z_7 Z_8 Z_9$. It is easy to show that each of the 27 different errors that can affect the nine carriers corresponds to a different syndrome (and therefore maps the logical states into orthogonal subspaces). The decoding should be done by measuring the above eight operators that reveal the syndrome and allow us to know the error that took place enabling us to correct it. A decoding circuit for this code can be easily constructed following the same discussion presented above for the three qubit. It is interesting to note that the code presented by Shor is by no means the most efficient way to correct errors. In fact, we notice that we are using an enormous Hilbert space of dimension $2^9 = 512$, but we would only need a space with enough room to accommodate for all the subspaces where we would map independent errors (in this case we require for this purpose only $2(1+3 \times 9) = 56$). Smaller codes have been developed, and the smallest one that corrects general one-qubit errors requires five qubits [77], because $n = 5$ saturates the identity $2^n = 2(3n + 1)$. This is the so-called “perfect” QECC and has the following symmetry operators $M_1 = Z_2 Z_3 Z_4 Z_5$, $M_2 = Y_1 Z_3 X_4 Y_5$, $M_3 = Z_1 X_2 Z_3 X_5$, and $M_4 = Z_1 Y_3 Y_4 Z_5$. To show that these symmetry operators constitute a good QECC requires showing that all independent errors produce a different anticommutation pattern with the M_i operator (this is left as an exercise). The construction of an

encoding–decoding circuit for this code can also be done by generalizing the ideas we have described before.

7.3 Stabilizer quantum error-correcting codes

A more formal description of the principles underlying the theory of quantum error–correcting codes can be given (following the presentation of [78]) we restrict ourselves to discuss a rather wide class of codes known as stabilizer codes (for more general codes and for a more thorough discussion of QECC we refer the reader to [79–81]). We can consider codes that protect k qubits by encoding them into n carriers. Here, the code space $\mathcal{H}_k$ (or logical space) is a 2^k dimensional subspace of the total Hilbert space of the n carriers. $\mathcal{H}_n$ is a tensor product of n two–dimensional factors and has a natural basis whose elements are product states of the individual carriers. This is the “physical basis” that can be formed with the common eigenstates of the operators $\{Z_1, \dots, Z_n\}$ (for convenience, we label states of this basis not by the eigenvalues of the corresponding operators, which are ± 1 , but by the eigenvalues of the projectors onto the -1 subspace, which are 0 or 1: thus, the label $z_j = 0$ ($z_j = 1$) corresponds to a $+1$ (-1) eigenvalue of the operator Z_j). Furthermore, we order the n carriers in such a way that the last k qubits are the ones whose state we encode, and the first $n - k$ are the ancillary carriers. Therefore, states of the physical basis are of the form $|s, z\rangle_P = |s\rangle_P \otimes |z\rangle_P$ (where the strings $s = (s_1, \dots, s_{n-k})$, $z = (z_1, \dots, z_k)$ store the corresponding eigenvalues and the subscript P is used to identify the states of the physical basis).

An error–correcting code is a mapping from the physical product states $|0\rangle_P \otimes |\Psi\rangle_P$ onto the code space $\mathcal{H}_k$, which is formed by entangled states of n carriers. A rather general class of codes can be described in terms of their stabilizer group (see [80]). The stabilizer of the code is an Abelian group formed by all operators that are tensor products of Pauli matrices and have $\mathcal{H}_k$ as an eigenspace with an eigenvalue equal to $+1$. Every element of the stabilizer, which is a finite group with 2^{n-k} elements, can be obtained by appropriately multiplying $n - k$ generators, which will be denoted as $M_1, \dots, M_{n-k}$. The elements of the stabilizer are completely degenerate in the code space $\mathcal{H}_k$ (since all states in $\mathcal{H}_k$ are eigenstates with eigenvalue $+1$ of all M_j). To define a basis in the code space, we choose k extra operators $L_1, \dots, L_k$, which being tensor products of Pauli matrices commute with all elements of the stabilizer. These operators $L_{j'}$, $j' = 1, \dots, k$ are the “logical pointers” because they define the directions in $\mathcal{H}_k$ associated with the logical states $|0\rangle_L, \dots, |2^k - 1\rangle_L$ (logical pointers belong to the group of operators that commute with the stabilizer, known as the normalizer).

The $n - k$ generators of the stabilizer together with the k logical pointers are a Complete Set of Commuting Operators (CSCO) whose common eigenstates form a complete basis of the Hilbert space $\mathcal{H}_n$. Elements of

this “logical basis”, labeled by n quantum numbers, are denoted as $|m, l\rangle_L$, where the bit strings $m = (m_1, \dots, m_{n-k})$, and $l = (l_1, \dots, l_k)$ identify the corresponding eigenvalues, and the subscript L refers to logical states. The CSCO formed by the generators of the stabilizer and the logical pointers defines a prescription for decomposing the original Hilbert space of the n -carriers into a tensor product of a 2^k -dimensional logical space $\mathcal{L}$ and a 2^{n-k} -dimensional syndrome space $\mathcal{Y}$. In fact, elements of the logical basis (which are entangled states of the n -carriers) are tensor products of states belonging to $\mathcal{L}$ and $\mathcal{Y}$: $|m, l\rangle_L = |m\rangle_L \otimes |l\rangle_L$. Encoded states, which belong to $\mathcal{H}_k$, are also product states of the form $|\Psi\rangle = |0\rangle_L \otimes \sum_l c_l |l\rangle_L$.

The code protects quantum states against any error E_a whose action on states of the logical basis is to change the logical syndrome and, eventually, rotate the logical state in $\mathcal{L}$ in a syndrome-dependent way,

$$E_a |m\rangle_L \otimes |l\rangle_L = e^{i\phi_{ma}} |m + c_a\rangle_L \otimes U_a |l\rangle_L . \quad (7.4)$$

Here, U_a is a unitary operator acting on the collective logical space $\mathcal{L}$, and ϕ_{ma} is a phase that may depend on the syndrome and the error. The error E_a changes the syndrome from m to $m + c_a$ where c_a is the bit string storing the commutation pattern between the error and the generators of the stabilizer (the j -th bit of this string is one if the error anticommutes with M_j and is zero otherwise). The reason for this is that when acting on a logical state, the error E_a changes the eigenvalue of the operator M_j only if $\{M_j, E_a\} = 0$. The label a used to identify errors is arbitrary and, for the case of nondegenerate codes (which are the only ones we will consider here) it is always possible to label errors E_a using simply the commutation pattern c_a (*i.e.*, we can choose $a = c_a$).

To correct against the action of any of the errors E_a (or against any linear superposition of them) one can first detect the error by measuring the collective syndrome (*i.e.*, measuring the observables M_j , $j = 1, \dots, n - k$) and later recover from the error by applying the corresponding operator $U_a^\dagger$. This detection-recovery process can be conveniently described as a quantum operation defined by the following mapping from the erroneous density matrix ρ_{in} into the corrected one ρ_{out} ,

$$\rho_{\text{out}} = \sum_{m=0}^N R_m \rho_{\text{in}} R_m^\dagger , \quad (7.5)$$

where the sum runs over all syndromes ($N = 2^{n-k} - 1$), and the recovery operator for each syndrome is

$$R_m = |0\rangle_L \otimes \langle m| \otimes U_m^\dagger . \quad (7.6)$$

By construction, these operators satisfy the identity $\sum_{m=0}^N R_m^\dagger R_m = I$.

Because our description of error detection–recovery process is entirely formulated on the logical basis, it does not involve so far any reference to encoding or decoding operations that can be simply defined as a change of basis. The encoding operator C is a unitary operator mapping the physical basis, formed by product states of the n carriers, onto the logical basis, formed by entangled states. Accordingly, C transforms the operators Z_i (whose eigenvalues define states on the physical basis) into the operators $M_j, L_{j'}$ (that label states on the logical basis). Thus, the encoding operator C is such that $Z_j = C^\dagger M_j C$, $j = 1, \dots, n - k$, and $Z_{n-k+j'} = C^\dagger L_{j'} C$, $j' = 1, \dots, k$. Taking this into account, the action of the operator R_m can be described, in the physical basis, as the following sequence of operations: i) decode the state, ii) measure the syndrome in the physical basis by measuring Z_j in the first $(n - k)$ carriers, iii) if the result of the measurement is the string s , apply the syndrome–dependent recovery operator $U_s^\dagger$ resetting the syndrome back to zero, and iv) encode the resulting state.

Finding a stabilizer code correcting a given set of errors is a rather hard task that involves designing generators having appropriate commutation patterns with the errors. Once the generators are found and the logical pointers are chosen, an encoding or decoding operator can be constructed (strategies for designing encoding or decoding circuits from the stabilizer are known; see [82, 83]). The recovery operators depend on the encoding or decoding strategy and can be explicitly found from the encoding circuit by running errors through it.

As we mentioned above, the simplest code protecting $k = 1$ qubit using $n = 3$ carriers correcting against phase errors in any of the carriers can be understood as a particular example of this general stabilizer code class. In such a case, the basic errors to correct are $E_1 = Z_1$, $E_2 = Z_2$ and $E_3 = Z_3$. The stabilizer of the code can be chosen to be generated by $M_1 = X_1 X_2$ and $M_2 = X_1 X_3$. The commutation pattern associated with each error is $c_1 = 11$ (because the error Z_1 anticommutes with both M_1 and M_2), $c_2 = 10$, $c_3 = 01$ (note that we could relabel the errors ordering them according to their commutation pattern). The decoding circuits exhibited in Figure 7 has the properties

$$C^\dagger Z_1 C = X_1 X_2 X_3, \quad C^\dagger Z_2 C = X_2, \quad \text{and} \quad C^\dagger Z_3 C = X_3. \quad (7.7)$$

These properties entirely determine the action of the errors Z_i in the logical basis. For example, the last identity implies that $E_3|m\rangle_L|l\rangle_L = |m + c_3\rangle_L|l + 1\rangle_L$. Thus, the error E_3 not only changes the syndrome but also modifies the logical state by flipping it. This means that the recovery operator for this error is $U_3 = X$. Analogously, we can find how the other errors act on the logical basis, showing that $U_1 = U_2 = I$.

8 Discussion

We have seen “decoherence in action” in a variety of settings. Our aim was not to review all of the studies of decoherence done in recent years. Thus, we left aside from our review the discussion of some very interesting physical problems where the role of environment-induced decoherence is relevant. For example, in cosmology, the way in which decoherence can account for the quantum to classical transition of density fluctuations (and of spacetime itself) has been – and still is – a matter of debate (see [84] for an incomplete list of relevant papers). Fortunately, there are also other areas where decoherence can be analyzed and tested in the laboratory. Among them, the use of systems of trapped and cold atoms (or ions) may offer the possibility of engineering the environment (effectively choosing the pointer states) as proposed in [85]. Trapped atoms inside cavities were discussed [86] and the relation between decoherence and other cavity QED effects (such as Casimir effect) was analyzed [87]. On the mesoscopic scale, the nature of decoherence may receive increasing attention specially in the context of BEC both as a key ingredient in the phenomenological description [88] and as a threat to the longevity of BEC Schrödinger cats [89]. Moreover, the nature of decoherence is being studied experimentally in the context of condensed matter systems (see, for example [90]).

The aim of this section is to describe briefly what is (and point out what is not) accomplished by decoherence, and to show how it facilitates understanding the transition from quantum to classical. Environment-induced superselection is clearly the key interpretational benefit arising from decoherence. The quantum principle of superposition does not apply to open quantum systems. States in the Hilbert space are no longer “equal”. Under a broad variety of realistic physical assumptions, one is now forced to conclude that for macroscopic objects only a small subset of states can ever contribute to the “familiar classical reality”. Only the einselected pointer states will persist for long enough to retain useful (stable) correlations with – say – the memories of the observers, or, more generally, with other stable states. By contrast, their superpositions will degrade into mixtures that are diagonal in the pointer basis.

The precondition for “perception” (as in “perception of classical reality”) is the ability of the state to persist, or to evolve in a more or less predictable manner during a time interval over which the observer is monitoring it. This time interval can occasionally be quite short, but it should not be as unreasonably short as the typical decoherence time for the macroscopic systems. Thus, the only states that have a chance of being perceived as “real” are the preferred (pointer) states. Indeed, given the limited accuracy of the observer’s efforts, it may be more precise to say that broad superpositions of pointer states are definitely ruled out.

It is important to emphasize that the environment-induced superselection leads to a probability distribution that is diagonal in the preferred basis, and not to a single pointer state. Thus, the uniqueness of perceptions of the observer has its roots in the stability of the correlations between the states of the macroscopic objects in the outside world and the records in the observer's memory (which, incidentally, must also use preferred states of, say, neurons to store records of the observations).

The information possessed by the observer is not an abstract, esoteric entity. Rather, "information is physical" [30] and "there is no information without representation" [3]. In practice, this means that the state of the observer is in part determined by what he knows about the rest of the universe. Thus, the physical existence of long-lasting records underlies the essence of the process of perception. Observers will be aware of their own records, and of the external universe in a state consistent with these records. This viewpoint known as the *existential interpretation* [3, 17] accounts for the apparent collapse, but is consistent with either the Many Worlds or Copenhagen Interpretation.

The nature of the preferred states is dynamically negotiated in the course of the interaction between the system and the environment, but, as we have already seen, the self-Hamiltonian of the system plays an important role. Truly realistic models are difficult to treat, but lessons of the predictability sieve applied to simple models allow one to infer with some confidence that, in general, pointer states will be localized in position. After all, most interactions depend on distance. Thus, localization is an inescapable consequence [2, 14]. Nevertheless, as we have already seen in perhaps the most relevant exactly solvable case of a decohering harmonic oscillator, preferred states tend to be localized in both position and momentum and can be regarded as quantum counterparts of classical points.

Investigation of the coexistence of decoherence with chaos is an example of a bit more complicated case. There, we have seen that localization is effectively enforced (even if such systems cannot be treated analytically, and extensive numerical studies are required).

An exciting "corollary" of decoherence in the setting of quantum chaos is the quantum derivation of the classically anticipated entropy production rate, given by the sum of positive Lyapunov exponents. This suggests a quantum origin of the second law of thermodynamics. Indeed, it seems that the resolution of the two outstanding puzzles of physics – the arrow of time and the apparent classicality – may originate from the same essentially quantum source, from decoherence and einselection.

The study of decoherence and einselection over the past two decades has yielded a new paradigm of emergent, effective classicality. It leads to a new understanding of the quantum origins of the classical. To be sure, not all of the interpretational questions have been settled, and much further work

is required. Nevertheless, as a result of this paradigm shift, the quantum-to-classical transition has become a subject of experimental investigations, while previously it was mostly a domain of philosophy.

Acknowledgements

This research was supported in part by NSA. We gratefully acknowledge Isaac Newton Institute in Cambridge, England, where much of this manuscript was prepared. JPP was also supported by grants from ANPCyT (PICT 01014) and Ubacyt (TW23).

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COURSE 9

**CAVITY QED EXPERIMENTS, ENTANGLEMENT
AND QUANTUM MEASUREMENT**

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CAVITY QED EXPERIMENTS, ENTANGLEMENT AND QUANTUM MEASUREMENT

M. Brune

1 Introduction

The theory of measurement is one of the most important part of quantum mechanics. It introduces at a fundamental level an intrinsic randomness in single measurement results. This randomness becomes even stranger when considering composite quantum systems. The correct description of statistical results of joined measurements performed on two parts of the system then involves a purely quantum feature named entanglement. It originates from the impossibility to factorize a composite system's wavefunction as a direct product of two individual wavefunctions (non-separability) once the two parts of the system have interacted. It manifests itself in non-local correlations while observing the two parts of the system after separation by a macroscopic distance. Entanglement makes it impossible to interpret these correlations in the light of classical logic.

This point is at the heart of a debate initiated in the early days of quantum mechanics by the EPR (Einstein Podolsky Rosen) argument [1]. Since then, it has been a challenging goal to design experiments demonstrating the difference between quantum and classical logic. The evidence of the violation of Bell's inequalities in the 70's was an essential step in this respect [2,3]. New perspectives have been opened by advances in the manipulation of isolated particles allowing the preparation of tailored entangled states. In particular, the degree of control of quantum systems is now high enough for preparing entangled states involving 3 to 4 two-level systems. These new possibilities are at the heart of the emerging field of quantum information processing [4]. Even if the goal of preparing sophisticated enough entangled states for building a quantum computer seems speculative, simple operations that process and transfer elements of information coded into quantum states (qubits) such as cryptographic key distribution [5] and state teleportation [6] have been performed. Beyond this aspect, it seems that improving our understanding of the behavior of "large" samples of entangled particles is of fundamental interest.

The understanding of entanglement in mesoscopic systems sits at the center of the quantum theory of measurement. This has been recognized since the early days of quantum mechanics and has been illustrated by the famous “Schrödinger cat” [7,8] metaphor which was emphasizing vividly the problem of the emergence of the classicality of meters out of the quantum structure of the underlying microscopic objects. More recently, the interplay between entanglement and dissipation, the so called decoherence process [9,10], has been recognized as playing a central role in this problem. The preparation of mesoscopic entangled states involving quasi-classical systems of adjustable size is thus of great interest for exploring the mechanisms involved in the transition between the quantum and classical worlds.

Various techniques are presently used for investigating quantum features related to entanglement in highly controlled systems. The key point is the degree of isolation of the system with respect to the environment. Pioneering experiments were performed with correlated photons. Once entangled, these particles propagate over large distances without interaction with the environment, thereby preserving entanglement until detection. Strongly entangled photon pairs are spontaneously produced by atomic cascades or parametric down-conversion. They have been used to demonstrate the violation of Bell inequalities [2,3] as well as to implement quantum cryptography [11] and teleportation [12–14]. Triplets of entangled photons have also been generated and used for non-locality tests [15,16]. This way of getting entangled particles relies however on random irreversible processes. In these experiments, one uses the entangled states that nature gives spontaneously in very specific situations. The method is thus limited to the demonstration of entanglement in relatively simple situations.

Progresses in the manipulation of single isolated massive particles have opened new perspectives by allowing to “synthesize” deterministically complex multiparticle entangled states. The key feature here is the use of strong interactions at the single particle level for generation of entanglement in controlled reversible Hamiltonian processes. Strongly interacting particles however, are also very often strongly coupled to the environment. The difficulty then consists in minimizing this coupling which is responsible for decoherence while preserving strong mutual interactions inside the system. This is presently achieved in two different fields: ion trapping [17,18] and microwave Cavity Quantum Electrodynamics (CQED) [19].

This course is devoted to the physics of entanglement in microwave CQED experiments. The heart of this system is a microwave photon trap, made of superconducting mirrors, which stores a few-photon field in a small volume of space for times as long as milliseconds. This field interacts with “circular” Rydberg atoms [20] injected one by one into the cavity. They combine a huge dipole coupling to a single photon with a lifetime (30 ms) three orders of magnitude larger than the cavity crossing time (20 μ s).

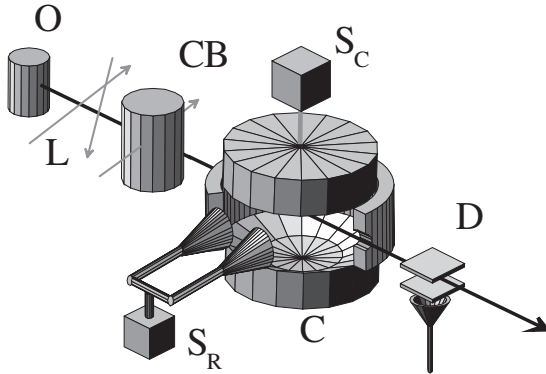


Fig. 1. Experimental set-up.

In this system, coupling to the environment is weak enough so that coherent atom-field interaction overwhelms dissipative processes achieving the so called “strong coupling regime”.

Section 2 of this course is devoted to the description of the strong coupling regime in Rydberg atom CQED [21–24]. The tools of the experiment are briefly presented at the beginning of this section as well as the main characteristics of the strong coupling regime [25–27]. We then show in Section 3 how to use the strong interaction with a single photon to perform a non-destructive detection of a single photon with a single atom as a meter [28]. In Section 4, we show that the achieved QND measurement process corresponds to the operation of a quantum phase gate [29]. It allows, in principle, to prepare arbitrary atom + field entangled states. Various methods will be presented for preparing entangled states such as a two atom EPR pair [30] as well as a GHZ (Greenberger *et al.* [15]) triplet [31]. Entanglement involving more and more complex systems will then be investigated in Section 5 where the preparation of a “Schrödinger cat state” of the cavity field is presented [32]. We especially address in this last section the problem of entanglement between the system and the meter which occurs during any quantum measurement process.

2 Microwave CQED experiments: The strong coupling regime

The microwave CQED experiments described in this course all rely on the strong coupling between single two level atoms and a few microwave photons stored in a high Q superconducting cavity. We will recall here the essential properties of the various element of the setup as sketched in Figure 1. A thermal beam of Rubidium atoms originating from oven O is promoted to highly excited circular Rydberg states in the circularization

box CB . The excitation scheme is made velocity-selective by a combination of velocity selective optical pumping performed by the lasers L and time of flight techniques [27]. The monokinetic atomic beam then crosses a high Q superconducting cavity mode C tuned close to transition between two circular levels e and g . A small classical field can be injected into C by the classical source S_C . Before and after interaction with C , the atoms can be exposed to microwave pulses generated by the source S_R . These pulses are used for preparation or detection of arbitrary two level superposition states. After leaving C , the atoms are detected one by one in a state selective ionization detector D allowing one to measure whether the atom eventually is in state e or g . Because of the use of superconducting material as well as to the high sensitivity of circular Rydberg atoms to blackbody radiation, all the elements of the set-up, from the circularization to the detection of the atoms, must be cooled down between 1.2 and 0.6 K in a ^3He cryostat.

2.1 *The experimental tools and orders of magnitude*

2.1.1 Circular Rydberg atoms

They combine a large principal quantum number N with maximal orbital and magnetic quantum numbers $l = |m| = N - 1$. A circular state with principal quantum number N will be referenced as N_c . The wavefunction of the Rydberg electron is a torus whose diameter is $a_0 N^2$. This “large” wavefunction results in a very large dipole coupling between adjacent circular levels. In the experiments described here, the levels e and g are respectively the 51_c and 50_c states. The dipole matrix element between these levels is $d = qa_0 N^2 / 2 = 1250 \text{ a.u.}$ The frequency of this transition is $\nu_{eg} = 51.099 \text{ GHz}$.

The circular atomic levels are prepared by exciting the valence electron of Rubidium atoms into the 52_c state in a complex process involving 52 photons [20]. The 51_c or 50_c levels are then prepared selectively by a last microwave pulse resonant either on the $52_c \rightarrow 51_c$ one-photon or $52_c \rightarrow 50_c$ two-photon transition at 48.195 GHz and 49.647 GHz, respectively. This process prepares up to 400 circular atoms per preparation pulse. The selectivity of the last microwave transition in a large dc electric field allows the elimination of spurious elliptical levels (all other values of l and m). The purity of the prepared state, measured by a selective spectroscopic method is better than 98%. The stability of circular atoms requires the application of a small electric field providing a physical quantization axis everywhere in the set-up [33]. Under this condition, the atoms prepared in e or g behave as ideal long lived two level atoms while they interact with a nearly resonant cavity mode.

Circular atoms are easily detected by ionization in a relatively small static electric field. As the ionization threshold increases with the binding

energy of the levels, one can selectively ionize either e or g in two different detectors. This detection scheme, relies on electron counting. It is extremely sensitive and behave as a meter for the energy of a single atom. It allows measurements on a single realization of the experiment as well as to measure average values of the atomic energy by resuming the same experiment until significant statistics is obtained. The regime of single atom interaction with the cavity is achieved at the expense of low counting rates of typically 0.1 to 0.2 detected atom per preparation pulse (detection efficiency 40%(10)). In this limit, the Poissonian statistic of the number of excited atoms results in a small probability to excite two atoms at the same time.

A pulsed velocity selective optical pumping scheme prepares monokinetic Rubidium atoms [27] in the state $5s_{1/2} F = 3$ just after they leave the oven O . This level is the starting point of the circular atoms preparation. The width of the velocity distribution obtained in this way is 10 m/s. It is reduced to 1.5 m/s by time of flight selection between optical pumping and circularization which is also a pulsed process. Due to the control of the atomic velocity and of the time of preparation of Rydberg atoms, one knows the position of the circular atoms inside the setup with a precision of ± 1 mm. This is used for applying to each atom the proper sequence of controlled interactions with the cavity mode and the auxiliary classical microwave pulses. In particular, the atom-cavity interaction time is adjusted by switching on and off an electric field of about 1 V/cm between the cavity mirrors. The atoms are then tuned in and out of resonance by Stark effect at user controlled programmable times while they cross the cavity.

2.1.2 The photon box

The cavity is made of two massive Niobium mirrors in a Fabry-Perot geometry depicted in Figure 1. The two spherical mirrors have a radius of curvature of 40 mm. The distance between the mirrors at center is 27.5 mm. The atoms are nearly resonantly coupled to the TEM_{900} Gaussian mode whose resonance frequency is close to $\nu_{eg} = 51.099$ GHz. The mode waist, $w_0 = 5.96$ mm, is close to the wavelength, $\lambda = 6$ mm. The corresponding mode volume [21] is relatively small ($V \simeq 700$ mm³). The microwave electric field amplitude at cavity center $E_0 = \sqrt{\hbar\nu_{eg}/2\epsilon_0 V} = 1.5$ mV/m is the essential parameter characterizing the coupling with the atomic dipole.

A quality factor as high as 3×10^8 corresponding to a photon lifetime of 1 ms can be obtained by careful polishing and processing of the mirrors. It is limited by diffusion of photons out of the aperture between the mirrors due to the residual roughness of their surface. These losses do not occur in a closed cavity [34]. However, the closed geometry is not compatible with the electric field needed for stabilizing circular atoms [33]. Diffusion losses are reduced by inserting an aluminum ring nearly closing the opening between the mirrors. The atoms enter the cavity through 3 mm diameter holes in this

ring. Inhomogeneous electric fields in these holes destroy atomic coherence but they do not affect the populations of Rydberg states. An external microwave source is coupled into the cavity mode through small 0.2 mm diameter holes at the center of the mirrors.

2.2 Resonant atom-field interaction: The vacuum Rabi oscillation

A detailed description of the atom-cavity interaction can be found in various review papers [21–24]. It relies on the Jaynes-Cummings hamiltonian [35] whose eigenstates are the so called “dressed states” [36] of the atom-field system. The non-degenerate ground state of the system is $|g, 0\rangle$ where 0 stands for the photon number. We are interested here in the dynamics of the two first excited states of the system $|g, 1\rangle$ and $|e, 0\rangle$ which are coupled by an electric dipole transition. This coupling results in a splitting $\hbar\Omega_0 = -2dE_0$ of the first dressed states $|+, 0\rangle$ and $|-, 0\rangle$. An atom initially in state e crossing an empty cavity thus experiences a “vacuum Rabi oscillation”: atom and field exchange periodically one photon at the Rabi frequency $\Omega_0/2\pi = 47$ kHz.

The corresponding Rabi oscillation signal [26] is presented in Figure 2. It shows the measured average atomic excitation as a function of the atom-field interaction time. The cavity is tuned at resonance with the 51_c to 50_c transition. The mode Q factor is 7×10^7 , corresponding to a photon lifetime of $220 \mu\text{s}$. Up to four cycles of Rabi oscillations are clearly observed demonstrating the strong coupling regime. The decay of the oscillation signal is due to various imperfections (dark counts, atoms detected in the wrong channel, inhomogeneous stray electric or magnetic fields). The observed $20 \mu\text{s}$ period of the Rabi oscillation is one order of magnitude shorter than the cavity damping time.

If the cavity contains initially n photons, the Rabi oscillation frequency is $(\Omega_0/2\pi)\sqrt{n+1}$ [37]. By observing the Rabi oscillation in a small coherent field [38] stored in C , a discrete spectrum of Rabi frequencies has been observed [22, 26]. Note that this spectrum is a direct manifestation of field energy quantization in the cavity mode. This feature has also been used for measuring the photon number distribution of small fields stored in C [26]. The Rabi oscillation in the $n = 0, 1$ or 2 photons Fock states has also been observed recently [34, 39].

2.3 “Quantum logic” operations based on the vacuum Rabi oscillation

The vacuum Rabi oscillation provides the essential tools for basic logic operations which will be combined step by step in our experiments. We present briefly now these basic operations.

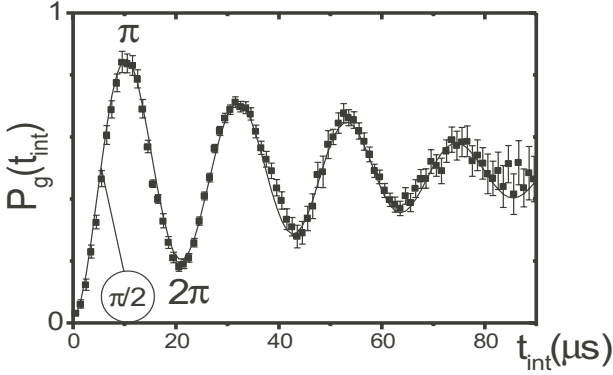


Fig. 2. Rabi oscillation signal: A single atom emits and reabsorbs a single photon. Up to 4 oscillation cycles are observed. Interaction times corresponding to $\pi/2$, π and 2π pulses are marked by labels.

For an atom and a field initially prepared either in $|e, 0\rangle$ or $|g, 1\rangle$, the atom-field wavefunctions after the interaction time t_{int} read respectively:

$$|\psi_e(t_{\text{int}})\rangle = \cos(\Omega_0 t_{\text{int}}/2)|e, 0\rangle + \sin(\Omega_0 t_{\text{int}}/2)|g, 1\rangle \quad (2.1)$$

$$|\psi_g(t_{\text{int}})\rangle = \cos(\Omega_0 t_{\text{int}}/2)|g, 1\rangle - \sin(\Omega_0 t_{\text{int}}/2)|e, 0\rangle. \quad (2.2)$$

Three basic functions are realized by adjusting the atom-cavity interaction time to specific values corresponding to $\Omega_0 t_{\text{int}} = \pi/2$, π or 2π . The π pulse can be used to exchange one excitation between the atom and the cavity mode. In this way, an atom in e can be used to *write* a one-photon field in the cavity. If the atom is prepared in the arbitrary superposition state $c_e|e\rangle + c_g|g\rangle$, it will, after a π pulse, always end up in g and prepare the field in the state: $c_e|1\rangle + c_g|0\rangle$. All the quantum information encoded in the atom by a classical microwave pulse is transferred and stored in the cavity. This writing process being reversible, the stored quantum information can be *read* by another atom prepared in g which is performing an absorbing π pulse. In these processes, the cavity acts as a quantum memory as demonstrated in [27].

In case of an atom in e performing $\pi/2$ pulse in the cavity, the prepared atom-field state is:

$$|\psi_{\text{EPR}}\rangle = 1/\sqrt{2}(|e, 0\rangle + |g, 1\rangle). \quad (2.3)$$

It is a maximally entangled state analogous to the singlet state of a pair of spin 1/2. As the atom leaves the cavity after interaction, this state exhibits the non-local quantum correlations which are at the heart of the EPR [1] situation and which characterize vividly the difference between quantum

and classical logic through the Bell theorem [2]. Section 4 will be devoted to the experimental characterization of this state [30].

Let us finally consider the 2π Rabi pulse. When the atom is prepared in g the atom-field wavefunction transforms in the following way:

$$\begin{aligned} |g, 1\rangle &\rightarrow -|g, 1\rangle \\ |g, 0\rangle &\rightarrow |g, 0\rangle. \end{aligned} \quad (2.4)$$

For a field containing one photon, the 2π pulse leads to a π phase shift of the atom-field state as seen on equation (2.4). A similar π -phase shift occurs when performing a 2π rotation on a spin $1/2$ system [40, 41]. Now if the cavity is initially empty, the system is in the ground state $|g, 0\rangle$. It does not evolve and does not experience any phase shift. In both cases, the field energy (*i.e.* 0 or 1 photon) is unchanged but the phase of the final state carries information on the photon number. This provides the principle of the QND (quantum non demolition) method of measurement of a 0 or 1 photon field that will be presented in the next section [28]. This photon number measurement scheme will also be shown to behave as a *quantum gate* [29]. This gate, which is very similar to a XOR quantum gate first realized with a single ion [42], provides the needed quantum logic operation for synthesizing arbitrary N particle entangled state. Section 4 will present an experiment where this gate is used to turn the $|\psi_{\text{EPR}}\rangle$ state into an entangled triplet involving the cavity mode and two atoms [31].

3 Quantum non-demolition detection of a single photon

3.1 Quantum non-demolition strategies

Quantum systems are usually strongly perturbed by measurements. Although it is possible to detect single elementary particles, the detection methods are very often destructive. As an example, photon counting with a photomultiplier relies on photon absorption. It is thus usually impossible to “see” a photon twice. Yet this is not a fundamental limitation imposed by quantum laws. According to quantum mechanics, a system can be ideally measured without any modification, provided it is in an “eigenstate” of the measured quantity. Real meters are usually far from performing such ideal measurements. In the 1970’s, in the context of gravitational waves detection, this has been recognized as introducing non-fundamental technical limitations to the ultimate accuracy of measurements [43–45].

So-called quantum non-demolition (QND) measurement strategies [46] were designed to overcome these limitations by allowing repeated measurements of the same physical quantity without affecting the system more than what is implied by the quantum rule of wave packet reduction. They are characterized by repeatability and allow successive measurements of one observable on a single quantum system.

These strategies have been first implemented in quantum optics in order to measure photon fluxes [46–56]. The intensity of a *signal* light beam is measured by coupling it to a *meter* beam in a non-linear medium whose refractive index depends on light intensity. The *meter* phase depends on the *signal* intensity. Measuring this phase by an interferometric procedure amounts to a non-destructive measurement of the *signal* photon number. These experiments, based on non-linear phenomena which usually require high intensities, are only sensitive to macroscopic photon fluxes. When considering single trapped microwave photons instead of large propagating optical fields, the strength of the interaction with single Rydberg atoms is large enough to push the sensitivity of QND strategies down to the one photon level.

The principle of the cavity QED single-photon quantum non demolition (SP-QND) scheme [28] was presented in the previous section. It relies on the measurement of the π phase-shift experienced by an atom prepared in g and performing a 2π resonant Rabi pulse while crossing the cavity containing one photon. The phase-shift of level g is measured with a Ramsey interferometer involving a third circular state i (49_c circular state). The $g \rightarrow i$ transition, at frequency $\nu_{gi} = 54.259$ GHz, is far from resonance with C , so that the level i does not couple to the cavity field.

3.2 The Ramsey interferometer for detecting a single photon

The principle of the experiment is illustrated in Figure 3a. The three relevant atomic levels (e, g and i) are shown in the inset. The field to be measured is stored in the resonant mode C of the cavity. *Meter* atoms, initially prepared in g are crossing C one at a time. The cavity field is tuned to exact resonance with the $e \rightarrow g$ transition.

The Ramsey interferometer consists in two $\pi/2$ pulses R_1 and R_2 induced before and after the atom crosses C with a microwave source S_R of frequency ν_R close to resonance with the $g \rightarrow i$ transition. The pulses are separated by the time interval t_R . The Ramsey set-up was first introduced as a powerful tool for high resolution spectroscopy [57]. We recall here that in this set-up, the transfer from g to i results from a quantum interference between two indistinguishable paths.

An atom resonantly coupled to a classical field performs Rabi oscillations. In the interaction picture and with an appropriate choice of the phase of S_R , the unitary transformation corresponding to a $\pi/2$ pulse induced at time t is:

$$\begin{aligned} |g\rangle &\rightarrow 1/\sqrt{2}(|g\rangle + e^{i\phi(t)}|i\rangle) \\ |i\rangle &\rightarrow 1/\sqrt{2}(|i\rangle - e^{-i\phi(t)}|g\rangle) \end{aligned} \quad (3.1)$$

where $\phi(t) = (\nu_R - \nu_{gi})t$. In this expression, the approximation of small detuning ($\delta_R = \nu_R - \nu_{gi} \ll 1/\tau_R$, where τ_R is the duration of each pulse) has

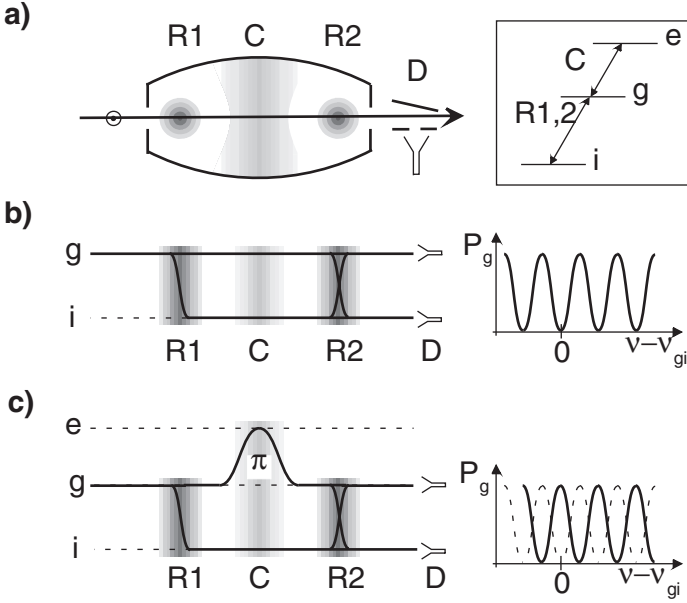


Fig. 3. The Ramsey Interferometer. a) The Ramsey setup: the atomic beam is submitted to two $\pi/2$ Ramsey pulses R_1 and R_2 separated by a time delay t_R . b) Symbolic representation of the Ramsey interferometer in case of zero photon in C . The Ramsey pulses act as the beam splitters of a two-wave interferometer. c) C contains one photon, the π phase shift experienced by the atom in the upper arm of the interferometer results in a π phase shift of the Ramsey fringes as shown by the solid line.

been taken into account. Under this assumption, the atomic wavefunction after interaction with R_1 at $t = 0$ is:

$$|\psi_{at,1}\rangle = 1/\sqrt{2}(|g\rangle + |i\rangle). \quad (3.2)$$

The action of R_1 on $|g\rangle$ can be seen as a splitting of the internal atomic state into two components. After application of the pulse R_2 at time $t = t_R$, the atomic wavefunction becomes:

$$|\psi_{at,2}\rangle = 1/2[(1 - e^{-i\phi_R})|g\rangle + (1 + e^{i\phi_R})|i\rangle], \quad (3.3)$$

where $\phi_R = \phi(t_R)$. The final probability amplitudes for finding the atom in g or i are the sum of two terms, originating from the two components of $|\psi_{at,1}\rangle$. The probability for detecting the atom in i , $P_i(\nu_R) = 1/2(1 + \cos(\phi_R))$ as a function of ϕ_R (or of ν_R) is the Ramsey fringes signal. It is an oscillatory function of ϕ_R . These oscillations originate from a two-wave interference process between two indistinguishable paths from g to

i as depicted in Figure 3b. Note that the two interfering paths (the two “arms” of the interferometer) correspond to the atom crossing the cavity either in g or i .

The principle of the QND detection of a single photon is then straightforward: introducing one photon in C amounts to adding a π phase shift in the g arm of the interferometer without changing the field nor the atom energy. As i is not coupled to C , the other arm of the interferometer is not affected and acts as a phase reference. Finally one expects a π phase shift of the Ramsey fringe pattern when C stores one photon as shown on the right of Figure 3c. Setting ϕ_R (or equivalently ν_R) at a fringe extremum thus results in a perfect correlation between the detected state of the *meter* (g or i) and the photon number (0 or 1). Ideally, the detection of the state of a single *meter* atom thus provides an unambiguous measurement of the photon number.

3.3 Experimental realization

In this experiment, the quality factor of the cavity was increased to 3×10^8 by the use of new mirrors and the addition of a nearly closed ring between them as mentioned in Section 2.2. The atomic velocity $v = 503 (\pm 2.5)$ m/s, corresponds to an effective interaction time $t_{\text{int}} = \sqrt{\pi} w_0 / v$ satisfying the condition $\Omega_0 t_{\text{int}} = 2\pi$.

We apply the Ramsey pulses inside the closed cavity structure, by injecting the Ramsey field through an additional hole in the ring. This field does not couple with the cavity mode, whose frequency is different by 3.2 GHz. It produces a standing-wave pattern, which we have mapped by performing time-resolved microwave spectroscopy of the Rydberg states. This standing-wave exhibits two field maxima before and after the cavity mode waist respectively (R_1 and R_2 pulses in Fig. 3a). Since we know the position of each atom as a function of time, we can apply to him well controlled R_1 and R_2 $\pi/2$ pulses when it is in the field maxima. The resulting Ramsey fringes, detected by accumulating statistics of atom counts in levels g and i , have a 72% contrast (g and i states probabilities oscillating between 0.86 and 0.14).

An experimental sequence consists in preparing a small field in C , then measuring it by sending one *meter* atom across the interferometer, finally checking the result with another atom after a delay. Statistics are accumulated over an ensemble of elementary sequences. Since each circular state sample has a 0.1 – 0.2 probability for yielding a signal, we detect an atomic pair in only 1 – 4% of the double pulse sequences. To limit data acquisition time, sequences are repeated after 1.5 ms, without waiting complete cavity relaxation. A *photon erasing* procedure [28] is used to get rid of the residual photons at the beginning of each sequence. Photon erasing is also important for another reason. The waveguide injecting the Ramsey pulses leaks a

small thermal field, corresponding to an average of 0.7 photons in the mode C (this photon number is deduced from a measurement of the $g \rightarrow e$ transfer rate of an atom absorbing the radiation in C). We start each sequence by sending five pulses of atoms in level g . Each of these *eraser* pulses contains three to nine atoms. These atoms absorb efficiently the remaining field and cool the mode down to 0.12 photon on average. The experimental sequence is then performed within 400 μs , to limit the build-up of the thermal field.

The characterization of the SP-QND scheme has been achieved by performing three experiments. In the first one, we demonstrate the expected π phase shift of the Ramsey fringes when C contains one photon by measuring a controlled initial one-photon “input” field. The second experiment consists in the QND detection of an initially unknown field. The QND information on the photon number provided by the *meter* atom is checked by absorbing the field left in the cavity after interaction with the *meter* (“output” field). The last experiment, involving the manipulation of three atoms allows a quantitative determination of the efficiency of the SP-QND scheme.

3.3.1 Input-meter: Demonstrating the single photon phase shift

In this experiment, we use a *source* atom to generate a single photon [27]. This atom, prepared in e , is sent across C 100 μs after the last *photon eraser* pulse. The interaction of the *source* atom with the cavity mode is shortened by Stark-tuning the transition into resonance only after the atom has already crossed half of the cavity mode. The atom-field system thus undergoes a π Rabi pulse and is prepared in the state $|g, 1\rangle$. The detection of the *source* atom in g ideally corresponds to the preparation of one photon in C .

We then send after a 100 μs delay the *meter* atom across the set-up. It is submitted to the Ramsey pulses R_1 and R_2 . The interaction time with C is reset to the value corresponding to a 2π pulse in a 1 photon field. This 2π pulse is slightly imperfect with a 20% residual probability to absorb the photon for an atom prepared in g . As the *meter* atom crosses C in the superposition state of equation (3.2), its probability to absorb 1 photon is only 10%. The conditional probability $P_{g_2/g_1}(\nu_R)$ for detecting the *meter* in level g , provided the *source* atom has been detected in g , is reconstructed as a function of the Ramsey frequency ν_R . Ideally, this probability is equal to the conditional probability for detecting the *meter* in g if there is 1 photon in C . The fringe pattern $P_{g_2/0}(\nu_R)$ corresponding to zero photon in C is monitored in the same way without sending the *source* atom after the photon erasing procedure. The results are displayed in Figure 4. As expected, we obtain two sinusoidal fringe patterns, π phase-shifted with respect to each other. These signals demonstrate that the interferometer works properly. The fringe contrast is limited to 51% by various known imperfections: 72%

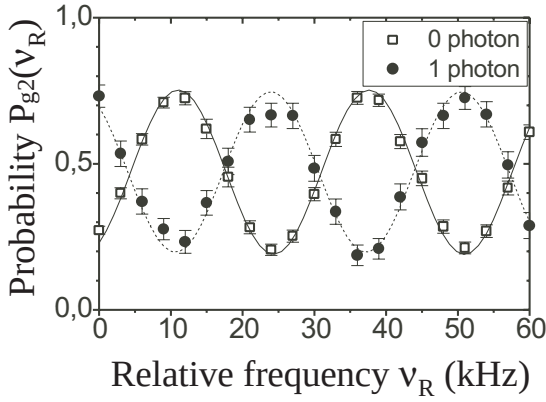


Fig. 4. Ramsey fringe pattern with 0 (open squares) or 1 photon (solid dots) in C .

contrast of the Ramsey interferometer, imperfections of the π and 2π Rabi pulses, detection errors mixing levels e and g , samples containing two atoms, residual thermal field building up in C after the erasing procedure, photon decay between the *source* and the *meter* atoms. The solid lines in Figure 4 correspond to a simulation taking these imperfections into account.

3.3.2 *Meter*-output correlation: Detecting the same photon twice

So far we have measured the conditional probability to find a given *meter* state provided the field contains 0 or 1 photon. In a real measurement situation, however, we are rather interested in the inverse question: what is the probability for having 0 or 1 photon in C after the measurement, provided the *meter* has been found in a given quantum state? We have performed a second experiment to measure this probability. The measured field is now a small thermal field (average photon number $n = 0.26$) which builds-up in C during a $300 \mu\text{s}$ delay between the last *photon eraser* pulse and the *meter* atom. The probabilities for finding 0 or 1 photon are now respectively $P_0 = 0.77$ and $P_1 = 0.18$, the probability for having more than one photon (0.05) is negligible.

Following the *meter* atom which performs the QND measurement, we send a second atom to absorb the field left in C . This *probe* atom is prepared in g , $75 \mu\text{s}$ after the first, and does not undergo any Ramsey pulse. Its interaction time with C corresponds to a π Rabi pulse in the field of a single photon. Hence, the probability for detecting it in e ideally equals to the probability for finding one photon in C after the QND measurement.

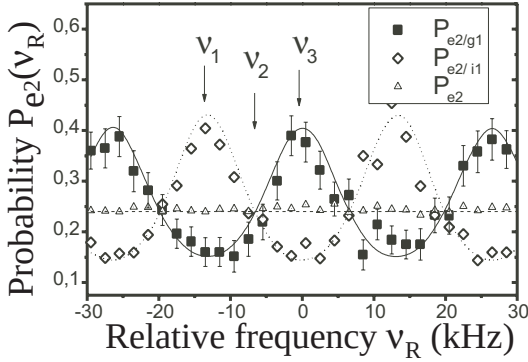


Fig. 5. Absorption rate of the probe atom. Triangles: no *meter* atom; squares: *Meter* detected in *g*; diamonds: *Meter* detected in *i*.

We have plotted in Figure 5 the conditional probabilities $P_{e2/g1}(\nu_R)$ and $P_{e2/i1}(\nu_R)$ for detecting the *probe* atom in *e*, provided the *meter* is respectively detected in *g* (squares) or *i* (diamonds), as a function of the Ramsey frequency ν_R applied to the *meter*. We have also recorded the probability P_{e2} for detecting the absorbing atom in *e*, when no *meter* atom is sent across *C* (triangles). The lines in Figure 5 are obtained by a numerical simulation including the imperfections discussed above and are in very good agreement with the experiment.

Ideally, $P_{e2/g1}$ and $P_{e2/i1}$ would be equal to $P_{1/g1}$ and $P_{1/i1}$, the conditional probabilities that there is one photon left in *C* after the *meter* atom has been detected in *g* or *i*. A simple application of Bayes laws yields:

$$P_{1/a} = P_1 \cdot P_{a/1} / [P_1 \cdot P_{a/1} + P_0 \cdot P_{a/0}] \quad (3.4)$$

where *a* stands for *g* or *i*. The probabilities $P_{a/1}$ and $P_{a/0}$ are those measured in the first experiment, *i.e.* sine functions of ν_R . Thus, $P_{1/g1}$ and $P_{1/i1}$ are non-sinusoidal periodic functions of ν_R , ideally varying between 0 and 1.

A qualitative discussion of the results is instructive. The triangle base line represents the average atomic absorption rate of the initial thermal field. The difference between the observed value of P_{e2} , 0.24, and P_1 is accounted for by the apparatus imperfections and the saturation of single atom absorption. The square and diamond curves show that the probability for having one photon in *C* after reading the *meter* can be either smaller or larger than P_1 , depending upon the outcome of the measurement and upon the frequency ν_R .

Let us consider three frequencies ν_{R1} , ν_{R2} and ν_{R3} (arrows in Fig. 5). At ν_{R1} , 1 photon in *C* results in a maximum probability for finding the *meter*

in i and a minimum probability for finding it in g . If the *meter* is found in i , it is thus likely that there is 1 photon left in C afterwards. The *a posteriori* probability for finding 1 photon in C is then much larger than the *a priori* probability P_1 . The probability that the *probe* atom will be excited to e is larger than the average probability measured by the triangle base line. If the *meter* is found in g , there is conversely a large probability that C is empty after the measurement and the second atom excitation probability falls below the base line. At ν_{R_2} , the *meter* indication is ambiguous and the *a posteriori* probabilities for exciting the second atom, which are equal for both *meter* states, correspond to the *a priori* probabilities. At ν_{R_3} , level g indicates 1 photon, and the conclusions are opposite to the ones for ν_{R_1} .

Some essential features of a QND measurement are revealed here. First, we have demonstrated the non-demolition feature. When the *meter* determines that there is 1 photon, it does so without destroying it, leaving it with a high probability behind for exciting the subsequent atom. The process by which the second atom detects the field is quite different. It absorbs the photon, leaving the cavity empty. The difference between normal (absorptive) and QND measuring schemes is clearly exhibited by comparing the effects of the two atoms on the field.

Another feature of this experiment is striking. The *meter*, injected in the lower state of the transition resonant with the cavity, cannot add any energy to the mode. However, after the *meter* has been detected in the state correlated to one photon, the probability for the second atom to absorb energy is greatly increased. This may at first sight seem paradoxical. In fact, our information about the thermal field (initially described by P_1) is modified by the *meter* reading and the change in the second atom's absorption rate merely reflects the fact that we have gained information on the field. Averaging the absorption rate of the second atom weighted by the respective probabilities for finding the *meter* in its two possible positions is equivalent to neglecting the *meter* information. This average recovers the value corresponding to P_1 .

We have also performed a repeated QND measurement, sending two identical *meter* atoms, 75 μ s apart, to detect twice a thermal field with $P_1 = 0.16$. The interferometer was set at frequencies ν_{R_1} , ν_{R_2} and ν_{R_3} and, in each case, 1000 coincidence events were recorded. At ν_{R_1} and ν_{R_3} , the conditional probability for finding the second atom in the same state as the first one is larger than the *a priori* probability for finding the first atom in this state. For example, at ν_{R_1} , the *a priori* probability for finding the atom in i is $0.32(\pm 0.01)$, whereas the conditional probability P_{i_2/i_1} is increased to the value $0.48(\pm 0.02)$. Ideally, these figures should be equal to 0.16 and 1. The observed values are correctly predicted by the numerical model.

3.3.3 Input–output correlation: Quantifying the QND performance

The two previous experiments demonstrate *input-field/meter* as well as *meter/output-field* correlations. From an analysis of the two experiments presented above, one also expects *input-field/output-field* correlations. This is an essential feature for a QND detection process. These *input-output* correlations can also be directly measured by performing a third experiment involving the *source*, the *meter* and the *probe* atoms in a single experimental sequence.

We first get rid of the 0.7 photon residual thermal field by the field erasing procedure. The initial field state is then produced by the *source* atom, prepared in e . It enters C 75 μs after the end of the cooling sequence and undergoes a $\pi/2$ spontaneous emission pulse in it. Either it is detected in e (50% of the cases), leaving C empty, or in g , preparing a single photon. The *meter* and *probe* are sent 100 μs and 175 μs after the *source*. The phase of the Ramsey interferometer is set so that the final meter state is i (g) when the photon number is 0 (1) (frequency ν_{R_3}). The *probe* is prepared in g . It undergoes a π Rabi rotation in $|1\rangle$. Hence, ideally, the *probe* is detected in g if C is empty and in e if C contains one photon. When the detected states of the *source* and *probe* agree (either e_1g_3 or g_1e_3), the probability of a photon number change induced by cavity relaxation is considerably reduced. In this way, by selecting *a posteriori* the two channels corresponding to no damping events, one can get rid of relaxation in the analysis of the SP-QND scheme. Let us stress that this post-selection is only made possible by a non-destructive measurement of the field by the *meter*.

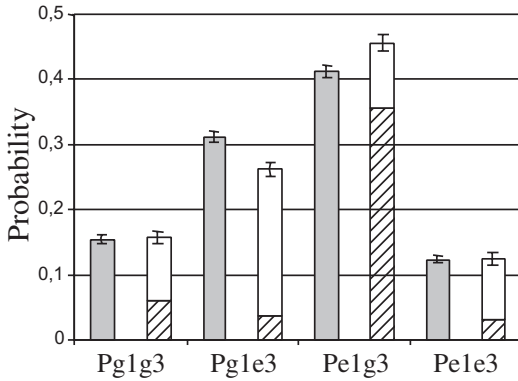


Fig. 6. Joined *Meter-probe* detection probability. Black: no *meter* atom; hatched and white: *meter* respectively detected in i_2 or g_2 .

Figure 6 presents the observed atomic correlations. The black histograms give the probabilities for the detection of the *source* and *probe*

in the four possible channels *when no meter atom is sent*. One thousand two-atom coincidences have been recorded in about twenty minutes. Ideally, channels g_1e_3 and e_1g_3 should have identical 0.5 probabilities. The populations of the other channels (g_1g_3 and e_1e_3) mainly originate from cavity relaxation. Photon decay populates g_1g_3 from g_1e_3 (the probability of a decay between the *source* and the *probe* is 16%). The appearance of a thermal photon accounts in part for the population of the channel e_1e_3 (the corresponding probability is 13%). Other imperfections contribute also (thermal photon already present in C before the *source*, two-atoms events in one sample, detectors imperfections...).

The results obtained when the *meter* is sent through C are displayed by the hatched and white histograms. About 1000 three-atom coincidences have been recorded in 2 hours. These histograms give the probabilities for getting one of the eight possible outcomes. The two bars corresponding to the two detected states of the *meter* atom are stacked. White bars correspond to a *meter* detected in g_2 , while the hatched ones correspond to a *meter* in i_2 .

We observe that, within statistical errors (error bars in Fig. 6), the stacked hatched and white boxes have the same height as the corresponding grey one. Hence, the *meter* does not alter the detection probabilities for the *source* and the *probe* and thus leaves the photon number unchanged. This demonstrates nearly perfect input-output correlations for a 0 or 1 photon state, under the operation of the SP-QND detection. For the g_1e_3 case (1 photon in C), the *meter* is detected mainly in g_2 , in agreement with the settings of the Ramsey pulses. Alternatively, it is detected most often in i_2 in the e_1g_3 case (empty cavity). The spurious channels mainly correspond to the absorption (g_1g_3) or to the creation (e_1e_3) of a photon. This occurs with equal probabilities before or after the *meter* has crossed C . In these cases, the *meter* is detected with almost equal probabilities in g_2 or i_2 .

The conditional probabilities relevant for characterizing the SP-QND scheme are easily computed. The probability for detecting the *meter* in g_2 provided the cavity contains one photon (g_1e_3 case) is $P(g_2|g_1e_3) = 0.83(4)$. In a similar way, the probability for detecting the *meter* in g_2 in the empty cavity case (e_1g_3 case) is found to be $P(g_2|e_1g_3) = 0.22(3)$. The measured average success rate (probability for detecting the *meter* in the expected channel for a known 0 or 1 photon field) is thus about 80%. This figure is in a good agreement with the 84% value predicted by the numerical simulation.

From these figures, we infer that, after a single atom QND measurement of an unknown field containing 0 or 1 photon (photon number probabilities $P_0 = P_1 = 0.5$), the photon number probability corresponding to the *meter* reading increases to 0.82 ± 0.02 . In addition to the 10% measured residual absorption rate of the *meter*, these two figures completely characterize the SP-QND scheme. A comparison with the absorptive measurement method

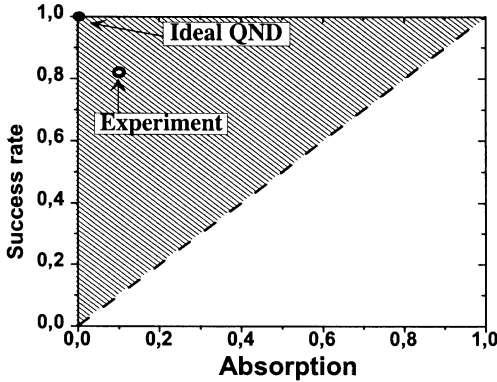


Fig. 7. SP-QND performance (open dot) as compared with the ideal QND situation (solid dot) and absorptive strategy (dashed line).

is instructive. Let us assume that the 1 photon state is detected by an atom prepared in g whose interaction time is set so that the absorption probability of 1 photon is P . The success rate of the single photon detection is then also equal to P . The SP-QND scheme can be graphically compared with this absorptive strategy using a two dimensional diagram (see Fig. 7) representing the success rate as a function of absorption rate. The absorptive method is represented by the diagonal whereas the perfect QND strategy is the solid dot. The hatched triangle corresponds to the QND zone, where the amount of information one gets by detecting the *meter* is larger than the amount of absorption. The experimental performance clearly lies in this area, close to the ideal QND case.

The achieved QND measurement of a photon with a single *meter* atom, satisfies the criteria of non-demolition and repeatability. A single photon QND measurement based on a similar 2π Rabi pulse was already suggested in [58]. The scheme relied however on the difficult observation of a tiny deflection of the atomic trajectory and not on a large interference effect as discussed here. Note also that multiple of 2π Rabi pulses leaving the photon number unchanged are the essential ingredients to generate ideally photon-number states in the micromaser (“trapping states”) [59].

QND detection strategies have also been extended to larger numbers of excitations. QND measurement of the excitation of the cyclotron motion of a single trapped electron was realized recently [60]. The four first excited motional state of the electron were successfully detected and quantum jumps between the first excited states of the system observed. It would be interesting to generalize our QND detection method to larger photon numbers. The SP-QND method presented above is based on the completion of a 2π Rabi pulse by the *meter* atom and is restricted to single photon fields.

For an n -photon field, the resonant Rabi frequency becomes $\Omega_0\sqrt{n}$ [26, 37] and photon number conservation cannot be enforced for all n values. By slightly detuning the cavity from the $e \rightarrow g$ transition, it is however possible to completely suppress the *meter* absorption, thus avoiding photon demolition, even if $n > 1$. The dispersive phase shift [61] experienced by the *meter* in the non-resonant case can again be used to perform a QND measurement of the photon number by Ramsey interferometry [62, 63]. In that case, the information will be extracted from a sequence of *meter* atoms, since each detection provides only one bit of information. Various strategies for optimizing the measurement sequences are discussed in [63, 64].

4 Step-by-step synthesis of a three-particle entangled state

The experiments described above rely on the combination of various controlled operations based on the resonant interaction of a single atom either with a classical Ramsey pulse or with a single photon stored in the cavity. We have been interested up to now in combining them in order to prepare and detect a single photon field in various ways. All these elementary steps are also coherent and reversible operations. They realize unitary operators involving either one atom (Ramsey pulses) or one atom plus the cavity field. We will show now that they provide the universal tools for preparing tailored many particle entangled states flying between the cavity and the detector.

Using the language of *quantum information processing*, these operations realize elementary *quantum gates* acting either on one or two *qubits* (*i.e.* a two level systems). Although these techniques cannot apply to the realization of a large scale *quantum computer* [65], it is convenient to use here the language of quantum information manipulation in order to emphasize the link between this work and other experiments or proposals involving the control and the use of quantum entanglement.

In this respect, the SP-QND scheme presented above realizes one of the simplest two-qubit gate the so-called quantum phase gate, (QPG) [66, 67]. The next section is devoted to the experimental demonstration of the coherence of our gate. The application to the controlled preparation of a three particle entangled state [31] is then presented in Section 4.2 [68].

4.1 The SP-QND scheme as a quantum phase gate

The QPG transformation simply reads:

$$|a, b\rangle \longrightarrow \exp(i\phi\delta_{a,1}\delta_{b,1})|a, b\rangle \quad (4.1)$$

where $|a\rangle$, $|b\rangle$ stand for the basis states ($|0\rangle$ or $|1\rangle$) of the two qubits and $\delta_{a,1}$, $\delta_{b,1}$ are the usual Kronecker symbols. The QPG leaves the initial state

unchanged, except if both qubits are 1, in which case the state is phase-shifted by an angle ϕ . The transformation corresponding to the 2π Rabi pulse in C involved in the SP-QND scheme is:

$$\begin{aligned} |i, 0\rangle &\longrightarrow |i, 0\rangle \\ |i, 1\rangle &\longrightarrow |i, 1\rangle \\ |g, 0\rangle &\longrightarrow |g, 0\rangle \\ |g, 1\rangle &\longrightarrow -|g, 1\rangle. \end{aligned} \quad (4.2)$$

When mapping the atomic states i and g on the 0 or 1 value of the atomic qubit, it exactly realizes the $\phi = \pi$ QPG.

The demonstration of the SP-QND scheme obviously amounts to check the last line of this “truth” table (the other lines are trivial). We now operate the QPG with both input qubits in a state superposition. In this case, the QPG operation generates entanglement as shown below. The atomic qubit state, $(1/\sqrt{2})(|i\rangle + |g\rangle)$, is produced, as above, by a $\pi/2$ pulse R_1 . The field qubit superposition, $c_0|0\rangle + c_1|1\rangle$, is generated by injecting into C a small coherent field [38] (average number of photons $n_{\text{coh}} = 0.18$). For that purpose, the strongly attenuated classical microwave source S_C shown on fig. 1 is coupled to C during a $10 \mu\text{s}$ time interval. The exact state of the field (amplitude $\alpha = \sqrt{n_{\text{coh}}}$) writes $|\alpha\rangle = c_0|0\rangle + c_1|1\rangle + \sum_{n>1} c_n|n\rangle$ with $c_0 = 1 - n_{\text{coh}}/2 = 0.91$, $c_1 = \sqrt{n_{\text{coh}}} = 0.4$ and c_n negligible for $n > 1$. To a good approximation it is thus a superposition of 0 and 1 photon states. The initial product state of the two qubits, $(1/\sqrt{2})(|i\rangle + |g\rangle)(c_0|0\rangle + c_1|1\rangle)$, is transformed by the gate operation into an entangled state $|\Psi\rangle$ which can be expressed in two equivalent forms:

$$|\Psi\rangle = \{c_0|0\rangle(|i\rangle + |g\rangle) + c_1|1\rangle(|i\rangle + e^{i\phi}|g\rangle)\}/\sqrt{2} \quad (4.3)$$

$$= \{|i\rangle(c_0|0\rangle + c_1|1\rangle) + |g\rangle(c_0|0\rangle + e^{i\phi}c_1|1\rangle)\}/\sqrt{2}. \quad (4.4)$$

Equations (4.3) and (4.4) exhibit the symmetry of the QPG: either the field in state 1 can be considered as the control qubit which produces a phase shift of the atom in state g (Eq. (4.3)) or, conversely, the atom in g is the control qubit which dephases the 1 photon state (Eq. (4.4)).

The correlations implied by equation (4.3) have been demonstrated in the presentation of the SP-QND scheme by showing that the phase of the atomic coherence is correlated to the photon number in C . In order to verify the correlations described by equation (4.4), we analyze the phase of the field in C by means of a “homodyning” method: we inject, after the atom has left C , a field with the amplitude $\alpha \exp(i\theta)$. It adds coherently to the field already present in C . The phase $\theta = T\Delta\nu$ depends upon the detuning $\Delta\nu$ between S_C and C ($T = 100 \mu\text{s}$ is the delay between the two field injections). The amplitude of the resulting field ideally varies between 0 and 2α as a function of the phase difference between the homodyning

pulse and the field left in C after the interaction with the atomic qubit. In this experiment, we set the atom-cavity detuning δ to zero and vary the phase θ by sweeping the frequency of S_C . The final field is probed by

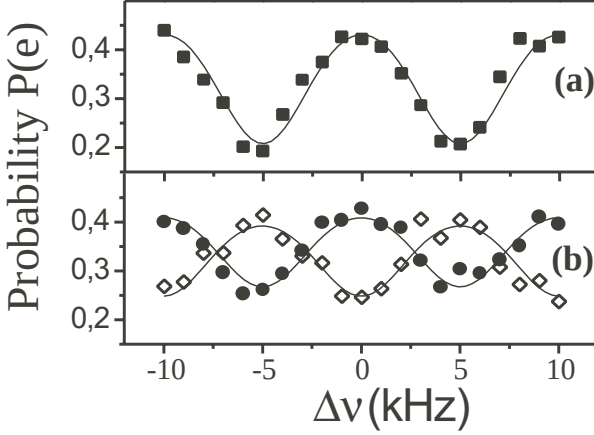


Fig. 8. Probing qubit entanglement: a small coherent field (amplitude $\alpha = \sqrt{0.18}$) is used as *field* qubit. Its phase is shifted according to the states (g or i) of a first atom acting as a control qubit. The final field phase is measured by adding a homodyning field $\alpha \exp(i\Delta\nu T)$ in C and measuring the field energy by absorption with a probe atom. a) Probability $P(e)$ to detect probe in e without atomic qubit. b) Conditional probabilities $P(e/i)$ (circles) and $P(e/g)$ (diamonds) *versus* $\Delta\nu$ to detect probe in e if the atomic qubit has crossed C in i or g . Points are experimental and lines are fits based on a simple model.

sending an atom, initially in g , across C (R_1 and R_2 are switched off). This probe atom undergoes a π -Rabi pulse in the field of 1 photon. Hence, the probability $P(e)$ for detecting it in e is ideally equal to the probability for finding a single photon in C (the latter being approximately the average photon number).

Figure 8a shows $P(e)$ *versus* $\Delta\nu$ when no atomic qubit is sent across C . In this case, the probe absorption is maximum for $\Delta\nu = 0$ since the amplitudes of the two injected fields then add with the same phase. The modulation of $P(e)$ when $\Delta\nu$ is tuned reflects the interference of these two fields with different phases. Figure 8b shows the conditional probabilities $P(e/i)$ and $P(e/g)$ for finding the probe in e provided the atomic qubit was found in i (circles) or in g (diamonds) *versus* $\Delta\nu$. The lines are obtained by a simple model which accounts for the experimental imperfections by adjustable contrasts and offsets. The signals in Figure 8b clearly exhibit the phase correlations of equation (4.4): the atomic qubit in i leaves the

field phase unchanged (the circle line in Fig. 8b has the same phase as the line in Fig. 8a) while the atomic qubit in g shifts the phase of the field by π (the diamond line in Fig. 8b has a phase opposite to the line in Fig. 8a). The phase correlations shown in Figure 8 thus prove that our cavity-QED QPG operates in a symmetrical and coherent way. It generates the expected output qubit entanglement when the input qubits are in state superpositions. Note additionally that by varying the atom-cavity detuning, the operation of a QPG with adjustable values of ϕ has been realized [29].

It is also a universal gate [69], since any quantum computation can be realized by combining QPGs and rotations of individual qubits. For example, a π -shift QPG and appropriate rotations of the second qubit realize a controlled-not or XOR gate which performs the transformation [70]:

$$|a, b\rangle \longrightarrow |a, a \oplus b\rangle \quad (4.5)$$

where $\oplus$ represents the addition modulo two. This gate is in fact realized in the SP-QND scheme by the association of the QPG with the Ramsey interferometer. Another method for realizing the XOR gate was also proposed in [71].

4.2 Building step-by-step three-particle entanglement: Principle

We present now an experiment where we prepare a set of three entangled qubits consisting of two atoms and a 0 or 1 photon field stored in C [31] by combining elementary quantum gate operations. It is the first example of preparation of a tailored three particle entangled state by a programmed sequence of quantum gates. This experiment is close to the three-atom experiment presented in Section 3.4. This section is devoted to the demonstration of entanglement in the prepared three particle state.

We first recall the sequence of operations used to prepare the three particle entangled state. It was proposed independently in [72] and [73]. The corresponding timing is sketched Figure 9a. We send across C , initially empty, an atom A_1 initially in e . A $\pi/2$ Rabi pulse prepares the state $|\psi_{\text{EPR}}\rangle$ described by equation (2.3). We then send a second atom A_2 . Initially in g , it is prepared, before C , in the state $(|g\rangle + |i\rangle)/\sqrt{2}$ by a Ramsey pulse P_2 . This atom interacts with C during its full cavity crossing time (2π Rabi pulse) and performs the QPG operation. Using equation (4.3), the resulting $A_1 - A_2 - C$ quantum state is:

$$|\Psi_{\text{triplet}}\rangle = \frac{1}{2} [|e_1\rangle(|i_2\rangle + |g_2\rangle)|0\rangle + |g_1\rangle(|i_2\rangle - |g_2\rangle)|1\rangle] \quad (4.6)$$

(the state indices correspond to the atom number). Equation (4.6) describes a three particle entangled state and can be rewritten as:

$$|\Psi_{\text{triplet}}\rangle = \frac{1}{2} [|i_2\rangle(|e_1, 0\rangle + |g_1, 1\rangle) + |g_2\rangle(|e_1, 0\rangle - |g_1, 1\rangle)], \quad (4.7)$$

describing an $A_1 - C$ EPR pair whose phase is conditioned to the A_2 state. Since $|\Psi_{\text{triplet}}\rangle$ involves two levels for each subsystem, it is equivalent to

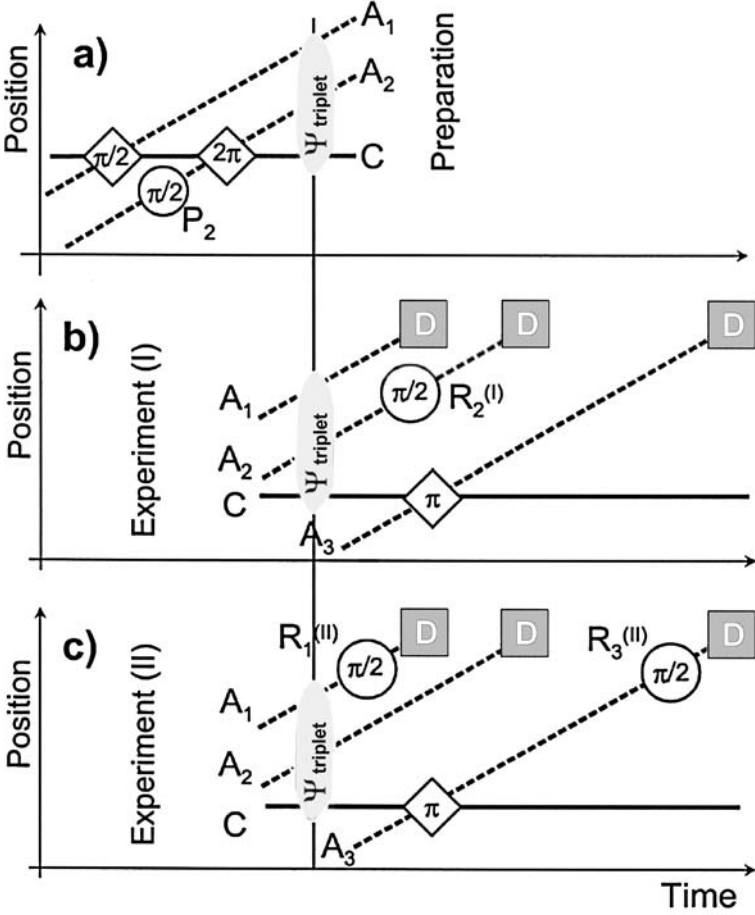


Fig. 9. The entanglement procedure. Qualitative representation of the atoms and cavity space lines during the experiments. The diamonds depict the atom-cavity interactions and the circles the classical pulses produced by S_R . The dark squares are the detection events. a) Preparation of the entangled state $|\Psi_{\text{triplet}}\rangle$ sketched by the grey oval. b) Experiment (I): detection of “longitudinal” correlations. c) Experiment (II): detection of “transverse” correlations.

an entangled state of three spins $1/2$. Let us define the states $|+i\rangle$ ($|-i\rangle$) (with $i = 1, 2$) as $|+1\rangle = |e_1\rangle$ ($|-1\rangle = |g_1\rangle$), $|\pm_2\rangle = (|g_2\rangle \pm |i_2\rangle)/\sqrt{2}$ and $|+c\rangle = |0\rangle$ ($|-c\rangle = |1\rangle$). With these notations, $|\Psi_{\text{triplet}}\rangle$ takes the form of

the Greenberger, Horne and Zeilinger (GHZ) spin triplet [15]:

$$|\Psi_{\text{triplet}}\rangle = \frac{1}{\sqrt{2}} (|+1, +2, +C\rangle - |-1, -2, -C\rangle), \quad (4.8)$$

Other schemes have been proposed to realize many particle atom-cavity entanglement [74, 75].

4.3 Detection of the three-particle entanglement

In order to characterize the state $|\Psi_{\text{triplet}}\rangle$, we are able to detect the atomic energy states, but not directly the cavity field. It can, however, be copied onto a third atom A_3 and detected afterwards [27]. The $A_3 - C$ interaction is set so that A_3 , initially in g , is not affected if C is empty, but undergoes a π Rabi pulse in a single photon field: $|g, 0\rangle \rightarrow |g, 0\rangle$ and $|g, 1\rangle \rightarrow -|e, 0\rangle$. Within a phase, A_3 maps the state of C . Thus, by detecting A_1 , A_2 and A_3 , we measure a set of observable belonging to the three parts of the entangled triplet. If A_3 crosses C before A_1 exits the ring, a three-atom entangled state $|\Psi'_{\text{triplet}}\rangle$ would be created between these two events:

$$|\Psi'_{\text{triplet}}\rangle = \frac{1}{2} [|e_1\rangle(|i_2\rangle + |g_2\rangle)|g_3\rangle - |g_1\rangle(|i_2\rangle - |g_2\rangle)|e_3\rangle] \quad (4.9)$$

$$= \frac{1}{2} [|i_2\rangle(|e_1, g_3\rangle - |g_1, e_3\rangle) + |g_2\rangle(|e_1, g_3\rangle + |g_1, e_3\rangle)]. \quad (4.10)$$

Even if A_3 is delayed, its correlations with A_1 and A_2 , which reflect those of C , are the same as those described in equation (4.10). In the following discussion, we thus refer equivalently to C or A_3 .

Checking the $A_1 - A_2 - C$ entanglement involves measurements in two different bases. A microwave pulse, after the interaction with C , followed by energy detection in D allows us to probe each atom's pseudo-spin along an arbitrary "quantization axis". In a first experiment (I), whose timing is sketched Figure 9b, we check "longitudinal" correlations by detecting the "spins" along what we define as the " z -axis" (eigenstates $|\pm_i\rangle$ for $i = \{1, 2\}$ and $|+3\rangle = |e_3\rangle$ and $|-3\rangle = |g_3\rangle$ for A_3). For A_1 and C (*i.e.* A_3), this is a direct energy detection. For A_2 , a $\pi/2$ analysis pulse $R_2^{(I)}$ on the $i \rightarrow g$ transition transforms $|+2\rangle$ (resp. $|-2\rangle$) into $|i_2\rangle$ (resp. $|g_2\rangle$). The three atoms should thus be detected in $\{e_1, i_2, g_3\}$ or $\{g_1, g_2, e_3\}$, with equal probabilities. However, these correlations, taken alone, can be explained classically (statistical mixture of $|e_1, i_2, g_3\rangle$ and $|g_1, g_2, e_3\rangle$ states).

A second experiment (II) is required to test the quantum nature of the superposition. We study "transverse correlations" by detecting A_1 and A_2 along the " x -axis" (eigenstates $|\pm_{x,i}\rangle = (|+i\rangle \pm |-i\rangle)/\sqrt{2}$). A_3 is detected along an axis in the horizontal plane at an angle ϕ from the x direction (eigenstates $|\pm_{\phi,i}\rangle = (|+i\rangle \pm \exp(+i\phi)|-i\rangle)/\sqrt{2}$). The timing of experiment

(II) is sketched Figure 9c. Atom A_2 is directly detected in D , since $|\pm_{x,2}\rangle$ coincide with $|g_2\rangle$ and $|i_2\rangle$. A_1 and A_3 undergo, after C , two analysis $\pi/2$ pulses $R_1^{(\text{II})}$ and $R_3^{(\text{II})}$ on the $e \rightarrow g$ transition, with a phase difference ϕ . A detection in g amounts to a detection in $|+_x\rangle$ or $|+_phi\rangle$ for A_1 and A_3 respectively at the exit of C .

For sake of clarity, let us first consider the case of only two atoms (1 and 3) in state:

$$|\Psi'_{\text{EPR}}\rangle = \frac{1}{\sqrt{2}}(|e_1, g_3\rangle - |g_1, e_3\rangle). \quad (4.11)$$

These atoms are analyzed along the x and ϕ directions respectively. When A_1 is detected in $|+_x,1\rangle$ (*i.e.* g_1 in D), A_3 is projected onto $|-_{x,3}\rangle$, since $|\Psi'_{\text{EPR}}\rangle$ is the rotation-invariant spin singlet. The detection probability of A_3 in $|+_phi,3\rangle$ (*i.e.* g_3 in D) thus oscillates *versus* ϕ between 1 for $\phi = \pm\pi$ and 0 for $\phi = 0, 2\pi$: “fringes” observed in the joint detection probabilities of the two atoms [30] show that quantum coherence has been transferred between them through the EPR correlations. The phase of the fringes would be shifted by π if the minus sign in equation (4.11) was changed into a plus. Returning to the three system case, equation (4.10) shows that similar fringes are expected for the joint detection of A_1 and A_3 corresponding to a given state for A_2 . They have the same phase as the EPR fringes described by equation (4.11) when A_2 is in i_2 . They are shifted by π when A_2 is in g_2 . This shift results from the action of the $A_2 - C$ phase gate [29] on the $A_1 - C$ EPR pair.

A tight timing is required to have A_1 and A_2 simultaneously inside the ring so that $|\psi_{\text{triplet}}\rangle$ is prepared before A_1 losses its coherence in the exit hole of the cavity (it was not the case in the experiments described in Sect. 3.4). A_2 interacts with C for the full atom–cavity interaction time. The π Rabi pulse condition for A_3 is realized with the Stark switching technique. Atom A_1 couples to C 75 μs after the erasing sequence, and should undergo a $\pi/2$ Rabi rotation. It is followed by A_2 after a delay of 25 μs . The separation between A_1 and A_2 is 1.2 cm, twice the cavity waist. Nevertheless, A_1 still interacts with C when A_2 starts its 2π Rabi rotation. Even in this case, an appropriate adjustment of the atom cavity Stark tuning allows to prepare $|\psi_{\text{triplet}}\rangle$ with a high fidelity as shown in [31]. Atom A_1 has exited the ring however before A_3 has crossed C , following A_2 after a delay of 75 μs . This timing thus does not permit to prepare $|\Psi'_{\text{triplet}}\rangle$ (Eq. (4.10)). As discussed above, the $A_1 - A_2 - A_3$ correlations nevertheless demonstrate the $A_1 - A_2 - C$ entanglement.

In the same way as in Section 3, we apply the pulses when the atom is in an antinode of the standing wave created inside the cavity ring by the classical microwave source S_R . The distance between A_1 and A_2 is such that one is in a node of this wave when the other is in an antinode. In this way, selective pulses may be applied on A_1 and A_2 even if both are simultaneously

in the ring. In experiment (I), P_2 and $R_2^{(I)}$ are applied on A_2 on the 54.3 GHz $g \rightarrow i$ transition. In experiment (II), $R_1^{(II)}$ and $R_3^{(II)}$ are used to probe the $|\pm_{x,1}\rangle$ and $|\pm_{\phi,3}\rangle$ states. A pulse resonant on the $e \rightarrow g$ transition would couple in C through scattering on the mirrors imperfections. A field would then build up in C and spoil quantum correlations. To avoid this, we first apply a π pulse on the $g \rightarrow i$ transition transforming the $e - g$ coherence into an $e - i$ one. A $\pi/2$ pulse on the two-photon $e \rightarrow i$ transition at 52.7 GHz, which does not feed any field in C , is then used to probe this coherence. States $|+_{x,1}\rangle$ ($|-_{x,1}\rangle$) and $|+_{\phi,3}\rangle$ ($|-_{\phi,3}\rangle$) are mapped by this effective three-photon $\pi/2$ pulse onto i_1 (e_1) and i_3 (e_3) respectively. The results of experiment (I), Figure 10, are presented as histograms giving

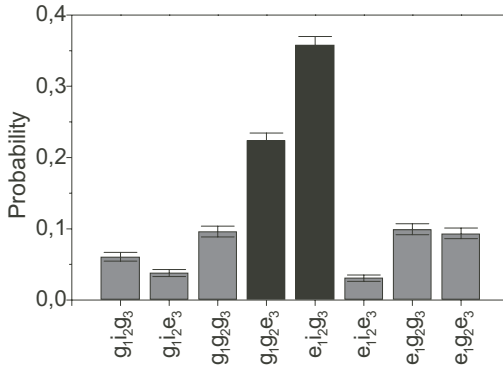


Fig. 10. Longitudinal correlations (experiment I). Histograms of the detection probabilities for the eight relevant detection channels. The two expected channels (g_1, g_2, e_3 and e_1, i_2, g_3 , black bars) clearly dominate the others (grey bars), populated by spurious processes. The error bars are statistical.

the probabilities for detecting the atoms in the eight relevant channels. As expected, the $\{e_1, i_2, g_3\}$ and $\{g_1, g_2, e_3\}$ channels dominate. The total probability of these channels is $P_{||} = 0.58 \pm 0.02$. The difference between them is due to experimental imperfections. Channel $\{g_1, g_2, e_3\}$ corresponds to one photon stored in the cavity between A_1 and A_3 . It is thus sensitive to field relaxation, and leaks into the other $\{g_1\}$ channels. Events with two atoms in the same sample, residual thermal fields, detection errors also contribute to the population of the parasitic channels. Note also that since the experiment involves three levels for each atom, there are altogether 27 detection channels. Figure 10 presents the channels corresponding to the relevant transitions for each atom: $e \rightarrow g$ for A_1 and A_3 ; $g \rightarrow i$ for A_2 . The other channels are weakly populated by spurious effects (spontaneous emission outside C , residual thermal photons, influence of the $R_3^{(I)}$ or P_2

pulses on the other atoms, absorption of the cavity field by A_2 due to imperfect 2π Rabi rotation...). The total contribution of these transfer processes is below 15%.

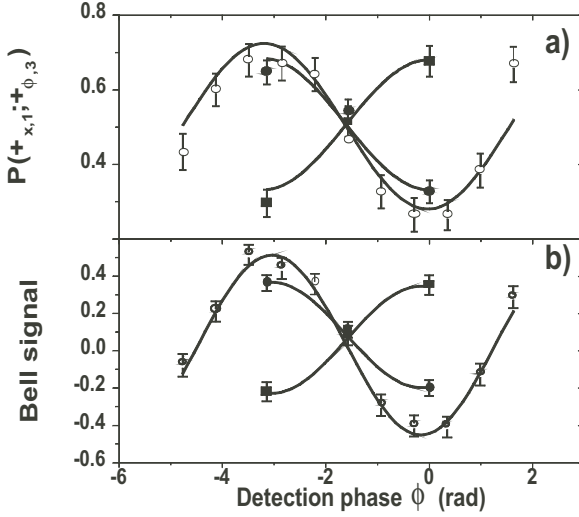


Fig. 11. Transverse correlations (experiment II).

For the signals of experiment (II) presented in Figure 11, the relative phase ϕ of $R_3^{(\text{II})}$ and $R_1^{(\text{II})}$ is adjusted by tuning the frequency of the source inducing the $e \rightarrow i$ two-photon transition. Figure 11a presents *versus* ϕ the probability $P(+_{\phi,3}; +_{x,1})$ for detecting A_3 in i (i.e. $|+_{\phi,3}\rangle$) provided A_1 has also been detected in i (i.e. $|+_{x,1}\rangle$). The open circles give the conditional probability when A_2 is not sent. The observed fringes correspond to the two-atom EPR pair situation. The solid circles give the corresponding conditional probability when A_2 is detected in i . Due to very long acquisition times (eight hours for the data in Fig. 11), signals have been recorded only for three phase values. The squares correspond to a detection of A_2 in g . The $A_1 - A_3$ correlations are not modified when A_2 is detected in i . When A_2 is detected in g , the $A_1 - A_3$ EPR fringes are shifted by π , as expected. All joint probabilities corresponding to the four possible outcomes for A_1 and A_3 are combined to produce the “Bell signal” [3] which is the expectation value $\langle \sigma_{x,1} \sigma_{\phi,3} \rangle = P_{i,1,i,3} + P_{e,1,e,3} - P_{i,1,e,3} - P_{e,1,i,3}$, where the σ 's are Pauli matrices associated to the pseudo-spins and $P_{a,1,b,3}$ is the probability for detecting A_1 in a and A_3 in b ($\{a, b\} = \{i, e\}$). We plot Figure 11b the Bell signal *versus* ϕ . The open circles correspond again to no A_2 atom sent, the solid circles and squares to A_2 detected in i or g , respectively. The π

phase shift of the $A_1 - A_3$ EPR correlations, conditioned to the A_2 state, is conspicuous. The fringes visibility is $2V_\perp = 0.28 \pm 0.04$.

Due to experimental imperfections, the first stage Figure 9a of our experiment does not prepare the pure state $|\Psi_{\text{triplet}}\rangle$, but rather a mixed state described by a density matrix ρ . The set-up efficiency is thus characterized by a fidelity $F = \langle \Psi_{\text{triplet}} | \rho | \Psi_{\text{triplet}} \rangle$. If the detection stages (Figs. 9b and 9c) were perfect, F would be equal to the sum $P_\parallel/2 + V_\perp$ [18]. The value of this quantity, 0.43, is however affected by known detection errors and F is actually larger. Trivial imperfections can occur at three different stages: The mapping of the cavity state onto A_3 , the classical microwave pulses $R_2^{(I)}$, $R_1^{(II)}$ and $R_3^{(II)}$, and the energy state-selective atom counting. We have determined these errors independently by additional single atom experiments. Taking them into account, we determine a fidelity $F = 0.54 \pm 0.03$. The three kinds of errors listed above account respectively for corrections of 0.03, 0.05 and 0.03 to the raw 0.43 value. The fact that F is larger than 0.5 ensures that genuine three particle entanglement is prepared here [18].

The combined results of experiments (I) and (II) demonstrate the step by step engineered entanglement of three qubits, manipulated and addressed individually. By adjusting the various pulses, the experiment could be programmed to prepare other tailored multiparticle state. In particular, the generalization of our experiment for preparing multiparticle generalizations of the GHZ triplet [76] are straightforward. These states are generated by a simple iteration of the present scheme [73, 74]. After having prepared the $A_1 - C$ pair in the state described by equation (4.6), one sends a stream of atoms $A_2 - A_3 - \dots - A_n$ all prepared in $(|i\rangle + |g\rangle)/\sqrt{2}$ and undergoing, if in g , a 2π Rabi rotation in a single photon field. Since this rotation does not change the photon number, the 0 photon (resp. 1 photon) part of the $A_1 - C$ system gets correlated to an $A_2 - A_3 - \dots - A_n$ state with all $n - 1$ atoms in $(|i\rangle + |g\rangle)/\sqrt{2}$ (resp $(|i\rangle - |g\rangle)/\sqrt{2}$), preparing the entangled state:

$$|\Psi\rangle = \frac{1}{\sqrt{2}} (|+1, +2, \dots, +C\rangle - |-1, -2, \dots, -C\rangle). \quad (4.12)$$

This state presents non-local $n + 1$ particles correlations which could be investigated by the techniques presented here.

Similar controlled and reversible manipulations of many particle entanglement can be performed with other systems. Complex spin manipulations have been demonstrated with nuclear magnetic resonance [77]. These experiments involve however macroscopic samples near thermal equilibrium without clear-cut entanglement [78]. Reversible entanglement with massive particles has also been realized with trapped ions [42]. The generation of an EPR pair [79] and, recently, of four ion entanglement [18] have been reported. In these experiments, strong coupling requires the ions to be only a few micrometers apart and the difficulty is to address them individually.

The entangled multi-particle state is prepared in a collective process, involving all qubits at once. Individual addressing of ions is possible in larger ions traps as demonstrated with calcium [80] but controlled quantum logic operations have not yet been demonstrated in this context. In contrast to ion traps, our CQED experiment manipulates particles at centimeter-scale distances, ideal conditions for separate qubit control.

5 Decoherence and quantum measurement

Our CQED experiment also allows for the preparation of another class of entangled states involving a single atom and a small (3 to 10 photons) coherent field [38]. This field is injected in the cavity with the classical source S_C . By using non-resonant atom-field interaction, one can prepare mesoscopic entangled states where the classical phase of the field is correlated with the atomic state e or g [32]. In such a configuration, the cavity field acts as a meter “pointer” determining the atomic energy. By varying the size of the pointer (*i.e.* the photon number), one can observe the decoherence stage of a quantum measurement which turns mesoscopic coherent superpositions into statistical mixtures. After a brief reminder of quantum measurement theory, we analyze the evolution of the mesoscopic entanglement prepared in the experiment and discuss some of the aspects of the decoherence approach introduced by Zurek [9, 10].

5.1 Quantum measurement theory

5.1.1 The postulates

In the orthodox interpretation of quantum mechanics, quantum measurements are described at a very conceptual level, independently of the precise nature of meters. Measured quantities are represented by hermitian operators whose eigenvalues constitute the list of possible results for a single measurement. An elementary measurement appears as the random choice of one of these possible results according to a probability law completely defined by the system’s wavefunction. For ideal quantum measurements, the final state of the system depends only on the measured eigenvalue and results from the projection of the initial state on the corresponding eigenvector.

These simple mathematical rules are powerful enough to describe interactions with meters independently of their detailed structure. In spite of their simplicity, these rules are remarkably efficient for all practical purposes. The price of this simplicity is however the introduction of two mutually exclusive ways of describing the evolution of quantum systems depending whether a measurement is performed or not. Between measurements, one has to apply hamiltonian evolution to all interacting parts of the system.

This is a deterministic, reversible and continuous evolution process. It is “interrupted” from time to time, when interaction with a meter occurs, an event which deserves a special treatment. Meters are postulated to behave classically: They are known to give results and not superpositions of results. It would then lead to deep inconsistencies not to assign them a particular status in the quantum theory. As a consequence, pure Hamiltonian evolution cannot apply any more when considering macroscopic objects such as meters. The orthodox prescription then consists in abruptly projecting the system’s state on the measurement result when a measurement is performed. The difficulty arises while wondering at which scale an interaction becomes a measurement.

In order to investigate this point and to get a more physical definition of what a meter is, it is instructive to follow Von Neumann in a deeper analysis of the quantum measurement process.

5.1.2 Von Neumann’s analysis of meters

Meters are obviously made of atoms, all submitted to the same quantum rules basically consisting in Hamiltonian evolutions. Following Von Neumann [8,81], it is then quite natural to try to infer the rules governing quantum measurements from the underlying microscopic quantum structure of meters. The first step then consists in enlarging considerably the considered quantum system in order to treat, in principle, the system-meter interaction quantum mechanically through Hamiltonian evolution. To be more specific, let us consider a meter M designed so that it measures the z component of a spin $1/2$ designed by S . Equation (5.1) represents the expected evolution of the $S + M$ system after interaction for S initially polarized along the z -axis:

$$\begin{aligned} |+\rangle; \uparrow &\rightarrow |+\rangle; \nearrow \\ |-\rangle; \uparrow &\rightarrow |-\rangle; \nwarrow \end{aligned} \quad (5.1)$$

Note that the arrows inside the ket symbolizes the position of the pointer on the meter. These equations exhibit correlations between the meter and well defined initial value of S_z . If the two considered states of the pointer are separated enough to be orthogonal, this situation characterizes an ideal measurement. Let us now consider the interaction of the meter with the spin prepared in the state $|+\rangle_x = 1/\sqrt{2}(|+\rangle + |-\rangle)$ corresponding to a spin polarized in the x direction. As a result of linearity, Hamiltonian evolution prepares in this case a superposition state:

$$|\psi_{S+M}\rangle = 1/\sqrt{2}(|+\rangle; \nearrow + |-\rangle; \nwarrow). \quad (5.2)$$

This state involves two positions of the pointer at the same time. $S + M$ are entangled and form an EPR pair where the needle of the meter replaces

one of the two usual spins. The strangeness of this state is manifest when rewriting it in the basis of eigenstates of S_x :

$$|\psi_{S+M}\rangle = 1/2[|+_x\rangle(|\nearrow\rangle + |\nwarrow\rangle) + |-_x\rangle(|\nearrow\rangle - |\nwarrow\rangle)]. \quad (5.3)$$

As well as $|\pm_z\rangle$, the states $|\pm_x\rangle$ are perfectly correlated to two orthogonal states of the meter. This is true for any choice of the quantization axis. These correlations are reminiscent of the perfect anticorrelation of two spins in the singlet state as discussed in the EPR argument. They make it impossible at this point to assign a particular status to the z -direction and to define which observable is measured. In other words, an entangled wavefunction carries too many correlations for describing the result of a real measurement. This point was vividly emphasized in the famous Schrödinger cat metaphor [7] where the animal plays the role of the pointer. At that point it appears that the Hilbert space describing $S + M$ contains Schrödinger cat states and is thus larger than the set of “legal” classical states of the system.

Following Von Neumann, the difficulty is evacuated by postulating that, “at some point” during a quantum measurement process, the pure state

$$\rho_{\text{pure}} = |\psi_{S+M}\rangle\langle\psi_{S+M}| = 1/2 \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}, \quad (5.4)$$

collapses into the density matrix ρ_{mix} defined by the expression:

$$\rho_{\text{mix}} = 1/2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (5.5)$$

in the *preferred* (or *pointer*) basis $\{|+_z, \nearrow\rangle; |-_z, \nwarrow\rangle\}$. The state ρ_{mix} represents a mere statistical mixture of the two possible classical results of the measurement: A meter pointing either left or right. The off-diagonal matrix elements of ρ_{pure} have canceled in the measurement process and classically meaningless spin-meter correlations have disappeared. The existence of a preferred basis is postulated and it is chosen according to our intuition of what a classical state should be. This amounts finally to come back to the orthodox point of view where meters are postulated to behave classically. However, it is important to formally identify the second step of a measurement as a transition between two well defined objects: A pure state and a classical statistical mixture.

The most unsatisfying aspect of this analysis is the apparent need to introduce by hand classical objects without reference to any physical argument. This point was formally addressed much later in the “decoherence” approach introduced notably by Zurek [9,10]. It basically consists in going one step further with respect to Von Neumann by taking the environment E of the meter under consideration. Spin and meter behave then as a subsystem and are naturally described by a density matrix obtained by tracing

over the environment degrees of freedom [82]. This is the mechanism for providing the required damping of the non-diagonal part of ρ_{pure} . Classical states of the meter are then defined as the most robust ones with respect to dissipation. In this basis, populations have a much longer lifetime than coherences. This is why the “good” classical $S - M$ correlations which carry the measured information are preserved, while the quantum entanglement is washed out.

It is out of the scope of this course to analyze extensively this decoherence approach. The reader will find a detailed presentation of the ideas in the contribution of Zurek and Paz in this book. We will rather focus on the analysis of a CQED experiment where the two main steps of a quantum measurement, system-meter correlation and decoherence have been observed successively. The general results of the decoherence approach will then be discussed in the light of this experiment.

5.2 *Observing progressive decoherence during a measurement process*

From any reasonable model of real meters, decoherence times are expected to be infinitely short for any practical purpose. This is one of the most important features of the decoherence approach. The decoherence rate usually increases proportionally to the distance between different final states of the classical pointers in units of elementary quantum. Observing the dynamics of decoherence thus requires the use of a mesoscopic meter with a high enough insulation with respect to the environment. In the experiment, we “measure” the state e or g of a single Rydberg atom with a pointer consisting in a small coherent field [38] stored in the cavity mode [32]. The photon number in the high Q cavity is small enough for observing decoherence while it proceeds.

5.2.1 Measuring the atom state with the field phase

Let us consider the non-resonant interaction (detuning δ) between an atom and a small coherent field $|\alpha\rangle$ (average photon number $n_{\text{coh}} = |\alpha|^2$) injected in the cavity mode with a classical source. The atom and the field cannot exchange energy but undergo only $1/\delta$ dispersive frequency shifts (single atom index effect). The atom-field coupling during the interaction produces an atomic-level dependent accumulated phase shift of the field. For an atom crossing C in e (resp. g) the field dephasing is $\phi = \Omega_0^2 t_{\text{eff}}/4\delta$ (resp. $-\phi$) [21]. The effective interaction time is $t_{\text{eff}} = 19 \mu\text{s}$ for atoms crossing the cavity at 400 m/s. It is obtained by integration over the Gaussian profile of the mode. Using the usual pictorial representation of coherent states by vectors in phase space, the dispersive interaction with an atom amounts to a rotation by an angle $\pm\phi$ of the vector representing the field amplitude depending whether the atom crosses C in e or g (see Fig. 12). Quantum fluctuations

make the tip of these vectors uncertain, with a circular Gaussian distribution of radius unity as represented in Figure 12. The field phase ideally measures the atomic state when the phase shift ϕ is larger than phase fluctuations. In terms of the distance $D = 2\sqrt{n} \sin \phi$ between the meter states, this condition reads $D > 1$.

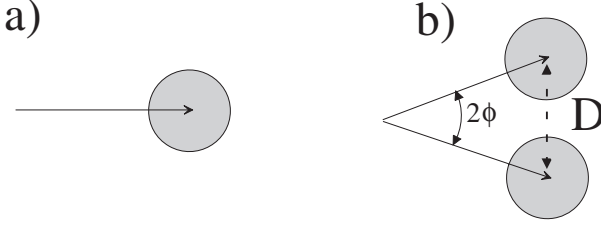


Fig. 12. (a) Pictorial representation in phase space of a coherent state of a field mode. (b) the two components separated by a distance D of a “Schrödinger cat” corresponding to equation (5.6).

When the atom is prepared in the superposition of states $1/\sqrt{2}(|e\rangle + |g\rangle)$ by a resonant $\pi/2$ Ramsey pulse, the interaction with C prepares a “phase Schrödinger cat” state:

$$|\Psi_{\text{cat}}\rangle = \frac{1}{\sqrt{2}} (|e, \alpha e^{i\phi}\rangle + |g, \alpha e^{-i\phi}\rangle). \quad (5.6)$$

This state is similar to the $S+M$ entangled state described by equation (5.2). The measurement result is carried by the phase of a small field whose amplitude can be varied easily by adjusting an attenuator. This is an essential feature for observing the emergence of the classical rules as the pointer become “larger”. Note that a similar entangled state has been prepared in an experiment involving a single trapped ion [83]. In this case however, the meter and the measured system were carried by the same particle.

5.2.2 Characterizing the Schrödinger cat state

The experiment is performed in two steps. We first demonstrate that the prepared state involves two fields with distinguishable phases. We then measure the mesoscopic coherence of the prepared superposition state.

These experiments were performed in an older version of the set-up. The quality factor was limited to 5.1×10^7 due to higher absorption losses on the mirror surface (corresponding damping time: $\tau_{\text{cav}} = 160 \mu\text{s}$). This moderate Q is compatible with large holes in the cavity ring allowing for propagating atomic superpositions outside C . External low Q cavities sandwiching C are used for the Ramsey pulses. The setup was cooled to 0.6 K making

thermal radiation negligible (mean steady state blackbody photon number in C : 0.02).

In this experiment, each circular atom is prepared in a superposition of e and g by a resonant microwave $\pi/2$ pulse R_1 . It crosses C in which a small coherent field with an average photon number n_{coh} varying from 0 to 10 is injected by a pulsed source. The field, which evolves freely while each atom crosses C , relaxes to vacuum before being regenerated for the next experimental sequence. We make sure that the field is coherent by checking that n_{coh} is proportional to the square of the injection pulse duration. After leaving C , each atom undergoes another $\pi/2$ pulse R_2 . R_1 and R_2 are fed by a source whose frequency ν is swept across ν_{eg} . The atoms are finally counted in e or g . With 50 000 events recorded in 10 min, the probability $P_g^{(1)}(\nu)$ to find the atom in g as a function of ν is reconstructed.

Figure 13a shows the signal obtained when C is empty ($\delta/2\pi = 712$ kHz). $P_g^{(1)}(\nu)$ exhibits Ramsey fringes typical of atoms subjected to two pulses separated by a time interval $T = 230 \mu\text{s}$. Let us remind that the fringes result from a quantum interference. The $e \rightarrow g$ transition can occur either in R_1 or in R_2 (atom crossing C in g or e). These two “paths” are indistinguishable, leading, in the final transition rate, to an interference term between the corresponding probability amplitudes. The fringe contrast, ideally 100%, is reduced to $55 \pm 5\%$ by various imperfections. Figures 13b to d show the fringes for $\delta = 712, 347$ and 104 kHz when there is a field in C ($n_{\text{coh}} = 9.5$; $|\alpha| = 3.1$). Two features are striking: when δ is reduced, the contrast of the fringes decreases and their phase is shifted.

The fringe contrast reduction demonstrates the separation of the field state into two components whose phase space representation are shown in the insets in Figure 13. When an atom leaves C , the system is prepared in the entangled state of equation (5.6), so that the field phase “points” towards e and g at the same time. For large value of δ (small ϕ), the measurement of the field phase would give no information on the state of the atom in C (large overlap of the field components). The two “paths” (atom crosses C in e or g) are still indistinguishable and the contrast remains large (Fig. 13b). When δ is reduced (ϕ increases), the field contains more information about the atomic state in C . The two “paths” thus become partially distinguishable and the fringe contrast decreases (Fig. 13c). It vanishes when the field components do not overlap at all (Fig. 13d).

It does not matter that the field is actually not measured. The mere fact that C stores information which *could* be read out destroys the interference. We recognize the ingredients of a “which path” experiment illustrating the basic aspect of complementarity [84, 85]. A simple quantitative analysis [32] confirms this discussion and shows that the fringe contrast is reduced by a factor equal to the modulus of the overlap integral $\langle \alpha e^{-i\phi} | \alpha e^{i\phi} \rangle = \exp(-D^2/2) \exp(in_{\text{coh}} \sin 2\phi)$. The same analysis shows that

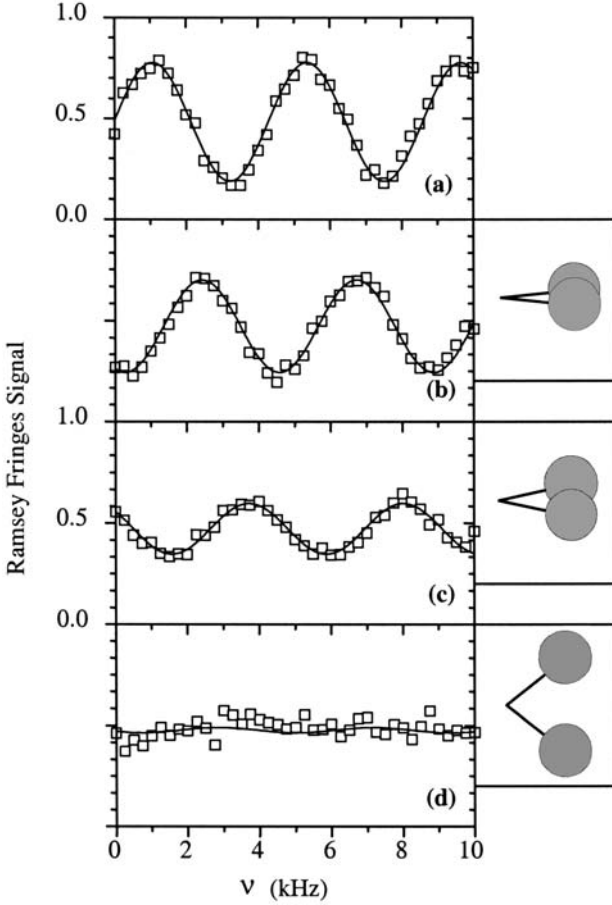


Fig. 13. $P_g^{(1)}(\nu)$ signal exhibiting Ramsey fringes: (a) C empty, $\delta/2\pi = 712$ kHz; (b) to (d) C stores a coherent field with $|\alpha| = \sqrt{9.5} = 3.1$, $\delta/2\pi = 712$, 347 and 104 kHz respectively. Points are experimental and curves are sinusoidal fits. Inserts show the phase space representation of the field components left in C .

the phase of the fringes is shifted by an angle $n_{\text{coh}} \sin 2\phi$ equal to the phase of $\langle \alpha e^{-i\phi} | \alpha e^{i\phi} \rangle$. The fringe phase shift is proportional to n_{coh} [32,61], which is determined from this set of data. The best fitted value is $n_{\text{coh}} = 9.5 \pm 0.2$.

The previous measurements demonstrate the correlations between the field phase and the atomic state. These correlations however could be correctly described by a statistical mixture of the two distinguishable positions of the pointer. The coherence between these two components of the state is revealed by a two-atom correlation experiment, whose principle follows

closely a proposal described in [86]. A first atom creates a superposition state of equation (5.6). A second “probe” atom crosses C with the same velocity after a short delay τ . It is also submitted to the pulses R_1 and R_2 , and dephases again the field by an angle $\pm\phi$ turning the two field components into three, with phases $\pm 2\phi$ and zero. The “zero-phase” component is obtained *via* two different “paths” since the atoms may have crossed C either in the (e, g) or in the (g, e) configurations. The probe atom “undoes” the phase splitting produced by the first one and recombines partially the state components. Since the atomic states are mixed after C in R_2 , the (e, g) and (g, e) “paths” are indistinguishable. As a result, an interference term related to the cat state coherence appears in the two atom correlation signal $\eta = P(e_2/e_1) - P(e_2/g_1)$. $P(a_2/a_1)$ is the conditional probability of detecting the second atom in a_2 provided the first one is detected in a_1 ($a_i = e$ or g).

Let us call $\rho(\tau)$ the “cat state” density matrix just before interaction with the probe atom. In the basis $\{|e, \alpha e^{i\phi}\rangle; |g, \alpha e^{-i\phi}\rangle\}$ this density matrix takes the form:

$$\rho(\tau) = 1/2 \begin{pmatrix} 1 & c \\ c & 1 \end{pmatrix}. \quad (5.7)$$

Provided ϕ is not too close from 0 or $\pi/2$, a straightforward calculation shows that: $\eta = 1/2 \operatorname{Re}(c)$. η is thus equal to 0.5 at short times τ when the quantum coherence is fully preserved, and decays to 0 when the “atom 1-field” system has evolved into a fully incoherent statistical mixture.

We measure η by detecting pairs of atoms separated by a delay τ varying from 30 to 250 μs . Figure 14 shows η *versus* τ (expressed in units of τ_{cav}) for $n_{\text{coh}} = 3.3$ and two different detunings ($\delta/2\pi = 170$ and 70 kHz). The points are experimental and the curves theoretical (see below).

The correlation signal measured with a short delay τ clearly demonstrate the coherence of the prepared superposition state. At this time, we have prepared a meter pointing “at the same time” in two different directions. This is the first observation of the first step of a quantum measurement: the entanglement between the system and the meter.

For larger values of τ , the correlation signal decrease with time revealing directly the dynamics of quantum decoherence. The prepared coherent superposition turns into a mere statistical mixture. We also observe that decoherence proceeds at a faster rate when the distance between the two state components is increased. An effective decoherence time of $0.24 \tau_{\text{cav}}$, much shorter than the photon decay time, is found for $\delta = 70$ kHz.

5.3 Theoretical analysis

The theoretical curves presented in Figure 14 can be obtained by an analytical solution of the standard master equation describing energy damping

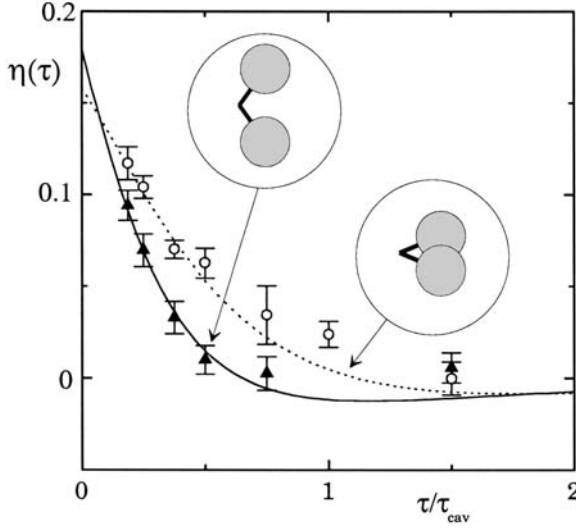


Fig. 14. Two-atom correlation signal η versus τ/T_r for $\delta/2\pi = 170$ kHz (circles) and $\delta/2\pi = 70$ kHz (triangles). Dashed and solid lines are theoretical. Inserts: pictorial representations of corresponding field components separated by 2ϕ .

for an harmonic oscillator [21, 86]. We present here a more intuitive analysis derived in [87], which coincides with the experimental data with the same accuracy and gives a better physical insight into the interplay between entanglement, complementarity and decoherence during a quantum measurement.

Let us model field energy damping by linear coupling between C and a quasi-continuum of modes C_i acting as an environment E at zero temperature. Just after preparation of $|\psi_{\text{cat}}\rangle$, E is assumed to be in the vacuum state $|0\rangle_E$, and the atom-cavity-environment wavefunction is:

$$|\psi_{\text{tot}}(0)\rangle = \frac{1}{\sqrt{2}} (|e, \alpha e^{i\phi}\rangle + |g, \alpha e^{-i\phi}\rangle) \otimes |0\rangle_E. \quad (5.8)$$

As a result of linear coupling with E , the cavity field amplitudes $\alpha e^{\pm i\phi}$ leaks in modes C_i small coherent amplitudes $\beta_i(\tau)e^{\pm i\phi}$. The field amplitude in C , $\alpha(\tau)$, thus decays as $\exp(-\tau/\tau_{\text{cav}})$. After a damping time τ , the system's wavefunction become:

$$\frac{1}{\sqrt{2}} (|e, \alpha(\tau)e^{i\phi}\rangle \prod_i |\beta_i(\tau)e^{i\phi}\rangle_E + |g, \alpha(\tau)e^{-i\phi}\rangle \prod_i |\beta_i(\tau)e^{-i\phi}\rangle_E). \quad (5.9)$$

A new entangled state builds up involving the atom, the cavity and the environment. Provided ϕ is not too close from 0 or π , the reduced

atom-cavity density matrix at time τ has the form of equation (5.7) with [87]:

$$\begin{aligned} c(\tau) &= \prod_i \langle \beta_i(\tau) e^{i\phi} | \beta_i(\tau) e^{-i\phi} \rangle \\ &= \exp \left(- \sum_i |\beta_i(\tau)|^2 (1 - e^{2i\phi}) \right). \end{aligned} \quad (5.10)$$

Due to energy conservation, $\sum_i |\beta_i(\tau)|^2$ is the average number of photons having escaped from C_0 at time τ , *i.e.* $n_{\text{coh}}(1 - e^{-\tau/\tau_{\text{cav}}})$. The coherence c writes finally:

$$c(\tau) = e^{-2n(1 - e^{-\tau/\tau_{\text{cav}}} \sin^2 \phi)} \cos(n(1 - e^{-\tau/\tau_{\text{cav}}} \sin 2\phi)). \quad (5.11)$$

From which one gets directly the decoherence signal $\eta = 1/2 \Re(c)$. The theoretical signal plotted in Figure 14 is obtained by a simple renormalization of this expression of η by a factor of 0.36 which takes into account the finite contrast of the Ramsey interferometer. Note that this expression coincides, in the frame of our approximations, with the result of the exact calculation adapted from [86]. The agreement with experimental data is excellent.

From this analysis, the mechanism governing the damping of mesoscopic coherences is intimately related to entanglement between the meter and the environment. An essential feature of Zurek's approach, the interpretation of decoherence in term of leak of information from the meter into the environment, is now straightforward. The initial atom-cavity superposition state turns into a statistical mixture as soon as the two field components building in E have an amplitude large enough to make them distinguishable.

In this case, the probe atom which interacts with the cavity field recombines its two phase components and makes them interfere. However, it does not recombine the two states building in the environment. As a consequence, the observed decay of the decoherence signal η results from the which path information on the meter state which is left in E and not erased by the probe atom.

From equation (5.11), in the limit of $\tau \ll \tau_{\text{cav}}$ decoherence proceeds exponentially with the time constant:

$$\tau_{\text{dec}} = \frac{\tau_{\text{cav}}}{2 \sin^2(\phi) n_{\text{coh}}} = \frac{2\tau_{\text{cav}}}{D^2}. \quad (5.12)$$

The decoherence time appears thus to vanish when the distance D between the positions of the pointer become macroscopic. The meter is thus characterized by a dissipative dynamic involving two timescales. The shortest one decreases with the size of the meter and describes the dissipation of

mesoscopic coherences. The other one is the classical damping time of the system. It does not depend on D and can be interpreted as the storage time of the measurement result in the meter. The existence of these two timescales is an essential feature of the decoherence approach.

The emergence of the pointer basis, the coherent states in our case, also originates from the cavity-environment dissipative coupling. The pointer basis is now defined as the basis in which the diagonal matrix elements of ρ have the smallest decay rate. In the above analysis, it corresponds to the states which are not sensitive to entanglement with E . This criteria thus provides the physical definition of the classical states of the meter introduced intuitively by Von Neumann. These states are now objectively defined by their maximal robustness with respect to damping. In our case they are the coherent states and any other field states will decay faster. Note that defining classical states on the basis of the decoherence approach thus finally leads to the usual definition of classical field states.

5.4 *Decoherence and interpretation of a quantum measurement*

On the basis of the analysis of the CQED experiment presented above, it is instructive to come back to some of the questions raised by the orthodox quantum description of measurement discussed in the introduction of this section. The first remark is that, even if it introduces a physical definition of the pointer states of the meter, the decoherence approach is still within the orthodox interpretation of quantum mechanics. Tracing over the unread degrees of freedom of the environment does not add anything fundamental to the usual quantum postulates.

It remains however interesting to remark that the decoherence point of view introduces irreversibility into quantum theory in the same way as statistical mechanics does in classical mechanics. In this sense, there is a strong analogy between the identification of the accessible information in an enormous entangled system + meter + environment wavefunction and the identification of the relevant thermodynamical parameters in a classical macroscopic system. In other words trying to describe quantum systems using huge Schrödinger cat states is equivalent to the description of a classical gas by the position and velocity of all the molecules. Even if, in principle, such a description contains all the information on the system, it contains much more information than one can access in any experiment. Note also that this kind of information is useless for any practical purpose. It is much more efficient to describe the system by focusing on relevant macroscopic parameters such as the volume, pressure or temperature of the gas. What decoherence tells us is that, by looking at damping dynamics, one can efficiently identify the relevant macroscopic parameters characterizing a meter and forget about Schrödinger cat wavefunctions.

In the light of this analysis, the question of the existence of “Schrödinger cat state” can thus be rephrased in the following way. Although there is no fundamental reason not to consider the universe as described by a huge “Schrödinger cat” quantum state, this is useless for describing statistically significant events.

From this statistical mechanics point of view, one can also reconsider the wavepacket projection postulate. It appears as the cheapest way to introduce the fact that we learn something about a system by measuring it. After a measurement, the wavefunction of the system, which can be seen as a table of the probability distribution of all possible results, has to be updated according to the additional knowledge we get. This occurs with classical probabilities as well. Of course, the origin of quantum randomness which manifests even with single isolated particles is not the same as in the case of classical systems. What Zurek’s approach tells us however, is that once decoherence has occurred, the system+meter wavefunction has been replaced by a much simpler object, a statistical mixture of classical states. At this level, the concept of probability amplitudes is not any more relevant. The effective readout of the results amounts then to the readout of a classical random variable. This readout is always achieved well after decoherence occurs and there is no need to suppose that some mysterious discontinuity happens to the system at any point during a measurement.

6 Conclusion and perspectives

Rydberg atoms interacting with small trapped microwave fields now appear as efficient tools to perform a variety of tests of quantum mechanics. A nearly ideal non-destructive detection of a single photon has been realized. The generalization of such an ideal detection scheme to larger photon number is still an experimental challenge which seems of great interest [62–64]. It is at the heart of a method proposed in [88] for measuring the Wigner distribution of the field inside the cavity. This distribution provides two-dimensional “pictures” of the field state. Various methods have been proposed in order to measure it [88,89]. They should provide the most powerful way of characterizing the quantum state of various non-classical fields prepared in the cavity. In particular, it would be extremely useful for exploring more deeply the domain where the decoherence rate of cat states scales as the inverse of the photon number.

In the field of engineered N particle entanglement, the CQED system offers the elementary operations needed for preparing complex entangled states. The present degree of fidelity of these operations is high enough for preparing three particle entanglement. We have also recently been able to involve a second resonant mode of the cavity in the entanglement procedure, adding one more degree of freedom to the system. For going further,

the realization of a new cavity without the closed ring is the most critical issue. It will allow for propagating atomic coherences over larger distance and increase the number of accessible entangled states. Teleportation experiments [6] operating for the first time on massive particles instead of photons will be within reach with such an improved version of the set-up [90].

The main present limitation is however that circular atoms are prepared with a Poisson statistics with a low mean value, requiring long data acquisition times. Circular states preparation techniques generating on demand exactly one atom could be implemented. For instance, the fluorescence from a weak atomic beam may be used to image a single atom and excite it deterministically to the circular state in a fully adiabatic process. With these improvements, the techniques described here could be extended to the manipulation of large controlled chains of atoms such as multiparticle generalizations of the GHZ triplet [76]. New fascinating tests of quantum non-locality in mesoscopic entangled systems should then become accessible to the experiments.

Acknowledgments

I warmly thank the colleagues, postdocs, students and visitors involved in the work presented here. I am very grateful to Serge Haroche, Jean-Michel Raimond and Arno Rauschenbeutel for many fruitful discussions and careful reading of this manuscript.

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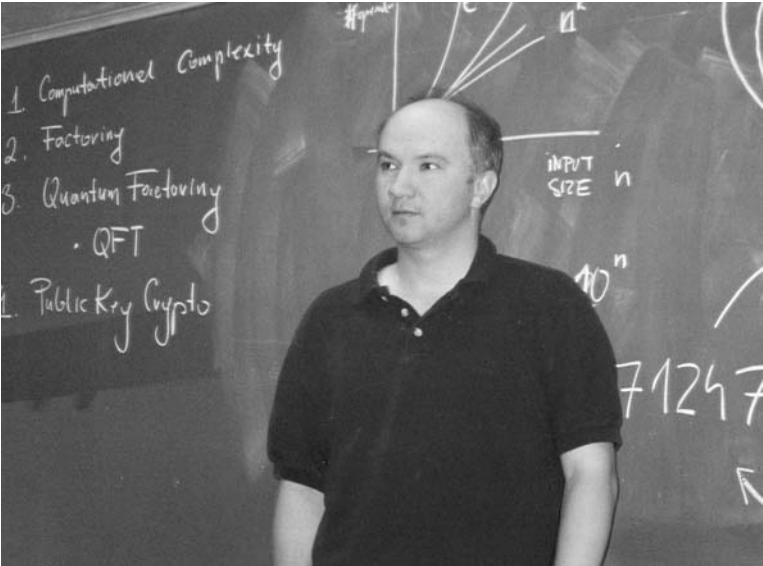
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COURSE 10

BASIC CONCEPTS IN QUANTUM COMPUTATION

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BASIC CONCEPTS IN QUANTUM COMPUTATION

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1 Qubits, gates and networks

Consider the two binary strings,

$$011, \tag{1.1}$$

$$111. \tag{1.2}$$

The first one can represent, for example, the number 3 (in binary) and the second one the number 7. In general three physical bits can be prepared in $2^3 = 8$ different configurations that can represent, for example, the integers from 0 to 7. However, a register composed of three classical bits can store only one number at a given moment of time. Enter qubits and quantum registers:

A *qubit* is a quantum system in which the Boolean states 0 and 1 are represented by a prescribed pair of normalised and mutually orthogonal quantum states labeled as $\{|0\rangle, |1\rangle\}$ [1]. The two states form a “computational basis” and any other (pure) state of the qubit can be written as a superposition $\alpha|0\rangle + \beta|1\rangle$ for some α and β such that $|\alpha|^2 + |\beta|^2 = 1$. A qubit is typically a microscopic system, such as an atom, a nuclear spin, or a polarised photon. A collection of n qubits is called a *quantum register* of size n .

We shall assume that information is stored in the registers in binary form. For example, the number 6 is represented by a register in state $|1\rangle \otimes |1\rangle \otimes |0\rangle$. In more compact notation: $|a\rangle$ stands for the tensor product $|a_{n-1}\rangle \otimes |a_{n-2}\rangle \dots |a_1\rangle \otimes |a_0\rangle$, where $a_i \in \{0, 1\}$, and it represents a quantum register prepared with the value $a = 2^0 a_0 + 2^1 a_1 + \dots 2^{n-1} a_{n-1}$. There are 2^n states of this kind, representing all binary strings of length n or numbers from 0 to $2^n - 1$, and they form a convenient computational basis. In the following $a \in \{0, 1\}^n$ (a is a binary string of length n) implies that $|a\rangle$ belongs to the computational basis.

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Thus a quantum register of size three can store individual numbers such as 3 or 7,

$$|0\rangle \otimes |1\rangle \otimes |1\rangle \equiv |011\rangle \equiv |3\rangle, \quad (1.3)$$

$$|1\rangle \otimes |1\rangle \otimes |1\rangle \equiv |111\rangle \equiv |7\rangle, \quad (1.4)$$

but, it can also store the two of them simultaneously. For if we take the first qubit and instead of setting it to $|0\rangle$ or $|1\rangle$ we prepare a superposition $1/\sqrt{2}(|0\rangle + |1\rangle)$ then we obtain

$$\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes |1\rangle \otimes |1\rangle \equiv \frac{1}{\sqrt{2}}(|011\rangle + |111\rangle), \quad (1.5)$$

$$\equiv \frac{1}{\sqrt{2}}(|3\rangle + |7\rangle). \quad (1.6)$$

In fact we can prepare this register in a superposition of all eight numbers – it is enough to put each qubit into the superposition $1/\sqrt{2}(|0\rangle + |1\rangle)$. This gives

$$\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle), \quad (1.7)$$

which can also be written in binary as (ignoring the normalisation constant $2^{-3/2}$),

$$|000\rangle + |001\rangle + |010\rangle + |011\rangle + |100\rangle + |101\rangle + |110\rangle + |111\rangle \quad (1.8)$$

or in decimal notation as

$$|0\rangle + |1\rangle + |2\rangle + |3\rangle + |4\rangle + |5\rangle + |6\rangle + |7\rangle, \quad (1.9)$$

or simply as

$$\sum_{x=0}^7 |x\rangle. \quad (1.10)$$

These preparations, and any other manipulations on qubits, have to be performed by unitary operations. A *quantum logic gate* is a device which performs a fixed unitary operation on selected qubits in a fixed period of time and a *quantum network* is a device consisting of quantum logic gates whose computational steps are synchronised in time [2]. The outputs of some of the gates are connected by wires to the inputs of others. The *size* of the network is the number of gates it contains.

The most common quantum gate is the Hadamard gate, a single qubit gate H performing the unitary transformation known as the Hadamard transform. It is defined as

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \quad |x\rangle \longrightarrow \boxed{H} \longrightarrow (-1)^x |x\rangle + |1-x\rangle$$

The matrix is written in the computational basis $\{|0\rangle, |1\rangle\}$ and the diagram on the right provides a schematic representation of the gate H acting on a qubit in state $|x\rangle$, with $x = 0, 1$.

And here is a network, of size three, which affects the Hadamard transform on three qubits. If they are initially in state $|000\rangle$ then the output is the superposition of all eight numbers from 0 to 7.

$$\left. \begin{array}{l} |0\rangle \text{---} \boxed{H} \text{---} \frac{|0\rangle+|1\rangle}{\sqrt{2}} \\ |0\rangle \text{---} \boxed{H} \text{---} \frac{|0\rangle+|1\rangle}{\sqrt{2}} \\ |0\rangle \text{---} \boxed{H} \text{---} \frac{|0\rangle+|1\rangle}{\sqrt{2}} \end{array} \right\} \begin{array}{l} \text{IN BINARY} \\ = \frac{1}{2^{3/2}} \left\{ \begin{array}{l} |000\rangle + |001\rangle + |010\rangle + |011\rangle + \\ + |100\rangle + |101\rangle + |110\rangle + |111\rangle \end{array} \right\} \\ = \frac{1}{2^{3/2}} \left\{ \begin{array}{l} |0\rangle + |1\rangle + |2\rangle + |3\rangle + \\ + |4\rangle + |5\rangle + |6\rangle + |7\rangle \end{array} \right\} \\ \text{IN DECIMAL} \end{array}$$

If the three qubits are initially in some other state from the computational basis then the result is a superposition of all numbers from 0 to 7 but exactly half of them will appear in the superposition with the minus sign, for example,

$$|101\rangle \mapsto \frac{1}{2^{3/2}} \left\{ \begin{array}{l} |000\rangle - |001\rangle + |010\rangle - |011\rangle + \\ - |100\rangle + |101\rangle - |110\rangle + |111\rangle \end{array} \right\}. \quad (1.11)$$

In general, if we start with a register of size n in some state $y \in \{0, 1\}^n$ then

$$|y\rangle \mapsto 2^{-n/2} \sum_{x \in \{0,1\}^n} (-1)^{y \cdot x} |x\rangle, \quad (1.12)$$

where the product of $y = (y_{n-1}, \dots, y_0)$ and $x = (x_{n-1}, \dots, x_0)$ is taken bit by bit:

$$y \cdot x = (y_{n-1}x_{n-1} + \dots + y_1x_1 + y_0x_0). \quad (1.13)$$

We will need another single qubit gate – the phase shift gate ϕ defined as $|0\rangle \mapsto |0\rangle$ and $|1\rangle \mapsto e^{i\phi}|1\rangle$, or, in matrix notation,

$$\phi = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{pmatrix} \quad |x\rangle \text{---} \bullet \text{---} e^{ix\phi} |x\rangle \quad (1.14)$$

The Hadamard gate and the phase gate can be combined to construct the following network (of size four), which generates the most general pure state of a single qubit (up to a global phase),

$$|0\rangle \text{---} \boxed{H} \text{---} \bullet^{2\theta} \text{---} \boxed{H} \text{---} \bullet^{\frac{\pi}{2} + \phi} \text{---} \cos \theta |0\rangle + e^{i\phi} \sin \theta |1\rangle. \quad (1.15)$$

Consequently, the Hadamard and phase gates are sufficient to construct *any* unitary operation on a single qubit.

Thus the Hadamard gates and the phase gates can be used to transform the input state $|0\rangle|0\rangle\ldots|0\rangle$ of the n qubit register into any state of the type $|\Psi_1\rangle|\Psi_2\rangle\ldots|\Psi_n\rangle$, where $|\Psi_i\rangle$ is an arbitrary superposition of $|0\rangle$ and $|1\rangle$. These are rather special n -qubit states, called the product states or the separable states. In general, a quantum register of size $n > 1$ can be prepared in states which are not separable – they are known as entangled states. For example, for two qubits ($n = 2$), the state

$$\alpha|00\rangle + \beta|01\rangle = |0\rangle \otimes (\alpha|0\rangle + \beta|1\rangle) \quad (1.16)$$

is separable, $|\Psi_1\rangle = |0\rangle$ and $|\Psi_2\rangle = \alpha|0\rangle + \beta|1\rangle$, whilst the state

$$\alpha|00\rangle + \beta|11\rangle \neq |\Psi_1\rangle \otimes |\Psi_2\rangle \quad (1.17)$$

is entangled ($\alpha, \beta \neq 0$), because it cannot be written as a tensor product.

In order to entangle two (or more qubits) we have to extend our repertoire of quantum gates to two-qubit gates. The most popular two-qubit gate is the controlled-NOT (C-NOT), also known as the XOR or the measurement gate. It flips the second (target) qubit if the first (control) qubit is $|1\rangle$ and does nothing if the control qubit is $|0\rangle$. The gate is represented by the unitary matrix

$$C = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \quad \begin{array}{c} |x\rangle \text{---} \bullet \text{---} |x\rangle \\ |y\rangle \text{---} \oplus \text{---} |x \oplus y\rangle \end{array} \quad (1.18)$$

where $x, y = 0$ or 1 and $\oplus$ denotes XOR or addition modulo 2. If we apply the C-NOT to Boolean data in which the target qubit is $|0\rangle$ and the control is either $|0\rangle$ or $|1\rangle$ then the effect is to leave the control unchanged while the target becomes a copy of the control, *i.e.*

$$|x\rangle|0\rangle \mapsto |x\rangle|x\rangle \quad x = 0, 1. \quad (1.19)$$

One might suppose that this gate could also be used to copy superpositions such as $|\Psi\rangle = \alpha|0\rangle + \beta|1\rangle$, so that

$$|\Psi\rangle|0\rangle \mapsto |\Psi\rangle|\Psi\rangle \quad (1.20)$$

for any $|\Psi\rangle$. This is not so! The unitarity of the C-NOT requires that the gate turns superpositions in the control qubit into *entanglement* of the control and the target. If the control qubit is in a superposition state $|\Psi\rangle = \alpha|0\rangle + \beta|1\rangle$, ($\alpha, \beta \neq 0$), and the target in $|0\rangle$ then the C-NOT generates the entangled state

$$(\alpha|0\rangle + \beta|1\rangle)|0\rangle \mapsto \alpha|00\rangle + \beta|11\rangle. \quad (1.21)$$

Let us notice in passing that it is impossible to construct a universal quantum cloning machine effecting the transformation in equation (1.20), or even the more general

$$|\Psi\rangle|0\rangle|W\rangle \mapsto |\Psi\rangle|\Psi\rangle|W'\rangle \quad (1.22)$$

where $|W\rangle$ refers to the state of the rest of the world and $|\Psi\rangle$ is *any* quantum state [3]. To see this take any two normalised states $|\Psi\rangle$ and $|\Phi\rangle$ which are non-identical ($|\langle\Phi|\Psi\rangle| \neq 1$) and non-orthogonal ($\langle\Phi|\Psi\rangle \neq 0$), and run the cloning machine,

$$|\Psi\rangle|0\rangle|W\rangle \mapsto |\Psi\rangle|\Psi\rangle|W'\rangle \quad (1.23)$$

$$|\Phi\rangle|0\rangle|W\rangle \mapsto |\Phi\rangle|\Phi\rangle|W''\rangle. \quad (1.24)$$

As this must be a unitary transformation which preserves the inner product hence we must require

$$\langle\Phi|\Psi\rangle = \langle\Phi|\Psi\rangle^2 \langle W'|W''\rangle \quad (1.25)$$

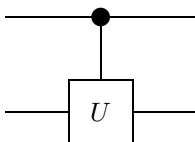
and this can only be satisfied when $|\langle\Phi|\Psi\rangle| = 0$ or 1 , which contradicts our assumptions. Thus states of qubits, unlike states of classical bits, cannot be faithfully cloned. This leads to interesting applications, quantum cryptography being one such.

Another common two-qubit gate is the controlled phase shift gate $B(\phi)$ defined as

$$B(\phi) = \left(\begin{array}{cccc} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{i\phi} \end{array} \right) \quad \left. \begin{array}{c} |x\rangle \text{---} \bullet \text{---} \\ |y\rangle \text{---} \bullet \text{---} \end{array} \right\} e^{ixy\phi} |x\rangle |y\rangle. \quad (1.26)$$

Again, the matrix is written in the computational basis $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$ and the diagram on the right shows the structure of the gate.

More generally, these various 2-qubit controlled gates are all of the form controlled- U , for some single-qubit unitary transformation U . The controlled- U gate applies the identity transformation to the auxiliary (lower) qubit when the control qubit is in state $|0\rangle$ and applies an arbitrary prescribed U when the control qubit is in state $|1\rangle$. The gate maps $|0\rangle|y\rangle$ to $|0\rangle|y\rangle$ and $|1\rangle|y\rangle$ to $|1\rangle(U|y\rangle)$, and is graphically represented as



The Hadamard gate, all phase gates, and the C-NOT, form an infinite *universal set of gates i.e.* if the C-NOT gate as well as the Hadamard and all phase gates are available then any n -qubit unitary operation can be simulated exactly with $O(4^n n)$ such gates [4]. (Here and in the following we use the asymptotic notation – $O(T(n))$ means bounded above by $cT(n)$ for some constant $c > 0$ for sufficiently large n .) This is not the only universal set of gates. In fact, almost any gate which can entangle two qubits can be used as a universal gate [6, 8]. Mathematically, an elegant choice is a pair of the Hadamard and the controlled- V (C- V) where V is described by the unitary matrix

$$V = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}. \quad (1.27)$$

The two gates form a finite universal set of gates – networks containing only a finite number of these gates can approximate any unitary transformation on two (and more) qubits. More precisely, if U is any two-qubit gate and $\varepsilon > 0$ then there exists a quantum network of size $O(\log^d(1/\varepsilon))$ (where d is a constant) consisting of only H and C- V gates which computes a unitary operation U' that is within distance ε from U [50]. The metric is induced by the Euclidean norm - we say that U' is within distance ε from U if there exists a unit complex number λ (phase factor) such that $\|U - \lambda U'\| \leq \varepsilon$. Thus if U' is substituted for U in a quantum network then the final state $\sum_x \alpha'_x |x\rangle$ approximates the final state of the original network $\sum_x \alpha_x |x\rangle$ as follows: $\sqrt{\sum_x |\lambda \alpha'_x - \alpha_x|^2} \leq \varepsilon$. The probability of any specified measurement outcome on the final state is affected by at most ε .

A *quantum computer* will be viewed here as a quantum network (or a family of quantum networks) and quantum computation is defined as a unitary evolution of the network which takes its initial state “input” into some final state “output”. We have chosen the network model of computation, rather than Turing machines, because it is relatively simple and easy to work with and because it is much more relevant when it comes to physical implementation of quantum computation.

2 Quantum arithmetic and function evaluations

Let us now describe how quantum computers actually compute, how they add and multiply numbers, and how they evaluate Boolean functions by means of unitary operations. Here and in the following we will often use the modular arithmetic [9]. Recall that

$$a \bmod b \quad (2.1)$$

denotes the remainder obtained by dividing integer b into integer a , which is always a number less than b . Basically $a = b \bmod n$ if $a = b + kn$ for some integer k . This is expressed by saying that a is *congruent* to b modulo n or that b is the *residue* of a modulo n . For example, $1 \bmod 7 = 8 \bmod 7 = 15 \bmod 7 = 50 \bmod 7 = 1$. Modular arithmetic is commutative, associative, and distributive.

$$(a \pm b) \bmod n = ((a \bmod n) \pm (b \bmod n)) \bmod n \quad (2.2)$$

$$(a \times b) \bmod n = ((a \bmod n) \times (b \bmod n)) \bmod n \quad (2.3)$$

$$(a \times (b + c)) \bmod n = (((ab) \bmod n + ((ac) \bmod n)) \bmod n. \quad (2.4)$$

Thus, if you need to calculate, say, $3^8 \bmod 7$ do not use the naive approach and perform seven multiplications and one huge modular reduction. Instead, perform three smaller multiplications and three smaller reductions,

$$((3^2 \bmod 7)^2 \bmod 7)^2 \bmod 7 = (2^2 \bmod 7)^2 \bmod 7 = 16 \bmod 7 = 2. \quad (2.5)$$

This kind of arithmetic is ideal for computers as it restricts the range of all intermediate results. For l -bit modulus n , the intermediate results of any addition, subtraction or multiplication will not be more than $2l$ bits long. In quantum registers of size n , addition modulo 2^n is one of the most common operations; for all $x \in \{0, 1\}^n$ and for any $a \in \{0, 1\}^n$,

$$|x\rangle \mapsto |(x + a) \bmod 2^n\rangle \quad (2.6)$$

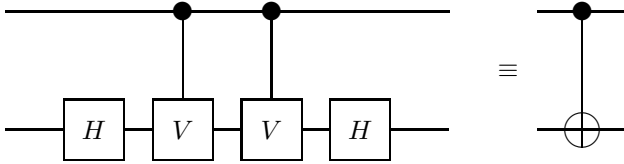
is a well defined unitary transformation.

The tricky bit in the modular arithmetic is the inverse operation, and here we need some basic number theory. An integer $a \geq 2$ is said to be *prime* if it is divisible only by 1 and a (we consider only positive divisors). Otherwise, a is called *composite*. The greatest common divisor of two integers a and b is the greatest positive integer d denoted $d = \gcd(a, b)$ that divides both a and b . Two integers a and b are said to be *coprime* or *relatively prime* if $\gcd(a, b) = 1$. Given two integers a and n that are coprime, it can be shown that there exists a unique integer $d \in \{0, \dots, n-1\}$ such that $ad = 1 \bmod n$ [9]. The integer d is called *inverse modulo n* of a , and denoted a^{-1} . For example, modulo 7 we find that $3^{-1} = 5 \bmod n$, since $3 \times 5 = 15 = 2 \times 7 + 1 = 1 \bmod 7$.

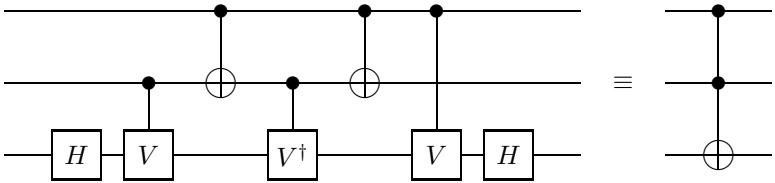
In quantum computers addition, multiplication, and any other arithmetic operation have to be embedded in unitary evolution. We will stick to the Hadamard and the controlled- V (C- V), and use them as building blocks for all other gates and eventually for quantum adders and multipliers.

If we apply C- V four times we get identity, so any three subsequent applications of C- V give the inverse of C- V , which will be called C- $V^\dagger$.

Now, if we have a couple of the C-V gates and a couple of the Hadamard gates we can build the C-NOT as follows



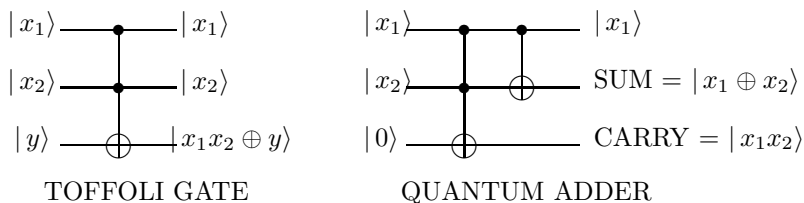
A single qubit operation NOT can be performed *via* a C-NOT gate if the control qubit is set to $|1\rangle$ and viewed as an auxiliary qubit. This is not to say that we want to do it in practice. The C-NOT gate is much more difficult to build than a single qubit NOT. Right now we are looking into the mathematical structure of quantum Boolean networks and do not care about practicalities. Our two elementary gates also allow us to construct a very useful gate called the controlled-controlled-NOT gate (c^2 -NOT) or the Toffoli gate [10]. The construction is given by the following network,



This gate has two control qubits (the top two wires on the diagram) and one target qubit which is negated only when the two controls are in the state $|1\rangle|1\rangle$. The c^2 -NOT gate gives us the logical connectives we need for arithmetic. If the target is initially set to $|0\rangle$ the gate acts as a reversible AND gate - after the gate operation the target becomes the logical AND of the two control qubits.

$$|x_1, x_2\rangle |0\rangle \mapsto |x_1, x_2\rangle |x_1 \wedge x_2\rangle. \quad (2.7)$$

Once we have in our repertoire operations such as NOT, AND, and C-NOT, all of them implemented as unitary operations, we can, at least in principle, evaluate any Boolean function $\{0, 1\}^n \rightarrow \{0, 1\}^m$ which map n bits of input into m bits of output. A simple concatenation of the Toffoli gate and the C-NOT gives a simplified quantum adder, shown below, which is a good starting point for constructing full adders, multipliers and more elaborate networks.



We can view the Toffoli gate and the evolution given by equation (2.7) as a quantum implementation of a Boolean function $f: \{0, 1\}^2 \rightarrow \{0, 1\}$ defined by $f(x_1, x_2) = x_1 \wedge x_2$. The operation AND is not reversible, so we had to embed it in the reversible operation c^2 -NOT. If the third bit is initially set to 1 rather than 0 then the value of $x_1 \wedge x_2$ is negated. In general we write the action of the Toffoli gate as the function evaluation,

$$|x_1, x_2\rangle |y\rangle \mapsto |x_1, x_2\rangle | (y + (x_1 \wedge x_2)) \bmod 2 \rangle. \quad (2.8)$$

This is how we compute any Boolean function $\{0, 1\}^n \rightarrow \{0, 1\}^m$ on a quantum computer. We require at least two quantum registers; the first one, of size n , to store the arguments of f and the second one, of size n , to store the values of f . The function evaluation is then a unitary evolution of the two registers,

$$|x, y\rangle \mapsto |x, (y + f(x)) \bmod 2^m\rangle \quad (2.9)$$

for any $y \in \{0, 1\}^m$. (In the following, if there is no danger of confusion, we may simplify the notation and omit the mod suffix.)

For example, a network computing $f: \{0, 1\}^2 \rightarrow \{0, 1\}^3$ such that $f(x) = x^2$ acts as follows

$$|00\rangle|000\rangle \mapsto |00\rangle|000\rangle, \quad |10\rangle|000\rangle \mapsto |10\rangle|100\rangle \quad (2.10)$$

$$|01\rangle|000\rangle \mapsto |01\rangle|001\rangle, \quad |11\rangle|000\rangle \mapsto |11\rangle|001\rangle \quad (2.11)$$

which can be written as

$$|x, 0\rangle \mapsto |x, x^2 \bmod 8\rangle, \quad (2.12)$$

e.g. $3^2 \bmod 2^2 = 1$ which explains why $|11\rangle|000\rangle \mapsto |11\rangle|001\rangle$.

In fact, for these kind of operations we also need a third register with the so-called working bits which are set to zero at the input and return to zero at the output but which can take non-zero values during the computation.

What makes quantum function evaluation really interesting is its action on a superposition of different inputs x , for example,

$$\sum_x |x, 0\rangle \mapsto \sum_x |x, f(x)\rangle \quad (2.13)$$

produces $f(x)$ for all x in a single run. The snag is that we cannot get them all from the entangled state $\sum_x |x, f(x)\rangle$ because any bit by bit measurement on the first register will yield one particular value $x' \in \{0, 1\}^n$ and the second register will then be found with the value $f(x') \in \{0, 1\}^m$.

3 Algorithms and their complexity

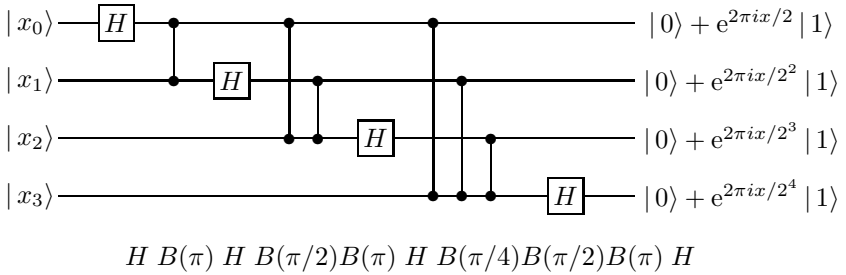
In order to solve a particular problem, computers, be it classical or quantum, follow a precise set of instructions that can be mechanically applied to yield the solution to any given instance of the problem. A specification of this set of instructions is called an algorithm. Examples of algorithms are the procedures taught in elementary schools for adding and multiplying whole numbers; when these procedures are mechanically applied, they always yield the correct result for any pair of whole numbers. Any algorithm can be represented by a family of Boolean networks $(N_1, N_2, N_3, \dots)$, where the network N_n acts on all possible input instances of size n bits. Any useful algorithm should have such a family specified by an example network N_n and a *simple rule* explaining how to construct the network N_{n+1} from the network N_n . These are called *uniform* families of networks [11]¹.

The quantum Hadamard transform defined by equation (1.12) has a uniform family of networks whose size is growing as n with the number of input qubits. Another good example of a uniform family of networks is the quantum Fourier transform (QFT) [12] defined in the computational basis as the unitary operation

$$|y\rangle \mapsto 2^{-n/2} \sum_x e^{i\frac{2\pi}{2^n}yx} |x\rangle. \quad (3.1)$$

Suppose we want to *construct* such a unitary evolution of n qubits using our repertoire of quantum logic gates. We can start with a single qubit and notice that in this case the QFT is reduced to applying a Hadamard gate. Then we can take two qubits and notice that the QFT can be implemented with two Hadamard gates and the controlled phase shift $B(\pi)$ in between. Progressing this way we can construct the three qubit QFT and the four qubit QFT, whose network looks like this:

¹This means that the network model is not a self-contained model of computation. We need an algorithm, a Turing machine, which maps each n into an explicit description of N_n .



(*N.B.* there are three different types of the $B(\phi)$ gate in the network above: $B(\pi)$, $B(\pi/2)$ and $B(\pi/4)$.)

The general case of n qubits requires a trivial extension of the network following the same sequence pattern of gates H and B . The QFT network operating on n qubits contains n Hadamard gates H and $n(n-1)/2$ phase shifts B , in total $n(n+1)/2$ elementary gates.

The big issue in designing algorithms or their corresponding families of networks is the optimal use of physical resources required to solve a problem. Complexity theory is concerned with the inherent cost of computation in terms of some designated elementary operations, memory usage, or network size. An algorithm is said to be fast or efficient if the number of elementary operations taken to execute it increases no faster than a polynomial function of the size of the input. We generally take the input size to be the total number of bits needed to specify the input (for example, a number N requires $\log_2 N$ bits of binary storage in a computer). In the language of network complexity - an algorithm is said to be *efficient* if it has a uniform and polynomial-size network family ($O(n^d)$ for some constant d) [11]. For example, the quantum Fourier transform can be performed in an efficient way because it has a uniform family of networks whose size grows only as a quadratic function of the size of the input, *i.e.* $O(n^2)$. Changing from one set of gates to another, *e.g.* constructing the QFT out of the Hadamard and the controlled- V gates with a prescribed precision ϵ , can only affect the network size by a multiplicative constant which does not affect the quadratic scaling with n . Thus the complexity of the QFT is $O(n^2)$ no matter which set of adequate gates we use. Problems which do not have efficient algorithms are known as hard problems.

Elementary arithmetic operations taught at schools, such as long addition, multiplication or division of n bit numbers require $O(n^2)$ operations. For example, to multiply $x = (x_{n-1} \dots x_1 x_0)$ and $y = (y_{n-1} \dots y_1 y_0)$ we successively multiply y by x_0, x_1 and so on, shift, and then add the result. Each multiplication of y by x_k takes about n single bit operations, the addition of the n products takes of the order of n^2 bit operations, which adds to the

total $O(n^2)$ operations. Knowing the complexity of elementary arithmetic one can often assess the complexity of other algorithms. For example, the greatest common divisor of two integers x and $y < x$ can be found using Euclid's algorithm; the oldest nontrivial algorithm which has been known and used since 300 BC². First divide x by y obtaining remainder r_1 . Then divide y by r_1 obtaining remainder r_2 , then divide r_1 by r_2 obtaining remainder r_3 , etc., until the remainder is zero. The last non-zero remainder is $\gcd(x, y)$ because it divides all previous remainders and hence also x and y (it is obvious from the construction that it is the *greatest* common divisor). For example, here is a sequence of remainders (r_j, r_{j+1}) when we apply Euclid's algorithm to compute $\gcd(12378, 3054) = 6$: (12378, 3054), (3054, 162), (162, 138), (138, 24), (24, 18), (18, 6), (6, 0). What is the complexity of this algorithm? It is easy to see that the largest of the two numbers is at least halved every two steps, so every two steps we need one bit less to represent the number, and so the number of steps is at most $2n$, where n is the number of bits in the two integers. Each division can be done with at most $O(n^2)$ operations hence the total number of operations is $O(n^3)$.

There are basically three different types of Boolean networks: classical deterministic, classical probabilistic, and quantum. They correspond to, respectively, deterministic, randomised, and quantum algorithms.

Classical deterministic networks are based on logical connectives such as AND, OR, and NOT and are required to always deliver correct answers. If a problem admits a deterministic uniform network family of polynomial size, we say that the problem is in the class P [11].

Probabilistic networks have additional “coin flip” gates which do not have any inputs and emit one uniformly-distributed random bit when executed during a computation. Despite the fact that probabilistic networks may generate erroneous answers they may be more powerful than deterministic ones. A good example is primality testing – given an n -bit number x decide whether or not x is prime. The smallest known uniform deterministic network family that solves this problem is of size $O(n^{d \log \log n})$, which is not polynomially bounded. However, there is a probabilistic algorithm, due to Solovay and Strassen [13], that can solve the same problem with a uniform probabilistic network family of size $O(n^3 \log(1/\epsilon))$, where ϵ is the probability of error. *N.B.* ϵ does not depend on n and we can choose it as small as we wish and still get an efficient algorithm.

The $\log(1/\epsilon)$ part can be explained as follows. Imagine a probabilistic network that solves a decision problem³ and that errs with probability

²This truly “classical” algorithm is described in Euclid's *Elements*, the oldest Greek treatise in mathematics to reach us in its entirety. Knuth (1981) provides an extensive discussion of various versions of Euclid's algorithm.

³A decision problem is a problem that admits only two answers: YES or NO.

smaller than $\frac{1}{2} + \delta$ for fixed $\delta > 0$. If you run r of these networks in parallel (so that the size of the overall network is increased by factor r) and then use the majority voting for the final YES or NO answer your overall probability of error will be bounded by $\epsilon = \exp(-\delta^2 r)$. (This follows directly from the Chernoff bound- see for instance, [14]). Hence r is of the order $\log(1/\epsilon)$. If a problem admits such a family of networks then we say the problem is in the class *BPP* (stands for “bounded-error probabilistic polynomial”) [11].

Last but not least we have quantum algorithms, or families of quantum networks, which are more powerful than their probabilistic counterparts. The example here is the factoring problem – given an n -bit number x find a list of prime factors of x . The smallest known uniform probabilistic network family which solves the problem is of size $O(2^{d\sqrt{n \log n}})$. One reason why quantum computation is such a fashionable field today is the discovery, by Peter Shor, of a uniform family of quantum networks of $O(n^2 \log \log n \log(1/\epsilon))$ in size, that solve the factoring problem [15]. If a problem admits a uniform quantum network family of polynomial size that for any input gives the right answer with probability larger than $\frac{1}{2} + \delta$ for fixed $\delta > 0$ then we say the problem is in the class *BQP* (stands for “bounded-error quantum probabilistic polynomial”).

We have

$$P \subseteq BPP \subseteq BQP. \quad (3.2)$$

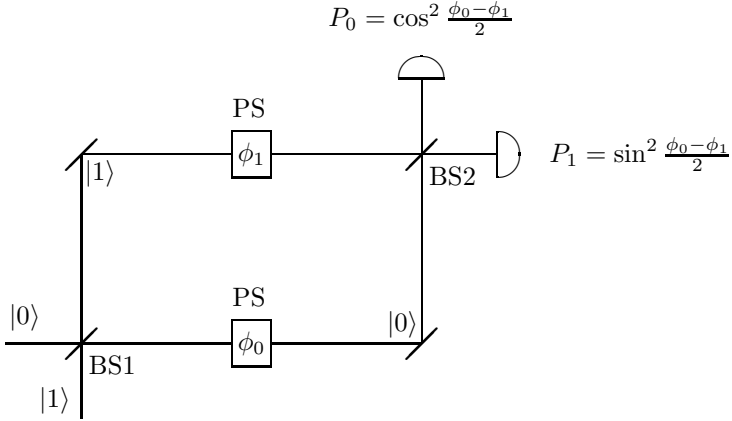
Quantum networks are potentially more powerful because of multiparticle quantum interference, an inherently quantum phenomenon which makes the quantum theory radically different from any classical statistical theory.

Richard Feynman [16] was the first to anticipate the unusual power of quantum computers. He observed that it appears to be impossible to simulate a general quantum evolution on a classical probabilistic computer in an *efficient* way *i.e.* any classical simulation of quantum evolution appears to involve an exponential slowdown in time as compared to the natural evolution since the amount of information required to describe the evolving quantum state in classical terms generally grows exponentially in time. However, instead of viewing this fact as an obstacle, Feynman regarded it as an opportunity. Let us then follow his lead and try to construct a computing device using inherently quantum mechanical effects.

4 From interferometers to computers

A single particle interference in the Mach-Zehnder interferometer works as follows. A particle, in this case a photon, impinges on a beam-splitter (BS1), and, with some probability amplitudes, propagates via two different paths to another beam-splitter (BS2) which directs the particle to one of

the two detectors. Along each path between the two beam-splitters, is a phase shifter (PS).



If the lower path is labeled as state $|0\rangle$ and the upper one as state $|1\rangle$ then the particle, initially in path $|0\rangle$, undergoes the following sequence of transformations

$$|0\rangle \xrightarrow{\text{BS1}} \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle) \xrightarrow{\text{PS}} \frac{1}{\sqrt{2}} (e^{i\phi_0} |0\rangle + e^{i\phi_1} |1\rangle) \quad (4.1)$$

$$= e^{i\frac{\phi_0+\phi_1}{2}} \frac{1}{\sqrt{2}} \left(e^{i\frac{\phi_0-\phi_1}{2}} |0\rangle + e^{i\frac{-\phi_0+\phi_1}{2}} |1\rangle \right)$$

$$\xrightarrow{\text{BS2}} e^{i\frac{\phi_1+\phi_0}{2}} \left(\cos \frac{1}{2}(\phi_0 - \phi_1) |0\rangle + i \sin \frac{1}{2}(\phi_0 - \phi_1) |1\rangle \right), \quad (4.2)$$

where ϕ_0 and ϕ_1 are the settings of the two phase shifters and the action of the beam-splitters is defined as

$$|0\rangle \mapsto \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle), \quad |1\rangle \mapsto \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle). \quad (4.3)$$

(We have ignored the phase shift in the reflected beam.) The global phase shift $e^{i\frac{\phi_0+\phi_0}{2}}$ is irrelevant as the interference pattern depends on the difference between the phase shifts in different arms of the interferometer. The phase shifters in the two paths can be tuned to effect any prescribed relative phase shift $\phi = \phi_0 - \phi_1$ and to direct the particle with probabilities

$$P_0 = \cos^2 \left(\frac{\phi}{2} \right) = \frac{1}{2} (1 + \cos \phi) \quad (4.4)$$

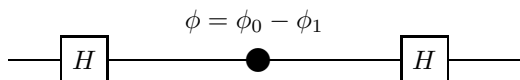
$$P_1 = \sin^2 \left(\frac{\phi}{2} \right) = \frac{1}{2} (1 - \cos \phi) \quad (4.5)$$

respectively to detectors “0” and “1”.

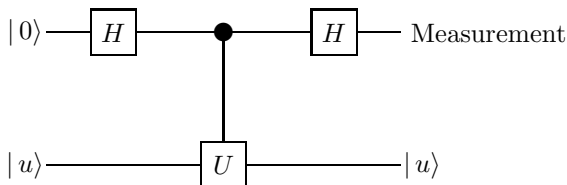
The roles of the three key ingredients in this experiment are clear. The first beam splitter prepares a superposition of possible paths, the phase shifters modify quantum phases in different paths and the second beam-splitter combines all the paths together erasing all information about which path was actually taken by the particle between the two beam-splitters. This erasure is very important as we shall see in a moment.

Needless to say, single particle interference experiments are not restricted to photons. One can go for a different “hardware” and repeat the experiment with electrons, neutrons, atoms or even molecules. When it comes to atoms and molecules both external and internal degrees of freedom can be used.

Although single particle interference experiments are worth discussing in their own right, here we are only interested in their generic features simply because they are all “isomorphic” and once you know and understand one of them you, at least for our purposes, understand them all (modulo experimental details, of course). Let us now describe any single particle interference experiment in more general terms. It is very convenient to view this experiment in a diagrammatic way as a *quantum network* with three quantum logic gates [17]. The beam-splitters will be now called the Hadamard gates and the phase shifters the phase shift gates. In particular any single particle quantum interference can be represented by the following simple network,



In order to make a connection with a quantum function evaluation let us now describe an alternative construction which simulates the action of the phase shift gate. This construction introduces a phase factor ϕ using a controlled- U gate. The phase shift ϕ is “computed” with the help of an auxiliary qubit in a prescribed state $|u\rangle$ such that $U|u\rangle = e^{i\phi}|u\rangle$.



In our example, shown above, we obtain the following sequence of transformations on the two qubits

$$\begin{aligned} |0\rangle|u\rangle &\xrightarrow{H} \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)|u\rangle \xrightarrow{c-U} \frac{1}{\sqrt{2}}(|0\rangle + e^{i\phi}|1\rangle)|u\rangle \\ &\xrightarrow{H} \left(\cos \frac{\phi}{2} |0\rangle + i \sin \frac{\phi}{2} |1\rangle \right) |u\rangle. \end{aligned} \quad (4.6)$$

We note that the state of the auxiliary qubit $|u\rangle$, being an eigenstate of U , is not altered along this network, but its eigenvalue $e^{i\phi}$ is “kicked back” in front of the $|1\rangle$ component in the first qubit. The sequence (4.6) is the exact simulation of the Mach-Zehnder interferometer and, as we shall see later on, the kernel of quantum algorithms.

Some of the controlled- U operations are special - they represent quantum function evaluations! Indeed, a unitary evolution which computes $f: \{0, 1\}^n \mapsto \{0, 1\}^m$,

$$|x\rangle|y\rangle \mapsto |x\rangle|(y + f(x)) \bmod 2^m\rangle, \quad (4.7)$$

is of the controlled- U type. The unitary transformation of the second register, specified by

$$|y\rangle \mapsto |(y + f(x)) \bmod 2^m\rangle, \quad (4.8)$$

depends on x – the state of the first register. If the initial state of the second register is set to

$$|u\rangle = \frac{1}{2^{m/2}} \sum_{y=0}^{2^m-1} \exp\left(-\frac{2\pi i}{2^m}y\right) |y\rangle, \quad (4.9)$$

by applying the QFT to the state $|111\dots 1\rangle$, then the function evaluation generates

$$|x\rangle|u\rangle = \frac{1}{2^{m/2}}|x\rangle \sum_{y=0}^{2^m-1} \exp\left(-\frac{2\pi i}{2^m}y\right) |y\rangle \quad (4.10)$$

$$\mapsto \frac{1}{2^{m/2}}|x\rangle \sum_{y=0}^{2^m-1} \exp\left(-\frac{2\pi i}{2^m}y\right) |f(x) + y\rangle \quad (4.11)$$

$$= \frac{e^{\frac{2\pi i}{2^m}f(x)}}{2^{m/2}}|x\rangle \sum_{y=0}^{2^m-1} \exp\left(-\frac{2\pi i}{2^m}(f(x) + y)\right) |f(x) + y\rangle \quad (4.12)$$

$$= \frac{e^{\frac{2\pi i}{2^m}f(x)}}{2^{m/2}}|x\rangle \sum_{y=0}^{2^m-1} \exp\left(-\frac{2\pi i}{2^m}y\right) |y\rangle \quad (4.13)$$

$$= e^{\frac{2\pi i}{2^m}f(x)}|x\rangle|u\rangle, \quad (4.14)$$

where we have relabelled the summation index in the sum containing 2^m terms

$$\sum_{y=0}^{2^m-1} \exp\left(-\frac{2\pi i}{2^m}(f(x) + y)\right) |f(x) + y\rangle = \sum_{y=0}^{2^m-1} \exp\left(-\frac{2\pi i}{2^m}y\right) |y\rangle. \quad (4.15)$$

Again, the function evaluation effectively introduces the phase factors in front of the $|x\rangle$ terms in the first register.

$$|x\rangle |u\rangle \mapsto \exp\left(\frac{2\pi i}{2^m}f(x)\right) |x\rangle |u\rangle. \quad (4.16)$$

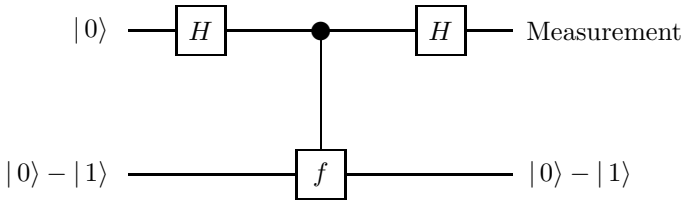
Please notice that the resolution in $\phi(x) = \frac{2\pi}{2^m}f(x)$ is determined by the size m of the second register. For $m = 1$ we obtain $\phi(x) = \pi f(x)$, *i.e.* the phase factors are $(-1)^{f(x)}$. Let us see how this approach explains the internal working of quantum algorithms.

5 The first quantum algorithms

The first quantum algorithms showed advantages of quantum computation without referring to computational complexity measured by the scaling properties of network sizes. The computational power of quantum interference was discovered by counting how many times certain Boolean functions have to be evaluated in order to find the answer to a given problem. Imagine a “black box” (also called an *oracle*) computing a Boolean function and a scenario in which one wants to learn about a given property of the Boolean function but has to pay for each use of the “black box” (often referred to as a *query*). The objective is to minimise number of queries.

Consider, for example, a “black box” computing a Boolean function $f: \{0,1\} \mapsto \{0,1\}$. There are exactly four such functions: two constant functions ($f(0) = f(1) = 0$ and $f(0) = f(1) = 1$) and two “balanced” functions ($f(0) = 0, f(1) = 1$ and $f(0) = 1, f(1) = 0$). The task is to deduce, by queries to the “black box”, whether f is constant or balanced (in other words, whether $f(0)$ and $f(1)$ are the same or different).

Classical intuition tells us that we have to evaluate both $f(0)$ and $f(1)$, which involves evaluating f twice (two queries). We shall see that this is not so in the setting of quantum information, where we can solve this problem with a single function evaluation (one query), by employing an algorithm that has the same mathematical structure as the Mach-Zehnder interferometer. The quantum algorithm that accomplishes this is best represented as the quantum network shown below, where the middle operation is the “black box” representing the function evaluation [17].



The initial state of the qubits in the quantum network is $|0\rangle(|0\rangle - |1\rangle)$ (apart from a normalization factor, which will be omitted in the following). After the first Hadamard transform, the state of the two qubits has the form $(|0\rangle + |1\rangle)(|0\rangle - |1\rangle)$. To determine the effect of the function evaluation on this state, first recall that, for each $x \in \{0, 1\}$,

$$|x\rangle(|0\rangle - |1\rangle) \xrightarrow{f} (-1)^{f(x)} |x\rangle(|0\rangle - |1\rangle). \quad (5.1)$$

Therefore, the state after the function evaluation is

$$[(-1)^{f(0)} |0\rangle + (-1)^{f(1)} |1\rangle](|0\rangle - |1\rangle). \quad (5.2)$$

That is, for each x , the $|x\rangle$ term acquires a phase factor of $(-1)^{f(x)}$, which corresponds to the eigenvalue of the state of the auxiliary qubit under the action of the operator that sends $|y\rangle$ to $|y + f(x)\rangle$. The second qubit is of no interest to us any more but the state of the first qubit

$$(-1)^{f(0)} |0\rangle + (-1)^{f(1)} |1\rangle \quad (5.3)$$

is equal either to

$$\pm(|0\rangle + |1\rangle), \quad (5.4)$$

when $f(0) = f(1)$, or

$$\pm(|0\rangle - |1\rangle), \quad (5.5)$$

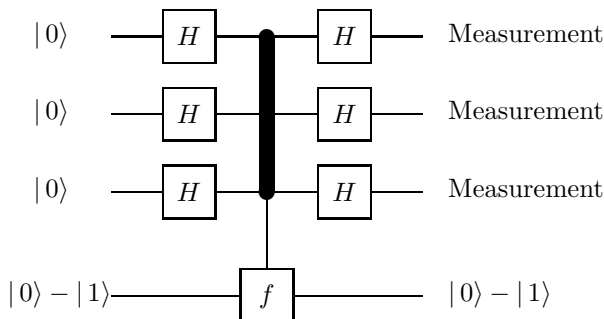
when $f(0) \neq f(1)$. Hence, after applying the second Hadamard gate the state of the first qubit becomes $|0\rangle$ if the function f is constant and $|1\rangle$ if the function is balanced! A bit-value measurement on this qubit distinguishes these cases with certainty.

This example [17] is an improved version of the first quantum algorithm proposed by Deutsch [18] (The original Deutsch algorithm provides the correct answer with probability 50%.) Deutsch's result laid the foundation for the new field of quantum computation, and was followed by several other quantum algorithms.

Deutsch's original problem was subsequently generalised to cover "black boxes" computing Boolean functions $f: \{0, 1\}^n \mapsto \{0, 1\}$. Assume that, for

one of these functions, it is “promised” that it is either constant or balanced (*i.e.* has an equal number of 0’s outputs as 1’s), and the goal is to determine which of the two properties the function actually has. How many queries to f are required to do this? Any classical algorithm for this problem would, in the worst-case, require $2^{n-1} + 1$ queries before determining the answer with certainty. There is a quantum algorithm that solves this problem with a single evaluation of f .

The algorithm is illustrated by a simple extension of the network which solves Deutsch’s problem.



The control register, now composed out of n qubits ($n = 3$ in the diagram above), is initially in state $|00 \cdots 0\rangle$ and an auxiliary qubit in the second register starts and remains in the state $|0\rangle - |1\rangle$.

Stepping through the execution of the network, the state after the first n -qubit Hadamard transform is applied is

$$\sum_x |x\rangle (|0\rangle - |1\rangle), \quad (5.6)$$

which, after the function evaluation, is

$$\sum_x (-1)^{f(x)} |x\rangle (|0\rangle - |1\rangle). \quad (5.7)$$

Finally, after the last Hadamard transform, the state is

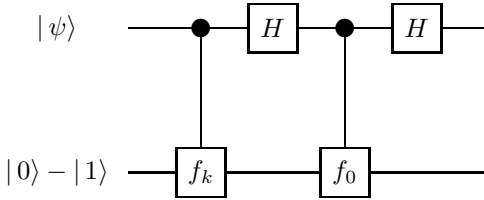
$$\sum_{x,y} (-1)^{f(x)+(x \cdot y)} |y\rangle (|0\rangle - |1\rangle). \quad (5.8)$$

Note that the amplitude of $|00 \cdots 0\rangle$ is $\sum_x \frac{(-1)^{f(x)}}{2^n}$ which is $(-1)^{f(0)}$ when f is constant and 0 when f is balanced. Therefore, by measuring the first n qubits, it can be determined with certainty whether f is constant or balanced. The algorithm follows the same pattern as Deutsch’s algorithm: the Hadamard transform, a function evaluation, the Hadamard transform (the H-f-H sequence). We recognize it as a generic interference pattern.

6 Quantum search

The generic H-f-H sequence may be repeated several times. This can be illustrated, for example, with Grover's data base search algorithm [19]. Suppose we are given, as an oracle, a Boolean function f_k which maps $\{0, 1\}^n$ to $\{0, 1\}$ such that $f_k(x) = \delta_{xk}$ for some k . Our task is to find k . Thus in a set of numbers from 0 to $2^n - 1$ one element has been "tagged" and by evaluating f_k we have to find which one. In order to find k with probability of 50% any classical algorithm, be it deterministic or randomised, will need to evaluate f_k a minimum of 2^{n-1} times. In contrast, a quantum algorithm needs only $O(2^{n/2})$ evaluations.

Unlike the algorithms studied so far, Grover's algorithm consists of *repeated* applications of the *same* unitary transformation many ($O(2^{n/2})$) times. The initial state is chosen to be the one that has equal overlap with each of the computational basis states: $|S\rangle = 2^{-n/2} \sum_{i=0}^{2^n-1} |i\rangle$. The operation applied at each individual iteration, referred to as the Grover iterate, can be best represented by the following network:



The components of the network are by now familiar: Hadamard transforms (H) and controlled- f gates. It is important to notice that in drawing the network we have used a shorthand notation: the first register (with the $|\psi\rangle$ input) actually consists of n qubits. The Hadamard transform is applied to each of those qubits and the controlled- f gates act on all of them simultaneously. Also, the input to the second register is always $|0\rangle - |1\rangle$ but the input to the first register, denoted $|\psi\rangle$ changes from iteration to iteration, as the calculation proceeds. As usual, the second register will be ignored since it remains constant throughout the computation.

To begin, consider only the controlled- f_k gate. This is just the phase-kickback construction that was introduced in Section 4 but for the specific function f_k . In particular, the transformation does nothing to any basis elements except for $|k\rangle$, which goes to $-|k\rangle$. Geometrically, this is simply a reflection in the hyperplane perpendicular to $|k\rangle$ so let us call it R_k .

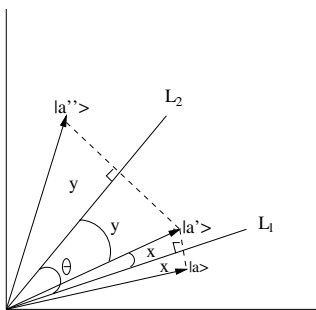
Similarly, with respect to the first register only, the controlled- f_0 operation sends $|0\rangle$ to $-|0\rangle$ and fixes all other basis elements, so it can be written R_0 . Now consider the sequence of operations HR_0H . Since $H^2 = I$, we can rewrite the triple as HR_0H^{-1} which is simply R_0 performed in a different

basis. More specifically, it is reflection about the hyperplane perpendicular to

$$H|0\rangle = \frac{1}{2^{n/2}} \sum_{x=0}^{2^n-1} |x\rangle = |S\rangle \quad (6.1)$$

so we will simply write the triple as R_S .

We can therefore rewrite the Grover iterate in the simple form $G = R_S R_k$. Now, since each reflection is an orthogonal transformation with negative determinant, their composition must be an orthogonal transformation with unit determinant, in other words, a rotation. The question, of course, is which rotation. To find the answer it suffices to consider rotations in the plane spanned by $|k\rangle$ and $|S\rangle$ since all other vectors are fixed by the Grover iterate. The generic geometrical situation is then illustrated in the following diagram.



If the vector $|a\rangle$ is reflected through the line L_1 to produce the vector $|a'\rangle$ and then reflected a second time through line L_2 to produce the vector $|a''\rangle$, then the net effect is a rotation by the total subtended angle between $|a\rangle$ and $|a''\rangle$, which is $2x + 2y = 2(x + y) = 2\theta$.

Therefore, writing $|k^\perp\rangle$ and $|S^\perp\rangle$ for plane vectors perpendicular to $|k\rangle$ and $|S\rangle$ respectively, the Grover iterate performs a rotation of twice the angle from $|k^\perp\rangle$ to $|S^\perp\rangle$. Setting, $\sin \phi = \frac{1}{2^{n/2}}$, this is easily seen to be a rotation by

$$2\left(3\frac{\pi}{2} - \phi\right) = \pi - 2\phi \bmod 2\pi. \quad (6.2)$$

Thus, up to phases, the Grover iterate rotates the state vector by an angle 2ϕ towards the desired solution $|k\rangle$. Normally, the initial state for the first

register is chosen to be $|S\rangle$. Since this initial state $|S\rangle$ is already at an angle ϕ to $|k\rangle$, the iterate should be repeated m times, where

$$(2m+1)\phi \approx \frac{\pi}{2}, \quad (6.3)$$

giving

$$m \approx \frac{\pi}{4\phi} - \frac{1}{4} \quad (6.4)$$

to get a probability of success bounded below by $\cos^2(2\phi)$, which goes to 1 as $n \mapsto \infty$. For large n , $\frac{1}{2^{n/2}} = \sin \phi \approx \phi$, so

$$m \approx \frac{\pi}{4} \frac{1}{2^{n/2}}. \quad (6.5)$$

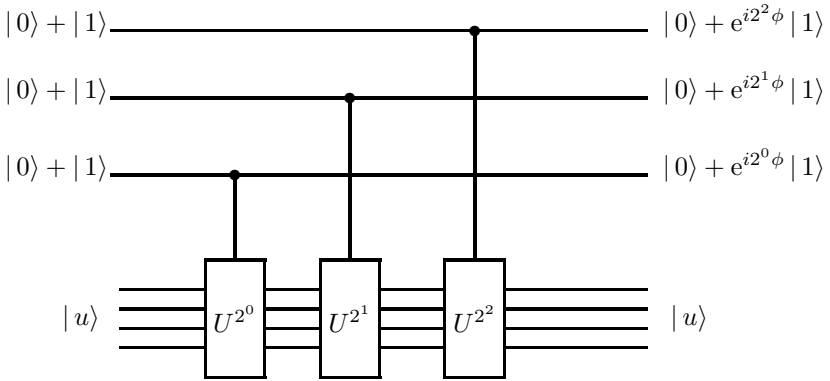
This is an astounding result: any search of an unstructured database can be performed in time proportional to the square-root of the number of entries in the database. Subsequent work extended the result to searches for multiple items [20], searches of structured databases [21], and many other situations. Also, Zalka [22], Boyer *et al.* [20] and others have demonstrated that Grover's algorithm is optimal, in the sense that any other quantum algorithm for searching an unstructured database must take time at least $O(2^{n/2})$.

7 Optimal phase estimation

Query models of quantum computation provided a natural setting for subsequent discoveries of “real quantum algorithms”. The most notable example is Shor's quantum factoring algorithm [15] which evolved from the the order-finding problem, which was originally formulated in the language of quantum queries. Following our “interferometric approach” we will describe this algorithm in the terms of multiparticle quantum interferometry. We start with a simple eigenvalue or phase estimation problem.

Suppose that U is any unitary transformation on m qubits and $|u\rangle$ is an eigenvector of U with eigenvalue $e^{i\phi}$ and consider the following scenario. We do not explicitly know U or $|u\rangle$ or $e^{i\phi}$, but instead we are given devices that perform controlled- U , controlled- U^{2^1} , controlled- U^{2^2} and so on until we reach controlled- $U^{2^{n-1}}$. Also, assume that we are given a single preparation

of the state $|u\rangle$. Our goal is to obtain an n -bit estimator of ϕ . We start by constructing the following network,



The second register of m qubits is initially prepared in state $|u\rangle$ and remains in this state after the computation, whereas the first register of n qubits evolves into the state,

$$\left(|0\rangle + e^{i2^{n-1}\phi} |1\rangle\right) \left(|0\rangle + e^{i2^{n-2}\phi} |1\rangle\right) \cdots \left(|0\rangle + e^{i\phi} |1\rangle\right) = \sum_{y=0}^{2^n-1} e^{2\pi i \frac{\phi y}{2^n}} |y\rangle. \quad (7.1)$$

Consider the special case where $\phi = 2\pi x/2^n$ for $x = \sum_{i=0}^{n-1} 2^i x_i$, and recall the quantum Fourier transform (QFT) introduced in Section 2. The state which gives the binary representation of x , namely, $|x_{n-1} \cdots x_0\rangle$ (and hence ϕ) can be obtained by applying the inverse of the QFT, that is by running the network for the QFT in the backwards direction (consult the diagram of the QFT). If x is an n -bit number this will produce the exact value ϕ .

However, ϕ does not have to be a fraction of a power of two (and may not even be a rational number). For such a ϕ , it turns out that applying the inverse of the QFT produces the best n -bit approximation of ϕ with probability at least $4/\pi^2 \approx 0.405$.

To see why this is so, let us write $\phi = 2\pi(a/2^n + \delta)$, where $a = (a_{n-1} \cdots a_0)$ is the best n -bit estimate of $\frac{\phi}{2\pi}$ and $0 < |\delta| \leq 1/2^{n+1}$. Applying the inverse QFT to the state in equation (7.1) now yields the state

$$\frac{1}{2^n} \sum_{x=0}^{2^n-1} \sum_{y=0}^{2^n-1} e^{\frac{2\pi i}{2^n} (a-x)y} e^{2\pi i \delta y} |x\rangle \quad (7.2)$$

and the coefficient in front of $|x = a\rangle$ in the above is the geometric series

$$\frac{1}{2^n} \sum_{y=0}^{2^n-1} (e^{2\pi i \delta})^y = \frac{1}{2^n} \left(\frac{1 - (e^{2\pi i \delta})^{2^n}}{1 - e^{2\pi i \delta}} \right). \quad (7.3)$$

Since $|\delta| \leq \frac{1}{2^{n+1}}$, it follows that $2^n |\delta| \leq 1/2$, and using the inequality $2z \leq \sin \pi z \leq \pi z$ holding for any $z \in [0, 1/2]$, we get $|1 - e^{2\pi i \delta 2^n}| = 2|\sin(\pi \delta 2^n)| \geq 4|\delta|2^n$. Also, $|1 - e^{2\pi i \delta}| = 2|\sin \pi \delta| \leq 2\pi \delta$. Therefore, the probability of observing $a_{n-1} \cdots a_0$ when measuring the state is

$$\left| \frac{1}{2^n} \left(\frac{1 - (e^{2\pi i \delta})^{2^n}}{1 - e^{2\pi i \delta}} \right) \right|^2 \geq \left(\frac{1}{2^n} \left(\frac{4\delta 2^n}{2\pi \delta} \right) \right)^2 = \frac{4}{\pi^2}, \quad (7.4)$$

which proves our assertion. In fact, the probability of obtaining the best estimate can be made $1 - \delta$ for any $0 < \delta < 1$, by creating the state in equation (7.1) but with $n + O(\log(1/\delta))$ qubits and rounding the answer off to the nearest n bits [17].

8 Periodicity and quantum factoring

Amazingly, the application of optimal phase estimation to a very particular unitary operator will allow us to factor integers efficiently. In fact, it will allow us to solve a more general class of problems related to the periodicity of certain integer functions.

Let N be an m -bit integer, and let a be an integer smaller than N , and coprime to N . Define a unitary operator U_a acting on m qubits such that for all $y < N$

$$|y\rangle \mapsto U_a |y\rangle = |ay \bmod N\rangle. \quad (8.1)$$

This unitary operation can be called multiplication by a modulo N . Since a is coprime to N , as discussed in Section 2, there exists a least strictly positive r such that $a^r = 1 \bmod N$. This r is called the *order* of a modulo N . Equivalently, r is the period of the function $f(x) = a^x \bmod N$, i.e. the least $r > 0$ such that $f(x) = f(x + r)$ for all x . We are after the optimal n -bit estimate of this period, given some specified precision n .

Now let the vectors $|u_k\rangle$ ($k \in \{1, \dots, r\}$) be defined by

$$|u_k\rangle = r^{-1/2} \sum_{j=0}^{r-1} e^{-\frac{2\pi i k j}{r}} |a^j \bmod N\rangle. \quad (8.2)$$

It is easy to check [23] that for each $k \in \{1, \dots, r\}$, $|u_k\rangle$ is an eigenvector with eigenvalue $e^{2\pi i \frac{k}{r}}$ of the modular multiplication operator U_a defined above.

It is important to observe that one can efficiently construct a quantum network for controlled multiplication modulo some number N . Moreover, for any j , it is possible to efficiently implement a controlled- $U_a^{2^j}$ gate [24, 25]. Therefore, we can apply the techniques for optimal phase estimation discussed in Section 7. For any $k \in \{1, \dots, r\}$, given the state $|u_k\rangle$ we can obtain the best n -bit approximation to $\frac{k}{r}$. This is tantamount to determining r itself. Unfortunately, there is a complication.

Our task is: given an m bit long number N and randomly chosen $a < N$ coprime with N , find the order of a modulo N . The problem with the above method is that we are aware of no straightforward efficient way to prepare any of the states $|u_k\rangle$. However, the state

$$|1\rangle = r^{-1/2} \sum_{k=1}^r |u_k\rangle \quad (8.3)$$

is most definitely an easy state to prepare.

If we start with $|1\rangle$ in place of the eigenvector $|u_k\rangle$, apply the phase estimation network and measure the first register bit by bit we will obtain n binary digits of x such that, with probability exceeding $4/\pi^2$, $\frac{x}{2^n}$ is the best n -bit estimate of $\frac{k}{r}$ for a randomly chosen k from $\{1, \dots, r\}$. The question is: given x how to compute r ? Let us make few observations:

- k/r is unique, given x .

Value $x/2^n$, being the n -bit estimate, differs by at most $1/2^n$ from k/r . Hence, as long as $n > 2m$, the n bit estimate x determines a unique value of $\frac{k}{r}$ since r is an m -bit number;

- Candidate values for k/r are all convergents to $x/2^m$.

For any real number θ , there is a unique sequence of special rationals $(\frac{p_n}{q_n})_{n \in \mathbb{N}}$ ($\gcd(p_n, q_n) = 1$) called the *convergents* to θ that tend to θ as n grows. A theorem [9] states that if p and q are integers with $|\theta - \frac{p}{q}| < \frac{1}{2q^2}$ then p/q is a convergent to θ . Since we have $\frac{1}{2^n} \leq \frac{1}{2(2^m)^2} \leq \frac{1}{2r^2}$, this implies $|\frac{x}{2^n} - \frac{k}{r}| < \frac{1}{2r^2}$ and k/r is a convergent to $x/2^n$;

- Only one convergent is eligible.

It is easy to show that there is at most one fraction a/b satisfying both $b \leq r$ and $|\frac{x}{2^n} - \frac{a}{b}| < \frac{1}{2r^2}$.

Convergents can be found efficiently using the well-known *continued fraction* method [9]. Thus we employ continued fractions and our observations above to find a fraction a/b such that $b \leq 2^m$ and $|\frac{x}{2^n} - \frac{a}{b}| < \frac{1}{2^n}$. We get the rational k/r , and $k = a, r = b$, provided k and r are coprime. For randomly chosen k , this happens with probability greater than or equal to $1/\ln r$ [26].

Finally, we show how order-finding can be used to factor a composite number N . Let a be a randomly chosen positive integer smaller than N such that $\gcd(a, N) = 1$. Then the order of a modulo N is defined, and we can find it efficiently using the above algorithm. If r is even, then we have:

$$a^r = 1 \bmod N \tag{8.4}$$

$$\Leftrightarrow (a^{r/2})^2 - 1^2 = 0 \bmod N \tag{8.5}$$

$$\Leftrightarrow (a^{r/2} - 1)(a^{r/2} + 1) = 0 \bmod N. \tag{8.6}$$

The product $(a^{r/2} - 1)(a^{r/2} + 1)$ must be some multiple of N , so unless $a^{r/2} = \pm 1 \bmod N$ at least one of terms must have a nontrivial factor in common with N . By computing the greatest common divisor of this term and N , one gets a non-trivial factor of N .

Furthermore, if N is odd with prime factorisation

$$N = p_1^{\alpha_1} p_2^{\alpha_2} \cdots p_s^{\alpha_s}, \tag{8.7}$$

then it can be shown [26] that if $a < N$ is chosen at random such that $\gcd(a, N) = 1$ then the probability that its order modulo N is even and that $a^{r/2} \neq \pm 1 \bmod N$ is:

$$\Pr(r \text{ is even AND } a^{r/2} \neq \pm 1 \bmod N) \geq 1 - \frac{1}{2^{s-1}}. \tag{8.8}$$

Thus, combining our estimates of success at each step, with probability greater than or equal to

$$\frac{4}{\pi^2} \frac{1}{\ln r} \left(1 - \frac{1}{2^{s-1}} \right) \geq \frac{2}{\pi^2} \frac{1}{\ln N} \tag{8.9}$$

we find a factor of N^4 . (Here we have used that N is composite and $r < N$.) If N is $\log N = n$ bits long then by repeating the whole process $O(n)$ times, or by a running $O(n)$ computations in parallel by a suitable extension of a quantum factoring network, we can then guarantee that we will find a factor of N with a fixed probability greater than $\frac{1}{2}$. This, and the fact that the quantum network family for controlled multiplication modulo some number is uniform and of size $O(n^2)$, tells us that factoring is in the complexity class BQP .

But why should anybody care about efficient factorisation?

⁴*N.B.* by equation (8.8), the method fails if N is a prime power, $N = p^\alpha$, but prime powers can be efficiently recognised and factored by classical means.

9 Cryptography

Human desire to communicate secretly is at least as old as writing itself and goes back to the beginnings of our civilisation. Methods of secret communication were developed by many ancient societies, including those of Mesopotamia, Egypt, India, and China, but details regarding the origins of cryptology⁵ remain unknown [27].

Originally the security of a cryptosystem or a cipher depended on the secrecy of the entire encrypting and decrypting procedures; however, today we use ciphers for which the algorithm for encrypting and decrypting could be revealed to anybody without compromising their security. In such ciphers a set of specific parameters, called a *key*, is supplied together with the plaintext as an input to the encrypting algorithm, and together with the cryptogram as an input to the decrypting algorithm [28]. This can be written as

$$\hat{E}_k(P) = C, \text{ and conversely, } \hat{D}_k(C) = P, \quad (9.1)$$

where P stands for plaintext, C for cryptotext or cryptogram, k for cryptographic key, and $\hat{E}$ and $\hat{D}$ denote an encryption and a decryption operation respectively.

The encrypting and decrypting algorithms are publicly known; the security of the cryptosystem depends entirely on the secrecy of the key, and this key must consist of a *randomly chosen*, sufficiently long string of bits. Probably the best way to explain this procedure is to have a quick look at the Vernam cipher, also known as the one-time pad [29].

If we choose a very simple digital alphabet in which we use only capital letters and some punctuation marks such as

A	B	C	D	E	...	...	X	Y	Z		?	,	.
00	01	02	03	04	...	...	23	24	25	26	27	28	29

we can illustrate the secret-key encrypting procedure by the following simple example (we refer to the dietary requirements of 007):

S	H	A	K	E	N		N	O	T		S	T	I	R	R	E	D
18	07	00	10	04	13	26	13	14	19	26	18	19	08	17	17	04	03
15	04	28	13	14	06	21	11	23	18	09	11	14	01	19	05	22	07
03	11	28	23	18	19	17	24	07	07	05	29	03	09	06	22	26	10

In order to obtain the cryptogram (sequence of digits in the bottom row) we add the plaintext numbers (the top row of digits) to the key numbers (the middle row), which are randomly selected from between 0 and 29, and take

⁵The science of secure communication is called cryptology from Greek *kryptos* hidden and *logos* word. Cryptology embodies cryptography, the art of code-making, and cryptanalysis, the art of code-breaking.

the remainder after division of the sum by 30, that is we perform addition modulo 30. For example, the first letter of the message “S” becomes a number “18” in the plaintext, then we add $18 + 15 = 33$; $33 = 1 \times 30 + 3$, therefore we get 03 in the cryptogram. The encryption and decryption can be written as $P_i + k_i \pmod{30} = C_i$ and $C_i - k_i \pmod{30} = P_i$ respectively for the symbol at position i .

The cipher was invented in 1917 by the American AT&T engineer Gilbert Vernam. It was later shown, by Claude Shannon [30], that as long as the key is truly random, has the same length as the message, and is never reused then the one-time pad is perfectly secure. So, if we have a truly unbreakable system, what is wrong with classical cryptography?

There is a snag. It is called *key distribution*. Once the key is established, subsequent communication involves sending cryptograms over a channel, even one which is vulnerable to total passive eavesdropping (*e.g.* public announcement in mass-media). This stage is indeed secure. However in order to establish the key, two users, who share no secret information initially, must at a certain stage of communication use a reliable and a very secure channel. Since the interception is a set of measurements performed by an eavesdropper on this channel, however difficult this might be from a technological point of view, *in principle* any classical key distribution can always be passively monitored, without the legitimate users being aware that any eavesdropping has taken place.

In the late 1970s Whitfield Diffie and Martin Hellman [31] proposed an interesting solution to the key distribution problem. It involved two keys, one public key π for encryption and one private key κ for decryption:

$$\hat{E}_\pi(P) = C, \text{ and } \hat{D}_\kappa(C) = P. \quad (9.2)$$

In these systems users do not need to share any private key before they start sending messages to each other. Every user has his own two keys; the public key is publicly announced and the private key is kept secret. Several public-key cryptosystems have been proposed since 1976; here we concentrate our attention on the most popular one namely the RSA [32]. In fact the techniques were first discovered at CESG in the early 1970s by James Ellis, who called them “Non-Secret Encryption” [33]. In 1973, building on Ellis’ idea, C. Cocks designed what we now call RSA [34], and in 1974 M. Williamson proposed what is essentially known today as the Diffie-Hellman key exchange protocol.

Suppose that Alice wants to send an RSA encrypted message to Bob. The RSA encryption scheme works as follows:

Key generation Bob picks randomly two distinct and large prime numbers p and q . We denote $n = pq$ and $\phi = (p-1)(q-1)$. Bob then picks a random integer $1 < e < \phi$ that is coprime with ϕ , and computes the inverse d of e modulo ϕ ($\gcd(e, \phi) = 1$). This inversion can be achieved

efficiently using for instance the extended Euclidean algorithm for the greatest common divisor [9]. Bob's private key is $\kappa = d$ and his public key is $\pi = (e, n)$.

Encryption Alice obtains Bob's public key $\pi = (e, n)$ from some sort of yellow pages or an RSA public key directory. Alice then writes her message as a sequence of numbers using, for example, our digital alphabet. This string of numbers is subsequently divided into blocks such that each block when viewed as a number P satisfies $P \leq n$. Alice encrypts each P as

$$C = \hat{E}_\pi(P) = P^e \bmod n \quad (9.3)$$

and sends the resulting cryptogram to Bob.

Decryption Receiving the cryptogram C , Bob decrypts it by calculating

$$\hat{D}_\kappa(C) = C^d \bmod n = P \quad (9.4)$$

where the last equality will be proved shortly.

The mathematics behind the RSA is a lovely piece of number theory which goes back to the XVI century when a French lawyer Pierre de Fermat discovered that if a prime p and a positive integer a are coprime, then

$$a^{p-1} = 1 \bmod p. \quad (9.5)$$

The cryptogram $C = P^e \bmod n$ is decrypted by $C^d \bmod n$ because $ed = 1 \bmod \phi$, implying the existence of an integer k such that $ed = k\phi + 1 = k(p-1)(q-1) + 1$. If $P \neq 0 \bmod p$, using equation (9.5) this implies

$$P^{ed} \bmod p = \left(P^{(p-1)}\right)^{k(q-1)} P \bmod p = P \bmod p. \quad (9.6)$$

The above equality holds trivially in the case $P = 0 \bmod p$. By identical arguments, $P^{ed} \bmod q = P \bmod q$. Since p and q are distinct primes, it follows that

$$P^{ed} \bmod n = P. \quad (9.7)$$

For example, let us suppose that Bob's public key is $\pi = (e, n) = (179, 571247)^6$. He generated it following the prescription above choosing $p = 773$, $q = 739$ and $e = 179$. The private key d was obtained by solving $179d = 1 \bmod 772 \times 738$ using the extended Euclidean algorithm which yields $d = 515627$. Now if we want to send Bob encrypted "SHAKEN NOT

⁶Needless to say, number n in this example is too small to guarantee security, do not try this public key with Bob.

STIRRED” we first use our digital alphabet to obtain the plaintext which can be written as the following sequence of six digit numbers

$$180700 \quad 100413 \quad 261314 \quad 192618 \quad 190817 \quad 170403.$$

Then we encipher each block P_i by computing $C_i = P_i^e \bmod n$; *e.g.* the first block $P_1 = 180700$ will be enciphered as

$$P_1^e \bmod n = 180700^{179} \bmod 571247 = 141072 = C_1, \quad (9.8)$$

and the whole message is enciphered as:

$$141072 \quad 253510 \quad 459477 \quad 266170 \quad 286377 \quad 087175.$$

The cryptogram C composed of blocks C_i can be send over to Bob. He can then decrypt each block using his private key $d = 515627$, *e.g.* the first block is decrypted as

$$141072^{515627} \bmod 571247 = 180700 = P_1. \quad (9.9)$$

In order to recover plaintext P from cryptogram C , an outsider, who knows C , n , and e , would have to solve the congruence

$$P^e \bmod n = C, \quad (9.10)$$

for example, in our case,

$$P_1^{179} \bmod 571247 = 141072. \quad (9.11)$$

Solving such an equation is believed to be a hard computational task for classical computers. So far, no classical algorithm has been found that computes the solution efficiently when n is a large integer (say 200 decimal digits long or more). However, if we know the prime decomposition of n it is a piece of cake to figure out the private key d : we simply follow the key generation procedure and solve the congruence $ed = 1 \bmod (p-1)(q-1)$. This can be done efficiently even when p and q are very large. Thus, in principle, anybody who knows n can find d by factoring n . The security of RSA therefore relies among others on the assumption that factoring large numbers is computationally difficult. In the context of classical computation, such difficulty has never been proved. Worse still, we have seen in Section 8 that there is a quantum algorithm that factors large number efficiently. This means that the security of the RSA cryptosystem will be completely compromised if large-scale quantum computation becomes one day practical. This way, the advent of quantum computation rules out public cryptographic schemes commonly used today that are based on the “difficulty” of factoring or the “difficulty” of another mathematical operation called discrete logarithm [9].

On the other hand, quantum computation provides novel techniques to generate a shared private key with perfect confidentiality, regardless the computational power (classical or quantum) of the adversaries. Such techniques are referred to as *quantum key distribution* protocols. Discussion on quantum key distribution is outside the scope of this lecture. Interested readers are referred to [35–37]. A comprehensive bibliography on this subject can be found in [38].

10 Conditional quantum dynamics

Quantum gates and quantum networks provide a very convenient language for building any quantum computer or (which is basically the same) quantum multiparticle interferometer. But can we build quantum logic gates?

Single qubit quantum gates are regarded as relatively easy to implement. For example, a typical quantum optical realisation uses atoms as qubits and controls their states with laser light pulses of carefully selected frequency, intensity and duration; any prescribed superposition of two selected atomic states can be prepared this way.

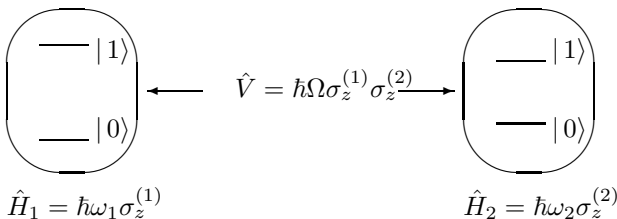
Two-qubit gates are much more difficult to build.

In order to implement two-qubit quantum logic gates it is sufficient, from the experimental point of view, to induce a conditional dynamics of physical bits, *i.e.* to perform a unitary transformation on one physical subsystem conditioned upon the quantum state of another subsystem,

$$U = |0\rangle\langle 0| \otimes U_0 + |1\rangle\langle 1| \otimes U_1 + \cdots + |k\rangle\langle k| \otimes U_k, \quad (10.1)$$

where the projectors refer to quantum states of the control subsystem and the unitary operations U_i are performed on the target subsystem [6]. The simplest non-trivial operation of this sort is probably a conditional phase shift such as $B(\phi)$ which we used to implement the quantum Fourier transform and the quantum controlled-NOT (or XOR) gate.

Let us illustrate the notion of the conditional quantum dynamics with a simple example. Consider two qubits, *e.g.* two spins, atoms, single-electron quantum dots, which are coupled via a $\sigma_z^{(1)}\sigma_z^{(2)}$ interaction (*e.g.* a dipole-dipole interaction):



The first qubit, with resonant frequency ω_1 , will act as the control qubit and the second one, with resonant frequency ω_2 , as the target qubit. Due to the coupling $\hat{V}$ the resonant frequency for transitions between the states $|0\rangle$ and $|1\rangle$ of one qubit *depends on the neighbour's state*. The resonant frequency for the first qubit becomes $\omega_1 \pm \Omega$ depending on whether the second qubit is in state $|0\rangle$ or $|1\rangle$. Similarly the second qubit's resonant frequency becomes $\omega_2 \pm \Omega$, depending on the state of the first qubit. Thus a π -pulse at frequency $\omega_2 + \Omega$ causes the transition $|0\rangle \leftrightarrow |1\rangle$ in the second qubit only if the first qubit is in $|1\rangle$ state. This way we can implement the quantum controlled-NOT gate.

11 Decoherence and recoherence

Thus in principle we know how to build a quantum computer; we can start with simple quantum logic gates and try to integrate them together into quantum networks. However, if we keep on putting quantum gates together into networks we will quickly run into some serious practical problems. The more interacting qubits are involved the harder it tends to be to engineer the interaction that would display the quantum interference. Apart from the technical difficulties of working at single-atom and single-photon scales, one of the most important problems is that of preventing the surrounding environment from learning about which computational path was taken in the multi-particle interferometer. This “welcher Weg” information can destroy the interference and the power of quantum computing.

Consider the following qubit-environment interaction, known as *decoherence* [39],

$$|0\rangle, |m\rangle \mapsto |0, m_0\rangle, \quad |1, m\rangle \mapsto |1, m_1\rangle, \quad (11.1)$$

where $|m\rangle$ is the initial state and $|m_0\rangle, |m_1\rangle$ are the two final states of the environment. This is basically a measurement performed by the environment on a qubit. Suppose that in our single qubit interference experiment (see Eqs. (4.1)) a qubit in between the two Hadamard transformation is “watched” by the environment which learns whether the qubit is in state $|0\rangle$ or $|1\rangle$. The evolution of the qubit and the environment after the first Hadamard and the phase gate is described by the following transformation,

$$|0\rangle |m\rangle \xrightarrow{H} \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle) |m\rangle \xrightarrow{\phi} \frac{1}{\sqrt{2}} \left(e^{i\phi/2} |0\rangle + e^{-i\phi/2} |1\rangle \right) |m\rangle. \quad (11.2)$$

We write the decoherence action as

$$\frac{1}{\sqrt{2}} \left(e^{i\frac{\phi}{2}} |0\rangle + e^{-i\frac{\phi}{2}} |1\rangle \right) |m\rangle \mapsto \frac{1}{\sqrt{2}} \left(e^{i\frac{\phi}{2}} |0\rangle |m_0\rangle + e^{-i\frac{\phi}{2}} |1\rangle |m_1\rangle \right). \quad (11.3)$$

The final Hadamard gate generates the output state

$$\frac{1}{\sqrt{2}}(e^{i\frac{\phi}{2}}|0\rangle|m_0\rangle + e^{-i\frac{\phi}{2}}|1\rangle|m_1\rangle) \quad (11.4)$$

$$\begin{aligned} &\xrightarrow{H} \frac{1}{2}|0\rangle\left(e^{i\frac{\phi}{2}}|m_0\rangle + e^{-i\frac{\phi}{2}}|m_1\rangle\right) \\ &+ \frac{1}{2}|1\rangle\left(e^{i\frac{\phi}{2}}|m_0\rangle - e^{-i\frac{\phi}{2}}|m_1\rangle\right). \end{aligned} \quad (11.5)$$

Taking $|m_0\rangle$ and $|m_1\rangle$ to be normalised and $\langle m_0|m_1\rangle$ to be real we obtain the probabilities P_0 and P_1 ,

$$P_0 = \frac{1}{2}(1 + \langle m_0|m_1\rangle \cos \phi), \quad (11.6)$$

$$P_1 = \frac{1}{2}(1 - \langle m_0|m_1\rangle \cos \phi). \quad (11.7)$$

It is instructive to see the effect of decoherence on the qubit alone when its state is written in terms as a density operator. The decoherence interaction entangles qubits with the environment,

$$(\alpha|0\rangle + \beta|1\rangle)|m\rangle \mapsto \alpha|0\rangle|m_0\rangle + \beta|1\rangle|m_1\rangle. \quad (11.8)$$

Rewriting in terms of density operators and tracing over the environment's Hilbert space on the both sides, we obtain

$$\begin{pmatrix} |\alpha|^2 & \alpha\beta^* \\ \alpha^*\beta & |\beta|^2 \end{pmatrix} \mapsto \begin{pmatrix} |\alpha|^2 & \alpha\beta^*\langle m_0|m_1\rangle \\ \alpha^*\beta\langle m_1|m_0\rangle & |\beta|^2 \end{pmatrix}. \quad (11.9)$$

The off-diagonal elements, originally called by atomic physicists coherences, vanish as $\langle m_1|m_0\rangle \mapsto 0$, that is why this particular interaction with the environment is called decoherence.

How does decoherence affect, for example, Deutsch's algorithm? Substituting 0 or π for ϕ in equation (11.6) we see that we obtain the correct answer only with some probability, which is

$$\frac{1 + \langle m_0|m_1\rangle}{2}. \quad (11.10)$$

If $\langle m_0|m_1\rangle = 0$, the perfect decoherence case, then the network outputs 0 or 1 with equal probabilities, *i.e.* it is useless as a computing device. It is clear that we want to avoid decoherence, or at least diminish its impact on our computing device.

In general when we analyse *physically realisable* computations we have to consider errors which are due to the computer-environment coupling and from the computational complexity point of view we need to assess how these

errors scale with the input size n . If the probability of an error in a single run, $\delta(n)$, grows exponentially with n , *i.e.* if $\delta(n) = 1 - A \exp(-\alpha n)$, where A and α are positive constants, then the randomised algorithm cannot technically be regarded as efficient any more regardless of how weak the coupling to the environment may be. Unfortunately, the computer-environment interaction leads to just such an unwelcome exponential increase of the error rate with the input size. To see this consider a register of size n and assume that each qubit decoheres separately,

$$\begin{aligned} |x\rangle |M\rangle &= |x_{n-1} \dots x_1 x_0\rangle |m\rangle \dots |m\rangle |m\rangle \\ \mapsto & |x_{n-1} \dots x_1 x_0\rangle |m_{x_{n-1}}\rangle \dots |m_{x_1}\rangle |m_{x_0}\rangle = |x\rangle |M_x\rangle, \end{aligned} \quad (11.11)$$

where $x_i \in \{0, 1\}$. Then a superposition $\alpha |x\rangle + \beta |y\rangle$ evolves as

$$(\alpha |x\rangle + \beta |y\rangle) |M\rangle \mapsto \alpha |x\rangle |M_x\rangle + \beta |y\rangle |M_y\rangle, \quad (11.12)$$

but now the scalar product $\langle M_x | M_y \rangle$ which reduces the off-diagonal elements of the density operator of the whole register and which affects the probabilities in the interference experiment is given by

$$\langle M_x | M_y \rangle = \langle m_{x_0} | m_{y_0} \rangle \langle m_{x_1} | m_{y_1} \rangle \dots \langle m_{x_{n-1}} | m_{y_{n-1}} \rangle \quad (11.13)$$

which is of the order of

$$\langle M_x | M_y \rangle = \langle m_0 | m_1 \rangle^{H(x,y)}, \quad (11.14)$$

where $H(x, y)$ is the Hamming distance between x and y , *i.e.* the number of binary places in which x and y differ (*e.g.* the Hamming distance between 101101 and 111101 is 1 because the two binary strings differ only in the second binary place). Hence there are some coherences which disappear as $\langle m_0 | m_1 \rangle^n$ and therefore in some interference experiments the probability of error may grow exponentially with n .

It is clear that for quantum computation of any reasonable length to ever be physically feasible it will be necessary to incorporate some efficiently realisable stabilisation scheme to combat the effects of decoherence. Deutsch was the first one to discuss this problem. During the Rank Prize Funds Mini-Symposium on Quantum Communication and Cryptography, Broadway, England in 1993 he proposed “recoherence” based on a symmetrisation procedure (for details see [40]). The basic idea is as follows. Suppose we have a quantum system, we prepare it in some initial state $|\Psi_i\rangle$ and we want to implement a prescribed unitary evolution $|\Psi(t)\rangle$ or just preserve $|\Psi_i\rangle$ for some period of time t . Now, suppose that instead of a single system we can prepare R copies of $|\Psi_i\rangle$ and subsequently we can project the state of the combined system into the symmetric subspace *i.e.* the subspace containing all states which are invariant under any permutation of the sub-systems. The claim is that frequent projections into the

symmetric subspace will reduce errors induced by the environment. The intuition behind this concept is based on the observation that a prescribed error-free storage or evolution of the R independent copies starts in the symmetric sub-space and should remain in that sub-space. Therefore, since the error-free component of any state always lies in the symmetric subspace, upon successful projection it will be unchanged and part of the error will have been removed. Note however that the projected state is generally not error-free since the symmetric subspace contains states which are not of the simple product form $|\Psi\rangle|\Psi\rangle\ldots|\Psi\rangle$. Nevertheless it has been shown that the error probability will be suppressed by a factor of $1/R$ [40].

More recently projections on symmetric subspaces were replaced by more complicated projections on carefully selected subspaces. These projections, proposed by Shor [41], Calderbank and Shor [42], Steane [43] and others [44–48], are constructed on the basis of classical error-correcting methods but represent intrinsically new quantum error-correction and stabilisation schemes; they are the subject of much current study.

Let us illustrate the main idea of recoherence by describing a simple method for protecting an unknown state of a single qubit in a noisy quantum register. Consider the following scenario: we want to store in a computer memory one qubit in an unknown quantum state of the form $|\phi\rangle = \alpha|0\rangle + \beta|1\rangle$ and we know that any single qubit which is stored in a register undergoes a decoherence type entanglement with an environment described by equation (11.8). To see how the state of the qubit is affected by the environment, we calculate the fidelity of the decohered state at time t with respect to the initial state $|\phi\rangle$

$$F(t) = \langle\phi|\rho(t)|\phi\rangle, \quad (11.15)$$

where $\rho(t)$ is given by equation (11.9). It follows that

$$F(t) = |\alpha|^4 + |\beta|^4 + 2|\alpha|^2|\beta|^2\text{Re}[\langle m_0(t)|m_1(t)\rangle]. \quad (11.16)$$

The expression above depends on the initial state $|\phi\rangle$ and clearly indicates that some states are more vulnerable to decoherence than others. In order to get rid of this dependence we consider the average fidelity, calculated under the assumption that any initial state $|\phi\rangle$ is equally probable. Taking into account the normalisation constraint the average fidelity is given by

$$\bar{F}(t) = \int_0^1 F(t) \, d|\alpha|^2 = \frac{1}{3}(2 + \text{Re}[\langle m_0(t)|m_1(t)\rangle]). \quad (11.17)$$

If we assume an exponential-type decoherence, where $\langle m_0(t)|m_1(t)\rangle = e^{-\gamma t}$, the average fidelity takes the simple form

$$\bar{F}(t) = \frac{1}{3}(2 + e^{-\gamma t}). \quad (11.18)$$

In particular, for times much shorter than the decoherence time $t_d = 1/\gamma$, the above fidelity can be approximated as

$$\bar{F}(t) \simeq 1 - \frac{1}{3}\gamma t + O(\gamma^2 t^2). \quad (11.19)$$

Let us now show how to improve the average fidelity by quantum encoding. Before we place the qubit in the memory register we *encode* it: we can add two qubits, initially both in state $|0\rangle$, to the original qubit and then perform an encoding unitary transformation

$$|000\rangle \mapsto |\bar{0}\bar{0}\bar{0}\rangle = (|0\rangle + |1\rangle)(|0\rangle + |1\rangle)(|0\rangle + |1\rangle), \quad (11.20)$$

$$|100\rangle \mapsto |\bar{1}\bar{1}\bar{1}\rangle = (|0\rangle - |1\rangle)(|0\rangle - |1\rangle)(|0\rangle - |1\rangle), \quad (11.21)$$

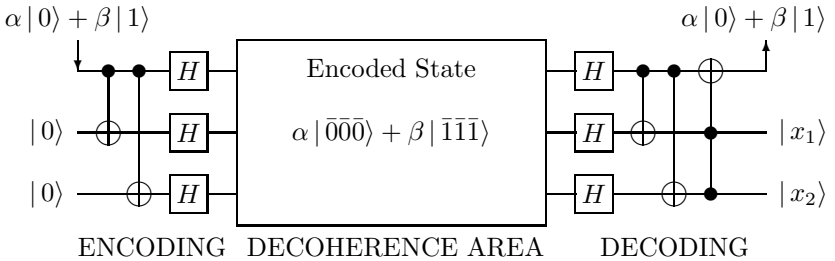
generating state $\alpha|\bar{0}\bar{0}\bar{0}\rangle + \beta|\bar{1}\bar{1}\bar{1}\rangle$, where $|\bar{0}\rangle = |0\rangle + |1\rangle$ and $|\bar{1}\rangle = |0\rangle - |1\rangle$. Now, suppose that only the second stored qubit was affected by decoherence and became entangled with the environment:

$$\begin{aligned} & \alpha(|0\rangle + |1\rangle)(|0\rangle|m_0\rangle + |1\rangle|m_1\rangle)(|0\rangle + |1\rangle) + \\ & \beta(|0\rangle - |1\rangle)(|0\rangle|m_0\rangle - |1\rangle|m_1\rangle)(|0\rangle - |1\rangle), \end{aligned} \quad (11.22)$$

which can also be written as

$$(\alpha|\bar{0}\bar{0}\bar{0}\rangle + \beta|\bar{1}\bar{1}\bar{1}\rangle)(|m_0\rangle + |m_1\rangle) + (\alpha|\bar{0}\bar{1}\bar{0}\rangle + \beta|\bar{1}\bar{0}\bar{1}\rangle)(|m_0\rangle - |m_1\rangle). \quad (11.23)$$

The decoding unitary transformation can be constructed using a couple of quantum controlled-NOT gates and the Toffoli gate, thus completing the error-correcting network:



Careful inspection of the network shows that any single phase-flip $|\bar{0}\rangle \leftrightarrow |\bar{1}\rangle$ will be corrected and the environment will be effectively disentangled from the qubits. In our particular case we obtain

$$(\alpha|0\rangle + \beta|1\rangle)[|00\rangle(|m_0\rangle + |m_1\rangle) + |10\rangle(|m_0\rangle - |m_1\rangle)]. \quad (11.24)$$

The two auxiliary outputs carry information about the error syndrome - 00 means no error, 01 means the phase-flip occurred in the third qubit, 10 means the phase-flip in the second qubit and 11 signals the phase flip in the first qubit.

Thus if only one qubit in the encoded triplet decoheres we can recover the original state perfectly. In reality all three qubits decohere simultaneously and, as the result, only partial recovery of the original state is possible. In this case lengthy but straightforward calculations show that the average fidelity of the reconstructed state after the decoding operation for an exponential-type decoherence is

$$\bar{F}_{\text{ec}}(t) = \frac{1}{6} [4 + 3e^{-\gamma t} - e^{-3\gamma t}] . \quad (11.25)$$

For short times this can be written as

$$\bar{F}_{\text{ec}}(t) \simeq 1 - \frac{1}{2}\gamma^2 t^2 + O(\gamma^3 t^3). \quad (11.26)$$

Comparing equation (11.18) with equation (11.25), we can easily see that for all times t ,

$$\bar{F}_{\text{ec}}(t) \geq \bar{F}(t). \quad (11.27)$$

This is the essence of recoherence via encoding and decoding. There is much more to say (and write) about quantum codes and the reader should be warned that we have barely scratched the surface of the current activities in quantum error correction, neglecting topics such as group theoretical ways of constructing good quantum codes [46, 47], concatenated codes [48], quantum fault tolerant computation [49] and many others.

12 Concluding remarks

Research in quantum computation and in its all possible variations has become vigorously active and any comprehensive review of the field must be obsolete as soon as it is written. Here we have decided to provide only some very basic knowledge, hoping that this will serve as a good starting point to enter the field. Many interesting papers in these and many related areas can be found at the Los Alamos National Laboratory e-print archive (<http://xxx.lanl.gov/archive/quant-ph>) and on the web site of the Center for Quantum Computation (www.qubit.org).

Acknowledgements

This work was supported in part by the European TMR Research Network ERP-4061PL95-1412, The Royal Society London, and Elsas plc. PH acknowledges the support of the Rhodes Trust.

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COURSE 11

COHERENT BACKSCATTERING OF LIGHT FROM A COLD ATOMIC CLOUD

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COHERENT BACKSCATTERING OF LIGHT FROM A COLD ATOMIC CLOUD

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C. Mueller, C. Miniatura and R. Kaiser

Abstract

We report the first observation of coherent backscattering of light from a sample of laser-cooled atoms. Rubidium 85 atoms are captured from a room-temperature vapor in a magneto-optical trap, and illuminated with a laser probe. The angular intensity distribution of the backscattered light is recorded on a cooled CCD detector. We observe a small enhancement factor in all polarization channels, including the “helicity preserving” channel where the enhancement is only 1.08. This surprising observation is attributed to the existence of contrast reduction processes involving the atom’s internal structure.

1 Introduction

The field of wave propagation in random media has gained a renewed attention in the 80s when it was realized that the concepts of weak and strong localization, originating from condensed matter physics, could also apply to any linear wave such as light [1]. A wave propagating in a strongly scattering medium experiences many scattering events which rapidly randomize the initial propagation direction, on a typical scale length l^* known as the transport mean free path. On larger scales, the propagation can be described by a diffusion process. This description yields the well-known Ohm’s law: the transmission of a slab of thickness L evolves according to l^*/L . However, it does not take into account an important phenomenon: the interference between multiply scattered waves. Indeed, it is now known that interferences can profoundly alter the wave transport [2]. An extreme situation is that of the Anderson (or strong) localization regime [3], where the propagation is brought to a halt and the wave remains “trapped” inside the medium. In the intermediate regime of weak localization, one spectacular manifestation of interference effects in multiple scattering is coherent backscattering (CBS) [4]. Some other important interference effects have been observed

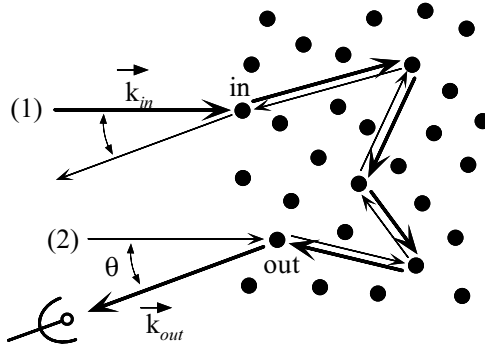


Fig. 1. Interpretation of coherent backscattering.

such as universal conductance fluctuations [5], random laser [6] and strong localization of light [7].

Atoms in a gas exhibit some peculiar properties as far as scattering of light is concerned, and open a new area for the study of multiple scattering. The now well-established techniques of laser cooling [8] allow one to fully exploit the potentialities of this atomic scattering medium.

2 Coherent backscattering

2.1 Principle of CBS

To understand the origin of CBS, let us consider the situation depicted in Figure 1. A sample of randomly distributed scatterers is illuminated by a plane wave (wavelength λ). The quantity we are interested in is the angular distribution of the scattered light in the backward direction. If the scatterers respective positions are fixed, the light intensity scattered at angle θ results from the interference of many partially scattered waves, and the intensity distribution is a well-known speckle pattern. Let us now imagine that a configuration averaging is performed: the respective positions of the scatterers in the sample are modified many times, and the corresponding speckle patterns added to each other to obtain an averaged intensity distribution. In experiments, this is obtained either automatically due to the scatterer's motion (*e.g.* in liquid samples), or by simply rotating the sample. As a result of this averaging process, we expect the speckle pattern to smooth out to give a relatively angle-independent intensity distribution. This is indeed what happens, except in a narrow angular range of order λ/l^* around the exact backscattering direction, where a sharp peak of scattered intensity, known as the “CBS cone”, is observed. This surprising observation can be interpreted as the result of the constructive interference between

the reciprocal waves shown in Figure 1. These waves follow the same multiple scattering path but in a reversed order (“time reversal”). The phase difference φ between these two waves clearly depends only on θ and the respective positions of the “input” and “output” scatterers (position vectors $\vec{r}_{\text{in}}$ and $\vec{r}_{\text{out}}$), namely:

$$\varphi = (\vec{r}_{\text{in}} - \vec{r}_{\text{out}}) \cdot (\vec{k}_{\text{in}} + \vec{k}_{\text{out}}). \quad (2.1)$$

In the particular case $\theta = 0$ (exact backscattering, $\vec{k}_{\text{in}} + \vec{k}_{\text{out}} = 0$), this phase difference is always zero, regardless of the specific scattering path considered. Thus, reciprocal waves always add up constructively in the backscattering direction, and this interference survive the averaging process due to the motion of the scatterers (this property is of course not verified for $\theta \neq 0$). As a result, the averaged intensity distribution exhibits a peak centered at $\theta = 0$, whose height can be a factor of 2 above the “incoherent background” obtained at $\theta \gg \lambda/l^*$. The angular width of the CBS cone is inversely proportional to the transport mean free path of the wave in the medium. To better understand this width, one can see the reciprocal waves of Figure 1 as originating from a Young’s slits experiment (the slits playing the role of the input and output scatterers). The fringe spacing is such a system is proportional to λ/d , where d is the distance between the slits. Thus we understand why the cone gets narrower when l^* increases. Considering now a given scattering order N ($N = 5$ in the case of Fig. 1), the average distance between the input and output scatterers grows as $\sqrt{N} l^*$ (random walk of step l^*): thus, high scattering orders give narrower cones. In a semi-infinite medium where all scattering orders contribute, the resulting cone is obtained by adding up the cones associated to each scattering order. The shape of this cone around the tip is a cusp, and the cone FWHM is given by:

$$\Delta\theta \approx 0.1 \frac{\lambda}{l^*}. \quad (2.2)$$

2.2 CBS with cold atoms

CBS has been observed in a variety of different media, ranging from dust particles in Saturn’s rings to biological tissues [9]. However, cold atoms exhibit some unusual properties that make them of great interest for studies of multiple scattering of light. Firstly, atoms are point scatterers, whose interaction with the electromagnetic field is intrinsically quantum. In addition, the atom’s scattering cross-section is highly resonant ($Q \approx 10^8$) and the resonance frequency is identical for all the scatterers in the sample (assuming a negligible Doppler effect, which implies laser cooling). Such a situation would be very difficult to achieve with classical resonators. As a consequence, the light mean free path in the atomic medium can be varied

by orders of magnitude by shifting the wave frequency by a few megahertz. It is also possible to manipulate the properties of the atomic medium to introduce orientation (through optical pumping) or gain. Thus atoms in a gas appear like promising candidates for interesting new studies.

Several reasons motivate the use of cold atoms for this experiment. Firstly, Doppler broadening is then strongly reduced and all the atoms have the same resonant scattering cross-section, characterized by the natural width of the atomic transition (about 6 MHz for rubidium). However, the atom's motion has a more important consequence on CBS: if the atoms are "too fast", the phase shift induced by the Doppler effect can destroy the constructive interference leading to CBS [10]. A time picture of this effect gives the following rough criterion: during the "characteristic time" in the problem, the atoms should move by less than an optical wavelength. The time involved here is the so-called delay time, which is for rubidium of the order of 50 ns when the laser is resonant with the atomic transition. This imposes rms velocities for the atoms in the sample below a few m/s, a regime easily reached by standard laser-cooling techniques.

3 Description of the experiment

3.1 *Preparation of the atomic sample*

The first step in our experiment is to prepare an atomic sample dense enough to reach the multiple scattering regime. The relevant parameter is the optical thickness of the atomic cloud $\xi = \varnothing/l$, where $\varnothing$ is the diameter of the cloud and l the light scattering mean free path. The multiple scattering regime corresponds roughly to $\xi \geq 1$. A magneto-optical trap (MOT) is loaded from a room-temperature vapor of rubidium atoms in a quartz cell, as shown in Figure 2. The atoms are trapped by six independent laser beams (instead of the usual three retro-reflected beams configuration) to reduce the imbalance due to shadow effects. The beams parameters are: wavelength $\lambda = 780$ nm, detuning from resonance $\delta = -3\Gamma$ (where Γ is the natural width of the transition), diameter 2.8 cm and power per beam 30 mW. The large beam size increases the number of trapped atoms. A magnetic field gradient of about 7 G/cm is applied to spatially confine the cold atoms.

The MOT contains approximately 10^9 atoms with a quasi-gaussian spatial distribution of fwhm between 5 and 7 mm. Transmission measurements using the $F = 3 \rightarrow 4$ transition of the D2 line yield an optical thickness of about 4. The rms velocity of the atoms, measured by time-of-flight, is 10 cm/s. We are not able to record the CBS cone while the MOT is operating. This is because the fluorescence of the atoms excited by the trapping lasers is much brighter than the light scattered from the probe. Also, it seems preferable to avoid perturbations of the atoms by the trapping lasers

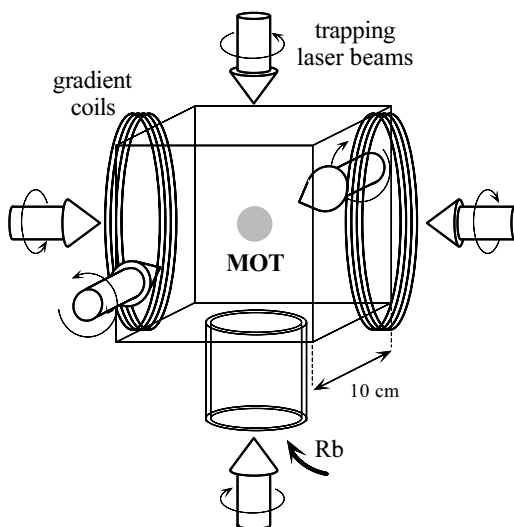


Fig. 2. Schematic view of the MOT setup.

during the CBS measurement. Thus, we alternate a “MOT” phase (duration 20 ms) where the atoms are trapped, with a “CBS” phase (2–3 ms) where the trapping beams and magnetic field are shut down and the CBS signal recorded; this phase is sufficiently short so that all the atoms remain in the capture zone and are efficiently recaptured when the MOT is switched back on.

3.2 CBS detection setup

The CBS detection setup is schematically represented in Figure 3. The sample is illuminated by a collimated laser probe. Part of the backscattered light is collected by a beam-splitter, and its angular distribution is recorded on a cooled CCD placed in the focal plane of an analysis lens. The angular resolution of the setup is about 0.1 mrad. As usual in CBS experiments, great care must be taken to shield the detector against stray light; the alternative paths that can be followed by the light (incident beam reflected by the beam-splitter and beam transmitted by the sample) must also be carefully blocked to avoid any unwanted backscattering.

The incident and detected polarizations can be selected using a quarter-wave plate and a polarizer. The choice of the appropriate polarization channel makes it possible, at least for spherical and Rayleigh scatterers [11], to remove the single scattering contribution to the detected light. Indeed, single scattering does not contribute to CBS but adds up to the signal as a background, and thus reduces the apparent enhancement factor (defined

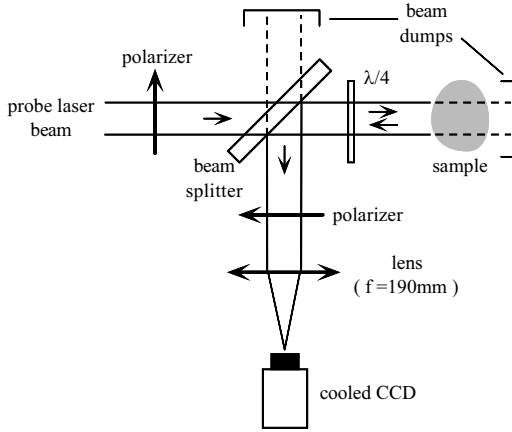


Fig. 3. The CBS detection setup.

as the ratio of the detected intensities at $\theta = 0$ and $\theta \gg \lambda/l^*$). Thus, CBS experiments are usually performed in the “helicity preserving” channel (incident and detected polarizations both circular with the same helicity, *i.e.* sign of rotation of electric field referenced to the direction of propagation), where the enhancement factor is 2 for spherical and Rayleigh scatterers.

To avoid blinding of the CCD during the “MOT” phase, a chopper (not represented in Fig. 3) is inserted in the detection path and synchronized with the signal driving the trap operation so as to transmit light only during the “CBS” phase. In order to record the CBS cone from the MOT with a satisfactory signal to noise ratio, we repeat the sequence “MOT”+“CBS” about 3000 times (total duration 1 min). The typical detected light flux is about 1 800 photons/s/pixel. A “background” image is also recorded, in the same conditions but without the MOT, and subtracted from the signal to remove residual stray light.

4 Results

Figure 4 shows a profile of the atomic CBS cone in the “orthogonal helicity” channel, obtained after an angular average is performed on the CCD image (this smoothing procedure is valid as long as the CBS cone is isotropic, which is the case in the circular channels).

The light mean free path, estimated from optical thickness and cloud size measurements, is about 1.5 mm. The measured cone width is 0.5 mrad FWHM. This value is about 10 times larger than what is obtained with the formula: $\Delta\theta \approx 0.1 \lambda/l^*$ valid for a semi-infinite medium. Because of the spherical symmetry and rather modest optical thickness of the sample, low

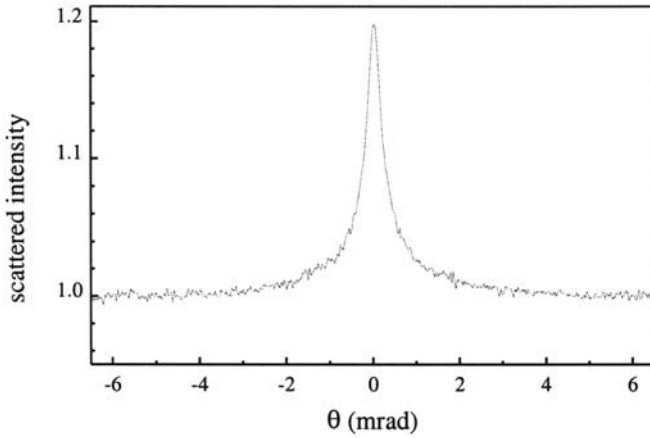


Fig. 4. CBS cone from the atomic cloud in the “orthogonal helicity” channel.

orders of multiple scattering are dominant yielding a broader cone than in the semi-infinite situation. We are currently developing a MonteCarlo simulation to quantitatively address the width and shape of the atomic CBS cone. The most striking feature of the curve shown in Figure 4 is the small value (≈ 1.2) of the enhancement factor; the contrast is even lower in the other polarization channels, with 1.08 in the circular “helicity preserving” channel, 1.14 and 1.12 in the linear “parallel” and “orthogonal” channels respectively. This comes as a major surprise since one would expect, for “classical” Rayleigh scatterers, an enhancement factor of 2 in the circular helicity preserving channel. However, several mechanisms could contribute to the reduction of the cone contrast in our experiment. Some are purely experimental (resolution, geometry) while others are more interesting because they arise from the internal structure of the atoms.

1) **Experimental resolution and transverse size effect.** The cone width is only 5 times larger than the estimated experimental resolution, so the cone contrast is affected by the convolution with the angular response of the apparatus. However this reduction should not exceed 5 to 10 per cent. As a confirmation we report in Figure 5 a CBS cone from a sample of polystyrene foam (spherical shape, $\varnothing = 10$ mm) in the circular helicity preserving channel. Its width is close to that of the atomic cone, but the enhancement factor is about 1.94 (limited by the experimental resolution).

Another effect is due to the inhomogenous intensity distribution of the probe. If the “input” and “output” scatterers of Figure 1 are not illuminated by the same laser intensity, the two waves that interfere to give rise to the cone are not balanced and the contrast is reduced. We have not yet estimated the magnitude of this reduction, but it should remain small in

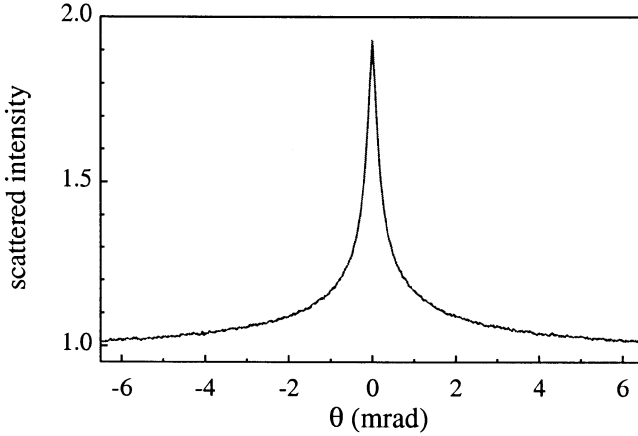


Fig. 5. CBS cone from a spherical sample of polystyrene foam in the “helicity preserving” channel.

our case since the atomic cloud is smaller than the probe diameter (9 mm FWHM).

2) **Single scattering.** As already mentioned, it is possible with classical (and spherical) scatterers to get rid of single scattering by choosing the helicity preserving channel. With our multi-level atomic scatterer, this is no longer possible because of (spontaneous) “Raman” scattering where the atom’s internal state (here the Zeeman sublevel) is modified. During such an event the polarization of the scattered light differs from the incident and thus can not be totally eliminated by polarization tricks. A similar behavior would be obtained for classical non-spherical scatterers.

3) **Effects due to the atom’s internal structure.** In this subsection we group some mechanisms that are intrinsically linked to the existence of an internal structure for the atomic scatterer. The first one is an imbalance between the waves which interfere to give the cone. An example involving double scattering is illustrated in Figure 6: two atoms (a $1/2 \rightarrow 1/2$ transition was chosen for the sake of simplicity, but the argument is not restricted to this transition), both in different Zeeman sublevels, are illuminated by a σ^+ wave. The atom on the left can scatter a photon at 90 degrees towards the atom on the right, with a linear polarization (projection of the incident polarization on the plane orthogonal to the propagation). This is seen by atom 2 as a combination of σ^+ and σ^- radiations. This atom can only make a σ^- transition, so this is the polarization that is backscattered, and detected in the helicity preserving channel. The counterpart which is first scattered by atom 2 has a zero amplitude since no σ^+ transition is available. Thus, in this extreme situation, there is no interference.

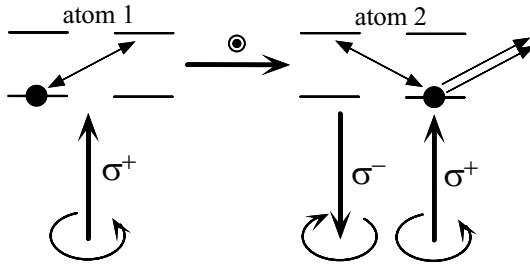


Fig. 6. CBS contrast reduction mechanism due to the atom's internal structure.

We stress that, as in the example illustrated in Figure 6, this contrast reduction mechanism occurs even if no Raman scattering is involved. We believe that this mechanism, new for the community of multiple scattering, accounts for most of the contrast reduction observed in our experiment in the helicity preserving channel. Indeed, preliminary calculations involving only single and double scattering yield a contrast of 1.16 only, quite close to what is observed. It also predicts enhancement factors in the other channels that are in fair agreement with the experiment (in particular the hierarchy of the enhancements in the various channels is reproduced). A more detailed theoretical analysis of this contrast reduction mechanism will be reported elsewhere [12]. A second possible source of contrast loss is inelastic scattering. In the simplest case of a two level atom, it is well known that the fluorescence light exhibits some inelastic spectral components in addition to the elastic one [13]. In the limit of weak saturation, these components vanish and the scattering is mostly elastic. However, in our situation of a multi-level atom, the “Raman” scattering events contribute to the inelastic spectrum [14], even in the limit of weak saturation. We still have to address the rather subtle question of the effect of inelastic scattering in our situation.

5 Conclusion

We have realized the first experimental observation of coherent backscattering of light from a cloud of cold atoms. We observe a CBS cone contrast much smaller than 2 even in the helicity preserving channel, contrary to what is usually obtained with classical samples. This contrast reduction is attributed to a new imbalance effect due to the internal structure of the atoms. We are currently setting up numerical simulations to address the specificities of our sample (atomic internal structure, cloud geometry). We then plan to study the effect of inelastic scattering and of an external magnetic field on the CBS cone.

Acknowledgements

We would like to thank the CNRS and PACA Region for financial support. We also thank D. Delande, B. van Tiggelen and D. Wiersma for many stimulating discussions.

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