THE SCHWINGER ACTION PRINCIPLE AND EFFECTIVE ACTION

This book is an introduction to the Schwinger action principle in quantum mechanics and quantum field theory, with applications to a variety of different models, not only those of interest to particle physics. The book begins with a brief review of the action principle in classical mechanics and classical field theory. It then moves on to quantum field theory, focusing on the effective action method. This is introduced as simply as possible by using the zero-point energy of the simple harmonic oscillator as the starting point. This allows the utility of the method, and the process of regularization and renormalization of quantum field theory, to be demonstrated with a minimum of formal development. The book concludes with a more complete definition of the effective action, and demonstrates how the provisional definition used earlier is the first term in the systematic loop expansion.

Several applications of the Schwinger action principle are given, including Bose–Einstein condensation, the Casimir effect, and trapped Fermi gases. The renormalization of interacting scalar field theory is presented to two-loop order. This book will interest graduate students and researchers in theoretical physics who are familiar with quantum mechanics.

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Preface

Then Jurgen mounted this horse and rode away from the plowed field wherein nothing grew as yet. As they left the furrows they came to a signboard with writing on it, in a peculiar red and yellow lettering.

Jurgen paused to decipher this.

'Read me!' was written on the signboard: 'read me, and judge if you understand! So you stopped in your journey because I called, scenting something unusual, something droll. Thus, although I am nothing, and even less, there is no one that sees me but lingers here. Stranger, I am a law of the universe. Stranger, render the law what is due the law!'

Jurgen felt cheated. 'A very foolish signboard, indeed! for how can it be 'a law of the universe', when there is no meaning to it!' says Jurgen. 'Why, for any law to be meaningless would not be fair.'

(James Branch Cabell)

The quantum theory of fields is now a mature and well-developed subject with a wide range of applications to physical systems. The predominant approach that is taught to students today is the Feynman path integral. There is another approach that receives much less attention due to Schwinger, and his method is the main emphasis of the present book.

The intention of this book is to present the material in a manner that is accessible to final-year undergraduates or beginning postgraduate students. The prospective reader is expected to already have had an exposure to classical mechanics, quantum mechanics, and statistical mechanics; the present book is not to be viewed as an introduction to any of these subjects. The assumed background is that found in a typical physics undergraduate in the UK at the end of the third year. Some material that is included here will already be familiar to a suitably prepared student and is intended as a refresher. Other material goes beyond that typically taught at the undergraduate level, but is presented in a way that leads on directly from the more familiar material. The necessary mathematical background is also typical of that found in the third-year physics undergraduate. I have included some of the necessary background material in appendices

at the end of the book, particularly on some of the mathematical topics that the physics student may not have seen, or met only in passing (like the Γ-function, ζ-function, or how to sum series using contour integral methods).

The idea for writing this book originated when I was invited to give some lectures[1] on quantum field theory at the 15th Symposium on Theoretical Physics held in Seoul, Korea, in 1996. Because this was intended to be a short course of lectures, rather than spend an inordinate amount of time developing formal aspects of the subject, I chose to introduce the energy ζ-function method at an early stage, and using the simple harmonic oscillator as a basis, to concentrate on some simple applications of one-loop quantum field theory at both zero and finite temperature. This enables the basics of renormalization of interacting fields to be introduced at an early stage without the full apparatus of perturbation theory being brought to bear. Because of the limitations of the method (to one-loop effects), although the initial chapters of the present book give the simpler one-loop calculations, later chapters describe the development of the general effective action in some depth. This can be done at the stage when the student has already been exposed to the basic idea and seen it at work in some simple applications.

I would like to thank Professor Choonkyu Lee who invited me to lecture in Seoul, Korea; the act of preparing for these lectures led me to think that a greatly expanded version could form the basis of an interesting book. Some of the material in the first few chapters was used as a basis for a series of lectures given to final-year undergraduates in theoretical physics at Newcastle, and the experience of giving the lectures, with student feedback, led to some improvements in presentation. Sam James managed to read through most of a draft version and pointed out numerous typographical errors, inconsistencies, and poor explanations. I am grateful to all my collaborators, past and present, for helping me to understand the beauty of quantum field theory. As is becoming standard practice, I will keep an up-to-date list of any errors that slip through the proofreading on my website (www.staff.ncl.ac.uk/d.j.toms).

I would like to dedicate this book to my parents, without whose help and support I would never have been able to reach the point of writing the book, and especially to Linda without whom there would simply be no point.

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[1] See Toms (1997), or http://xxx.soton.ac.uk/pdf/cond-mat/9612003.

1
Action principle in classical mechanics

1.1 Euler–Lagrange equations

In classical mechanics we are usually interested in solving the equations of motion of a point particle under the action of some prescribed force. A method for doing this in a systematic way is given by Newton's equation $\mathbf{F} = m\mathbf{a}$, where $\mathbf{F}$ is the force applied, m is the mass, and $\mathbf{a}$ is the acceleration.[1] Since the force is often a function of time t and the position $\mathbf{x}$ of the particle (it may also depend on velocity in some cases), and the acceleration $\mathbf{a}$ is given in terms of the vector $\mathbf{x}$ specifying the position of the particle by $\mathbf{a} = \ddot{\mathbf{x}}$, Newton's equations of motion result in a set of ordinary differential equations for the path $\mathbf{x}(t)$ followed by the particle. The motion is completely specified if we give the position $\mathbf{x}(t_0) = \mathbf{x}_0$ and the velocity $\dot{\mathbf{x}}(t_0) = \mathbf{v}_0$ at some initial time t_0. (Other conditions on the path are also possible. For example, we might specify the location of the particle at two different times.)

It is usually assumed that the path of the particle can be described by regarding $\mathbf{x}$ as a vector in the Euclidean space $\mathbb{R}^D$, and typically we are interested in the case $D = 3$. The components of $\mathbf{x}$ may be chosen to be the Cartesian coordinates of the curve $\mathbf{x}(t)$ that describes the motion of the particle parameterized by the time t. However, the choice of Cartesian coordinates is totally arbitrary, and any coordinates may be used.[2] This basic principle of relativity is used almost without comment all the time. Two independent observers looking at the same particle under the action

[1] Here and throughout boldfaced text will be used to denote a vector.

[2] The physics of the situation must be independent of this arbitrary choice of coordinates.

of a given force and who adopt different choices of coordinates should agree on the behaviour of the particle in any situation.[3]

We are often interested in a conservative force which can be derived from a potential using $\mathbf{F} = -\nabla V$. For such forces the work done on a particle moving in the field of force between two points in space, $\mathbf{x}_1$ and $\mathbf{x}_2$, is

$$\text{Work}(1 \to 2) = \int_{\mathbf{x}_1}^{\mathbf{x}_2} \mathbf{F} \cdot d\mathbf{x} = -(V_2 - V_1).$$

The work done is seen to depend only on the difference in potential between the two endpoints of the path. If we assume Cartesian coordinates, then Newton's equation $\mathbf{F} = m\mathbf{a}$ becomes

$$m\ddot{\mathbf{x}} = -\nabla V \tag{1.1}$$

when we use the definition of acceleration in terms of position, and write the force in terms of the potential. If we take the dot product of both sides of (1.1) with $\dot{\mathbf{x}}$, we find

$$m\dot{\mathbf{x}} \cdot \ddot{\mathbf{x}} = -\dot{\mathbf{x}} \cdot \nabla V = -\frac{d}{dt}V, \tag{1.2}$$

if we assume for simplicity that the potential V has no explicit time dependence. The result in (1.2) can be rearranged to read

$$\frac{d}{dt}\left(\frac{1}{2}m\,\dot{\mathbf{x}} \cdot \dot{\mathbf{x}} + V\right) = 0. \tag{1.3}$$

The expression in braces in this last result may be identified as the total energy of the particle. The two separate terms are

$$T = \frac{1}{2}m\dot{\mathbf{x}} \cdot \dot{\mathbf{x}}, \tag{1.4}$$

giving the kinetic energy, and V giving the potential energy.

There is another way of formulating Newton's laws which allows for a generalization. Instead of forming the combination $T + V$, which represents the total energy, form

$$L = T - V, \tag{1.5}$$

[3] The motion of the moon does not depend on whether you live in London or in Oshawa, or in how you choose to introduce a coordinate system to describe the motion.

which is called the Lagrangian. L is regarded as a function of the coordinates $\mathbf{x}$ and the velocities $\dot{\mathbf{x}}$, which are treated as independent variables. We have

$$L(\mathbf{x}, \dot{\mathbf{x}}) = \frac{1}{2} m \sum_{i=1}^{D} (\dot{x}^i)^2 - V(\mathbf{x}) \tag{1.6}$$

if we use (1.4) with the dot product between the velocities written out explicitly in terms of the components.[4] It is now easy to see that because $\mathbf{x}$ and $\dot{\mathbf{x}}$ are viewed as independent variables, we have

$$\frac{\partial L}{\partial x^i} = -\frac{\partial V}{\partial x^i}$$
$$\frac{\partial L}{\partial \dot{x}^i} = m\dot{x}^i.$$

It therefore follows that

$$0 = \frac{\partial L}{\partial x^i} - \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}^i}\right) \tag{1.7}$$

for $i = 1, \ldots, D$ are completely equivalent to Newton's equations of motion. We call (1.7) the Euler–Lagrange equations.

It is worth describing what happens if Cartesian coordinates are not used. First of all we would expect that the work done in moving a particle in a given force field should not depend on the choice of coordinates. This is most easily achieved if the potential energy does not depend on the coordinate choice. If we let $\mathbf{q}$ represent any set of coordinates, with $\mathbf{x}$ being reserved for Cartesian coordinates, then we will require

$$V(\mathbf{x}) = \tilde{V}(\mathbf{q}). \tag{1.8}$$

The tilde is necessary in this expression because the functional form of the potential energy may be different for the new and the old coordinates. For example, if $\mathbf{x} = (x, y)$ and we set $\mathbf{q} = (r, \theta)$ with $x = r\cos\theta$ and $y = r\sin\theta$, then for $V(x, y) = x^2 + y^2$ we find $x^2 + y^2 = r^2 = \tilde{V}(r, \theta)$. Clearly, $V(r, \theta) = r^2 + \theta^2 \neq V(x, y)$. If V satisfies (1.8) it is said to be a scalar function.

If we demand that the kinetic energy also be a scalar function of coordinates, then we will be assured that the total energy will be a scalar,

[4] We regard the components of the vector $\mathbf{x}$ in $\mathbb{R}^D$ as x^i with $i = 1, \ldots, D$.

and hence independent of the arbitrary coordinate choice. In Cartesian coordinates we have

$$\begin{aligned} T &= \frac{1}{2}m\sum_{i=1}^{D}(\dot{x}^i)^2 \\ &= \frac{1}{2}m\sum_{i=1}^{D}\sum_{j=1}^{D}\delta_{ij}\dot{x}^i\dot{x}^j. \end{aligned} \tag{1.9}$$

Here δ_{ij} is the Kronecker delta, defined to be equal to 1 if $i = j$ and equal to 0 if $i \neq j$. We regard $x^i = x^i(\mathbf{q})$, simply expressing the Cartesian coordinates $\mathbf{x}$ in terms of the general coordinates $\mathbf{q}$. The velocity becomes

$$\dot{x}^i = \frac{d}{dt}x^i(\mathbf{q}(t)) = \sum_{j=1}^{D}\frac{\partial x^i}{\partial q^j}\dot{q}^j. \tag{1.10}$$

(We have just used the chain rule for partial differentiation to obtain the last equality here.) Substitution of this expression into the result in (1.9) for the kinetic energy gives

$$\begin{aligned} T &= \frac{1}{2}m\sum_{i=1}^{D}\sum_{j=1}^{D}\delta_{ij}\left(\sum_{k=1}^{D}\frac{\partial x^i}{\partial q^k}\dot{q}^k\right)\left(\sum_{l=1}^{D}\frac{\partial x^j}{\partial q^l}\dot{q}^l\right) \\ &= \frac{1}{2}m\sum_{k=1}^{D}\sum_{l=1}^{D}g_{kl}(\mathbf{q})\dot{q}^k\dot{q}^l, \end{aligned} \tag{1.11}$$

where we have defined

$$g_{kl}(\mathbf{q}) = \sum_{i=1}^{D}\sum_{j=1}^{D}\delta_{ij}\frac{\partial x^i}{\partial q^k}\frac{\partial x^j}{\partial q^l}. \tag{1.12}$$

$g_{kl}(\mathbf{q})$ is called the metric tensor, and will be familiar to students of differential geometry. (See Laugwitz (1965) for example.)

Due to the proliferation of summation signs, it proves convenient to adopt the Einstein summation convention: any repeated index is summed over the appropriate range of values, in this case $1, 2, \ldots, D$. For example, we would write

$$\dot{x}^i = \sum_{j=1}^{D}\frac{\partial x^i}{\partial q^j}\dot{q}^j$$

as

$$\dot{x}^i = \frac{\partial x^i}{\partial q^j}\dot{q}^j$$

using the Einstein summation convention. The understanding is that because the index j occurs twice in $\left(\partial x^i/\partial q^j\right)\dot{q}^j$, it is summed over all values $1,\ldots,D$.[5] With this new notation we would then rewrite (1.11) and (1.12) as

$$T = \frac{1}{2} m\, g_{kl}(\mathbf{q})\dot{q}^k\dot{q}^l \tag{1.13}$$

and

$$g_{kl}(\mathbf{q}) = \delta_{ij}\,\frac{\partial x^i}{\partial q^k}\frac{\partial x^j}{\partial q^l}, \tag{1.14}$$

respectively. Because the repeated indices are arbitrary labels in a summation they can be relabelled at will. This means, for example, that $g_{ij}\dot{q}^i\dot{q}^j$ and $g_{nm}\dot{q}^n\dot{q}^m$ are both equivalent to $g_{kl}\dot{q}^k\dot{q}^l$. The indices of summation are often referred to as dummy indices or dummy labels.

1.2 Hamilton's principle

It is possible to reformulate classical mechanics in order to obtain the Euler–Lagrange equations as a result of a principle of stationary action. To do this we will define the action functional $S[\mathbf{q}(t)]$ as

$$S[\mathbf{q}(t)] = \int_{t_1}^{t_2} dt\, L(q^i(t), \dot{q}^i(t), t). \tag{1.15}$$

Here L is the Lagrangian described in the previous section that, for generality, we allow to have an explicit dependence on time. We allow the use of any coordinate choice here. The use of square brackets in this definition is to symbolize that the action S is a functional, which can be thought of as a function defined on a space of functions.[6] Given some path $\mathbf{q}(t)$, the action is just a real number. If $\mathcal{P}$ denotes the space of all possible paths then we regard $S : \mathcal{P} \to \mathbb{R}$. In contrast to normal functions, the domain of a functional is an infinite dimensional space.[7] Because of the infinite dimensional nature of $\mathcal{P}$, a rigorous treatment of functionals involves some subtle concepts. In particular the notions of differentiation and integration involve some thought. We will proceed in a heuristic manner without full mathematical rigour, as is conventional in physics.

[5] In contrast, the index i only occurs once in each term.

[6] That is the domain of a functional is some space of functions. For the action the domain is the space consisting of all possible particle paths for which the position of the particle is given at the times t_1 and t_2.

[7] Clearly there are an infinite number of paths connecting two points in space.

Hamilton's principle states that the actual motion of a particle whose Lagrangian is L is such that the action functional is stationary (i.e. assumes a maximum or a minimum value). In order to see that this principle is correct we must show that requiring the action to be stationary results in the Euler–Lagrange equations, and conversely that if we impose the Euler–Lagrange equations then the action functional is stationary. The technique for accomplishing this involves the calculus of variations. We will look at what happens to the action functional when the path is varied slightly. We are regarding the endpoints of the path as fixed here, although other choices are possible. Let $\mathbf{q}(t_1) = \mathbf{q}_1$ and $\mathbf{q}(t_2) = \mathbf{q}_2$ be the positions of the particle at the initial time t_1 and the final time t_2 respectively. Let $\mathbf{q}(t)$ be the classical path that the particle follows, and let $\bar{\mathbf{q}}(t)$ be any path with the same two endpoints as the classical path. Now form the difference

$$\delta\mathbf{q}(t) = \bar{\mathbf{q}}(t) - \mathbf{q}(t), \tag{1.16}$$

which represents the deviation of $\bar{\mathbf{q}}(t)$ from the classical path. Because both paths $\bar{\mathbf{q}}(t)$ and $\mathbf{q}(t)$ have the same endpoints, the deviation between the two paths $\delta\mathbf{q}(t)$ must vanish at the initial and final times: $\delta\mathbf{q}(t_1) = \delta\mathbf{q}(t_2) = 0$. The situation is pictured in Fig. 1.1.

We are aiming to show that the action is stationary for the classical path. One way to do this is to assume that the difference $\delta\mathbf{q}(t)$ is small and show that the action is unchanged to first order in the small quantity $\delta\mathbf{q}(t)$. Evaluating the action (1.15) using the arbitrary path $\bar{\mathbf{q}}(t)$ we find

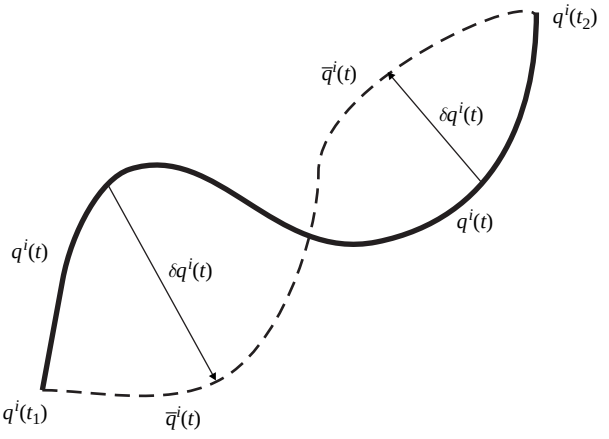

Fig. 1.1 This demonstrates the relationship between the classical path $q^i(t)$ (shown as a solid line), the arbitrary path $\bar{q}^i(t)$ (shown as a dashed line), and the deviation, or difference, $\delta q^i(t)$. The endpoints are held fixed, so that the difference $\delta q^i(t)$ vanishes at times t_1 and t_2.

$$S[\bar{\mathbf{q}}(t)] = \int_{t_1}^{t_2} dt\, L(\bar{q}^i(t), \dot{\bar{q}}^i(t), t)$$
$$= \int_{t_1}^{t_2} dt\, L(q^i(t) + \delta q^i(t), \dot{q}^i(t) + \delta \dot{q}^i(t), t). \tag{1.17}$$

The last equality has just used the definition in (1.16). The Lagrangian is an ordinary function of $q^i(t)$ and $\dot{q}^i(t)$, so may be expanded in an ordinary Taylor series:

$$L\left(q^i(t) + \delta q^i(t), \dot{q}^i(t) + \delta \dot{q}^i(t), t\right) = L\left(q^i(t), \dot{q}^i(t), t\right)$$
$$+ \frac{\partial L(q^i(t), \dot{q}^i(t), t)}{\partial q^i(t)} \delta q^i(t) + \frac{\partial L(q^i(t), \dot{q}^i(t), t)}{\partial \dot{q}^i(t)} \delta \dot{q}^i(t) + \cdots . \tag{1.18}$$

Note that the summation convention has been used here, and we have only calculated terms in the expansion up to and including those linear in $\delta q^i(t)$. There will be terms of quadratic and higher order in δq^i in the expansion (1.18), but we will not be concerned with them. Substitution of (1.18) into (1.17) leads to

$$S[\bar{\mathbf{q}}(t)] = S[\mathbf{q}(t)] + \int_{t_1}^{t_2} dt\, \left(\frac{\partial L}{\partial q^i} \delta q^i + \frac{\partial L}{\partial \dot{q}^i} \delta \dot{q}^i \right) + \cdots . \tag{1.19}$$

The second term in the integrand of (1.19) can be rewritten using the identity

$$\frac{\partial L}{\partial \dot{q}^i} \delta \dot{q}^i = \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}^i} \delta q^i \right) - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}^i} \right) \delta q^i .$$

This results in

$$S[\bar{\mathbf{q}}(t)] = S[\mathbf{q}(t)] + \int_{t_1}^{t_2} dt\, \left[\frac{\partial L}{\partial q^i} - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}^i} \right) \right] \delta q^i + \frac{\partial L}{\partial \dot{q}^i} \delta q^i \Big|_{t_1}^{t_2} + \cdots ,$$

if we perform the integration over the total time derivative. Because δq^i vanishes at t_1 and t_2, the last term in the line above disappears and we are left with

$$S[\bar{\mathbf{q}}(t)] = S[\mathbf{q}(t)] + \int_{t_1}^{t_2} dt\, \left[\frac{\partial L}{\partial q^i} - \frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}^i} \right) \right] \delta q^i , \tag{1.20}$$

to first order in δq^i. This is our main result.

If the Euler–Lagrange equations hold then (1.20) shows that $S[\bar{\mathbf{q}}(t)] = S[\mathbf{q}(t)]$ demonstrating that the action is stationary. Conversely, if

$S[\bar{\mathbf{q}}(t)] = S[\mathbf{q}(t)]$ then we must have the Euler–Lagrange equations holding.[8] This has demonstrated Hamilton's principle: *The action is stationary if and only if the path satisfies the classical equation of motion.* This provides an elegant formulation of classical mechanics with the action functional playing a key role.

1.3 Hamilton's equations

For systems of the type considered in Section 1.1 the Euler–Lagrange equations provide a set of second-order differential equations for the path. With $\mathbf{q} \in \mathbb{R}^D$ we have a set of D coupled equations. It is possible to reformulate these equations as a set of $2D$ coupled first-order differential equations, and this is the essential content of the Hamiltonian form of classical mechanics, along with a physical interpretation of the procedure.

Define the momentum canonically conjugate to the coordinate q^i by

$$p_i = \frac{\partial L}{\partial \dot{q}^i}. \tag{1.21}$$

p_i is usually called just the canonical momentum. Note that for L given by (1.6), $\mathbf{p} = m\dot{\mathbf{x}}$ is the normal definition for the momentum familiar from elementary mechanics. The aim now is to eliminate the dependence on the velocity components $\dot{q}^i$ in favour of the components of canonical momentum p_i. This requires being able to solve the set of equations (1.21) for $\dot{q}^i$ in terms of q^i and p_i. The necessary and sufficient conditions for this are given by the inverse function theorem which states that it is possible to solve (1.21) for $\dot{q}^i$ in terms of q^i and p_i if and only if $\det\left(\partial p_i/\partial \dot{q}^j\right) \neq 0$. A heuristic way to see this is to look at a small variation of (1.21) with q^i held fixed:

$$\delta p_i = \frac{\partial^2 L}{\partial \dot{q}^j \partial \dot{q}^i}\delta \dot{q}^j = \frac{\partial p_i}{\partial \dot{q}^j}\delta \dot{q}^j.$$

It is only possible to solve this for $\delta \dot{q}^j$ if the matrix $\frac{\partial p_i}{\partial \dot{q}^j}$ is invertible. A system which has $\det\left(\partial p_i/\partial \dot{q}^j\right) = 0$ is called singular. We will see examples of singular systems later. For now assume a non-singular system.

Given a non-singular system we can eliminate all dependence on $\dot{q}^i$ by a Legendre transformation:

$$H(\mathbf{q}, \mathbf{p}, t) = p_i \dot{q}^i - L(\mathbf{q}, \dot{\mathbf{q}}, t). \tag{1.22}$$

[8] Formally, if $S[\bar{\mathbf{q}}(t)] = S[\mathbf{q}(t)]$ the integral in (1.20) must vanish for arbitrary $\delta q^i(t)$. We can take $\delta q^i(t)$ to be zero everywhere except for an arbitrary time in the interval $[t_1, t_2]$; thus, the quantity in the integrand of (1.20) appearing in braces must vanish for all times between t_1 and t_2.

H is called the Hamiltonian, and as the notation in (1.22) suggests, it is regarded as a function of the independent variables $\mathbf{q}$ and $\mathbf{p}$, along with a possible time dependence. The Hamiltonian equations are obtained from considering the derivatives of the Hamiltonian with respect to p_i and q^i. To compute the derivative with respect to p_i we use (1.22) and note that apart from the explicit dependence on p_i in the first term, p_i only enters through $\dot{\mathbf{q}}$. This leads to (relabelling the dummy index i in (1.22) to j before differentiating with respect to p_i)

$$\begin{aligned}\frac{\partial H}{\partial p_i} &= \dot{q}^i + p_j \frac{\partial \dot{q}^j}{\partial p_i} - \frac{\partial L}{\partial \dot{q}^j}\frac{\partial \dot{q}^j}{\partial p_i} \\ &= \dot{q}^i, \end{aligned} \tag{1.23}$$

if it is noted that the second and third terms in the first line cancel upon use of (1.21). To compute the derivative of H with respect to q^i we note that $\mathbf{q}$ and $\mathbf{p}$ are the independent variables, and that q^i enters $\dot{q}^j$ through (1.21). This leads to (again relabelling the dummy index i in (1.22) to j)

$$\begin{aligned}\frac{\partial H}{\partial q^i} &= p_j \frac{\partial \dot{q}^j}{\partial q^i} - \frac{\partial L}{\partial q^i} - \frac{\partial L}{\partial \dot{q}^j}\frac{\partial \dot{q}^j}{\partial q^i} \\ &= -\frac{\partial L}{\partial q^i} \quad \text{(by (1.21))} \\ &= -\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}^i}\right) \quad \text{(by (1.7))} \\ &= -\dot{p}_i, \end{aligned} \tag{1.24}$$

where the last line has followed by using (1.21) again. The results contained in (1.23) and (1.24) are called Hamilton's equations. They are seen to consist of a set of first-order differential equations as promised.

Suppose that L takes the standard form

$$L = \frac{1}{2} m\, g_{ij}(\mathbf{q}) \dot{q}^i \dot{q}^j - V(\mathbf{q}),$$

considered in Section 1.1. We can compute p_i from (1.21) to be

$$p_i = \frac{\partial L}{\partial \dot{q}^i} = m\, g_{ij} \dot{q}^j.$$

It is easy to invert this result using the inverse metric g^{ij} defined by

$$g^{ij} g_{jk} = \delta^i{}_k,$$

with $\delta^i{}_k$ the Kronecker delta (i.e. $\delta^i{}_k$ is zero unless the indices i and k are equal, in which case it has the value 1). This gives

$$\dot{q}^i = \frac{1}{m} g^{ij} p_j.$$

The Hamiltonian is now computed from (1.22) to be

$$H = \frac{1}{2m} g^{ij} p_i p_j + V(\mathbf{q}), \tag{1.25}$$

which may be recognized as the sum of the kinetic and potential energies. The Hamiltonian in this case represents the total energy.

In Section 1.2 we showed how the Euler–Lagrange equations could be viewed as a consequence of Hamilton's principle of stationary action. The action functional was defined in (1.15). It is possible to modify the principle of stationary action so that Hamilton's equations (1.23) and (1.24) result. This can be done easily if we note that from (1.22) we have $L = p_i \dot{q}^i - H$. If this is substituted into (1.15) we obtain

$$S[\mathbf{q}, \mathbf{p}] = \int_{t_1}^{t_2} dt \left\{ p_i \dot{q}^i - H(\mathbf{q}, \mathbf{p}, t) \right\}, \tag{1.26}$$

with the action now regarded as a functional of both $\mathbf{q}$ and $\mathbf{p}$. We can now think of the action as a functional of a path in phase space parameterized by the independent coordinates and momenta. To see that Hamilton's equations result from Hamilton's principle of stationary action, perform a variation of (1.26) with independent variations $\delta\mathbf{q}$ and $\delta\mathbf{p}$. This gives

$$\delta S = \int_{t_1}^{t_2} dt \left(\delta p_i \dot{q}^i + p_i \delta \dot{q}^i - \frac{\partial H}{\partial p_i} \delta p_i - \frac{\partial H}{\partial q^i} \delta q^i \right). \tag{1.27}$$

If the second term of (1.27) is integrated by parts, and it is noted that δq^i vanishes at times t_1 and t_2 since the endpoints of the path are held fixed, it is easily seen that

$$\delta S = \int_{t_1}^{t_2} dt \left[\left(\dot{q}^i - \frac{\partial H}{\partial p_i} \right) \delta p_i - \left(\dot{p}_i + \frac{\partial H}{\partial q^i} \right) \delta q^i \right]. \tag{1.28}$$

This result is sufficient to show that Hamilton's equations follow directly from Hamilton's principle of stationary action.

Of course the formalism of Hamiltonian dynamics can be developed much further,[9] and we will consider one line of development in the next

[9] The interested reader should consult Goldstein (1950) or Lanczos (1971) for more details.

section. For our purposes at this stage, we only need to introduce the notion of Poisson brackets. Let $F(\mathbf{q}, \mathbf{p}, t)$ be any function of the canonical variables $(\mathbf{q}, \mathbf{p})$ with a possible explicit time dependence. If we compute the total time derivative of F then

$$\begin{aligned}\frac{dF}{dt} &= \frac{\partial F}{\partial t} + \frac{\partial F}{\partial q^i}\,\dot{q}^i + \frac{\partial F}{\partial p_i}\,\dot{p}_i \\ &= \frac{\partial F}{\partial t} + \frac{\partial F}{\partial q^i}\frac{\partial H}{\partial p_i} - \frac{\partial F}{\partial p_i}\frac{\partial H}{\partial q^i}\end{aligned}$$

where Hamilton's equations (1.23) and (1.24) have been used in the second line. The Poisson bracket is now defined by[10]

$$[F, H] = \frac{\partial F}{\partial q^i}\frac{\partial H}{\partial p_i} - \frac{\partial F}{\partial p_i}\frac{\partial H}{\partial q^i}. \tag{1.29}$$

We can therefore write

$$\frac{dF}{dt} = \frac{\partial F}{\partial t} + [F, H]. \tag{1.30}$$

Hamilton's equations can now be written in terms of the Poisson bracket as

$$\dot{q}^i = [q^i, H], \tag{1.31}$$
$$\dot{p}_i = [p_i, H]. \tag{1.32}$$

In addition, because q^i and p_i are regarded as independent variables we have the fundamental Poisson bracket relations

$$[q^i, q^j] = 0 = [p_i, p_j] \tag{1.33}$$

and

$$[q^i, p_j] = \delta^i{}_j, \tag{1.34}$$

among the canonical variables.

[10] This definition also holds if the Hamiltonian H is replaced with any other function of the canonical variables.

1.4 Canonical transformations

1.4.1 Infinitesimal transformations and generating functions

We have already considered the transformation from Cartesian to general coordinates in Section 1.1. If we adopt the Hamiltonian formulation (rather than the Lagrangian formulation) of classical mechanics, then we can consider the more general transformation from one set of canonical variables (q^i, p_i) to another set (q'^i, p'_i):

$$q'^i = q'^i(q, p, t), \tag{1.35}$$

$$p'_i = p'_i(q, p, t). \tag{1.36}$$

This transformation will lead to a transformation of the Hamiltonian from $H(q, p, t)$ to $H'(q', p', t)$. The requirement that the transformation be canonical consists of demanding that the Hamiltonian equations of motion (1.23) and (1.24) are obeyed in the transformed coordinates:

$$\dot{q}'^i = \frac{\partial H'}{\partial p'_i}, \tag{1.37}$$

$$\dot{p}'_i = -\frac{\partial H'}{\partial q'^i}, \tag{1.38}$$

as well as in the original coordinates. If we use Hamilton's principle to derive these equations, then (1.37, 1.38) should follow from

$$0 = \delta S'[q', p'] = \delta \int_{t_1}^{t_2} \Big[p'_i \dot{q}'^i - H'(q', p', t) \Big]. \tag{1.39}$$

Since Hamilton's equations in our original coordinates followed from

$$0 = \delta S[q, p] = \delta \int_{t_1}^{t_2} \Big[p_i \dot{q}^i - H(q, p, t) \Big], \tag{1.40}$$

we can conclude that the integrands of (1.39) and (1.40) differ by no more than a total time derivative of some function, called the 'generating function'.[11] However the form we choose to write this total time derivative is up to us, and depends on which of the canonical variables we choose to regard as independent. For our purposes the most important case arises if we choose to take our generating function to depend on q^i and p'_i (other common choices are discussed in Goldstein (1950)). With

[11] This must be true since a total time derivative integrates to a function which depends only on the endpoints, which we hold fixed when computing the variation.

our choice made, we regard q'^i as dependent variables. If we integrate the $p'_i\dot{q}'^i$ term in (1.39) by parts, we obtain

$$0 = \delta S' = \delta \int_{t_1}^{t_2} dt \Big[-\dot{p}'_i q'^i - H' \Big]. \tag{1.41}$$

The integration by parts is done so that the velocity term involves our choice of independent variables $\dot{p}'_i$ rather than the dependent variables q'^i. The integrated term vanishes since the endpoints are fixed. The velocity term of (1.40) involves the other dependent variables $\dot{q}^i$, so we can write

$$-\dot{p}'_i q'^i - H' = p_i \dot{q}^i - H + \frac{d}{dt} G(q^i, p'_i, t). \tag{1.42}$$

G is called the generating function. The total time derivative of G cannot affect the equations of motion since, as we have already discussed, the endpoints are fixed under the variation of path. If we abbreviate $G(q^i, p'_i, t)$ to simply $G(t)$ in order to save a bit of writing, then (1.42) results in

$$S' = S + G(t_2) - G(t_1). \tag{1.43}$$

In this form, it is seen that a canonical transformation is interpreted as the addition of a total time derivative to the Lagrangian. This addition cannot affect the equations of motion.

To find out how the dependent variables are fixed by the above procedure, we can compute the total time derivative of the generating function:

$$\frac{d}{dt} G(q^i, p'_i, t) = \frac{\partial G}{\partial t} + \dot{q}^i \frac{\partial G}{\partial q^i} + \dot{p}'_i \frac{\partial G}{\partial p'_i}. \tag{1.44}$$

The velocity terms in (1.42) involving $\dot{q}^i$ and $\dot{p}'_i$ must be independent. Equating coefficients on both sides of (1.42) when we use (1.44) yields

$$q'^i = -\frac{\partial G}{\partial p'_i}, \tag{1.45}$$

$$p_i = -\frac{\partial G}{\partial q^i}, \tag{1.46}$$

$$H' = H - \frac{\partial G}{\partial t}. \tag{1.47}$$

In the special case where the generating function has no explicit time dependence, (1.47) shows that $H' = H$; the Hamiltonian is invariant under a time-independent canonical transformation. Invariance of the Hamiltonian is not true in general though.

The identity transformation results from the simple choice

$$G = -p'_i q^i, \tag{1.48}$$

as is easy to verify from (1.45) and (1.46). If we choose the slightly more general transformation

$$G(q^i, p'_i, t) = -p'_i f^i(q), \tag{1.49}$$

then (1.45) and (1.46) become

$$q'^i = f^i(q), \tag{1.50}$$

$$p_i = p'_j \frac{\partial f^j}{\partial q^i}. \tag{1.51}$$

This shows that the case of a simple transformation of coordinates, such as the passage from Cartesian to polars for example, is a special case of a canonical transformation. A transformation like (1.50) is sometimes called a 'point transformation'.

Having shown that (1.48) generates the identity transformation, we can consider a canonical transformation defined by

$$G(q^i, p'_i, t) = -p'_i q^i + \delta G(q^i, p'_i, t), \tag{1.52}$$

where δG is infinitesimal. In fact, the restriction to infinitesimal canonical transformations is not actually a restriction at all, because any finite transformation can be built up out of successive infinitesimal ones.[12] From (1.45) we find

$$q'^i = q^i - \frac{\partial}{\partial p'_i} \delta G(q^i, p'_i, t). \tag{1.53}$$

From (1.46) we find

$$p'_i = p_i + \frac{\partial}{\partial q^i} \delta G(q^i, p'_i, t). \tag{1.54}$$

Because q^i and p_i only differ from q'^i and p'_i by infinitesimal terms, if we work to lowest order in small quantities, then we can replace p'_i in δG by p_i. This means that to lowest order in small quantities,

$$q'^i = q^i + \delta q^i, \tag{1.55}$$

$$p'_i = p_i + \delta p_i, \tag{1.56}$$

[12] This is most easily demonstrated by showing that the set of all canonical transformations forms a group, but we will not do this here.

where

$$\delta q^i = -\frac{\partial}{\partial p_i}\delta G(q^i, p_i, t), \tag{1.57}$$

$$\delta p_i = \frac{\partial}{\partial q^i}\delta G(q^i, p_i, t). \tag{1.58}$$

This gives the general form of the infinitesimal canonical transformation in terms of the generating function δG.

A special case occurs for the choice

$$\delta G(q^i, p_i, t) = -H(q^i, p_i, t)\delta t, \tag{1.59}$$

where δt is an infinitesimal time. Using this expression for δG in (1.57) and (1.58), we find

$$\delta q^i = \frac{\partial H}{\partial p_i}\,\delta t = \dot{q}^i \delta t, \tag{1.60}$$

$$\delta p_i = -\frac{\partial H}{\partial q^i}\,\delta t = \dot{p}_i \delta t, \tag{1.61}$$

upon use of Hamilton's equations. These last two results mean that the Hamiltonian is responsible for generating a canonical transformation which corresponds to the time development of the system. This central role played by the Hamiltonian will be useful later when we discuss quantum mechanics.

We can also consider what happens to any function of the canonical variables under a canonical transformation. Under (1.35) and (1.36) we will assume

$$A'(q'^i, p'_i, t) = A(q^i, p_i, t). \tag{1.62}$$

Specifically we are assuming that A transforms like a scalar under canonical transformations. The change in the functional form of A is defined by

$$\delta A = A(q'^i, p'_i, t) - A(q^i, p_i, t). \tag{1.63}$$

If we restrict ourselves to an infinitesimal transformation, and work to lowest order in small quantities, we have

$$\begin{aligned}
\delta A &= A(q^i + \delta q^i, p_i + \delta p_i, t) - A(q^i, p_i, t) \\
&= \delta q^i \frac{\partial A}{\partial q^i} + \delta p_i \frac{\partial A}{\partial p_i} \\
&= -\frac{\partial \delta G}{\partial p_i}\frac{\partial A}{\partial q^i} + \frac{\partial \delta G}{\partial q^i}\frac{\partial A}{\partial p_i} \\
&= -[A, \delta G]
\end{aligned} \tag{1.64}$$

where we have used (1.57, 1.58) and the definition of the Poisson bracket (1.29).

There is another issue related to Poisson brackets and canonical transformations which arises; namely, does it matter which set of canonical variables – (q^i, p_i) or (q'^i, p'_i) – is used? It is easy to demonstrate that the answer is no for infinitesimal transformations, and from our assertion that considering infinitesimal transformations is not a restriction, it must be the case that it does not matter which set of canonical variables is used to calculate the Poisson bracket. A direct proof for an arbitrary canonical transformation will be given in Section 1.4.3.

1.4.2 Hamilton–Jacobi equation

Canonical transformations play a pivotal role in the formal structure of classical mechanics. This can be used to provide the basis for a very beautiful approach. We will look for a canonical transformation such that in the new canonical variables the Hamiltonian is identically zero: $H' = 0$. If this is possible, then because (1.37) and (1.38) must hold, the new canonical variables are constant in time. This presents a general solution to Hamilton's equations for any mechanical system! The catch with the deceptive ease of this result is that in order for it to be useful, we must be able to find the transformation from our initial canonical variables to the new constant ones, and this is generally equivalent in difficulty to solving the original Hamiltonian equations. Nevertheless, there is a beauty in the elegance of this approach, called 'Hamilton–Jacobi theory'. In addition, there is an interesting parallel in quantum mechanics.

With the generating function $G(q^i, p'_i, t)$ defined as before, (1.47) becomes

$$H(q^i, p_i, t) = \frac{\partial}{\partial t} G(q^i, p'_i, t),$$

since we are requiring $H'(q', p', t) = 0$. If we use (1.46), we can write this last result as

$$H\left(q^i, -\frac{\partial G}{\partial q^i}, t\right) = \frac{\partial}{\partial t} G(q^i, p'_i, t). \tag{1.65}$$

Given a Hamiltonian H this equation, called the Hamilton–Jacobi equation, provides us with a single partial differential equation for the generating function (noting that p'_i is constant). Classical mechanics is reduced to a solution of this equation.

It is customary to define

$$S = -G, \tag{1.66}$$

and to call S Hamilton's principal function. The reader might worry that we have already used S to denote the action; however, it is easy to see that there is a close connection between Hamilton's principal function and the action. If we differentiate $G(q^i, p'_i, t)$ with respect to time we have

$$\begin{aligned}\frac{d}{dt}G(q^i, p'_i, t) &= \frac{\partial G}{\partial t} + \frac{\partial G}{\partial q^i}\,\dot{q}^i + \frac{\partial G}{\partial p'_i}\,\dot{p}'_i \\ &= \frac{\partial G}{\partial t} - p_i\dot{q}^i,\end{aligned}$$

using $\dot{p}'_i = 0$ and (1.46). Because of (1.65) we have

$$\frac{d}{dt}G = H - p_i\dot{q}^i = -L,$$

where L is the Lagrangian. Integrating both sides of this with respect to time gives

$$G(t_2) - G(t_1) = -\int_{t_1}^{t_2} L\,dt.$$

This is in complete agreement with our earlier result in (1.43).

1.4.3 Symplectic form and invariance of Poisson brackets

The distinction between what we call coordinates q^i and what we call momenta p_i becomes unimportant in the Hamiltonian formulation of classical mechanics. This should be evident from canonical transformations which mix up coordinates and momenta. In fact it is possible to perform a canonical transformation $q^i \to p_i$ and $p_i \to -q^i$ which effectively interchanges the role of coordinates and momenta. This motivates looking at a more unified approach in which we define a phase space variable z^α with $\alpha = 1, 2, \ldots, 2n$ by

$$z^\alpha = (q^1, p_1, q^2, p_2, \ldots, q^n, p_n). \tag{1.67}$$

Explicitly, we have

$$z^\alpha = \begin{cases} q^i & \text{for } \alpha = 2i-1, i = 1, \ldots, n, \\ p_i & \text{for } \quad \alpha = 2i, i = 1, \ldots, n. \end{cases} \tag{1.68}$$

The Hamiltonian equations of motion (1.23) and (1.24) become

$$\dot{z}^{2i-1} = \frac{\partial H}{\partial z^{2i}}, \tag{1.69}$$

$$\dot{z}^{2i} = -\frac{\partial H}{\partial z^{2i-1}}, \tag{1.70}$$

when written in terms of the phase space variable z. We now regard $H = H(z^\alpha, t)$.

The two equations (1.69) and (1.70) can be unified into the single equation

$$\dot{z}^\alpha = \omega^{\alpha\beta}\frac{\partial H}{\partial z^\beta}, \tag{1.71}$$

if we define the $2n \times 2n$ matrix $\omega^{\alpha\beta}$ by

$$\omega^{2i-1\,2i} = 1 = -\omega^{2i\,2i-1}, \tag{1.72}$$

with all other components zero. This definition makes $\omega^{\alpha\beta}$ antisymmetric:

$$\omega^{\beta\alpha} = -\omega^{\alpha\beta}. \tag{1.73}$$

If we define the 2×2 matrix J by

$$J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \tag{1.74}$$

then $\omega^{\alpha\beta}$ are the matrix elements of the matrix ω obtained by taking

$$\omega = \begin{pmatrix} J & 0 & \cdots & 0 \\ 0 & J & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & 0 & J \end{pmatrix}. \tag{1.75}$$

In this form it is easy to see that

$$\omega^2 = -I_{2n}, \tag{1.76}$$

where I_{2n} is the $2n \times 2n$ identity matrix.

It is possible to view (1.71) as the Euler–Lagrange equation resulting from the Lagrangian L_c defined by

$$L_c(z, \dot{z}, t) = \frac{1}{2}\dot{z}^\alpha \omega_{\alpha\beta} z^\beta - H(z, t). \tag{1.77}$$

We use the subscript c to denote that this is in the canonical formalism.[13] $\omega_{\alpha\beta}$ is identically equal to $\omega^{\alpha\beta}$ with the index placement made for consistency with the Einstein summation convention. The proof that (1.71) is the Euler–Lagrange equation for L_c follows from defining

$$S_c[z(t)] = \int_{t_1}^{t_2} dt\, L_c(z, \dot{z}, t), \tag{1.78}$$

[13] We will establish the relationship between L_c and the normal Lagrangian L in a moment.

and using Hamilton's principle. If we write out (1.77) in detail by splitting up the indices as in (1.68), we have

$$\begin{aligned} L_c(z,\dot{z},t) &= \frac{1}{2}\dot{z}^{2i}\omega_{2i\,2i-1}z^{2i-1} + \frac{1}{2}\dot{z}^{2i-1}\omega_{2i-1\,2i}z^{2i} - H(z,t) \\ &= -\frac{1}{2}\dot{p}_i q^i + \frac{1}{2}\dot{q}^i p_i - H(q,p,t) \\ &= L(q,\dot{q},t) - \frac{d}{dt}\left(\frac{1}{2}p_i q^i\right). \end{aligned} \tag{1.79}$$

The canonical Lagrangian L_c is observed to differ from the usual Lagrangian by a total time derivative.

Any dynamical variable $A(q,p,t)$ can be regarded as a function $A(z,t)$ of z and t in this new phase space formalism. By computing the total time derivative of $A(z,t)$ we have

$$\begin{aligned} \frac{d}{dt}A(z^\alpha,t) &= \frac{\partial A}{\partial t} + \frac{\partial A}{\partial z^\alpha}\,\dot{z}^\alpha \\ &= \frac{\partial A}{\partial t} + \frac{\partial A}{\partial z^\alpha}\,\omega^{\alpha\beta}\,\frac{\partial H}{\partial z^\beta}. \end{aligned} \tag{1.80}$$

This agrees with our previous definition (1.30) in terms of Poisson brackets if we take

$$[A,B] = \frac{\partial A}{\partial z^\alpha}\,\omega^{\alpha\beta}\,\frac{\partial B}{\partial z^\beta}, \tag{1.81}$$

for any two dynamical variables A and B.

A canonical transformation can be regarded as a transformation from z^α to $z'^\alpha = z'^\alpha(z,t)$ leaving Hamilton's equations invariant. From the viewpoint of Hamilton's principle of stationary action, this will be guaranteed if

$$L'_c(z',\dot{z}',t) = L_c(z,\dot{z},t) - \frac{d}{dt}G \tag{1.82}$$

for some generating function G. From (1.77) we find

$$\frac{1}{2}\dot{z}'^\alpha\,\omega_{\alpha\beta}\,z'^\beta - H'(z',t) = \frac{1}{2}\dot{z}^\alpha\,\omega_{\alpha\beta}\,z^\beta - H(z,t) - \frac{dG}{dt}.$$

Rearrangement of this last result gives

$$dG = \frac{1}{2}\left(dz^\alpha\,\omega_{\alpha\beta}\,z^\beta - dz'^\alpha\,\omega_{\alpha\beta}\,z'^\beta\right) + \left(H'(z',t) - H(z,t)\right)dt. \tag{1.83}$$

Because z' is a function of both z and t, we have

$$dz'^\alpha = \frac{\partial z'^\alpha}{\partial z^\gamma}\,dz^\gamma + \frac{\partial z'^\alpha}{\partial t}\,dt. \tag{1.84}$$

Substitution of (1.84) back into (1.83) gives us

$$dG = \frac{1}{2}\left(\omega_{\alpha\beta}\, z^{\beta} - \frac{\partial z'^{\,\gamma}}{\partial z^{\alpha}}\,\omega_{\gamma\beta}\, z'^{\,\beta}\right) dz^{\alpha} + \left(H'(z',t) - H(z,t) - \frac{1}{2}\,\frac{\partial z'^{\,\alpha}}{\partial t}\,\omega_{\alpha\beta}\, z'^{\,\beta}\right) dt. \tag{1.85}$$

If we regard G as a function of z^{α} and t, then

$$dG = \frac{\partial G}{\partial z^{\alpha}}\, dz^{\alpha} + \frac{\partial G}{\partial t}\, dt. \tag{1.86}$$

Comparing the coefficients of dz^{α} and dt between (1.85) and (1.86) leads to the conclusions

$$\frac{\partial G}{\partial z^{\alpha}} = \frac{1}{2}\,\omega_{\alpha\beta}\, z^{\beta} - \frac{1}{2}\,\frac{\partial z'^{\,\gamma}}{\partial z^{\alpha}}\,\omega_{\gamma\beta}\, z'^{\,\beta}, \tag{1.87}$$

$$\frac{\partial G}{\partial t} = H'(z',t) - H(z,t) - \frac{1}{2}\,\frac{\partial z'^{\,\alpha}}{\partial t}\,\omega_{\alpha\beta}\, z'^{\,\beta}. \tag{1.88}$$

The last equation (1.88) determines the transformed Hamiltonian in terms of the original one. The first condition (1.87) allows us to derive an important result. To do this, we begin by noting that the generating function should satisfy the condition

$$\frac{\partial^2 G}{\partial z^{\beta}\partial z^{\alpha}} = \frac{\partial^2 G}{\partial z^{\alpha}\partial z^{\beta}}, \tag{1.89}$$

if it is to be a smooth function, that we demand. Differentiating (1.87) with respect to z^{β} results in

$$\frac{\partial^2 G}{\partial z^{\beta}\partial z^{\alpha}} = \frac{1}{2}\,\omega_{\alpha\beta} - \frac{1}{2}\,\frac{\partial^2 z'^{\,\gamma}}{\partial z^{\beta}\partial z^{\alpha}}\,\omega_{\gamma\delta}\, z'^{\,\delta} - \frac{1}{2}\,\frac{\partial z'^{\,\gamma}}{\partial z^{\alpha}}\,\omega_{\gamma\delta}\,\frac{\partial z'^{\,\delta}}{\partial z^{\beta}}. \tag{1.90}$$

Using this result in (1.89), along with the same expression with the indices α and β interchanged, and noting that because the transformation $z \to z'$ is assumed to be smooth,

$$\frac{\partial^2 z'^{\,\gamma}}{\partial z^{\beta}\partial z^{\alpha}} = \frac{\partial^2 z'^{\,\gamma}}{\partial z^{\alpha}\partial z^{\beta}},$$

we have simply

$$\omega_{\alpha\beta} - \frac{\partial z'^{\,\gamma}}{\partial z^{\alpha}}\,\omega_{\gamma\delta}\,\frac{\partial z'^{\,\delta}}{\partial z^{\beta}} = \omega_{\beta\alpha} - \frac{\partial z'^{\,\gamma}}{\partial z^{\beta}}\,\omega_{\gamma\delta}\,\frac{\partial z'^{\,\delta}}{\partial z^{\alpha}}.$$

Because $\omega_{\alpha\beta}$ is antisymmetric (see (1.73)), it is easily shown from this last result upon relabelling indices that

$$\frac{\partial z'^{\gamma}}{\partial z^{\alpha}}\,\omega_{\gamma\delta}\,\frac{\partial z'^{\delta}}{\partial z^{\beta}} = \omega_{\alpha\beta}. \tag{1.91}$$

This is the condition that the canonical transformation must satisfy. Such a transformation is called a symplectic transformation, and the matrix ω is referred to as a symplectic matrix. It is straightforward to show from (1.87) and (1.88) that

$$\frac{\partial^2 G}{\partial t \partial z^{\alpha}} = \frac{\partial^2 G}{\partial z^{\alpha} \partial t}, \tag{1.92}$$

if (1.91) holds.

Having gone this far, it is now easy to prove that the Poisson bracket of any two functions of the canonical variables is invariant under a canonical transformation. To do this, we first write (1.91) in an equivalent form. Let

$$\mathsf{J}^{\alpha}{}_{\beta} = \frac{\partial z'^{\alpha}}{\partial z^{\beta}}, \tag{1.93}$$

and

$$\left(\mathsf{J}^{-1}\right)^{\alpha}{}_{\beta} = \frac{\partial z^{\alpha}}{\partial z'^{\beta}}. \tag{1.94}$$

J is regarded as a $2n \times 2n$ matrix whose elements are made up of the partial derivatives of the transformation. The determinant of J gives the Jacobian of the transformation. We can write (1.91) as

$$\mathsf{J}^{\gamma}{}_{\alpha}\,\omega_{\gamma\delta}\,\mathsf{J}^{\delta}{}_{\beta} = \omega_{\alpha\beta}, \tag{1.95}$$

It is easier to dispense with the index notation and write (1.95) in matrix form as

$$\mathsf{J}^{T}\,\omega\,\mathsf{J} = \omega, \tag{1.96}$$

where J^{T} is the transpose matrix.[14] If we take the inverse of (1.96) we obtain

$$\mathsf{J}^{-1}\,\omega^{-1}\,\left(\mathsf{J}^{T}\right)^{-1} = \omega^{-1}.$$

However, because of (1.76) we can see that the inverse of ω is simply the negative: $\omega^{-1} = -\omega$. If we use $\omega^{-1} = -\omega$ in the previous result it is easily seen that

$$\mathsf{J}^{-1}\,\omega\,\left(\mathsf{J}^{-1}\right)^{T} = \omega, \tag{1.97}$$

[14] The introduction of the transpose is necessary because the indices in the first factor on the left-hand side of (1.95) are not in the correct order for a matrix multiplication.

or reverting back to index notation,

$$\frac{\partial z^\alpha}{\partial z'^\gamma}\,\omega^{\gamma\delta}\,\frac{\partial z^\beta}{\partial z'^\delta} = \omega^{\alpha\beta}, \tag{1.98}$$

using (1.94). We write the indices on ω as shown for consistency with the summation convention.

Now suppose that $A_i(z,t)$, where $i = 1,\ldots,N$ are any functions of the canonical variables transforming like

$$A_i(z,t) = A'_i[z'(z,t),t], \tag{1.99}$$

under a canonical transformation. We can compute the Poisson bracket between any two of them using either the original coordinates z^α or the transformed coordinates z'^α. Using the transformed coordinates, we have from (1.81)

$$[A'_1, A'_2]' = \frac{\partial A'_1}{\partial z'^\alpha}\,\omega^{\alpha\beta}\,\frac{\partial A'_2}{\partial z'^\beta}. \tag{1.100}$$

Using the chain rule for partial derivatives on the right-hand side of (1.100), along with the assumption (1.99), we find

$$[A'_1, A'_2]' = \frac{\partial A_1}{\partial z^\gamma}\,\frac{\partial z^\gamma}{\partial z'^\alpha}\,\omega^{\alpha\beta}\,\frac{\partial z^\delta}{\partial z'^\beta}\,\frac{\partial A_2}{\partial z^\delta}. \tag{1.101}$$

The symplectic property (1.98) allows us to reduce the middle three terms on the right-hand side of (1.101) to give

$$\begin{aligned}[A'_1, A'_2]' &= \frac{\partial A_1}{\partial z^\gamma}\,\omega^{\gamma\delta}\,\frac{\partial A_2}{\partial z^\delta} \\ &= [A_1, A_2],\end{aligned} \tag{1.102}$$

where the definition (1.81) of the Poisson bracket has been used. This proves that the Poisson bracket of any two functions of the canonical variables is invariant under a canonical transformation.

1.5 Conservation laws and symmetries

1.5.1 Noether's theorem

There is a general systematic way to discuss symmetries of a classical mechanical system using the action and Hamilton's principle. This approach proves very useful when we consider continuous matter distributions, as in field theory. Because this is our intention, we will be slightly more general here than we need to be. The two subsections after this one

will show how the general framework we develop here can be applied to non-relativistic and relativistic particle mechanics respectively.

Our first task will be to define the transformation describing the symmetry. We will consider only an infinitesimal transformation and allow it to depend on a set of r infinitesimal parameters $\delta\epsilon^A$, with $A = 1, \ldots, r$. These parameters characterize the transformation and could include angles of rotation or a translation of axes for example, although we need not specify them at this stage. We will also allow the time coordinate to transform, since we will later wish to link invariance under such a transformation to energy conservation. Let the infinitesimal transformation be

$$t' = t + \delta t = t + \lambda_A(t)\delta\epsilon^A, \tag{1.103}$$

$$q'^i(t') = q^i(t) + \Phi^i{}_A[t, q^i(t)]\delta\epsilon^A. \tag{1.104}$$

Here $\lambda_A(t)$ and $\Phi^i{}_A(t, q^i)$ are sets of functions specific to, and defining, a given transformation.[15]

The next task is to state with precision what we mean by a symmetry of the system. A symmetry of the system will be defined as a transformation of the time and generalized coordinates whose infinitesimal form is given by (1.103) and (1.104) and which leaves the equations of motion invariant. Under the transformation (1.103) and (1.104), the action functional will change from $S[q(t)]$ to

$$S[q'(t')] = \int_{t'_1}^{t'_2} dt'\, L\left[t', q'^i(t'), \dot{q}'^i(t')\right]. \tag{1.105}$$

Upon application of Hamilton's principle of stationary action, from which the equations of motion follow, $S[q(t)]$ and $S[q'(t')]$ must give rise to the same equations of motion. A sufficient condition for this to be true occurs when $S[q(t)] = S[q'(t')]$, meaning that the action is invariant under the transformation. While this may be the case for certain classes of transformations, it is not a general requirement for invariance of the equations of motion; that is, invariance of the action is not a necessary condition for invariance of the equations of motion. This also becomes obvious if we recall that we can freely add a total time derivative to the Lagrangian without affecting the equations of motion, because they follow upon variation with respect to $q^i(t)$ with $q^i(t)$ fixed at the initial and final times. The general condition for $S[q'(t')]$ and $S[q(t)]$ to give rise to the same equations of motion is that

$$S[q'(t')] = S[q(t)] + F_2 - F_1, \tag{1.106}$$

[15] Examples will be given in the next two subsections.

where $F_2(F_1)$ depends only on the final (initial) time. When we vary (1.106) with the endpoints held fixed, we will have $\delta S[q'(t')] = \delta S[q(t)]$, and therefore will obtain the same equations of motion.

If we set $\delta\epsilon^A = 0$ in (1.103) and (1.104), this will correspond to the identity transformation (since nothing will change) and accordingly $F_2 - F_1$ in (1.106) must vanish. We therefore expect $F_2 - F_1$ to depend linearly on $\delta\epsilon^A$ to lowest order in the infinitesimal parameters. We will define a set of quantities Δ^A by

$$F_2 - F_1 = \int_{t_1}^{t_2} dt \, \frac{d}{dt} \left\{ \Delta_A[t, q^i(t)] \delta\epsilon^A \right\}. \tag{1.107}$$

A necessary and sufficient condition for a transformation to have a form-invariant action is for $\Delta_A = 0$. Given a transformation (1.103) and (1.104) we can calculate Δ_A from (1.106) and (1.107). We will see an application of this in Section 1.5.2. For the remainder of the section we proceed quite generally.

Our next task is to relate $S[q'(t')]$ to $S[q(t)]$ under the transformation (1.103) and (1.104). We will work to first order in the small quantities $\delta\epsilon^A$. If we change variables from t' to t in the integral of (1.105) we will find

$$\begin{aligned} S[q'(t')] - S[\,q(t)] = \textstyle\int_{t_1}^{t_2} dt \Big\{ \frac{dt'}{dt} \, L \left[t + \delta t, q'^i(t + \delta t), \dot{q}'^i(t + \delta t) \right] \\ - L \left[t, q^i(t), \dot{q}^i(t) \right] \Big\}. \end{aligned} \tag{1.108}$$

The change of time variable in $S[q'(t')]$ is motivated by the desire to write both terms on the left-hand side of (1.108) under the same integral.

Our objective is to expand the integral of (1.108) to first order in $\delta\epsilon^A$, and show that the result can be expressed as a total time derivative. When the result is used back in (1.106) with (1.107), this will lead to a set of conserved quantities.

From (1.103) we find

$$\frac{dt'}{dt} = 1 + \dot{\lambda}_A(t) \delta\epsilon^A. \tag{1.109}$$

For later use we also record

$$\frac{dt}{dt'} \simeq 1 - \dot{\lambda}_A(t) \delta\epsilon^A, \tag{1.110}$$

since $\frac{dt}{dt'} = \left(\frac{dt'}{dt}\right)^{-1}$ and we expand to first order in $\delta\epsilon^A$. Using (1.109) in (1.108) results in

$$\begin{aligned} S[q'(t')] - S[q(t)] \simeq \int_{t_1}^{t_2} dt \Big\{ & L\left[t+\delta t, q'^i(t+\delta t), \dot{q}'^i(t+\delta t)\right] \\ & + \dot{\lambda}_A(t)\delta\epsilon^A L\left[t, q^i(t), \dot{q}^i(t)\right] \\ & - L\left[t, q^i(t), \dot{q}^i(t)\right] \Big\}. \end{aligned} \tag{1.111}$$

The middle term has been obtained by noting that to first order in $\delta\epsilon^A$,

$$\delta\epsilon^A L\left[t+\delta t, q'^i(t+\delta t), \dot{q}'^i(t+\delta t)\right] \simeq \delta\epsilon^A L\left[t, q^i(t), \dot{q}^i(t)\right], \tag{1.112}$$

as should be obvious from (1.103) and (1.104).

The next step is to Taylor expand the first term in the integrand of (1.111). Expansion of the first two arguments of the Lagrangian follows quite simply from (1.103) and (1.104). We therefore only need to find out how the velocity term transforms under (1.103) and (1.104). By definition,

$$\begin{aligned} \dot{q}'^i(t') &= \frac{d}{dt'} q'^i(t') \\ &= \frac{dt}{dt'}\frac{d}{dt} q'^i(t+\delta t) \\ &\simeq \left[1 - \dot{\lambda}_A(t)\delta\epsilon^A\right] \frac{d}{dt}\left\{q^i(t) + \Phi^i{}_A[t, q^i(t)]\delta\epsilon^A\right\} \\ &\simeq \dot{q}^i(t) + \dot{\Phi}^i{}_A\delta\epsilon^A - \dot{\lambda}_A\delta\epsilon^A\dot{q}^i(t), \end{aligned} \tag{1.113}$$

if we use (1.110) and (1.104).[16] Expanding out the first term on the right-hand side of (1.111) using (1.103), (1.104), and (1.113) gives

$$\begin{aligned} S[q'(t')] - S[q(t)] \simeq \int_{t_1}^{t_2} dt\, \delta\epsilon^A \Bigg[& \lambda_A \frac{\partial L}{\partial t} + \Phi^i{}_A \frac{\partial L}{\partial q^i} + \dot{\lambda}_A L \\ & + \left(\dot{\Phi}^i{}_A - \dot{\lambda}_A \dot{q}^i\right) \frac{\partial L}{\partial \dot{q}^i} \Bigg]. \end{aligned} \tag{1.114}$$

where we do not write out the arguments of the functions for brevity.

[16] Note that $\dot{\Phi}^i{}_A = (d/dt)\,\Phi^i{}_A[t, q^i(t)]$ is the total time derivative, not just the partial derivative.

The final step is to show that the integrand in (1.114) can be expressed as a total time derivative. To this end, first note that

$$\begin{aligned}\frac{d}{dt}\left(\lambda_A L - \lambda_A \dot{q}^i \frac{\partial L}{\partial \dot{q}^i}\right) &= \dot{\lambda}_A L + \lambda_A \left(\frac{\partial L}{\partial t} + \dot{q}^i \frac{\partial L}{\partial q^i} + \ddot{q}^i \frac{\partial L}{\partial \dot{q}^i}\right) \\ &\quad - \dot{\lambda}_A \dot{q}^i \frac{\partial L}{\partial \dot{q}^i} - \lambda_A \ddot{q}^i \frac{\partial L}{\partial \dot{q}^i} - \lambda_A \dot{q}^i \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}^i}\right) \\ &= \dot{\lambda}_A L + \lambda_A \frac{\partial L}{\partial t} - \dot{\lambda}_A \dot{q}^i \frac{\partial L}{\partial \dot{q}^i}, \end{aligned} \tag{1.115}$$

if we use the Euler–Lagrange equations to simplify. Secondly,

$$\begin{aligned}\frac{d}{dt}\left(\Phi^i{}_A \frac{\partial L}{\partial \dot{q}^i}\right) &= \dot{\Phi}^i_A \frac{\partial L}{\partial \dot{q}^i} + \Phi^i{}_A \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}^i}\right) \\ &= \dot{\Phi}^i{}_A \frac{\partial L}{\partial \dot{q}^i} + \Phi^i_A \frac{\partial L}{\partial q^i}, \end{aligned} \tag{1.116}$$

again simplifying by using the Euler–Lagrange equations. The identities established in (1.115) and (1.116) may be used in (1.114) with the result

$$S[q'(t')] - S[q(t)] \simeq \int_{t_1}^{t_2} dt\, \delta\epsilon^A \frac{d}{dt}\left(\lambda_A L - \lambda_A \dot{q}^i \frac{\partial L}{\partial \dot{q}^i} + \Phi^i_A \frac{\partial L}{\partial \dot{q}^i}\right). \tag{1.117}$$

If we use the definition of the canonical momentum in (1.21) and the Hamiltonian in (1.22), this allows us to express

$$S[q'(t')] - S[q(t)] \simeq \int_{t_1}^{t_2} dt\, \delta\epsilon^A \frac{d}{dt}\left(\Phi^i_A p_i - \lambda_A H\right). \tag{1.118}$$

Using this result back in (1.106), with $F_2 - F_1$ given in (1.107), yields

$$0 = \int_{t_1}^{t_2} dt\, \frac{d}{dt}\left[\delta\epsilon^A \left(\Phi^i{}_A p_i - \lambda_A H - \Delta_A\right)\right]. \tag{1.119}$$

This proves that

$$G(t) = \delta\epsilon^A (\Phi^i{}_A p_i - \lambda_A H - \Delta_A), \tag{1.120}$$

is a constant of the motion. Since the infinitesimal parameters are arbitrary and independent, we have a set of N conserved quantities given by

$$G_A(t) = \Phi^i{}_A p_i - \lambda_A H - \Delta_A. \tag{1.121}$$

This is the essential content of Noether's theorem: For any continuous symmetry of the system there is a conserved quantity (i.e. a conservation law). Note that the theorem as proven does not apply to any

transformation which cannot be expressed in the form of (1.103) and (1.104). This includes all discrete symmetries, such as a reflection of coordinates for example, since discrete symmetries cannot be written in a form infinitesimally close to the identity.

1.5.2 Non-relativistic particle

We will now apply the general formalism of the previous subsection to the case of a system of non-relativistic interacting particles. Assume that the I^{th} particle has mass m_I and position vector $\mathbf{x}_I(t)$ at time t with respect to some origin of coordinates which can be arbitrary. Take the Lagrangian to be

$$L\left(t, \mathbf{x}_I(t), \dot{\mathbf{x}}_I(t)\right) = \sum_{I=1}^{N} \frac{1}{2}\, m_I\, \dot{\mathbf{x}}_I^2(t) - V\left(t, \mathbf{x}_I(t)\right). \tag{1.122}$$

Here $V\left(t, \mathbf{x}_I(t)\right)$ is the potential, which we assume depends at most on the time and position of the particles. The action is

$$S\left[\mathbf{x}_I(t)\right] = \int_{t_1}^{t_2} dt \left\{ \sum_{I=1}^{N} \frac{1}{2}\, m_I\, \dot{\mathbf{x}}_I^2(t) - V\left(t, \mathbf{x}_I(t)\right) \right\}, \tag{1.123}$$

from which the equations of motion

$$m_I \ddot{\mathbf{x}}_I(t) = -\nabla_I V\left(t, \mathbf{x}_I(t)\right) \tag{1.124}$$

may be found by using Hamilton's principle. (∇_I denotes the gradient with respect to $\mathbf{x}_I$.)

We will first look at invariance under a translation in time and show how this is related to the conservation of energy. Let

$$t' = t + \delta\epsilon, \tag{1.125}$$

$$\mathbf{x}_I'(t') = \mathbf{x}_I(t), \tag{1.126}$$

with $\delta\epsilon$ infinitesimal. Comparison with (1.103) shows that

$$\lambda_A = 1, \tag{1.127}$$

$$\Phi^i{}_A = 0. \tag{1.128}$$

It is easy to see from (1.123) that

$$S\left[\mathbf{x}_I'(t')\right] - S\left[\mathbf{x}_I(t)\right] \simeq -\int_{t_1}^{t_2} dt\, \delta\epsilon\, \frac{\partial V\left(t, \mathbf{x}_I(t)\right)}{\partial t}, \tag{1.129}$$

if (1.125) and (1.126) are used.

From the discussion leading up to (1.106) and (1.107), we will only have (1.125) and (1.126), a symmetry of the equations of motion if the integrand of (1.129) can be expressed as a total (rather than a partial) time derivative. This can happen in two cases. The first is if V has no dependence on the coordinates $\mathbf{x}_I(t)$, so that the only time dependence in V is an explicit dependence. A consequence of this is that V does not affect the equations of motion (1.124) and the particles do not interact, which is equivalent to taking $V = 0$. We may therefore specialize to $V = V(\mathbf{x}_I(t))$ only, since $V = 0$ is a special case of this. If the potential has no explicit time dependence, then the right-hand side of (1.129) vanishes and we have

$$\Delta_A = 0. \tag{1.130}$$

The action is therefore form-invariant in this case. It is obvious from the equations of motion (1.124) that they are only invariant under (1.125) and (1.126) if $\frac{\partial}{\partial t}V = 0$.

It is now a simple consequence of our general result (1.121) to link invariance of the system of particles under an infinitesimal time translation to conservation of energy (just use (1.127), (1.128), (1.130) in (1.121)). A necessary condition for conservation of energy to hold is that the Lagrangian, and hence the Hamiltonian, have no explicit dependence on the time. Admittedly, this is rather a long-winded and cumbersome way to deduce the conservation of energy; nevertheless, it is gratifying to see how it arises from the general framework embodied in Noether's theorem.

We turn next to invariance under an arbitrary translation of the spatial coordinates specified by

$$t' = t, \tag{1.131}$$

$$\mathbf{x}'_I(t') = \mathbf{x}_I(t) + \delta\epsilon. \tag{1.132}$$

Note that this corresponds to a translation of the origin of the coordinate system, so that the positions of all particles get shifted by the same amount. This will only be a symmetry of the equations of motion (1.124) if the potential is translationally invariant.[17] The most important case where this occurs is for potentials which only depend on the relative distances between the particles:

$$V = V(t, |\mathbf{x}_I - \mathbf{x}_J|). \tag{1.133}$$

[17] It can have an explicit time dependence in this case.

This includes particles under Newtonian gravity, and charged particles with Coulomb interactions. Because $|\mathbf{x}'_I - \mathbf{x}'_J| = |\mathbf{x}_I - \mathbf{x}_J|$ under a translation of the coordinate axes, for potentials of the form (1.133) it is easy to verify that the action is form-invariant, with Δ_A vanishing as in (1.130) again.

Using $\lambda_A = 0$ and $\mathbf{\Phi}_I = \delta\epsilon$ we find the conserved quantity

$$G(t) = \delta\epsilon \cdot \left(\sum_{I=1}^{N} \mathbf{p}_I \right), \tag{1.134}$$

showing that the total momentum of the system is constant. This provides a link between an invariance under translational symmetry and the conservation of momentum.

The next case we will look at is a symmetry transformation consisting of an infinitesimal rotation of the coordinate axes. To make things as simple as possible, we will adopt Cartesian coordinates in three spatial dimensions, and pick the axis of rotation to be the z-axis. The situation is pictured in Fig. 1.2.

$$x'_I = x_I \cos\delta\epsilon + y_I \sin\delta\epsilon \simeq x_I + \delta\epsilon\, y_I, \tag{1.135}$$
$$y'_I = y_I \cos\delta\epsilon - x_I \sin\delta\epsilon \simeq -\delta\epsilon\, x_I + y_I, \tag{1.136}$$
$$z'_I = z_I, \tag{1.137}$$
$$t' = t. \tag{1.138}$$

We again have $\lambda_A = 0$ since the time coordinate is unchanged. For potentials of the form (1.133), because the rotation of coordinates does not affect the relative distances between particles, the transformation

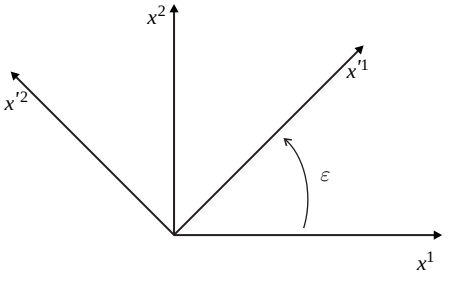

Fig. 1.2 This shows the transformation obtained by a rotation of coordinate axes by a finite angle ϵ about the z-axis in three spatial dimensions. We have called $x = x^1$ and $y = x^2$ here. The infinitesimal rotation is obtained by setting $\epsilon = \delta\epsilon$.

will be a symmetry of the equations of motion, and the action will be form-invariant: $\Delta_A = 0$ again. From (1.120) the conserved quantity corresponding to invariance under (1.135)–(1.138) is

$$G(t) = \sum_{I=1}^{N} \delta\epsilon \left(y_I p_I^1 - x_I p_I^2 \right) \tag{1.139}$$

$$= -\delta\epsilon \, L^3, \tag{1.140}$$

where L^3 is the z-component of the total angular momentum, and we denote the x and y components of linear momentum by superscripts 1 and 2 respectively. Thus invariance under a rotation about the z-axis corresponds to conservation of the z-component of the angular momentum. It should be obvious from this that invariance under a rotation about an arbitrary axis will be linked to the conservation of angular momentum about that axis.

One final symmetry transformation we wish to discuss is invariance under Galilean transformations. This corresponds to the transformation

$$t' = t, \tag{1.141}$$

$$\mathbf{x}_I'(t') = \mathbf{x}_I(t) - t\delta\epsilon, \tag{1.142}$$

which represents relative motion between two sets of coordinate axes with constant relative velocity $\delta\epsilon$, taken to be infinitesimal. For potentials of the form (1.133), this will be a symmetry of the equations of motion (1.124). The Galilean symmetry gives us our first case where the action is not invariant under the transformation. It is easy to see, working to first order in $\delta\epsilon$, that

$$S[\mathbf{x}_I'] - S[\mathbf{x}_I] \simeq -\int_{t_1}^{t_2} dt \, \sum_{I=1}^{N} m_I \, \delta\epsilon \cdot \dot{\mathbf{x}}_I. \tag{1.143}$$

Noting that

$$\mathbf{P} = \sum_{I=1}^{N} m_I \, \dot{\mathbf{x}}_I \tag{1.144}$$

is just the total momentum of the system, we see that the action is only form-invariant if $\mathbf{P} = 0$, which is not the case in general. However the right-hand side of (1.143) can be expressed as a total time derivative, and from comparison with (1.107) we have

$$\Delta_A \delta\epsilon^A = -\sum_{I=1}^{N} m_I \, \delta\epsilon \cdot \mathbf{x}_I. \tag{1.145}$$

The right-hand side of this expression has an interpretation as well, since

$$\mathbf{x}_{cm} = \frac{1}{M}\sum_{I=1}^{N} m_I\,\mathbf{x}_I \tag{1.146}$$

is the position of the centre of mass of the system. Here $M = \sum_{I=1}^{N} m_I$ is the total mass of the system. We can write

$$\Delta_A \delta\epsilon^A = -M\delta\epsilon\cdot\mathbf{x}_{cm}. \tag{1.147}$$

The conserved quantity under a Galilean transformation follows from (1.120) as

$$\begin{aligned} G(t) &= -\sum_{I=1}^{N} t\,\delta\epsilon\cdot\mathbf{p}_I + M\delta\epsilon\cdot\mathbf{x}_{cm} \\ &= \delta\epsilon\cdot\mathbf{G}, \end{aligned}$$

where

$$\mathbf{G}(t) = M\mathbf{x}_{cm} - t\mathbf{P}. \tag{1.148}$$

If we use the constancy of $\mathbf{P}$ as implied by invariance under spatial translations, this shows that invariance under Galilean transformations implies that the centre of mass moves with constant velocity given by

$$\mathbf{V}_{cm} = \frac{\mathbf{P}}{M}. \tag{1.149}$$

Recognizing that $\Delta_A \neq 0$, meaning that the action is not form-invariant under a Galilean transformation, is crucial in obtaining the correct conservation law. In the special case where $V = 0$, meaning that we have a system of free particles, it is easy to evaluate the action (1.123) exactly and verify this. This is because (1.124) implies that the velocity of each particle is constant, so we find

$$S = \sum_{I=1}^{N} \frac{m_I|\mathbf{x}_I(t_2) - \mathbf{x}_I(t_1)|^2}{2(t_2 - t_1)}. \tag{1.150}$$

This is manifestly invariant under a time translation, spatial translation, and rotation of axes, but not under a Galilean transformation, since

$$\mathbf{x}'_I(t_2) - \mathbf{x}'_I(t_1) = \mathbf{x}_I(t_2) - \mathbf{x}_I(t_1) - (t_2 - t_1)\delta\epsilon.$$

Using

$$|\mathbf{x}'_I(t_2) - \mathbf{x}'_I(t_1)|^2 \simeq |\mathbf{x}_I(t_2) - \mathbf{x}_I(t_1)|^2 - 2(t_2 - t_1)\delta\epsilon\cdot\left[\mathbf{x}_I(t_2) - \mathbf{x}_I(t_1)\right],$$

it is easy to reproduce (1.143).

1.5.3 Relativistic particle

In non-relativistic mechanics the Lagrangian L has always been taken as the difference between the kinetic and the potential energies. However, this may not always be the case as we will now see. We will consider the relativistic free particle in this section. A brief review of special relativity can be found in Appendix 2.

One way to proceed is to use the relativistic expressions for the energy and momentum which are

$$E = \gamma mc^2, \tag{1.151}$$

$$\mathbf{p} = \gamma m\mathbf{v}, \tag{1.152}$$

where

$$\gamma = \left(1 - \frac{v^2}{c^2}\right)^{-1/2}, \tag{1.153}$$

and m is the particle rest mass. We expect that the Hamiltonian for a free particle should be the total energy E, so that

$$H = \gamma mc^2 = \left(p^2c^2 + m^2c^4\right)^{1/2} \tag{1.154}$$

where the second equality is obtained by solving (1.152) and (1.153) for $v = |\mathbf{v}|$ in terms of $p = |\mathbf{p}|$. The Lagrangian can be defined in terms of H by the usual Legendre transformation

$$\begin{aligned} L &= \mathbf{p}\cdot\mathbf{v} - H \\ &= \gamma mv^2 - \gamma mc^2 \\ &= -mc^2\left(1 - \frac{v^2}{c^2}\right)^{1/2}. \end{aligned} \tag{1.155}$$

Naively, we would have expected that L should equal the relativistic kinetic energy $T = (\gamma - 1)mc^2$, and it is clear that this is not the case here. Note however that if $v << c$, then L in (1.155) becomes $L \simeq -mc^2 + \frac{1}{2}mv^2$. Apart from the constant rest mass energy term, we recover the non-relativistic result for the Lagrangian in this limit.

Another way to arrive at (1.155) is to require that

$$p_i = \frac{\partial L}{\partial \dot{x}^i}, \tag{1.156}$$

where p_i are the components of the relativistic momentum which we have defined in (1.152). Integration of (1.156) leads to (1.155), up to an additive constant of integration. Since this constant of integration cannot affect

the equation of motion, we can fix it how we like, and recover (1.155) by choosing it to vanish.

Given the Lagrangian (1.155) we can form the action functional in the usual way

$$S = \int_{t_1}^{t_2} dt\, L = -mc^2 \int_{t_1}^{t_2} dt \left(1 - \frac{v^2}{c^2}\right)^{1/2}. \tag{1.157}$$

Recalling the definition of the proper time interval

$$d\tau = dt \left(1 - \frac{v^2}{c^2}\right)^{1/2}, \tag{1.158}$$

it is observed that

$$S = -mc^2 \int_{\tau_1}^{\tau_2} d\tau. \tag{1.159}$$

Hamilton's principle states that the motion of the particle is such that the proper time is stationary.

It is possible to obtain other equivalent forms for the action of a relativistic particle. If we use the definition of the proper time in terms of the coordinate differentials

$$c^2 d\tau^2 = \eta_{\mu\nu} dx^\mu dx^\nu, \tag{1.160}$$

then we can choose

$$c d\tau = \left[\eta_{\mu\nu} dx^\mu dx^\nu\right]^{1/2}. \tag{1.161}$$

Now let λ be any parameter along the particle's worldline, so that we can write $x^\mu(\lambda)$ for the worldline.[18] Then we have

$$c d\tau = \left[\eta_{\mu\nu} \frac{dx^\mu}{d\lambda} \frac{dx^\nu}{d\lambda}\right]^{1/2} d\lambda, \tag{1.162}$$

and we see that (1.159) may be expressed as

$$S = -mc \int_{\lambda_1}^{\lambda_2} d\lambda \left[\eta_{\mu\nu} \frac{dx^\mu}{d\lambda} \frac{dx^\nu}{d\lambda}\right]^{1/2}. \tag{1.163}$$

In this form the action is seen to be invariant under an arbitrary change $\lambda \to \lambda'$ of the worldline parameter.[19] Variation of (1.163) with respect

[18] We assume that there is a 1-1 relationship between λ and τ.

[19] If we choose $\lambda = \tau$ we recover (1.159).

to $x^\mu(\lambda)$, keeping the endpoints of the path fixed, results in the Euler–Lagrange equation

$$\frac{d}{d\lambda}\left\{\left[\eta_{\mu\nu}\frac{dx^\mu}{d\lambda}\frac{dx^\nu}{d\lambda}\right]^{-1/2}\frac{dx^\sigma}{d\lambda}\right\}=0. \tag{1.164}$$

If we now identify $\lambda=\tau$ and use (1.160), this reduces to

$$\frac{d^2x^\sigma}{d\tau^2}=0, \tag{1.165}$$

which is the equation of motion for a relativistic free particle.

There is another form for the action which is frequently used because it does not have the square root present in (1.163):

$$\tilde{S}=-\frac{1}{2}m\int_{\lambda_1}^{\lambda_2}d\lambda\,\eta_{\mu\nu}\frac{dx^\mu}{d\lambda}\frac{dx^\nu}{d\lambda}. \tag{1.166}$$

This form for the action differs from (1.163) and is no longer invariant under an arbitrary change $\lambda\to\lambda'$ of the worldline parameter. When using this form, the understanding is that we vary the path first with λ arbitrary, and then set $\lambda=\tau$ at the end, so that (1.165) is regained.

We will now look at the invariance of the equations of motion for a relativistic free particle and the associated conservation laws. Instead of looking at time and spatial translations separately, in the spirit of special relativity we will look at

$$x'^\mu(\lambda)=x^\mu(\lambda)+\delta\epsilon^\mu. \tag{1.167}$$

The worldline parameter λ is analogous to the time in the non-relativistic case of Section 1.5.2, and we keep it fixed here.[20] Because $dx'^\mu=dx^\mu$ under (1.167), the action (1.163) is form-invariant, and we have $\Delta_A=0$. The conserved quantity corresponding to invariance under the spacetime translation (1.167) is seen to be

$$G(\lambda)=\delta\epsilon^\mu\,\frac{\partial L}{\partial\,(dx^\mu/d\lambda)}. \tag{1.168}$$

With the Lagrangian in (1.163) we find

$$\frac{\partial L}{\partial\,(dx^\mu/d\lambda)}=-mc\left[\eta_{\alpha\beta}\frac{dx^\alpha}{d\lambda}\frac{dx^\beta}{d\lambda}\right]^{-1/2}\eta_{\mu\nu}\frac{dx^\nu}{d\lambda}. \tag{1.169}$$

[20] It is easy to see that under the infinitesimal translation $\lambda'=\lambda+\delta\epsilon$, Noether's theorem applied to (1.163) does not give any new conservation law.

Identification of $\lambda = \tau$ reduces the right-hand side to give

$$\frac{\partial L}{\partial \left(dx^\mu/d\lambda\right)} = -m\eta_{\mu\nu}\frac{dx^\nu}{d\lambda}. \tag{1.170}$$

It is conventional to define the 4-velocity U^μ by

$$U^\mu = \frac{dx^\mu}{d\tau}, \tag{1.171}$$

and the 4-momentum P^μ by

$$P^\mu = mU^\mu. \tag{1.172}$$

The conservation of 4-momentum is therefore linked to the invariance under a spacetime translation. Note that

$$\begin{aligned} P^0 &= m\frac{dx^0}{d\tau} \\ &= mc\frac{dt}{d\tau} \\ &= \gamma\, mc \qquad (1.173) \\ &= E/c, \qquad (1.174) \end{aligned}$$

where $E = \gamma\, mc^2$ is the total energy of the particle. The spatial components of the 4-momentum are

$$\begin{aligned} P^i &= m\frac{dx^i}{d\tau} \\ &= m\frac{dt}{d\tau}\frac{dx^i}{dt} \\ &= \gamma\, mv^i \qquad (1.175) \end{aligned}$$

corresponding to the relativistic momentum in (1.152). Thus conservation of both energy and momentum are subsumed in the single conservation law for 4-momentum.

For the non-relativistic particle we showed that conservation of angular momentum was linked to invariance under rotations of the axes. The analogous symmetry here is invariance under Lorentz transformations. The general form for the Lorentz transformation is

$$x'^\mu = L^\mu{}_\nu x^\nu, \tag{1.176}$$

with

$$\eta_{\alpha\beta} = L^\mu{}_\alpha L^\nu{}_\beta \eta_{\mu\nu}. \tag{1.177}$$

We will specify an infinitesimal Lorentz transformation by

$$L^{\mu}{}_{\nu} = \delta^{\mu}{}_{\nu} + \delta\epsilon^{\mu}{}_{\nu}, \tag{1.178}$$

where $\delta\epsilon^{\mu}{}_{\nu}$ are the infinitesimal parameters of the transformation. Substitution of (1.178) into (1.177) leads to

$$\begin{aligned}\eta_{\alpha\beta} &= \left(\delta^{\mu}{}_{\alpha} + \delta\epsilon^{\mu}{}_{\alpha}\right)\left(\delta^{\nu}{}_{\beta} + \delta\epsilon^{\nu}{}_{\beta}\right)\eta_{\mu\nu} \\ &\simeq \delta^{\mu}{}_{\alpha}\delta^{\nu}{}_{\beta}\eta_{\mu\nu} + \delta^{\mu}{}_{\alpha}\delta\epsilon^{\nu}{}_{\beta}\eta_{\mu\nu} + \delta\epsilon^{\mu}{}_{\alpha}\delta^{\nu}{}_{\beta}\eta_{\mu\nu} \\ &= \eta_{\mu\nu} + \delta\epsilon^{\nu}{}_{\beta}\eta_{\alpha\nu} + \delta\epsilon^{\mu}{}_{\alpha}\eta_{\mu\beta},\end{aligned} \tag{1.179}$$

if we work only to first order in $\delta\epsilon^{\mu}{}_{\nu}$. We may use the definition of the metric tensor as an index lowering operator to write $\delta\epsilon^{\mu}{}_{\alpha}\eta_{\mu\beta}$ as $\delta\epsilon_{\beta\alpha}$. This leaves us with

$$0 = \delta\epsilon_{\alpha\beta} + \delta\epsilon_{\beta\alpha}, \tag{1.180}$$

from (1.179). If we regard $\delta\epsilon_{\alpha\beta}$ as the components of a matrix, (1.180) shows that this matrix is antisymmetric. In the spacetime with D spatial dimensions (so the spacetime is $(D+1)$-dimensional), there are $\frac{1}{2}D(D+1)$ independent parameters (corresponding to the number of independent components of a $(D+1)\times(D+1)$ antisymmetric matrix). The fact that $\delta\epsilon_{\alpha\beta}$ is antisymmetric will prove important later on.

Our symmetry transformation is therefore

$$x'^{\mu} = x^{\mu} + \delta\epsilon^{\mu}{}_{\nu}x^{\nu}, \tag{1.181}$$

corresponding to an infinitesimal Lorentz transformation. The action is invariant under this transformation in either the form (1.163) or (1.166). Thus we have $\Delta_A = 0$ in the expression of Noether's theorem. (We also have $\lambda_A = 0$ here.) The conserved quantity under the transformation (1.181) is, from (1.120) and (1.170),

$$\begin{aligned}G(\tau) &= -\delta\epsilon^{\mu}{}_{\nu}x^{\nu}P_{\mu} \\ &= \frac{1}{2}\delta\epsilon_{\mu\nu}L^{\mu\nu}\end{aligned} \tag{1.182}$$

where

$$L^{\mu\nu} = x^{\mu}P^{\nu} - x^{\nu}P^{\mu}. \tag{1.183}$$

We can conclude that $L^{\mu\nu}$ is a conserved quantity. It is important to use the fact that $\delta\epsilon_{\alpha\beta} = -\delta\epsilon_{\beta\alpha}$ here meaning that only the antisymmetric part of $x^{\nu}P^{\mu}$ in $G(\tau)$ contributes to the summation over the dummy indices in (1.182).

If we compare the conserved quantity (1.183) with the analogous expression (1.139, 1.140) for the conservation law under spatial rotations

for the non-relativistic case, there is seen to be a similarity. In fact if we take μ and ν in (1.183) to be spatial indices (as opposed to a time index), then $L^{ij} = x^i P^j - x^j P^i$ is precisely the relativistic expression for the angular momentum.[21] The L^{0i} component is clearly

$$L^{0i} = ct\, P^i - x^i \frac{E}{c}, \tag{1.184}$$

using $x^0 = ct, P^0 = E/c$. We already know that E and P^i are constant, so the constancy of L^{0i} shows that

$$\frac{dx^i}{dt} = c^2 \frac{P^i}{E} \tag{1.185}$$

which relates the velocity to the momentum and energy. If we use (1.173) and (1.175), it is easily seen that (1.185) holds. There is a resemblance between the conserved quantity (1.184) and the result we found for the non-relativistic particle corresponding to a symmetry under Galilean transformations (see (1.148)). This can be furthered if we consider a system of relativistic particles. To avoid confusion with spatial indices, we will again label the different particles with capital Latin letters. Suppose we have N particles of rest of masses m_I with spatial positions x_I^i, with $I = 1, 2, \ldots, N$ labelling the different particles. Invariance under an arbitrary spacetime translation[22]

$$x_I'^{\mu} = x_I^{\mu} + \delta\epsilon^{\mu}, \tag{1.186}$$

shows that

$$P^{\mu} = \sum_{I=1}^{N} P_I^{\mu} \tag{1.187}$$

is conserved, where P_I^{μ} is the 4-momentum of the I^{th} particle. Invariance under an infinitesimal Lorentz transformation

$$x_I'^{\mu} = x_I^{\mu} + \delta\epsilon^{\mu}{}_{\nu} x_I^{\nu}, \tag{1.188}$$

leads to

$$L^{\mu\nu} = \sum_{I=1}^{N} L_I^{\mu\nu} \tag{1.189}$$

[21] For D different from 3, the angular momentum is specified by a tensor, rather than a vector. For $D = 3$ there are three independent components L^{12}, L^{23}, and L^{31} which can be identified as three components of a vector, corresponding to the vector cross-product $\mathbf{x} \times \mathbf{P}$.

[22] $x_I^0 = ct$ is independent of I since we are recording the particle positions at a given time for a single observer.

as the conserved quantity, where

$$L_I^{\mu\nu} = x_I^\mu P_I^\nu - x_I^\nu P_I^\mu, \tag{1.190}$$

is the angular momentum tensor for the I^{th} particle as in (1.183). Now

$$L^{0i} = \sum_{I=1}^{N} \left(ctP_I^i - x_I^i \frac{E_I}{c} \right) \tag{1.191}$$

is constant. We can define something like the centre of mass in the non-relativistic case by

$$x_{cm}^i = \frac{1}{E} \sum_{I=1}^{N} x_I^i E_I. \tag{1.192}$$

(Note that $E = \sum_{I=1}^{N} E_I$ is the total energy.) It is more correct to call x_{cm}^i the centre of energy here, rather than the centre of mass. With this definition we find

$$L^{0i} = ct\, P^i - \frac{E}{c}\, x_{cm}^i \tag{1.193}$$

to be constant. Using the constancy of the total energy E and the total momentum P^i we obtain

$$\frac{dx_{cm}^i}{dt} = c^2 \frac{P^i}{E}. \tag{1.194}$$

This is the relativistic generalization of (1.149). Note that if $v_I << c$, where v_I is the speed of the I^{th} particle, then

$$E = \sum_{I=1}^{N} m_I c^2 \left(1 - \frac{v_I^2}{c^2} \right)^{-1/2} \simeq Mc^2,$$

where M is the total rest mass of the system. The relativistic result, following from invariance under infinitesimal Lorentz transformations, therefore reduces to (1.149) in the non-relativistic limit.[23]

Notes

The material presented in this chapter provides only a bare outline of the basics of classical mechanics needed for an understanding of field

[23] Note that the centre of energy reduces to the centre of mass if $v_I << c$.

theory. There are many excellent textbooks on classical mechanics, but my two favourites are Goldstein (1950) and Lanczos (1971). A particularly good discussion of the Hamilton–Jacobi equation is given in Lanczos (1971). Our treatment of invariance of the Poisson bracket under canonical transformations in Section 1.4.3 does not make use of the introduction of Lagrange brackets as an alternative to Goldstein (1950) and Lanczos (1971). A good reference for Noether's theorem is Hill (1951).

2

Action principle in classical field theory

2.1 Continuous systems

So far we have been concerned with a single point particle moving in some potential. The extension to a system of point particles is fairly obvious since for non-interacting particles the energy is additive. This means that in the absence of interactions the total Lagrangian, or Hamiltonian, is obtained simply by summing over the individual Lagrangians or Hamiltonians. If L_i is the Lagrangian for the ith particle on its own, then $L = \sum_i L_i$, with a similar result for the Hamiltonian. In classical field theory we are concerned with a continuous distribution of mass and energy. For example, the electromagnetic field of a point charge (the Coulomb field) extends over all space. We can describe such a system using a Lagrangian or Hamiltonian framework. To begin with, our initial model will be a one-dimensional vibrating string.

Consider a string of total length ℓ with ends fixed at $x = 0$ and $x = \ell$. Assume that the string undergoes a small displacement from equilibrium in such a way that the tension in the string remains constant. Focus attention on a small element of string of length ds at a given time t. By taking ds arbitrarily small, the small segment of string can be considered as a straight line segment. Let $\psi(x,t)$ and $\psi(x+dx,t)$ be the displacements of the two ends of the segment at the given time t. The situation is pictured in Fig. 2.1.

The Pythagorean theorem gives

$$\begin{aligned} ds &= \left\{ dx^2 + [\psi(x+dx,t) - \psi(x,t)]^2 \right\}^{1/2} \\ &\simeq \left\{ 1 + \left[\frac{\partial \psi(x,t)}{\partial x} \right]^2 \right\}^{1/2} dx, \end{aligned} \tag{2.1}$$

if we expand $\psi(x+dx,t) \simeq \psi(x,t) + [\partial\psi(x,t)/\partial x]dx$ and work to first order in the small quantity dx.

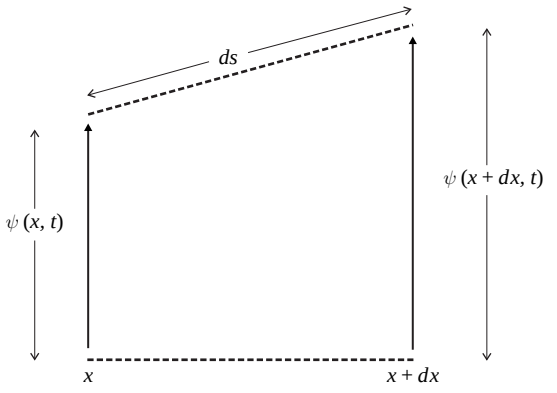

Fig. 2.1 This depicts the displacement of an infinitesimal element of string. For small displacements of the string from equilibrium the motion will be transverse to the direction of the length. If dx is the length of a small element when the string is at rest, ds represents the length of the stretched element.

The kinetic energy of the element of string is

$$dT = \frac{1}{2} dm \left(\frac{\partial \psi}{\partial t} \right)^2, \tag{2.2}$$

where dm is the mass of the element and $\partial\psi/\partial t$ is its velocity.[1] Let $dm = \rho(x)dx$ with $\rho(x)$ the mass per unit length. The total kinetic energy of the string is obtained by adding up the contribution from each little element over the whole length of the string:

$$T = \int_0^\ell \frac{1}{2} \rho(x) \left[\frac{\partial \psi(x,t)}{\partial t} \right]^2 dx. \tag{2.3}$$

The potential energy may be evaluated by considering the work done against the tension τ in increasing the length of the string from dx to ds. This results in an increase in potential energy of

$$\begin{aligned} dV &= \tau(ds - dx) \\ &= \tau \left\{ \left[1 + \left(\frac{\partial \psi}{\partial x} \right)^2 \right]^{1/2} - 1 \right\} dx \quad \text{(using (2.1))} \\ &\simeq \frac{1}{2} \tau \left(\frac{\partial \psi}{\partial x} \right)^2 dx, \end{aligned} \tag{2.4}$$

[1] Because we are only assuming small displacements of the string from the equilibrium position, the velocity should be perpendicular to the x-axis.

if we expand in powers of the small displacement ψ. The total potential energy is obtained by integrating the infinitesimal contribution in (2.4) over the whole length of the string:

$$V = \int_0^\ell \frac{1}{2}\tau \left(\frac{\partial\psi}{\partial x}\right)^2 dx. \tag{2.5}$$

The Lagrangian is therefore given as the difference between the kinetic energy (2.3) and the potential energy (2.5):

$$L = T - V = \int_0^\ell dx \frac{1}{2}\left[\rho\left(\frac{\partial\psi}{\partial t}\right)^2 - \tau\left(\frac{\partial\psi}{\partial x}\right)^2\right]. \tag{2.6}$$

We will now use Hamilton's principle to show that we obtain the wave equation.

The action functional is, using the basic definition (1.15) along with (2.6),

$$S[\psi] = \int_{t_1}^{t_2} dt\, L = \frac{1}{2}\int_{t_1}^{t_2} dt \int_0^\ell dx \left[\rho\left(\frac{\partial\psi}{\partial t}\right)^2 - \tau\left(\frac{\partial\psi}{\partial x}\right)^2\right], \tag{2.7}$$

which is regarded as a functional of the string displacement $\psi(x,t)$. If we vary S with respect to ψ, we have

$$\begin{aligned}\delta S &= S[\psi+\delta\psi] - S[\psi],\\ &= \int_{t_1}^{t_2} dt \int_0^\ell dx \left[\rho\frac{\partial\psi}{\partial t}\delta\left(\frac{\partial\psi}{\partial t}\right) - \tau\frac{\partial\psi}{\partial x}\delta\left(\frac{\partial\psi}{\partial x}\right)\right].\end{aligned} \tag{2.8}$$

Here $\delta\psi$ represents the variation in the displacement of the string and we work to first order in $\delta\psi$. We will require that

$$\delta\psi(x,t_1) = 0 = \delta\psi(x,t_2), \tag{2.9}$$

which expresses that the initial and final displacements of the varied string configuration are the same as the original string, and also that

$$\delta\psi(0,t) = 0 = \delta\psi(\ell,t), \tag{2.10}$$

to ensure that the varied displacement of the string has the same two endpoints as the original displacement. In order to work out $\delta\left(\partial\psi/\partial t\right)$ we note that it is just the difference in velocity between the varied displacement $\psi+\delta\psi$ and the original displacement ψ. Thus we have

$$\begin{aligned}\delta\left(\frac{\partial\psi}{\partial t}\right) &= \frac{\partial}{\partial t}(\psi+\delta\psi) - \frac{\partial}{\partial t}\psi\\ &= \frac{\partial}{\partial t}\delta\psi.\end{aligned} \tag{2.11}$$

A similar procedure applied to the partial derivative of ψ with respect to x gives

$$\delta\left(\frac{\partial\psi}{\partial x}\right) = \frac{\partial}{\partial x}\delta\psi. \tag{2.12}$$

Using (2.11) and (2.12) in (2.8) results in

$$\delta S = \int_{t_1}^{t_2} dt \int_0^\ell dx \left(\rho\frac{\partial\psi}{\partial t}\frac{\partial}{\partial t}\delta\psi - \tau\frac{\partial\psi}{\partial x}\frac{\partial}{\partial x}\delta\psi\right).$$

If we integrate by parts and use (2.9) and (2.10) we obtain

$$\delta S = \int_{t_1}^{t_2} dt \int_0^\ell dx \left(-\rho\frac{\partial^2\psi}{\partial t^2} + \tau\frac{\partial^2\psi}{\partial x^2}\right)\delta\psi. \tag{2.13}$$

Since this must vanish for arbitrary $\delta\psi$ (apart from the restrictions in Eqs (2.9) and (2.10)), we find the equation of motion

$$\rho\frac{\partial^2\psi}{\partial t^2} = \tau\frac{\partial^2\psi}{\partial x^2}. \tag{2.14}$$

This can be recognized as the one-dimensional wave equation.

The generalization from one to many spatial dimensions is straightforward. Let Σ be any bounded region of $\mathbb{R}^D$ (i.e. Σ is any region of D-dimensional Euclidean space which has a boundary). If we let $d\sigma_x$ represent the volume element for Σ, which if we used Cartesian coordinates would be simply $d\sigma_x = d^D x$, then we define

$$S[\psi] = \frac{1}{2}\int_{t_1}^{t_2} dt \int_\Sigma d\sigma_x \left[\rho\left(\frac{\partial\psi}{\partial t}\right)^2 - \tau\left|\nabla\psi\right|^2\right]. \tag{2.15}$$

The physical interpretation of this action is that it represents a vibrating membrane fixed on the boundary of the region Σ with ψ the displacement of the membrane from equilibrium. It is not difficult to show that Hamilton's principle leads to the wave equation in D spatial dimensions:

$$\rho\frac{\partial^2\psi}{\partial t^2} = \tau\nabla^2\psi. \tag{2.16}$$

2.2 Lagrangian and Hamiltonian formulation for continuous systems

In this section we wish to develop the general procedure for dealing with continuous systems described by a field variable $\psi(t, \mathbf{x})$. Instead of dealing with a Lagrangian, it is sometimes more convenient to deal with a Lagrangian density $\mathcal{L}$ defined by

$$S = \int_{t_1}^{t_2} dt \int_{\Sigma} d\sigma_x \, \mathcal{L}. \tag{2.17}$$

Again we are using Σ to denote any region of $\mathbb{R}^D$, possibly with boundary, and $d\sigma_x$ to be the volume element for this region. The relationship between the Lagrangian $L(t)$ and Lagrangian density $\mathcal{L}(t,\mathbf{x})$ is

$$L(t) = \int_{\Sigma} d\sigma_x \, \mathcal{L}(t, \mathbf{x}). \tag{2.18}$$

For example, for the one-dimensional string whose Lagrangian was given in (2.6) we have Σ given by the closed line interval $0 \leq x \leq \ell$, with ℓ the equilibrium length of the string. The boundary of Σ in this case consists of the two points representing the ends of this interval: $x = 0$ and $x = \ell$. The Lagrangian density is

$$\mathcal{L} = \frac{1}{2}\rho \left(\frac{\partial \psi}{\partial t}\right)^2 - \frac{1}{2}\tau \left(\frac{\partial \psi}{\partial x}\right)^2.$$

for the one-dimensional string.

In general we will be interested in a Lagrangian density $\mathcal{L}$ which depends on $\psi, \partial\psi/\partial t$ and $\nabla\psi$, so that

$$S[\psi] = \int_{t_1}^{t_2} dt \int_{\Sigma} d\sigma_x \, \mathcal{L}\left(\psi, \frac{\partial}{\partial t}\psi, \nabla\psi\right). \tag{2.19}$$

The Lagrangian density may also have an explicit dependence on the time or the spatial coordinates but we do not indicate this explicitly. There are many cases of physical interest in which the Lagrangian density depends upon more than just the first time or spatial derivatives of ψ, but as this is not the case usually dealt with in quantum field theory we will not consider this further here.

If we vary (2.19) with respect to ψ we find

$$\delta S = \int_{t_1}^{t_2} dt \int_{\Sigma} d\sigma_x \left[\frac{\partial \mathcal{L}}{\partial \psi}\delta\psi + \frac{\partial \mathcal{L}}{\partial \dot{\psi}}\delta\dot{\psi} + \frac{\partial \mathcal{L}}{\partial(\partial_i \psi)}\delta(\partial_i \psi)\right]. \tag{2.20}$$

Here ∂_i is shorthand for the partial derivative with respect to x^i. We may use $\delta\dot{\psi} = (\partial/\partial t)\delta\psi$ and $\delta(\partial_i\psi) = \partial_i \delta\psi$ as in (2.11) and (2.12). After performing an integration by parts using the facts that $\delta\psi$ is fixed on the boundary of the region Σ and that the initial and final configurations are fixed (see (2.9) and (2.10) for the one-dimensional string), we find

$$\delta S = \int_{t_1}^{t_2} dt \int_{\Sigma} d\sigma_x \left\{\frac{\partial \mathcal{L}}{\partial \psi} - \frac{\partial}{\partial t}\left(\frac{\partial \mathcal{L}}{\partial \dot{\psi}}\right) - \partial_i \left[\frac{\partial \mathcal{L}}{\partial(\partial_i \psi)}\right]\right\} \delta\psi. \tag{2.21}$$

Hamilton's principle of stationary action leads to the Euler–Lagrange equation

$$0 = \frac{\partial \mathcal{L}}{\partial \psi} - \frac{\partial}{\partial t}\left(\frac{\partial \mathcal{L}}{\partial \dot{\psi}}\right) - \partial_i \left[\frac{\partial \mathcal{L}}{\partial(\partial_i \psi)}\right]. \tag{2.22}$$

It is easily verified that when this result is applied to the one-dimensional string the wave equation (2.14) is regained.

In order to apply the Hamiltonian formalism we must be able first to define the notion of momentum for a continuous field variable. By complete analogy with the definition (1.21) in point particle mechanics define

$$\pi(\mathbf{x}, t) = \frac{\partial \mathcal{L}}{\partial \dot{\psi}(\mathbf{x}, t)}, \tag{2.23}$$

to be the momentum canonically conjugate to ψ. As in Section 1.3, we will assume that we are able to solve this for $\dot{\psi}(t, \mathbf{x})$ in terms of $\psi(t, \mathbf{x})$, the spatial derivatives $\nabla\psi(t, \mathbf{x})$ of ψ, and $\pi(t, \mathbf{x})$. The Hamiltonian density $\mathcal{H}(t, \mathbf{x})$ may be defined by

$$\mathcal{H}(t, \mathbf{x}) = \pi(t, \mathbf{x})\dot{\psi}(t, \mathbf{x}) - \mathcal{L}(t, \mathbf{x}). \tag{2.24}$$

This, like (1.22) for point-particle mechanics, involves a Legendre transformation. We can regard the Hamiltonian density as a function of $\psi(t, \mathbf{x})$, $\nabla\psi(t, \mathbf{x})$, and $\pi(t, \mathbf{x})$.

The action functional in Hamiltonian form reads

$$S[\psi, \pi] = \int_{t_1}^{t_2} dt \int_\Sigma d\sigma_x \left[\pi(t, \mathbf{x})\dot{\psi}(t, \mathbf{x}) - \mathcal{H}(t, \mathbf{x})\right]. \tag{2.25}$$

As was the case for the Hamiltonian form of point-particle classical mechanics in Section 1.3, the action is regarded as a functional of the basic variable ψ and its conjugate momentum π which are treated independently. With $\mathcal{H}$ depending on $\psi, \nabla\psi$, and π, taking the variation of (2.25) with independent variations ψ and π, we find

$$\delta S = \int_{t_1}^{t_2} dt \int_\Sigma d\sigma_x \left[\delta\pi\dot{\psi} + \pi\delta\dot{\psi} - \frac{\partial \mathcal{H}}{\partial \psi}\delta\psi - \frac{\partial \mathcal{H}}{\partial \pi}\delta\pi - \frac{\partial \mathcal{H}}{\partial(\partial_i \psi)}\delta(\partial_i \psi)\right].$$

After the usual integrations by parts, setting the terms multiplying the variations $\delta\psi$ and $\delta\pi$ separately to zero results in

$$\dot{\psi} = \frac{\partial \mathcal{H}}{\partial \pi}, \tag{2.26}$$

$$\dot{\pi} = -\frac{\partial \mathcal{H}}{\partial \psi} + \partial_i \left[\frac{\partial \mathcal{H}}{\partial(\partial_i \psi)}\right]. \tag{2.27}$$

These two equations are the Hamiltonian equations of motion for a theory described by a continuous field variable, and are the direct generalization of (1.23) and (1.24) for point-particle mechanics.

Before proceeding with a final development it may be helpful to illustrate the formalism for the one-dimensional string considered earlier. The Lagrangian density is

$$\mathcal{L} = \frac{1}{2}\rho(\dot{\psi})^2 - \frac{1}{2}\tau(\psi')^2, \tag{2.28}$$

where we have abbreviated ψ' as the partial derivative of ψ with respect to x. It is easy to see that

$$\frac{\partial \mathcal{L}}{\partial \psi} = 0, \qquad \frac{\partial \mathcal{L}}{\partial \dot{\psi}} = \rho\dot{\psi}, \qquad \frac{\partial \mathcal{L}}{\partial \psi'} = -\tau\psi'.$$

The Euler–Lagrange equation follows directly from (2.22) as

$$0 = -\rho\frac{\partial^2\psi}{\partial t^2} + \tau\frac{\partial^2\psi}{\partial x^2},$$

which is recognized as the one-dimensional wave equation in agreement with (2.14) found earlier. The momentum π conjugate to ψ is

$$\pi = \frac{\partial \mathcal{L}}{\partial \dot{\psi}} = \rho\dot{\psi},$$

from the definition (2.23). This is easily solved for $\dot{\psi} = \pi/\rho$. The Hamiltonian density $\mathcal{H}$ is found using (2.24) and eliminating $\dot{\psi}$ in favour of π. The result of this is

$$\mathcal{H} = \frac{1}{2\rho}\pi^2 + \frac{1}{2}\tau\left(\frac{\partial\psi}{\partial x}\right)^2, \tag{2.29}$$

which can be recognized as the energy density of the string. Finally we may compute the Hamiltonian equations of motion using (2.26) and (2.27) to be

$$\begin{aligned} \dot{\psi} &= \frac{\partial \mathcal{H}}{\partial \pi} = \frac{1}{\rho}\pi, \\ \dot{\pi} &= -\frac{\partial \mathcal{H}}{\partial \psi} + \frac{\partial}{\partial x}\left(\frac{\partial \mathcal{H}}{\partial \psi'}\right) = \tau\frac{\partial^2\psi}{\partial x^2}. \end{aligned} \tag{2.30}$$

These two equations, which are first order in time derivatives, are equivalent to the wave equation (2.14).

Many cases we will deal with involve relativistic field theories; that is, field theories invariant (or covariant) under the Lorentz spacetime transformations of special relativity. The basic concepts of special relativity needed for this book are summarized in Appendix 2. For such theories we can obtain the Lagrangian formulation in a relativistically covariant manner. Let x^μ where $\mu = 0, 1, 2, \ldots, D$ be the spacetime coordinates of Minkowski spacetime. Here $x^0 = ct$. It is convenient to adopt units in which the speed of light $c = 1$, so that $x^0 = t$. This means that time is measured in units of length with 1 second of time corresponding to about 3×10^8 m. Factors of c in any expression can always be restored later by dimensional analysis. Let $\varphi^I(t, \mathbf{x})$ where $I = 1, 2, \ldots, N$ denote a set of N real-valued field variables. The Lagrangian density $\mathcal{L}$ is taken to depend on φ^I and the spacetime derivatives $\partial_\mu \varphi^I$:

$$\mathcal{L} = \mathcal{L}\left[\varphi^I(x), \partial_\mu \varphi^I(x)\right]. \tag{2.31}$$

Here we are using the standard notation $\partial_\mu = \partial/\partial x^\mu$. The argument x of φ^I stands for the complete set x^μ of all spacetime coordinates. The action functional is

$$S[\varphi^I(x)] = \int_{t_1}^{t_2} dt \int_\Sigma d\sigma_x \mathcal{L}\left[\varphi^I(x), \partial_\mu \varphi^I(x)\right]. \tag{2.32}$$

$\mathcal{L}$ may have an explicit dependence on x, but we do not indicate this. The action, like the Lagrangian density, should be real. In addition, under the Lorentz transformations of special relativity it should transform like a scalar. Application of Hamilton's principle of stationary action to (2.32) leads to, after manipulations that should now be familiar,

$$0 = \frac{\partial \mathcal{L}}{\partial \varphi^I(x)} - \partial_\mu \left\{ \frac{\partial \mathcal{L}}{\partial[\partial_\mu \varphi^I(x)]} \right\}. \tag{2.33}$$

These are the Euler–Lagrange equations in covariant form, which could have been deduced from (2.22). The momentum conjugate to φ^I is defined by

$$\pi_I(x) = \frac{\partial \mathcal{L}}{\partial \dot{\varphi}^I(x)}, \tag{2.34}$$

exactly as in (2.23). The Hamiltonian density $\mathcal{H}$ is

$$\mathcal{H}(x) = \pi_I(x)\dot{\varphi}^I(x) - \mathcal{L}(x). \tag{2.35}$$

Note that we are using the summation convention here with the repeated index I summed over the range $1, 2, \ldots, N$. We will elaborate on the case of relativistic field theory in the next section, and illustrate the formalism with examples.

2.3 Some examples

2.3.1 Real scalar field

Let $\varphi(x)$ be a real-valued function of the spacetime coordinates. By defining $\varphi(x)$ to be a scalar field we mean that under a Lorentz transformation characterized by

$$x'^{\mu} = L^{\mu}{}_{\nu} x^{\nu} + a^{\mu}, \tag{2.36}$$

where $L^{\mu}{}_{\nu}$ and a^{μ} are constants, we have

$$\varphi'(x') = \varphi(x). \tag{2.37}$$

This means that when the field is written in terms of the new coordinates x'^{μ} to obtain $\varphi'(x')$, the field is identical to the original value $\varphi(x)$ expressed in terms of the original coordinates x^{μ}. This is the simplest possibility for a transformation of the field. Our sign convention for the metric tensor is that in Cartesian coordinates

$$\eta_{\mu\nu} = \mathrm{diag}(+1, -1, -1, \ldots, -1), \tag{2.38}$$

where by diag we mean a diagonal matrix with the components indicated in (2.38) down the diagonal and zero components elsewhere. A brief review of special relativity can be found in Appendix 2.

The Lagrangian density for a real scalar field $\varphi(x)$ will be defined to be

$$\mathcal{L} = \frac{1}{2}\eta^{\mu\nu}\partial_{\mu}\varphi\partial_{\nu}\varphi - \frac{1}{2}m^2\varphi^2 - U(\varphi), \tag{2.39}$$

where m is a constant and $U(\varphi)$ is some function of φ, usually taken to be a polynomial. The constant m is called the 'mass of the field', an interpretation which will be justified later. If we use the explicit form of $\eta_{\mu\nu}$ given in (2.38) it is seen that

$$\mathcal{L} = \frac{1}{2}\dot{\varphi}^2 - \frac{1}{2}\left|\nabla\varphi\right|^2 - \frac{1}{2}m^2\varphi^2 - U(\varphi). \tag{2.40}$$

Comparing this Lagrangian density with that for the vibrating string in (2.15) it can be seen that the real scalar field theory is a relativistic generalization of the string. $\mathcal{L}$ as expressed in (2.39) is manifestly invariant under a Lorentz transformation (i.e. $\mathcal{L}'(x') = \mathcal{L}(x)$).

The Euler–Lagrange equations are easily evaluated using (2.33). If we note that

$$\frac{\partial\mathcal{L}}{\partial(\partial_{\mu}\varphi)} = \eta^{\mu\nu}\partial_{\nu}\varphi \quad \text{and} \quad \frac{\partial\mathcal{L}}{\partial\varphi} = -m^2\varphi - U'(\varphi),$$

we find the equation of motion

$$0 = -m^2\varphi - U'(\varphi) - \eta^{\mu\nu}\partial_\mu\partial_\nu\varphi.$$

It is conventional to define the d'Alembertian, or wave operator, $\Box$ by

$$\Box = \eta^{\mu\nu}\partial_\mu\partial_\nu = \frac{\partial^2}{\partial t^2} - \nabla^2. \tag{2.41}$$

The equation of motion for the real scalar field can be written in terms of the d'Alembertian as

$$0 = (\Box + m^2)\varphi + U'(\varphi). \tag{2.42}$$

If the potential $U(\varphi)$ is set to zero, we obtain the Klein–Gordon equation

$$0 = (\Box + m^2)\varphi, \tag{2.43}$$

which describes a free scalar field. The momentum conjugate to φ follows from the general definition in (2.34). Using (2.40) for $\mathcal{L}$ we find

$$\pi = \frac{\partial\mathcal{L}}{\partial\dot{\varphi}} = \dot{\varphi}. \tag{2.44}$$

The Hamiltonian density may be computed from (2.35) to be

$$\mathcal{H} = \frac{1}{2}\pi^2 + \frac{1}{2}\left|\nabla\varphi\right|^2 + \frac{1}{2}m^2\varphi^2 + U(\varphi). \tag{2.45}$$

2.3.2 Complex scalar field

Let $\Phi(x)$ denote a complex-valued function of the spacetime coordinates which transforms like a scalar under the Lorentz transformation (2.36). Explicitly we have $\Phi'(x') = \Phi(x)$. Because $\Phi(x)$ is a complex number we can always decompose it into its real and imaginary parts. Define

$$\Phi(x) = \frac{1}{\sqrt{2}}\left[\varphi_1(x) + i\varphi_2(x)\right], \tag{2.46}$$

where $\varphi_1(x)$ and $\varphi_2(x)$ are independent real scalar fields representing the real and imaginary parts of Φ. The factor of $1/\sqrt{2}$ in (2.46) is a normalization factor included for later convenience. If we ignore the potential term $U(\varphi)$ in the real scalar field Lagrangian density considered in (2.39), a natural choice for the Lagrangian density for the complex scalar field is

$$\mathcal{L} = \mathcal{L}_1 + \mathcal{L}_2,$$

where $\mathcal{L}_1$ and $\mathcal{L}_2$ are the Lagrangian densities for real scalar fields φ_1 and φ_2:

$$\mathcal{L}_{1,2} = \frac{1}{2}\eta^{\mu\nu}\partial_\mu\varphi_{1,2}\partial_\nu\varphi_{1,2} - \frac{1}{2}m^2\varphi_{1,2}^2.$$

When written in terms of the complex field Φ, it is easy to show that

$$\mathcal{L} = \eta^{\mu\nu}\partial_\mu\Phi^*\partial_\nu\Phi - m^2\Phi^*\Phi. \tag{2.47}$$

Note that by choosing the mass term m^2 to be the same for both the real and imaginary parts φ_1 and φ_2 we ensured that the Lagrangian density was real. The factor of $1/\sqrt{2}$ in (2.46) meant that no numerical factors occurred in the terms of (2.47).

When computing the Euler–Lagrange equations we can treat $\delta\Phi$ and $\delta\Phi^*$ as independent variations. This is because the real and imaginary parts of Φ can be varied independently. From (2.47) we find

$$\frac{\partial\mathcal{L}}{\partial\Phi^*} = -m^2\Phi \quad \text{and} \quad \frac{\partial\mathcal{L}}{\partial(\partial_\mu\Phi^*)} = \eta^{\mu\nu}\partial_\nu\Phi,$$

which gives

$$(\Box + m^2)\Phi = 0. \tag{2.48}$$

In a similar way

$$\frac{\partial\mathcal{L}}{\partial\Phi} = -m^2\Phi^* \quad \text{and} \quad \frac{\partial\mathcal{L}}{\partial(\partial_\mu\Phi)} = \eta^{\mu\nu}\partial_\nu\Phi^*,$$

which gives

$$(\Box + m^2)\Phi^* = 0. \tag{2.49}$$

These two equations of motion could also have been obtained from the fact that φ_1 and φ_2 each satisfy the Klein–Gordon equation (2.43).

The momentum conjugate to Φ is

$$\Pi = \frac{\partial\mathcal{L}}{\partial\dot{\Phi}} = \dot{\Phi}^*. \tag{2.50}$$

The momentum conjugate to Φ^* is

$$\Pi^* = \frac{\partial\mathcal{L}}{\partial\dot{\Phi}^*} = \dot{\Phi}. \tag{2.51}$$

The Hamiltonian density is

$$\begin{aligned}\mathcal{H} &= \Pi\dot{\Phi} + \Pi^*\dot{\Phi}^* - \mathcal{L} \\ &= \Pi^*\Pi + (\nabla\Phi^*)\cdot(\nabla\Phi) + m^2\Phi^*\Phi.\end{aligned} \tag{2.52}$$

2.3.3 Schrödinger field

The Schrödinger equation is (with $\hbar = 1$)

$$-\frac{1}{2m}\nabla^2\Psi + V(\mathbf{x},t)\Psi = i\frac{\partial}{\partial t}\Psi. \tag{2.53}$$

Here $V(\mathbf{x},t)$ represents an arbitrary potential which may be time dependent. The Schrödinger field Ψ is a complex valued function of t and $\mathbf{x}$. As for the complex scalar field, we can treat Ψ and its complex conjugate Ψ^* as independent when performing variations. A suitable Lagrangian density which gives rise to (2.53) and its complex conjugate under independent variations of Ψ and Ψ^* is

$$\mathcal{L} = \frac{i}{2}\left(\Psi^*\dot{\Psi} - \dot{\Psi}^*\Psi\right) - \frac{1}{2m}(\nabla\Psi^*)\cdot(\nabla\Psi) - V\Psi^*\Psi, \tag{2.54}$$

which is manifestly real (i.e. $\mathcal{L}^* = \mathcal{L}$).

The momentum canonically conjugate to Ψ is

$$\Pi = \frac{\partial\mathcal{L}}{\partial\dot{\Psi}} = \frac{i}{2}\Psi^*. \tag{2.55}$$

The momentum canonically conjugate to Ψ^* is

$$\Pi^* = \frac{\partial\mathcal{L}}{\partial\dot{\Psi}^*} = -\frac{i}{2}\Psi. \tag{2.56}$$

This situation is quite unlike the case for the complex relativistic field. Here Π and Π^* are just simple multiples of the basic field variables Ψ and Ψ^*. This should not be surprising for the reader who has understood the passage from the Lagrangian to Hamiltonian description. The momentum was introduced as a device for obtaining equations of motion which were first order in time. However the Schrödinger equation is already first order in time. We will see that a similar situation occurs for the Dirac field, describing a relativistic electron, in Section 2.8.

The Hamiltonian density is

$$\begin{aligned}\mathcal{H} &= \Pi\dot{\Psi} + \Pi^*\dot{\Psi}^* - \mathcal{L}\\ &= \frac{i}{2}\left(\Psi^*\dot{\Psi} - \dot{\Psi}^*\Psi\right) - \mathcal{L}\\ &= \frac{1}{2m}(\nabla\Psi^*)\cdot(\nabla\Psi) + V\Psi^*\Psi.\end{aligned} \tag{2.57}$$

The Hamiltonian is

$$H(t) = \int_\Sigma d\sigma_x\mathcal{H} = \int_\Sigma d\sigma_x\Psi^*\left(-\frac{1}{2m}\nabla^2 + V\right)\Psi, \tag{2.58}$$

if we perform an integration by parts. In wave mechanics this is interpreted as the expectation value of the Hamiltonian operator. Thus, wave mechanics can be viewed as an example of a classical field theory.[2]

2.3.4 The Maxwell field

The usual form for Maxwell's equations of electromagnetism is (in SI units)

$$\nabla\cdot\mathbf{E} = \frac{1}{\epsilon_0}\rho, \tag{2.59}$$

$$\nabla\cdot\mathbf{B} = 0, \tag{2.60}$$

$$\nabla\times\mathbf{E} = -\frac{\partial}{\partial t}\mathbf{B}, \tag{2.61}$$

$$\nabla\times\mathbf{B} = \mu_0\mathbf{J} + \frac{1}{c^2}\frac{\partial}{\partial t}\mathbf{E}, \tag{2.62}$$

where $\epsilon_0\mu_0 = c^{-2}$. These equations are valid for free space in the presence of the sources ρ (the charge density) and $\mathbf{J}$ (the current density). We will choose units, as usual, with $c = 1$, which implies $\epsilon_0\mu_0 = 1$. In addition it is advantageous to adopt Heaviside–Lorentz rationalized units in which $\epsilon_0 = 1$ and $\mu_0 = 1$. This removes all dependence on the constants ϵ_0 and μ_0 from the Maxwell equations.

Rather than dealing directly with $\mathbf{E}$ and $\mathbf{B}$, a Lagrangian description is simpler if the potentials Φ and $\mathbf{A}$ defined by

$$\mathbf{E} = -\nabla\Phi - \frac{\partial}{\partial t}\mathbf{A}, \tag{2.63}$$

$$\mathbf{B} = \nabla\times\mathbf{A}, \tag{2.64}$$

are used. These potentials may be combined into a 4-vector $A^\mu = (\Phi, \mathbf{A})$. In a similar way we may form a 4-vector $J^\mu = (\rho, \mathbf{J})$ which is called the current density 4-vector. By lowering the spacetime index using $A_\mu = \eta_{\mu\nu}A^\nu$, with our choice of metric (2.38) we have $A_\mu = (\Phi, -\mathbf{A})$, and similarly $J_\mu = (\rho, -\mathbf{J})$. A second-rank antisymmetric tensor $F_{\mu\nu}$, called the 'field-strength tensor', may be defined by

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu. \tag{2.65}$$

[2] Using the word *classical* to describe wave mechanics may lead to some confusion. From the viewpoint of quantum field theory, because the wave function is a function, rather than an operator, wave mechanics is a classical field theory. To avoid this confusion, proceeding from classical mechanics to wave mechanics is sometimes called 'first quantization', and proceeding from wave mechanics to quantum field theory (where the wave function becomes a field operator) is called 'second quantization'.

In terms of the original **E** and **B** fields the components of $F_{\mu\nu}$ are easily seen to be

$$F_{\mu\nu} = \begin{pmatrix} 0 & E_1 & E_2 & E_3 \\ -E_1 & 0 & -B_3 & B_2 \\ -E_2 & B_3 & 0 & -B_1 \\ -E_3 & -B_2 & B_1 & 0 \end{pmatrix}. \tag{2.66}$$

The contravariant components are found using $F^{\mu\nu} = \eta^{\mu\alpha}\eta^{\nu\beta}F_{\alpha\beta}$. The Maxwell equations (2.59)–(2.62) may be summarized as

$$\partial_\nu F^{\mu\nu} = -J^\mu, \tag{2.67}$$

(and the definition of $F_{\mu\nu}$ in (2.65)).

An important point is that the potential A_μ is not uniquely defined by a given electromagnetic field. This is clear from the definition (2.65) where it can be seen that A'_μ is given by

$$A'_\mu = A_\mu + \partial_\mu \theta, \tag{2.68}$$

and A_μ give rise to the same field-strength $F_{\mu\nu}$ for any function θ. This is an example of a gauge transformation which will be discussed in more detail later.

So far we have been concerned with the theory of electromagnetism in the usual three-dimensional space. It is possible to define a theory of electromagnetism in an arbitrary dimension in a straightforward and simple manner by adopting (2.65) and (2.67) as the definition of the theory. As in three spatial dimensions, we can call F_{0i} the components of the electric field vector. The components F_{ij} with $i \neq j$ define the magnetic field. In D spatial dimensions F_{ij} is a $D \times D$ antisymmetric tensor, and it is not possible to describe the magnetic field as a vector for general D. (For example, if $D = 2$ then F_{ij} has only a single independent component F_{12}, since the other non-zero component $F_{21} = -F_{12}$. But a vector in $D = 2$ has two independent components, not one.) Only for $D = 3$ can the magnetic field be described by a vector field. This is easy to see by considering the number of independent components of F_{ij}. (The components of the vector can be identified with F_{32}, F_{13}, and F_{21} when $D = 3$.)

The classical action functional for the electromagnetic field may be taken to be

$$S[A] = \int_{t_1}^{t_2} dt \int_\Sigma d\sigma_x \left(-\frac{1}{4} F_{\mu\nu}F^{\mu\nu} - J_\mu A^\mu \right). \tag{2.69}$$

It is easy to show that (2.67) is recovered if $S[A]$ is varied with respect to A_μ with the definition (2.65) used. It can be noted from (2.66) that

$F_{\mu\nu}F^{\mu\nu} = -2(E^2 - B^2)$. It also follows that under the gauge transformation (2.68)

$$S[A'] = S[A] - \int_{t_1}^{t_2} dt \int_\Sigma d\sigma_x J^\mu \partial_\mu \theta.$$

If the last term above is integrated by parts we find

$$S[A'] = S[A] + \int_{t_1}^{t_2} dt \int_\Sigma d\sigma_x \theta \partial_\mu J^\mu.$$

Since J^μ is the 4-current density, $\partial_\mu J^\mu = 0$ is guaranteed by the conservation of charge. The classical action functional (2.69) is therefore gauge invariant.[3]

2.4 Functional differentiation and Poisson brackets for field theory

In the classical mechanics of a point particle we described the motion using a generalized coordinate $q^i(t)$. In field theory we used $\varphi^I(x)$. We can therefore think of the following correspondence between point-particle mechanics and classical field theory:

$$q^i(t) \Longleftrightarrow \varphi^I(t, \mathbf{x}), \tag{2.70}$$

$$i \Longleftrightarrow (I, \mathbf{x}). \tag{2.71}$$

In addition we had a metric tensor, which for Cartesian coordinates was δ_{ij}. If we take the correspondence between indices in (2.71) seriously, then there should be a counterpart of the metric tensor in field theory. Because one of the labels on the right-hand side of (2.71) involves the continuous spatial coordinate $\mathbf{x}$, we need to use the Dirac delta distribution in place of the Kronecker delta. We will define the Dirac delta distribution $\delta(\mathbf{x}, \mathbf{x}')$ by

$$\int_\Sigma d\sigma_{x'} \delta(\mathbf{x}, \mathbf{x}') f(\mathbf{x}') = f(\mathbf{x}), \tag{2.72}$$

for any function $f(\mathbf{x})$ defined on Σ. Because the left-hand side of (2.72) involves an integral of $f(\mathbf{x})$ over the whole of Σ, and the right-hand side involves only the value of $f(\mathbf{x})$ at the single point $\mathbf{x}$, we can think of $\delta(\mathbf{x}, \mathbf{x}')$ as being zero everywhere except at the single point $\mathbf{x} = \mathbf{x}'$. It is in this sense that the Dirac delta distribution is the analogue of the Kronecker delta for continuous variables. Strictly speaking, $\delta(\mathbf{x}, \mathbf{x}')$ is only

[3] In curved spacetime, or if non-Cartesian coordinates are used in flat spacetime, it is easy to show that the covariant divergence of J^μ is obtained.

defined when it occurs inside an integral, although in physics we often write it alone. We have been careful not to use the terminology 'function' to describe $\delta(\mathbf{x}, \mathbf{x}')$, since it is not really a function at all, but rather is an object referred to as a distribution. We will add the correspondence

$$\delta_{ij} \Longleftrightarrow \delta_{IJ}\delta(\mathbf{x}, \mathbf{x}') \tag{2.73}$$

to (2.70) and (2.71).

There are many ways to represent the Dirac delta distribution. One of the most useful for field theory involves the use of Fourier transforms. Take the case $\Sigma = \mathbb{R}^D$ here and use Cartesian coordinates so that $d\sigma_x = d^D x$. The Fourier transform of the function $f(\mathbf{x})$ is defined to be $\tilde{f}(\mathbf{p})$ where

$$f(\mathbf{x}) = \int \frac{d^D p}{(2\pi)^D}\, e^{i\mathbf{p}\cdot\mathbf{x}} \tilde{f}(\mathbf{p}). \tag{2.74}$$

The inverse Fourier transform is

$$\tilde{f}(\mathbf{p}) = \int d^D x'\, e^{-i\mathbf{p}\cdot\mathbf{x}'} f(\mathbf{x}'). \tag{2.75}$$

If we now substitute for $\tilde{f}(\mathbf{p})$ in (2.74) using (2.75) we obtain

$$\begin{aligned} f(\mathbf{x}) &= \int \frac{d^D p}{(2\pi)^D}\, e^{i\mathbf{p}\cdot\mathbf{x}} \int d^D x'\, e^{-i\mathbf{p}\cdot\mathbf{x}'} f(\mathbf{x}') \\ &= \int d^D x' \left[\int \frac{d^D p}{(2\pi)^D}\, e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{x}')} \right] f(\mathbf{x}'). \end{aligned}$$

Comparison of this result with the definition of the Dirac delta distribution in (2.72), noting $d\sigma_{x'} = d^D x'$, shows that we may identify

$$\delta(\mathbf{x}, \mathbf{x}') = \int \frac{d^D p}{(2\pi)^D}\, e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{x}')}. \tag{2.76}$$

This result agrees with our intuitive feeling for $\delta(\mathbf{x}, \mathbf{x}')$ since for $\mathbf{x} \neq \mathbf{x}'$ we would expect that the exponential function in (2.76) should oscillate equally between positive and negative values when integrated over all momentum space, and the result should average to zero; when $\mathbf{x} = \mathbf{x}'$ the right-hand side of (2.76) is seen to be infinite. This gives us all of the properties of the Dirac delta distribution we need for now.

In point-particle mechanics, the independence of the generalized coordinates can be expressed by

$$\frac{\partial q^i}{\partial q^j} = \delta^i{}_j. \tag{2.77}$$

Because q^i depends on time, this result should hold at any fixed time. We wish to know the analogue of (2.77) in field theory. To obtain this we need to know how to differentiate a function with respect to another function. This is called 'functional differentiation'.

First of all consider the case where φ^i and ψ^i are simply the components of vectors in a finite dimensional vector space. Taylor's theorem gives

$$f(\varphi+\psi)=f(\varphi)+\psi^i\frac{\partial f(\varphi)}{\partial\varphi^i}+\cdots, \tag{2.78}$$

for any continuous function $f(\varphi)$. In order to obtain the analogue of this for functionals, we can use our correspondence in (2.71) between i and $(I,\mathbf{x})$. The index i in the second term on the right-hand side of (2.78) is summed over all values; thus, using our correspondence between i and $(I,\mathbf{x})$, we will obtain a sum over I and over $\mathbf{x}$. The analogue of summing over $\mathbf{x}$ is an integral, motivating

$$F[\varphi(t,\mathbf{x})+\psi(t,\mathbf{x})]=F[\varphi(t,\mathbf{x})]+\int_\Sigma d\sigma_{x'}\psi^I(t,\mathbf{x}')\frac{\delta F\left[\varphi(t,\mathbf{x})\right]}{\delta\varphi^I(t,\mathbf{x}')}+\cdots, \tag{2.79}$$

as the analogue of (2.78) for functionals. We retain the summation convention on the index I which is a normal sum over the components of φ^I. We will call $\delta F[\varphi(t,\mathbf{x})]/\delta\varphi^I(t,\mathbf{x}')$ the functional derivative of $F[\varphi]$. The terms denoted by $+\cdots$ in (2.79) involve quadratic and higher powers of ψ^I. A more elegant definition which removes these higher-order terms is obtained by writing

$$\lim_{\epsilon\to0}\frac{F\left[\varphi(t,\mathbf{x})+\epsilon\psi(t,\mathbf{x})\right]-F\left[\varphi(t,\mathbf{x})\right]}{\epsilon}=\int_\Sigma d\sigma_{x'}\psi^I(t,\mathbf{x}')\frac{\delta F\left[\varphi(t,\mathbf{x})\right]}{\delta\varphi^I(t,\mathbf{x}')}. \tag{2.80}$$

The process of taking the limit removes all of the higher-order terms in the Taylor expansion. It should be clear that the left-hand side can be written in the equivalent form

$$\frac{d}{d\epsilon}F[\varphi(t,\mathbf{x})+\epsilon\psi(t,\mathbf{x})]\bigg|_{\epsilon=0}.$$

Because the functional derivative is defined under an integral sign, it would be expected to be a distribution in general.

We will look at some explicit examples of functional differentiation. First of all take $F[\varphi(t,\mathbf{x})]=\varphi^J(t,\mathbf{x})$. It is obvious that $F[\varphi+\epsilon\psi]=F[\varphi]+\epsilon\psi^J(t,\mathbf{x})$. In this case (2.80) gives us

$$\int_\Sigma d\sigma_{x'}\psi^I(t,\mathbf{x}')\frac{\delta\varphi^J(t,\mathbf{x})}{\delta\varphi^I(t,\mathbf{x}')}=\psi^J(t,\mathbf{x}).$$

By comparing this with the definition of the Dirac delta function we can read off

$$\frac{\delta\varphi^J(t,\mathbf{x})}{\delta\varphi^I(t,\mathbf{x}')} = \delta^J{}_I\delta(\mathbf{x},\mathbf{x}'). \tag{2.81}$$

This makes sense from (2.77) given our earlier correspondences in (2.70), (2.71) and (2.73) between point-particle mechanics and field theory.

We may also wish to work out functional derivatives of functionals which involve different time arguments. This is easily accommodated. We would define

$$\int_{t_1}^{t_2} dt' \int_\Sigma d\sigma_{x'}\psi^I(t',\mathbf{x}')\frac{\delta F[\varphi(t,\mathbf{x})]}{\delta\varphi^I(t',\mathbf{x}')} = \lim_{\epsilon\to 0}\frac{F[\varphi(t,\mathbf{x})+\epsilon\psi(t,\mathbf{x})]-F[\varphi]}{\epsilon} \tag{2.82}$$

$$= \frac{d}{d\epsilon}F[\varphi(t,\mathbf{x})+\epsilon\psi(t,\mathbf{x})]\bigg|_{\epsilon=0}. \tag{2.83}$$

In particular we find

$$\frac{\delta\varphi^I(t,\mathbf{x})}{\delta\varphi^J(t',\mathbf{x}')} = \delta^I{}_J\delta(t,t')\delta(\mathbf{x},\mathbf{x}'). \tag{2.84}$$

We cannot simply set $t=t'$ to regain our previous result in (2.81) due to the distributional nature of the functional derivative.

Consider the special case of the action functional. We can compute

$$\begin{aligned} S[\varphi+\epsilon\psi] &= \int_{t_1}^{t_2} dt \int_\Sigma d\sigma_x \mathcal{L}\left(\varphi+\epsilon\psi, \partial_\mu\varphi+\epsilon\partial_\mu\psi\right) \\ &= \int_{t_1}^{t_2} dt \int_\Sigma d\sigma_x \left[\mathcal{L}(\varphi,\partial_\mu\varphi) + \epsilon\psi^I\frac{\partial\mathcal{L}}{\partial\varphi^I} + \epsilon\partial_\mu\psi^I\frac{\partial\mathcal{L}}{\partial(\partial_\mu\varphi^I)} + \cdots\right] \\ &= S[\varphi] + \epsilon\int_{t_1}^{t_2} dt\int_\Sigma d\sigma_x\psi^I\left\{\frac{\partial\mathcal{L}}{\partial\varphi^I} - \partial_\mu\left[\frac{\partial\mathcal{L}}{\partial(\partial_\mu\varphi^I)}\right]\right\} + \cdots, \end{aligned}$$

where in the second line we expanded the Lagrangian density to order ϵ, and in the third line we performed an integration by parts. The definition (2.83) now shows that

$$\frac{\delta S[\varphi(x)]}{\delta\varphi^I(x)} = \frac{\partial\mathcal{L}}{\partial\varphi^I(x)} - \partial_\mu\left\{\frac{\partial\mathcal{L}}{\partial[\partial_\mu\varphi^I(x)]}\right\}. \tag{2.85}$$

Note that although the action was defined in terms of the Lagrangian density by an integral, the distributional nature of the functional derivative

has 'pulled off' the integral sign. Hamilton's principle and the Euler–Lagrange equations can be neatly summarized as

$$\frac{\delta S[\varphi(x)]}{\delta \varphi^I(x)} = 0. \tag{2.86}$$

The principle of stationary action states that the first functional derivative of the action vanishes, completely analogously to stating that a function $f(x)$ is stationary when $f'(x) = 0$.

The Lagrangian (as opposed to the Lagrangian density) is defined by

$$L(t) = L[\varphi^I(t,\mathbf{x}), \dot{\varphi}^I(t,\mathbf{x})] = \int_\Sigma d\sigma_x \mathcal{L}\left[\varphi^I(t,\mathbf{x}), \partial_\mu \varphi^I(t,\mathbf{x})\right].$$

By following an analysis similar to that which led to (2.85), except that the definition in (2.80) is used because we perform the differentiation with respect to fields occurring at the same time t as enters $L(t)$, we find

$$\frac{\delta L(t)}{\delta \varphi^I(t,\mathbf{x})} = \frac{\partial \mathcal{L}(t,\mathbf{x})}{\partial \varphi^I(t,\mathbf{x})} - \partial_j \left\{ \frac{\partial \mathcal{L}(t,\mathbf{x})}{\partial[\partial_j \varphi^I(t,\mathbf{x})]} \right\}, \tag{2.87}$$

$$\frac{\delta L(t)}{\delta \dot{\varphi}^I(t,\mathbf{x})} = \frac{\partial \mathcal{L}(t,\mathbf{x})}{\partial \dot{\varphi}^I(t,\mathbf{x})}. \tag{2.88}$$

The Euler–Lagrange equations can therefore be written in the form

$$0 = \frac{\delta L(t)}{\delta \varphi^I(t,\mathbf{x})} - \frac{\partial}{\partial t}\left[\frac{\delta L(t)}{\delta \dot{\varphi}^I(t,\mathbf{x})}\right]. \tag{2.89}$$

In this form the Euler–Lagrange equations for classical field theory resemble those for point-particle mechanics except that functional derivatives, rather than normal derivatives, occur.

The field momentum was defined in (2.34) to be

$$\pi_I(t,\mathbf{x}) = \frac{\partial \mathcal{L}(t,\mathbf{x})}{\partial \dot{\varphi}^I(t,\mathbf{x})} = \frac{\delta L(t)}{\delta \dot{\varphi}^I(t,\mathbf{x})}, \tag{2.90}$$

if we use (2.88). The Hamiltonian follows from (2.35) as

$$H(t) = \int_\Sigma d\sigma_x \pi_I(t,\mathbf{x}) \dot{\varphi}^I(t,\mathbf{x}) - L(t), \tag{2.91}$$

since the Hamiltonian is just the spatial integral of the Hamiltonian density. $H(t)$ may be regarded as a functional of φ^I and π_I. We can now

compute the functional derivatives of $H(t)$ with respect to φ^I and π_I. The derivative with respect to φ^I is

$$\frac{\delta H(t)}{\delta\varphi^I(t,\mathbf{x})} = \int_{\Sigma_x} d\sigma_{x'}\pi_J(t,\mathbf{x}')\frac{\delta\dot{\varphi}^J(t,\mathbf{x}')}{\delta\varphi^I(t,\mathbf{x})} - \frac{\delta L(t)}{\delta\varphi^I(t,\mathbf{x})} - \int_{\Sigma} d\sigma_{x'}\frac{\delta L(t)}{\delta\dot{\varphi}^J(t,\mathbf{x}')}\frac{\delta\dot{\varphi}^J(t,\mathbf{x}')}{\delta\varphi^I(t,\mathbf{x})}. \tag{2.92}$$

The presence of the last term requires some explanation. We are regarding π_I and φ^I as the independent variables in the Hamiltonian formalism, whereas we have φ^I and $\dot{\varphi}^I$ as the independent variables in the Lagrangian formalism. The definition of π_I gives an implicit relation for $\dot{\varphi}^I$ as a functional of φ^I and π_I. The last term in (2.92) therefore accounts for the dependence in $L(t)$ of $\dot{\varphi}^I$ on φ^I. More formally we could say that the last term is really the chain rule for functional differentiation. In any case, the first term in (2.92) is seen to cancel with the third term and we are left with

$$\begin{aligned}\frac{\delta H(t)}{\delta\varphi^I(t,\mathbf{x})} &= -\frac{\delta L(t)}{\delta\varphi^I(t,\mathbf{x})} \\ &= -\frac{\partial}{\partial t}\left[\frac{\delta L(t)}{\delta\dot{\varphi}^I(t,\mathbf{x})}\right] \text{ (by (2.89))} \\ &= -\dot{\pi}_I(t,\mathbf{x}),\end{aligned} \tag{2.93}$$

where in the last line we have used the definition (2.34) of the field momentum. In a similar way, if we differentiate the Hamiltonian with respect to the momentum we find

$$\begin{aligned}\frac{\delta H(t)}{\delta\pi_I(t,\mathbf{x})} &= \dot{\varphi}^I(t,\mathbf{x}) + \int_{\Sigma} d\sigma_{x'}\pi_J(t,\mathbf{x}')\frac{\delta\dot{\varphi}^J(t,\mathbf{x}')}{\delta\pi_I(t,\mathbf{x})} \\ &\quad - \int_{\Sigma} d\sigma_{x'}\frac{\delta L(t)}{\delta\dot{\varphi}^J(t,\mathbf{x}')}\frac{\delta\dot{\varphi}^J(t,\mathbf{x}')}{\delta\pi_I(t,\mathbf{x})} \\ &= \dot{\varphi}^I(t,\mathbf{x}).\end{aligned} \tag{2.94}$$

The results in (2.93) and (2.94) express the Hamiltonian equations of motion for field theory in a form resembling those for point-particle mechanics, except that functional derivatives occur.

The final development we wish to discuss in this section is the definition of a Poisson bracket for field theory. We can use the correspondence between field theory and point-particle mechanics discussed at the beginning of this section to motivate the definition

$$[F(t),G(t)] = \int_{\Sigma} d\sigma_x\left[\frac{\delta F(t)}{\delta\varphi^I(t,\mathbf{x})}\frac{\delta G(t)}{\delta\pi_I(t,\mathbf{x})} - \frac{\delta F(t)}{\delta\pi_I(t,\mathbf{x})}\frac{\delta G(t)}{\delta\varphi^I(t,\mathbf{x})}\right]. \tag{2.95}$$

Here $F(t)$ and $G(t)$ represent any two functionals of the canonical variables π_I and φ^I evaluated at the same time. In particular, it is easy to show that the Hamiltonian equations of motion may be written as

$$[\varphi^I(t,\mathbf{x}), H(t)] = \dot{\varphi}^I(t,\mathbf{x}), \tag{2.96}$$

$$[\pi_I(t,\mathbf{x}), H(t)] = \dot{\pi}_I(t,\mathbf{x}). \tag{2.97}$$

The Poisson bracket relations between the canonical variables are

$$[\varphi^I(t,\mathbf{x}), \pi_J(t,\mathbf{x}')] = \delta^I{}_J\delta(\mathbf{x},\mathbf{x}'), \tag{2.98}$$

and

$$[\varphi^I(t,\mathbf{x}), \varphi^J(t,\mathbf{x}')] = 0 = [\pi_I(t,\mathbf{x}), \pi_J(t,\mathbf{x}')]. \tag{2.99}$$

2.5 Noether's theorem

In Section 1.5 we discussed the relationship between symmetries of a point-particle system and conservation laws. The essential features were found from the results of Noether's theorem. The principal aim of this section is to consider the analogous development for classical field theory.

For relativistic field theory in Minkowski spacetime we will always have a set of conserved quantities because we will always demand that the theory be invariant under the Lorentz transformations of special relativity. In general, we might be interested in other more abstract symmetries, such as gauge invariance. As in Section 1.5, we will only consider an infinitesimal transformation which depends on r infinitesimal parameters $\delta\epsilon^A$, with $A = 1, \ldots, r$. For example, a Lorentz transformation in four-dimensional spacetime is characterized by ten parameters: three velocities, representing the uniform relative motion of the three spatial axes; three angles, representing the relative rotation of the three spatial axes; and four parameters representing a translation of the spacetime coordinates. If the set of infinitesimal transformations forms a group, as it does in the case of the Lorentz transformations, then there is no loss of generality in considering only infinitesimal ones because a finite transformation can always be built up from repeated infinitesimal ones.

In the case of particle mechanics we had the transformation of the time t and generalized coordinates $q^i(t)$ specified in (1.103) and (1.104). For field theory, we must consider our fields depending on spacetime coordinates x^μ, not just time, so we generalize (1.103) to

$$x^\mu \to x'^\mu = x^\mu + \delta x^\mu = x^\mu + \lambda^\mu{}_A(x)\delta\epsilon^A. \tag{2.100}$$

$\lambda^{\mu}{}_{A}(x)$ is a set of functions that characterize the transformation. The fields will be chosen to be a set of N real fields $\varphi^{I}(x)$ with $I = 1, \ldots, N$. In place of (1.104) we will take

$$\varphi^{I}(x) \to \varphi'^{I}(x') = \varphi^{I}(x) + \Phi^{I}{}_{A}[x, \varphi^{I}(x)]\delta\epsilon^{A}, \tag{2.101}$$

for some functions $\Phi^{I}{}_{A}[x, \varphi^{I}(x)]$. We will abbreviate $\Phi^{I}{}_{A}[x, \varphi^{I}(x)]$ to simply $\Phi^{I}{}_{A}(x)$ in what follows, but take care to remember that there is a dependence on the fields. If the spacetime coordinates change as in (2.100), then there are two main reasons why the fields must transform. First of all there is the obvious fact that the fields have an explicit dependence on the spacetime coordinates. Secondly, the transformation can mix up different components of the fields. This happens, for example, for a vector field if we perform a rotation of coordinates. It sometimes proves convenient to distinguish the first type of transformation from the second, although we will not need to do that here.

As before, we will define a symmetry of the system to be a transformation of the form (2.100), (2.101) which leaves the equations of motion invariant. Under the transformation (2.100), (2.101) the action functional $S[\varphi^{I}(x)]$ transforms to

$$S[\varphi'^{I}(x')] = \int_{t'_1}^{t'_2} dt' \int_{\Sigma'} d\sigma_{x'} \mathcal{L}\left[\varphi'^{I}(x'), \partial'_{\mu}\varphi'^{I}(x'), x'\right]. \tag{2.102}$$

We require $S[\varphi'^{I}(x')]$ and $S[\varphi^{I}(x)]$ to give rise to the same equations of motion. In the case of particle mechanics, this corresponded to the action functionals $S[\varphi'^{I}(x')]$ and $S[\varphi^{I}(x)]$ differing by terms which depended only on the initial and final times (see (1.106)). This in turn corresponded to the freedom to add a total time derivative to the Lagrangian. In the case of field theory, the integration extends over spacetime, so the natural generalization of adding a total time derivative to the Lagrangian is to add the spacetime divergence of a vector field Λ^{μ} to the Lagrangian density. We will show that this does not affect the equations of motion.

Let

$$\mathcal{L}' = \mathcal{L} + \partial_{\mu}\Lambda^{\mu}, \tag{2.103}$$

and consider the altered action

$$S' = S + \int_{t_1}^{t_2} dt \int_{\Sigma} d\sigma_x \partial_{\mu}\Lambda^{\mu}. \tag{2.104}$$

If we write out $\partial_{\mu}\Lambda^{\mu}$ explicitly, we have

$$\partial_{\mu}\Lambda^{\mu} = \frac{\partial}{\partial t}\Lambda^{0} + \partial_{i}\Lambda^{i}. \tag{2.105}$$

The last term in (2.105) can be recognized as $\vec{\nabla}\cdot\vec{\Lambda}$ in vector notation. We can use Gauss' theorem of vector calculus to express the volume integral of $\vec{\nabla}\cdot\vec{\Lambda}$ as a surface integral:

$$\int_\Sigma d\sigma_x\, \partial_i \Lambda^i = \int_{\partial\Sigma} da_x\, n_i \Lambda^i. \tag{2.106}$$

Here $\partial\Sigma$ denotes the boundary of the spatial region Σ, da_x is the element of area on $\partial\Sigma$, and n^i is the unit vector in the outwards normal direction to $\partial\Sigma$.[4] We can also write

$$\int_\Sigma d\sigma_x \frac{\partial}{\partial t}\Lambda^0 = \frac{d}{dt}\int_\Sigma d\sigma_x\, \Lambda^0,$$

from which we get

$$\int_{t_1}^{t_2} dt \int_\Sigma d\sigma_x \frac{\partial}{\partial t}\Lambda^0 = F(t_2) - F(t_1), \tag{2.107}$$

with

$$F(t) = \int_\Sigma d\sigma_x\, \Lambda^0(t, \mathbf{x}). \tag{2.108}$$

Combining the results of (2.104), (2.106), and (2.107) shows that

$$S' = S + F(t_2) - F(t_1) + \int_{t_1}^{t_2} dt \int_{\partial\Sigma} da_x\, n_i \Lambda^i \tag{2.109}$$

gives the change in the action functional corresponding to altering the Lagrangian density as in (2.103). If we now apply Hamilton's principle of stationary action, with the assumption (as before) that the fields are fixed at the initial and final times, as well as on the boundary of the region of integration, it is clear from (2.109) that S' and S will give rise to the same equations of motion.

If we return to our requirement that $S[\varphi']$ in (2.102) gives rise to the same equations of motion as $S[\varphi]$ under the transformation (2.100) and (2.101), we can conclude that

$$S[\varphi'] = S[\varphi] + \int_{t_1}^{t_2} dt \int_\Sigma d\sigma_x\, \partial_\mu \left\{ \Delta^\mu_A[x, \varphi^I(x)]\delta\epsilon^A \right\}, \tag{2.110}$$

[4] If Σ is compact, as in the case of a box in flat space with periodic boundary conditions on the fields, then $\partial\Sigma$ is the empty set, and the right-hand side of (2.106) vanishes.

for some function $\Delta^{\mu}_{A}[x,\varphi^{I}(x)]$. This is the field theory counterpart to (1.106) and (1.107). If $\Delta^{\mu}_{A}=0$, then the action functional will be form-invariant, but from our discussion above this is not a necessary requirement for invariance of the equations of motion.

All that we have to do now is follow through an analysis similar to that in Section 1.5.1. Begin by changing variables from $(t',\mathbf{x}')$ in (2.102) to $(t,\mathbf{x})$ giving

$$S[\varphi']-S[\varphi]=\int_{t_1}^{t_2}dt\int_{\Sigma}d\sigma_x\Big\{J\mathcal{L}[\varphi'^{I}(x+\delta x),\frac{\partial x^{\nu}}{\partial x'^{\mu}}\partial_{\nu}\varphi'^{I}(x+\delta x),x+\delta x] -\mathcal{L}[\varphi^{I}(x),\partial_{\mu}\varphi^{I}(x),x]\Big\}, \tag{2.111}$$

where

$$J=\det\left(\frac{\partial x'^{\mu}}{\partial x^{\nu}}\right) \tag{2.112}$$

is the Jacobian of the coordinate transformation we have just performed. Note that we have used the chain rule to write

$$\partial'_{\mu}\varphi'^{I}(x')=\frac{\partial x^{\nu}}{\partial x'^{\mu}}\partial_{\nu}\varphi'^{I}(x+\delta x), \tag{2.113}$$

and that because we have changed variables from x'^{μ} to x^{μ}, we must write the arguments of the functions appearing in the integrand in terms of x^{μ} and not x'^{μ}. The aim now is to expand the integrand of (2.111) to first order in $\delta\epsilon^{A}$, and to write the result as the divergence of a vector field.

We first evaluate the Jacobian (2.112). If we rewrite (2.100) as

$$x'^{\mu}=x^{\mu}+\delta x^{\mu},$$

with $\delta x^{\mu}=\lambda^{\mu}{}_{A}(x)\delta\epsilon^{A}$, then $J=\det(\delta^{\mu}{}_{\nu}+\partial_{\nu}\delta x^{\mu})$. To lowest order in δx^{μ} we have simply $J=1$. In order to compute the first-order change in J we can use the identity

$$\det A=e^{\mathrm{tr}\ln A}, \tag{2.114}$$

which is valid for any matrix A which can be expressed in upper triangular form.[5] Using this identity we find

$$\begin{aligned}J&=e^{\mathrm{tr}\ln(\delta^{\mu}{}_{\nu}+\partial_{\nu}\delta x^{\mu})}\\&\simeq e^{\mathrm{tr}(\partial_{\nu}\delta x^{\mu})}\quad\text{(by expanding ln in a Taylor series to first order)}\\&=e^{\partial_{\mu}\delta x^{\mu}}\\&\simeq 1+\partial_{\mu}\delta x^{\mu},\end{aligned} \tag{2.115}$$

where the last line has resulted from expanding the exponential.

[5] It is easy to prove (2.114) if A is a symmetric matrix by diagonalization of A.

An alternate way to compute the Jacobian makes use of the definition of the determinant of a matrix. Consider $J = \det(I + \epsilon M)$ where M is any $n \times n$ matrix, and ϵ is any infinitesimal parameter. The definition of the determinant gives

$$J = \sigma^{i_1 \cdots i_n}(\delta_{1i_1} + \epsilon M_{1i_1}) \cdots (\delta_{ni_n} + \epsilon M_{ni_n}), \tag{2.116}$$

where $\sigma^{i_1 \cdots i_n} = +1(-1)$ if $i_1 \cdots i_n$ is an even (odd) permutation of $1 \cdots n$ and is zero otherwise. The repeated indices $i_1 \cdots i_n$ are summed over $1, \ldots, n$. Expanding (2.116) to linear order in ϵ results in

$$\begin{aligned} J = &\sigma^{i_1 \cdots i_n}(\delta_{1i_1} \cdots \delta_{ni_n} + \epsilon M_{1i_1}\delta_{2i_2} \cdots \delta_{ni_n} + \epsilon \delta_{1i_1} M_{2i_2} \cdots \delta_{ni_n} \\ &+ \cdots + \epsilon \delta_{1i_1} \cdots \delta_{(n-1)i_{n-1}} M_{ni_n}) + \cdots \\ = &\sigma^{1 \cdots n} + \epsilon(M_{1i_1}\sigma^{i_1 2 \cdots n} + M_{2i_2}\sigma^{1i_2 3 \cdots n} + \cdots \\ &+ M_{ni_n}\sigma^{12 \cdots (n-1)i_n}) + \cdots . \end{aligned}$$

If we use $\sigma^{1 \cdots n} = 1$ and $\sigma^{i_1 2 \cdots n} = 0$ unless $i_1 = 1$ it is then easy to see that

$$\begin{aligned} J &= 1 + \epsilon(M_{11} + M_{22} + \cdots M_{nn}) + \cdots \\ &= 1 + \epsilon \operatorname{tr} M + \cdots . \end{aligned} \tag{2.117}$$

If we apply this to $J = \det(\delta^\mu{}_\nu + \partial_\nu \delta x^\mu)$ we again find (2.115).

We must now expand $\mathcal{L}\Big[\varphi'^I(x + \delta x), (\partial x^\nu / \partial x'^\mu)\partial_\nu \varphi'^I(x + \delta x), x + \delta x\Big]$ to first order in δx^μ. The first and third arguments of $\mathcal{L}$ are given directly by (2.100) and (2.101) respectively. Only the middle argument needs any discussion. If we differentiate (2.100) with respect to x^ν we find

$$\frac{\partial x'^\mu}{\partial x^\nu} = \delta^\mu{}_\nu + \partial_\nu \delta x^\mu.$$

Because $\partial x^\nu / \partial x'^\mu$ is the inverse of $\partial x'^\mu / \partial x^\nu$, and we only work to first order in δx^μ, it should be clear that

$$\frac{\partial x^\nu}{\partial x'^\mu} \simeq \delta^\nu{}_\mu - \partial_\mu \delta x^\nu \tag{2.118}$$

to this order. Combining (2.118) with (2.101) shows that

$$\frac{\partial x^\nu}{\partial x'^\mu}\partial_\nu \varphi'^I(x + \delta x) \simeq \partial_\mu \varphi^I(x) + \partial_\mu(\Phi^I_A \delta\epsilon^A) - \partial_\mu(\lambda^\nu_A \delta\epsilon^A)\partial_\nu \varphi^I(x) \tag{2.119}$$

to first order in $\delta\epsilon^A$. Utilizing (2.115) and (2.119) along with (2.100) and (2.101) to expand the integrand in (2.111) to first order in $\delta\epsilon^A$ shows that

$$S[\varphi'] - S[\varphi] \simeq \int_{t_1}^{t_2} dt \int_\Sigma d\sigma_x \Big\{ \partial_\mu(\lambda^\mu_A \delta\epsilon^A)\mathcal{L} + \Phi^I_A \delta\epsilon^A \frac{\partial \mathcal{L}}{\partial \varphi^I} + \lambda^\mu_A \delta\epsilon^A \frac{\partial \mathcal{L}}{\partial x^\mu} + \Big[\partial_\mu(\Phi^I_A \delta\epsilon^A) - \partial_\mu(\lambda^\nu_A \delta\epsilon^A)\partial_\nu \varphi^I\Big] \frac{\partial \mathcal{L}}{\partial(\partial_\mu \varphi^I)} \Big\}. \quad (2.120)$$

Here $\mathcal{L}$ is now understood to be $\mathcal{L}\Big[\varphi^I(x), \partial_\mu\varphi^I(x), x^\mu\Big]$. The first term on the last line of (2.120) represents the derivative of $\mathcal{L}$ with respect to its third argument only.

We now look at the terms in the integrand of (2.120) that depend on Φ^I_A, and note that

$$\Phi^I_A \delta\epsilon^A \frac{\partial \mathcal{L}}{\partial \varphi^I} + \partial_\mu(\Phi^I_A \delta\epsilon^A) \frac{\partial \mathcal{L}}{\partial(\partial_\mu \varphi^I)} = \partial_\mu \left[\Phi^I_A \delta\epsilon^A \frac{\partial \mathcal{L}}{\partial(\partial_\mu \varphi^I)} \right], \quad (2.121)$$

if we use the Euler–Lagrange equations. The terms in (2.120) that involve $\lambda^\mu_A \delta\epsilon^A$ can also be written as a divergence upon use of the Euler–Lagrange equations:

$$\begin{aligned} &\partial_\mu(\lambda^\mu_A \delta\epsilon^A)\mathcal{L} + \lambda^\mu_A \delta\epsilon^A \frac{\partial \mathcal{L}}{\partial x^\mu} - \partial_\mu(\lambda^\nu_A \delta\epsilon^A)\partial_\nu \varphi^I \frac{\partial \mathcal{L}}{\partial(\partial_\mu \varphi^I)} \\ &\qquad = \partial_\mu \left[\lambda^\mu_A \delta\epsilon^A \mathcal{L} - \lambda^\nu_A \delta\epsilon^A \partial_\nu \varphi^I \frac{\partial \mathcal{L}}{\partial(\partial_\mu \varphi^I)} \right]. \end{aligned} \quad (2.122)$$

The results of (2.121) and (2.122) when used in (2.120) give rise to

$$S[\varphi'^I(x')] - S[\varphi^I(x)] \simeq \int_{t_1}^{t_2} dt \int_\Sigma d\sigma_x \partial_\mu(\Lambda^\mu_A \delta\epsilon^A), \quad (2.123)$$

where

$$\Lambda^\mu_A = \Phi^I_A \frac{\partial \mathcal{L}}{\partial(\partial_\mu \varphi^I)} + \lambda^\nu_A \left[\delta^\mu_\nu \mathcal{L} - \partial_\nu \varphi^I \frac{\partial \mathcal{L}}{\partial(\partial_\mu \varphi^I)} \right]. \quad (2.124)$$

Finally, by using (2.123) back in (2.110) we find

$$0 = \int_{t_1}^{t_2} dt \int_\Sigma d\sigma_x \partial_\mu \left(\Lambda^\mu_A \delta\epsilon^A - \Delta^\mu_A \delta\epsilon^A \right). \quad (2.125)$$

This is the direct counterpart of (1.119). Using the divergence theorem, assuming that either $\partial\Sigma$ is empty, or else that the fields satisfy boundary conditions leading to the vanishing of the surface term, we conclude that

$$G(t) = \int_\Sigma d\sigma_x \, \delta\epsilon^A (\Lambda^0_A - \Delta^0_A) \quad (2.126)$$

is independent of time ($G(t_2) = G(t_1)$ for any two times t_1 and t_2). With $\delta\epsilon^A$ chosen to be constant, this gives a set of conserved Noether charges defined by

$$Q_A = \int_\Sigma d\sigma_x (\Lambda^0_A - \Delta^0_A) \tag{2.127}$$

$$= \int_\Sigma d\sigma_x \left[\lambda^0_A \mathcal{L} + (\Phi^I_A - \lambda^\nu_A \partial_\nu \varphi^I) \frac{\partial \mathcal{L}}{\partial \dot{\varphi}^I} - \Delta^0_A \right]$$

$$= \int_\Sigma d\sigma_x \left[\lambda^0_A \mathcal{L} + (\Phi^I_A - \lambda^\nu_A \partial_\nu \varphi^I) \pi_I - \Delta^0_A \right] \tag{2.128}$$

if we use (2.124) and the definition of the canonical momentum (2.23). In the special case where the symmetry transformations correspond to inhomogeneous Lorentz transformations, the usual requirement is that the Lagrangian density is invariant. This requires $\Delta^\mu_A = 0$, simplifying the conservation law.

2.6 The stress–energy–momentum tensor

If the Lagrangian density has no explicit dependence on the spacetime coordinates, then the spacetime translation

$$x'^\mu = x^\mu + \delta\epsilon^\mu \tag{2.129}$$

will be a symmetry of the equations of motion leaving the action invariant. We may therefore take $\Delta^\mu_A = 0$ here. Comparison of (2.129) with (2.100) shows that the index A in our general treatment is a spacetime index, say α, and that

$$\lambda^\mu_\alpha = \delta^\mu_\alpha. \tag{2.130}$$

Also, fields should transform like scalars under (2.129), meaning that

$$\varphi'^I(x') = \varphi^I(x). \tag{2.131}$$

Comparison with (2.101) allows us to conclude that

$$\Phi^I_\alpha = 0 \tag{2.132}$$

for a spacetime translation. The conserved Noether current corresponding to the symmetry (2.129) follows from (2.124) as

$$t^\mu{}_\alpha = \frac{\partial \mathcal{L}}{\partial(\partial_\mu \varphi^I)} \partial_\alpha \varphi^I - \delta^\mu_\alpha \mathcal{L}. \tag{2.133}$$

It obeys

$$\partial_\mu t^\mu{}_\alpha = 0 \tag{2.134}$$

as a consequence of Noether's theorem.[6] We have chosen to define $t^\mu{}_\alpha = -\Lambda^\mu{}_\alpha$ to facilitate the identification of the conserved charges given below.

The conserved Noether charges follow from (2.127) as

$$Q_\alpha = \int_\Sigma d\sigma_x t^0{}_\alpha. \tag{2.135}$$

If we take $\alpha = 0$, it follows from (2.133) that

$$\begin{aligned} t^0{}_0 &= \frac{\partial \mathcal{L}}{\partial \dot{\varphi}^I}\dot{\varphi}^I - \mathcal{L} \\ &= \pi_I \dot{\varphi}^I - \mathcal{L} \\ &= \mathcal{H} \end{aligned}$$

is the Hamiltonian density. Thus the Noether charge $Q_0 = H$ is the Hamiltonian. With $\alpha = i$ (corresponding to a spatial index) we have

$$t^0{}_i = \pi_I \partial_i \varphi^I. \tag{2.136}$$

The conserved charge is

$$Q_i = \int_\Sigma d\sigma_x \pi_I \partial_i \varphi^I. \tag{2.137}$$

Since this corresponds to invariance under a translation in space, we will identify Q_i with the linear momentum.

$t^\mu{}_\alpha$, as defined in (2.133), is called the 'canonical stress–energy–momentum tensor'.[7] The stress–energy–momentum tensor plays a central role in Einstein's theory of general relativity, acting as a source term in the gravitational field equations (see Weinberg (1972) for example). However, it is not $t^\mu{}_\alpha$ which plays this role, but rather a modified version of it. The basic problem with using $t^\mu{}_\alpha$ is that it is not symmetrical in general; that is, $t_{\mu\alpha} \neq t_{\alpha\mu}$. Einstein's theory of general relativity requires the source term to be symmetrical. Even without appealing to the authority of Einstein's general relativity, there are problems if $t_{\mu\alpha}$ is not symmetrical. One of these problems comes about if we compute $t_{\mu\alpha}$ for Maxwell's theory of

[6] This can also be verified directly from (2.133) by differentiation and use of the Euler–Lagrange equations.

[7] Sometimes it is called the 'stress–energy', or 'energy–momentum', or simply the 'stress tensor'.

electromagnetism (see Section 2.3.4). If we take $\mathcal{L} = -(1/4)F^{\mu\nu}F_{\mu\nu}$ and $\varphi^I \leftrightarrow A^\mu$, a simple calculation shows that

$$t^\mu{}_\alpha = \frac{1}{4}\delta^\mu_\alpha F_{\nu\sigma}F^{\nu\sigma} - F^{\mu\nu}\partial_\alpha A_\nu. \tag{2.138}$$

The problem with (2.138) is that the last term on the right-hand side is not invariant under the gauge transformation (2.68). The canonical stress–energy–momentum tensor is therefore not gauge-invariant and cannot represent a physical quantity. The second problem will come to light when we consider invariance under Lorentz transformations. This provides sufficient motivation to look for a symmetrical stress–energy–momentum tensor.

If we lower the index μ in (2.133), it is easily seen that the first term on the right-hand side is not manifestly symmetric. The most obvious thing to do whenever we encounter such a situation is to make the object symmetrical by hand, by defining

$$\tilde{t}_{\mu\alpha} = \frac{1}{2}(t_{\mu\alpha} + t_{\alpha\mu}). \tag{2.139}$$

This is clearly symmetric, but no longer satisfies a conservation law

$$\partial^\mu \tilde{t}_{\mu\alpha} = 0, \tag{2.140}$$

required for the existence of conserved charges.[8] We must find a symmetrical form for $t_{\mu\alpha}$ without sacrificing the conservation law (2.134). A way to do this was discussed by Belinfante (1939).[9] Belinfante's method, which we will follow, is reviewed in Wentzel (1949).

Suppose that we consider the infinitesimal Lorentz transformation defined in (1.178) with $\delta\epsilon_{\mu\nu} = -\delta\epsilon_{\nu\mu}$ as in (1.180). The Lagrangian density will be required to be invariant under this transformation. From (2.101), the fields obey[10]

$$\begin{aligned}\delta\varphi^I(x) &= \varphi'^I(x') - \varphi^I(x) \\ &= \Phi^I_{\mu\nu}(x)\delta\epsilon^{\mu\nu}.\end{aligned} \tag{2.141}$$

Because of the antisymmetry of $\delta\epsilon^{\nu\mu} = -\delta\epsilon^{\mu\nu}$, we can take

$$\Phi^I_{\nu\mu} = -\Phi^I_{\mu\nu} \tag{2.142}$$

[8] It also will not cure the gauge-dependence problem we found in (2.138).
[9] Rosenfeld (1940) showed how to obtain a symmetrized tensor in general relativity.
[10] Our index A on the parameters $\delta\epsilon^A$ must now refer to a pair of spacetime indices.

without any loss of generality.[11] Noting that $\delta x^\mu = \delta\epsilon^\mu{}_\nu x^\nu$ we see, by comparison with (2.100), that we have

$$\lambda^\mu_{\alpha\beta}\delta\epsilon^{\alpha\beta} = \delta\epsilon^\mu{}_\nu x^\nu. \tag{2.143}$$

Relabelling indices on the right-hand side to match those on the left-hand side, and noting that $\lambda^\mu_{\alpha\beta} = -\lambda^\mu_{\beta\alpha}$, by the same argument as we used leading up to (2.142), we find

$$\lambda^\mu_{\alpha\beta} = \frac{1}{2}\left(\delta^\mu_\alpha\eta_{\beta\nu} - \delta^\mu_\beta\eta_{\alpha\nu}\right)x^\nu. \tag{2.144}$$

The conserved Noether current follows from (2.124) as

$$\Delta^\mu_{\alpha\beta} = \Phi^I_{\alpha\beta}\frac{\partial\mathcal{L}}{\partial(\partial_\mu\varphi^I)} + \lambda^\nu_{\alpha\beta}\left[\delta^\mu_\nu\mathcal{L} - \partial_\nu\varphi^I\frac{\partial\mathcal{L}}{\partial(\partial_\mu\varphi^I)}\right]. \tag{2.145}$$

If we use the definition (2.133), and for convenience define

$$H^\mu{}_{\alpha\beta} = \Phi^I_{\alpha\beta}\frac{\partial\mathcal{L}}{\partial(\partial_\mu\varphi^I)}, \tag{2.146}$$

we can write (2.145) as

$$\Delta^{\mu\alpha\beta} = H^{\mu\alpha\beta} + \frac{1}{2}(x^\alpha t^{\mu\beta} - x^\beta t^{\mu\beta}), \tag{2.147}$$

after raising the indices α and β. Because we require the Lagrangian density to be Lorentz-invariant, we must have

$$\partial_\mu\Delta^{\mu\alpha\beta} = 0 \tag{2.148}$$

as a consequence of Noether's theorem. From (2.147), this requires

$$0 = \partial_\mu H^{\mu\alpha\beta} + \frac{1}{2}(t^{\alpha\beta} - t^{\beta\alpha}). \tag{2.149}$$

The result (2.149) is the crucial identity needed to construct a symmetrical stress–energy–momentum tensor. It is obvious that $t^{\alpha\beta}$ is symmetric if and only if $\partial_\mu H^{\mu\alpha\beta} = 0$. This turns out to be the case for a scalar field, but not for general fields. (For scalar fields we have $\varphi'^I(x') = \varphi^I(x)$ by definition, which results in $\Phi^I_{\alpha\beta} = 0$, and hence $H^\mu{}_{\alpha\beta} = 0$.)

[11] This is because if $\Phi^I_{\mu\nu}$ has a part which is symmetrical under the interchange of μ and ν, this symmetrical part would make no contribution to (2.141) due to the antisymmetry of $\delta\epsilon^{\mu\nu}$.

Define a new tensor $T_{\alpha\beta}$ by

$$T_{\alpha\beta} = t_{\alpha\beta} + \partial^\mu G_{\mu\alpha\beta} \tag{2.150}$$

for some $G_{\mu\alpha\beta}$ to be determined. Require $T_{\alpha\beta}$ to be symmetric

$$T_{\beta\alpha} = T_{\alpha\beta}, \tag{2.151}$$

and conserved,

$$\partial^\alpha T_{\alpha\beta} = 0. \tag{2.152}$$

Since we already know that $\partial^\alpha t_{\alpha\beta} = 0$ from (2.150), we must have

$$\partial^\alpha \partial^\mu G_{\mu\alpha\beta} = 0, \tag{2.153}$$

if (2.152) is to hold. The simplest way to ensure (2.153) is to require[12]

$$G_{\mu\alpha\beta} = -G_{\alpha\mu\beta}. \tag{2.154}$$

Demanding (2.151) requires

$$0 = t_{\alpha\beta} - t_{\beta\alpha} + \partial^\mu (G_{\mu\alpha\beta} - G_{\mu\beta\alpha}).$$

From (2.149) we find

$$0 = -2\partial^\mu H_{\mu\alpha\beta} + \partial^\mu (G_{\mu\alpha\beta} - G_{\mu\beta\alpha}),$$

leading us to choose[13]

$$G_{\mu\alpha\beta} - G_{\mu\beta\alpha} = 2H_{\mu\alpha\beta}. \tag{2.155}$$

All that remains is for us to solve for $G_{\mu\alpha\beta}$ and verify that our solution obeys (2.154) and (2.155).

To solve (2.155) we can use the following procedure. Write down the same equation with the indices $(\mu\alpha\beta)$ replaced with $(\alpha\beta\mu)$:

$$G_{\alpha\beta\mu} - G_{\alpha\mu\beta} = 2H_{\alpha\beta\mu}. \tag{2.156}$$

Now write down (2.156) with the indices $(\alpha\beta\mu)$ replaced with $(\beta\mu\alpha)$:

$$G_{\beta\mu\alpha} - G_{\beta\alpha\mu} = 2H_{\beta\mu\alpha}. \tag{2.157}$$

[12] It is easy to see that this antisymmetry condition implies (2.153) because $\partial^\alpha \partial^\mu = \partial^\mu \partial^\alpha$ is symmetric.

[13] Note that because $H_{\mu\beta\alpha} = -H_{\mu\alpha\beta}$, this is a consistent choice.

Add together (2.155) and (2.156), and subtract off (2.157):

$$G_{\mu\alpha\beta} - G_{\mu\beta\alpha} + G_{\alpha\beta\mu} - G_{\alpha\mu\beta} - G_{\beta\mu\alpha} + G_{\beta\alpha\mu} = 2(H_{\mu\alpha\beta} + H_{\alpha\beta\mu} - H_{\beta\mu\alpha}).$$

The left-hand side may be simplified using (2.154) to leave

$$\begin{aligned} G_{\mu\alpha\beta} &= H_{\mu\alpha\beta} + H_{\alpha\beta\mu} - H_{\beta\mu\alpha} \\ &= H_{\mu\alpha\beta} + H_{\alpha\beta\mu} + H_{\beta\alpha\mu}, \end{aligned} \tag{2.158}$$

where in the last line we have used $H_{\beta\mu\alpha} = -H_{\beta\alpha\mu}$.[14] We therefore have constructed a symmetric, conserved tensor $T_{\alpha\beta}$ given in terms of the canonical one $t_{\alpha\beta}$ by

$$T_{\alpha\beta} = t_{\alpha\beta} + \partial^{\mu}(H_{\mu\alpha\beta} + H_{\alpha\beta\mu} + H_{\beta\alpha\mu}). \tag{2.159}$$

It is possible to show that the conserved Noether charges defined in (2.135) are not affected by whether we use $t_{\alpha\beta}$ or $T_{\alpha\beta}$. First of all, taking $\alpha = \beta = 0$ in (2.159) we find

$$\begin{aligned} T_{00} &= t_{00} + \partial^{\mu}(H_{\mu 00} + H_{00\mu} + H_{00\mu}) \\ &= t_{00} + 2\partial^{\mu} H_{00\mu} \\ &= t_{00} + 2\partial^{i} H_{00i}. \end{aligned} \tag{2.160}$$

We have used the antisymmetry property $H_{\mu\alpha\beta} = -H_{\mu\beta\alpha}$ to conclude that $H_{\mu 00} = 0$ here. The second term on the right-hand side of (2.160) takes the form of a spatial divergence. This means that when we integrate over Σ to form Q_0, we can assume that this term vanishes. We also have

$$\begin{aligned} T_{0i} &= t_{0i} + \partial^{\mu}(H_{\mu 0i} + H_{0i\mu} + H_{i\mu 0}) \\ &= t_{0i} + \partial^{0}(H_{00i} + H_{0i0} + H_{i00}) + \partial^{j}(H_{j0i} + H_{0ij} + H_{ij0}) \\ &= t_{0i} + \partial^{j}(H_{j0i} + H_{0ij} + H_{ij0}) \end{aligned} \tag{2.161}$$

where the second term of the middle line vanishes identically using $H_{i00} = 0$ and $H_{00i} = -H_{0i0}$. This shows that T_{0i} and t_{0i} differ by a spatial divergence which vanishes upon integration over Σ to form Q_i.

Finally we will look at the conserved Noether charges arising from the current (2.147), and which correspond to invariance under Lorentz transformations. We define[15]

$$J^{\alpha\beta} = 2\int_{\Sigma} d\sigma_x \Delta^{0\alpha\beta}. \tag{2.162}$$

[14] As a check, it is simple to show that the result in (2.158) does satisfy (2.154) and (2.155).

[15] The factor of 2 is inserted here to remove the factor of 1/2 which occurs in (2.147) to facilitate the physical interpretation of the charges.

To obtain the last line, we have used $G^{00\beta} = 0$ which follows from (2.154) to note that the term in the summation over ν in the first line with $\nu = 0$ vanishes. Based on our previous experience with particle mechanics, we would expect $J^{\alpha\beta}$ to be related to the angular momentum tensor. Because the symmetric stress–energy–momentum tensor plays a more important role than the canonical one, we will define

$$\mathcal{I}^{\mu\alpha\beta} = \frac{1}{2}(x^\alpha T^{\mu\beta} - x^\beta T^{\mu\alpha}). \tag{2.163}$$

This tensor is easily seen to be conserved,

$$\partial_\mu \mathcal{I}^{\mu\alpha\beta} = 0, \tag{2.164}$$

by virtue of the properties (2.151) and (2.152).

If we can show that $\mathcal{I}^{0\alpha\beta}$ differs from $\Delta^{0\alpha\beta}$ by no more than a spatial divergence, this will be sufficient to conclude that $\mathcal{I}^{\mu\alpha\beta}$ and $\Delta^{\mu\alpha\beta}$ give rise to the same Noether charges (2.162). To do this, first use (2.150) to find

$$\mathcal{I}^{\mu\alpha\beta} = \frac{1}{2}(x^\alpha t^{\mu\beta} - x^\beta t^{\mu\alpha}) + \frac{1}{2}x^\alpha \partial_\nu G^{\nu\mu\beta} - \frac{1}{2}x^\beta \partial_\nu G^{\nu\mu\alpha}.$$

Next, use (2.147) to obtain

$$\mathcal{I}^{\mu\alpha\beta} = \Delta^{\mu\alpha\beta} - H^{\mu\alpha\beta} + \frac{1}{2}x^\alpha \partial_\nu G^{\nu\mu\beta} - \frac{1}{2}x^\beta \partial_\nu G^{\nu\mu\alpha}.$$

We can rewrite the last two terms on the right-hand side to give

$$\begin{aligned}\mathcal{I}^{\mu\alpha\beta} &= \Delta^{\mu\alpha\beta} - H^{\mu\alpha\beta} + \frac{1}{2}\partial_\nu(x^\alpha G^{\nu\mu\beta} - x^\beta G^{\nu\mu\alpha}) \\ &\quad -\frac{1}{2}(G^{\alpha\mu\beta} - G^{\beta\mu\alpha}) \\ &= \Delta^{\mu\alpha\beta} + \frac{1}{2}\partial_\nu(x^\alpha G^{\nu\mu\beta} - x^\beta G^{\nu\mu\alpha}),\end{aligned} \tag{2.165}$$

where we simplify the right-hand side using (2.154) and (2.155). Taking $\mu = 0$ in (2.165) yields

$$\begin{aligned}\mathcal{I}^{0\alpha\beta} &= \Delta^{0\alpha\beta} + \frac{1}{2}\partial_\nu(x^\alpha G^{\nu 0\beta} - x^\beta G^{\nu 0\alpha}) \\ &= \Delta^{0\alpha\beta} + \frac{1}{2}\partial_j(x^\alpha G^{j0\beta} - x^\beta G^{j0\alpha}).\end{aligned} \tag{2.166}$$

By our usual argument concerning spatial divergences, the last term of (2.166) makes no contribution to the conserved Noether charges $J^{\alpha\beta}$ defined in (2.162). We are therefore free to take

$$J^{\alpha\beta} = \int_\Sigma d\sigma_x (x^\alpha T^{0\beta} - x^\beta T^{0\alpha}) \tag{2.167}$$

as the Noether charges. If we regard $T^{0\alpha}$ as representing the density of 4-momentum, then (2.167) has an obvious comparison with (1.183).

We can further the comparison with what we found in Section 1.5.3 by looking at J^{0i}. From (2.167) we find

$$J^{0i} = \int_\Sigma d\sigma_x (x^0 T^{0i} - x^i T^{00}).$$

If we define the Noether charges

$$P^\alpha = \int_\Sigma d\sigma_x T^{0\alpha}$$

which we have already seen to be the 4-momentum, and define the centre of energy by

$$x^i_{cm} = \frac{\int_\Sigma d\sigma_x \, x^i T^{00}}{\int_\Sigma d\sigma_x \, T^{00}},$$

analogously to what we did in (1.192), we find

$$J^{0i} = x^0 P^i - x^i_{cm} P^0$$

conserved exactly as we had for the relativistic particle in (1.193). The conclusion (1.194) follows again.

2.6.1 Scalar field

The Lagrangian density for the real scalar field was given in (2.39). We have already remarked that a scalar field is characterized by $\varphi'(x') = \varphi(x)$ under a Lorentz (or in fact any) coordinate transformation. This means that

$$\Phi^I_{\alpha\beta} = 0,$$

and as a consequence

$$T_{\alpha\beta} = t_{\alpha\beta}.$$

A simple calculation shows that the stress–energy–momentum tensor is given by

$$T_{\alpha\beta} = t_{\alpha\beta} = \partial_\alpha \varphi \partial_\beta \varphi - \eta_{\alpha\beta} \mathcal{L}. \tag{2.168}$$

2.6.2 Maxwell field

We can now return to the problem encountered with the Maxwell field in (2.138). The canonical stress–energy–momentum tensor was gauge dependent. However, we are really interested in the symmetrical tensor $T_{\alpha\beta}$.

Under an infinitesimal Lorentz transformation, $A^\mu(x)$ transforms like x^μ, so we have

$$\delta A^\mu(x) = \delta\epsilon^\mu{}_\nu A^\nu(x).$$

Comparison with the general result (2.101), noting that $I = \mu$ is a space-time index here, shows that

$$\Phi^\mu_{\alpha\beta}\delta\epsilon^{\alpha\beta} = \delta\epsilon^\mu{}_\nu A^\nu, \tag{2.169}$$

leading to[16]

$$\Phi^\mu_{\alpha\beta} = \frac{1}{2}\left(\delta^\mu_\alpha A_\beta - \delta^\mu_\beta A_\alpha\right). \tag{2.170}$$

We can now use (2.146), along with $\mathcal{L} = -(1/4)F^{\mu\nu}F_{\mu\nu}$, to find

$$H_{\mu\alpha\beta} = \frac{1}{2}\left(A_\alpha F_{\mu\beta} - A_\beta F_{\mu\alpha}\right). \tag{2.171}$$

Using this result in (2.158) leads to

$$G_{\mu\alpha\beta} = A_\beta F_{\alpha\mu} \tag{2.172}$$

noting $F_{\nu\mu} = -F_{\mu\nu}$. We can compute

$$\begin{aligned}\partial^\mu G_{\mu\alpha\beta} &= \partial^\mu A_\beta F_{\alpha\mu} + A_\beta \partial^\mu F_{\alpha\mu} \\ &= \partial_\mu A_\beta F_\alpha{}^\mu\end{aligned}$$

using the Maxwell equations. (See (2.67) with $J^\mu = 0$, because we have no sources present here.) The symmetric conserved stress–energy– momentum tensor follows from (2.150) as

$$\begin{aligned}T_{\alpha\beta} &= t_{\alpha\beta} + \partial_\mu A_\beta F_\alpha{}^\mu \\ &= F_\alpha{}^\mu F_{\mu\beta} + \frac{1}{4}\eta_{\alpha\beta}F_{\mu\nu}F^{\mu\nu}\end{aligned} \tag{2.173}$$

using the canonical expression (2.138). Unlike our previous result for $t_{\alpha\beta}$, our new expression $T_{\alpha\beta}$ is gauge-invariant, since it involves only the gauge-invariant combination $F_{\mu\nu}$.

[16] Again care must be taken in cancelling off $\delta\epsilon^{\alpha\beta}$ from each side of (2.169) because of the antisymmetry in α and β.

It is simple to use the components of $F_{\mu\nu}$ given in (2.66) for three spatial dimensions to show that

$$T_{00} = \frac{1}{2}(E^2 + B^2), \tag{2.174}$$

$$T_{0i} = -(\mathbf{E} \times \mathbf{B})_i. \tag{2.175}$$

From electromagnetic theory (Jackson, 1962), T_{00} may be recognized as the energy density, and T_{0i} is related to the Poynting vector which describes the flow of energy.[17]

The conserved angular momentum may be found using (2.167). In the case of $D = 3$, we can define a vector $\mathbf{J}$ with components $\mathbf{J} = (J^{23}, J^{31}, J^{12})$, and it can then be seen from (2.175) that

$$\mathbf{J} = \int_\Sigma d\sigma_x \, \mathbf{x} \times (\mathbf{E} \times \mathbf{B}), \tag{2.176}$$

recognized as the standard expression for the angular momentum of electromagnetic radiation.[18]

The correspondence between our general results and the more familiar expressions from electromagnetism would not have been so evident had we not used the symmetric stress–energy–momentum tensor.

2.7 Gauge invariance

2.7.1 U(1) *symmetry*

The Lagrangian (or Hamiltonian) for the Schrödinger field is invariant under the transformation

$$\Psi(x) \to \Psi'(x) = e^{i\epsilon}\Psi(x), \tag{2.177}$$

where ϵ is an arbitrary real constant. This reflects the well-known property of wave mechanics that physically measurable quantities do not depend on the phase of the wave function. Suppose that we promote this from a rigid gauge symmetry to a local one by letting ϵ depend on t and $\mathbf{x}$. This means that we allow the phase of the Schrödinger field to vary from place to place as well as in time, and demand that the theory be invariant under this transformation. It should be clear that the

[17] The spatial components T_{ij} can be found easily, and describe the Maxwell stress tensor for electromagnetism.

[18] See for example the discussions in Heitler (1984) or Low (1997).

action functional obtained using (2.54) will not have this local symmetry because $\mathcal{L}$ involves derivatives of the field Ψ. We have

$$\partial_\mu \Psi \to \partial_\mu \Psi' = e^{i\epsilon}(\partial_\mu \Psi + i\partial_\mu \epsilon \Psi). \tag{2.178}$$

The presence of terms involving $\partial_\mu \epsilon$ spoils the invariance under the local transformation (2.177). If we wish to insist upon local invariance then the theory must be modified.

In order to see how to modify the theory to obtain local invariance, consider the infinitesimal form of (2.177):

$$\delta\Psi = i\delta\epsilon\Psi. \tag{2.179}$$

We also have

$$\delta\Psi^* = -i\delta\epsilon\Psi^*. \tag{2.180}$$

From the expression for $\mathcal{L}$ in (2.54) it is easy to show that to first order in $\delta\epsilon$ we have

$$\delta\mathcal{L} = -\dot{\delta\epsilon}\Psi^*\Psi + \frac{i}{2m}(\partial^i\delta\epsilon)(\Psi^*\partial_i\Psi - \partial_i\Psi^*\Psi), \tag{2.181}$$

under the transformations (2.179) and (2.180). Because $\mathcal{L}$ is invariant under a rigid transformation we would expect that $\delta\mathcal{L}$ should only depend on derivatives of $\delta\epsilon$ and this is the case in (2.181). We will define

$$J_0 = \Psi^*\Psi, \tag{2.182}$$

$$J_i = \frac{i}{2m}(\partial_i\Psi^*\Psi - \Psi^*\partial_i\Psi). \tag{2.183}$$

These two expressions should be familiar from wave mechanics where J_0 represents the probability density and J_i represents the probability current (see Schiff (1968), for example). We can write

$$\delta\mathcal{L} = -\dot{\delta\epsilon}J_0 - (\partial^i\delta\epsilon)J_i. \tag{2.184}$$

We will now modify the theory by adding on a term $B_\mu J^\mu$ to $\mathcal{L}$ where B_μ is a new vector field whose transformation law is to be determined and whose purpose is to lead to a new Lagrangian that is invariant under the local gauge transformation. Let

$$\mathcal{L}_1 = \mathcal{L} + B_\mu J^\mu. \tag{2.185}$$

Then we calculate

$$\begin{aligned}\delta\mathcal{L}_1 &= \delta\mathcal{L} + \delta B_\mu J^\mu + B_\mu \delta J^\mu \\ &= -\dot{\delta\epsilon}J_0 - (\partial_i\delta\epsilon)J^i + \delta B_0 J^0 + \delta B_i J^i + B_\mu \delta J^\mu\end{aligned}$$

if (2.184) is used. Suppose that we pick

$$\delta B_0 = \dot{\delta\epsilon}, \tag{2.186}$$

$$\delta B_i = \partial_i \delta\epsilon. \tag{2.187}$$

Then the result for $\delta\mathcal{L}_1$ simplifies to

$$\delta\mathcal{L}_1 = B^0 \delta J_0 + B^i \delta J_i. \tag{2.188}$$

We can compute δJ_0 and δJ_i from (2.182) and (2.183). It is easily shown that

$$\delta J_0 = 0, \tag{2.189}$$

$$\delta J_i = -\frac{1}{m}(\partial_i \delta\epsilon)\Psi^*\Psi. \tag{2.190}$$

We therefore have

$$\delta\mathcal{L}_1 = -\frac{1}{m} B^i (\partial_i \delta\epsilon)\Psi^*\Psi.$$

Since (2.187) holds we may write

$$\begin{aligned}\delta\mathcal{L}_1 &= -\frac{1}{m} B^i \delta B_i \Psi^*\Psi \\ &= -\frac{1}{2m}\delta(B^i B_i \Psi^*\Psi)\end{aligned}$$

if we note that $\delta(B^i B_i) = 2B^i \delta B_i$ and $\delta(\Psi^*\Psi) = 0$. Finally if we define

$$\mathcal{L}_2 = \mathcal{L}_1 + \frac{1}{2m} B^i B_i \Psi^*\Psi,$$

we have $\delta\mathcal{L}_2 = 0$. The Lagrangian density for a theory with local invariance corresponding to an arbitrary infinitesimal change in the phase of the field is therefore given by $\mathcal{L}_2$. We have

$$\begin{aligned}\mathcal{L}_2 = {} & \frac{i}{2}\left[\Psi^*(\partial_0 - iB_0)\Psi - (\partial_0\Psi^* + iB_0\Psi^*)\Psi\right] \\ & -\frac{1}{2m}(\partial^i\Psi^* + iB^i\Psi^*)(\partial_i\Psi - iB_i\Psi) - V\Psi^*\Psi,\end{aligned} \tag{2.191}$$

as the Lagrangian density for the theory with invariance under (2.179) and (2.180). It is easily verified that the theory (2.191) is also invariant under the finite transformation (2.177) which is called a 'local gauge transformation'.

It is convenient to rewrite (2.191) by introducing gauge-covariant derivatives. We will define

$$D_\mu \Psi = \partial_\mu \Psi - iB_\mu \Psi, \tag{2.192}$$

$$D_\mu \Psi^* = \partial_\mu \Psi^* + iB_\mu \Psi^*, \tag{2.193}$$

We can now write

$$\mathcal{L}_2 = \frac{i}{2}\left[\Psi^* D_0 \Psi - (D_0 \Psi^*)\Psi\right] - \frac{1}{2m}(\mathbf{D}\Psi^*)\cdot(\mathbf{D}\Psi) - V\Psi^*\Psi. \tag{2.194}$$

This is the same form as the original Lagrangian density $\mathcal{L}$ except that ∂_μ has been replaced with D_μ. It is easy to show that the transformations (2.186) and (2.187) may be written in a more covariant form as

$$\delta B_\mu = B'_\mu - B_\mu = \partial_\mu \epsilon. \tag{2.195}$$

Using this, under a finite gauge transformation specified in (2.177) we have

$$D'_\mu \Psi' = e^{i\epsilon} D_\mu \Psi, \tag{2.196}$$

$$D'_\mu \Psi'^* = e^{-i\epsilon} D_\mu \Psi^*. \tag{2.197}$$

The new modified derivatives in (2.192) and (2.193) transform in exactly the same way as the fields Ψ and Ψ' under a local gauge transformation. In fact with hindsight we can note that because it was the derivative terms in the original Lagrangian density which destroyed invariance under local gauge transformations, if we define new derivatives by (2.192) and (2.193) with the transformation properties (2.196) and (2.197) this would require B_μ to transform as in (2.195). We would arrive at (2.194) in a much simpler way than that presented above. Nevertheless the derivation we have given should give us some faith that we could have arrived at a locally gauge-invariant Lagrangian without being too clever.

We are now left with the task of identifying the physical significance of the field B_μ that has been introduced. Nature has provided us with a natural candidate, namely the gauge potential of electromagnetism. The Maxwell equations involve A_μ only through the combination

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu. \tag{2.198}$$

The theory is therefore invariant under the gauge transformation

$$A_\mu \to A'_\mu = A_\mu + \partial_\mu \theta, \tag{2.199}$$

for arbitrary function θ (see Section 2.3.4). The similarity between (2.199) and (2.195) should be obvious. We may therefore take

$$B_\mu = \kappa A_\mu, \tag{2.200}$$

for some constant κ. The constant κ is completely arbitrary, and the theory is invariant under the local gauge transformation for any choice of κ. We must therefore use the physics of the problem to fix κ. To do this we will add on the action for electromagnetism to $\mathcal{L}_2$ in (2.191) or (2.194). This gives

$$\begin{aligned}\mathcal{L} = &-\frac{1}{4}F_{\mu\nu}F^{\mu\nu} + \frac{i}{2}\left[\Psi^*(\partial_0 - i\kappa A_0)\Psi - (\partial_0\Psi^* + i\kappa A_0\Psi^*)\Psi\right] \\ &-\frac{1}{2m}(\partial^i\Psi^* + i\kappa A^i\Psi^*)(\partial_i\Psi - i\kappa A_i\Psi) - V\Psi^*\Psi.\end{aligned} \tag{2.201}$$

If we vary the action obtained from using (2.201) we find after a straightforward calculation

$$\delta S = \int_{t_1}^{t_2} dt \int_\Sigma d\sigma_x \left(\partial_\mu F^{\mu\nu}\delta A_\nu + \kappa\delta A_0\tilde{J}^0 + \kappa\delta A_i\tilde{J}^i\right), \tag{2.202}$$

where we have defined

$$\tilde{J}^0 = \tilde{J}_0 = \Psi^*\Psi, \tag{2.203}$$

$$\tilde{J}_i = \frac{i}{2m}\left[(\partial_i\Psi^* + i\kappa A_i\Psi^*)\Psi - \Psi^*(\partial_i\Psi - i\kappa A_i\Psi)\right]. \tag{2.204}$$

$\tilde{J}_i$ differs from (2.183) by the addition of terms in A_i. We find the Maxwell equations to be

$$\partial_\mu F^{0\mu} = \kappa\tilde{J}^0, \tag{2.205}$$

$$\partial_\mu F^{i\mu} = \kappa\tilde{J}^i. \tag{2.206}$$

From (2.67) we expect that the right-hand side of (2.205) should involve $-e\Psi^*\Psi$ since $e\Psi^*\Psi$ would be the charge density for a field describing particles of charge e. This will be the case if we choose $\kappa = -e$.

To conclude, we note that there is another way to introduce the field strength $F_{\mu\nu}$ defined in (2.198). Suppose that we consider the second covariant derivative of Ψ and form the commutator $[D_\mu, D_\nu]\Psi = D_\mu D_\nu\Psi - D_\nu D_\mu\Psi$. A straightforward computation shows that

$$[D_\mu, D_\nu]\Psi = -ieF_{\mu\nu}\Psi. \tag{2.207}$$

The electromagnetic field strength tensor enters in a natural way through the gauge-covariant derivative.

2.7.2 Non-Abelian gauge symmetry

This section assumes a basic knowledge of Lie algebras. Hopefully students who have never studied this subject formally will be familiar with the basic notions from their study of angular momentum in quantum mechanics (see Schiff (1968, p. 199) for example). The student who is not comfortable with this topic can omit this section.[19]

We start by noting that the transformation (2.177) involves the factor $U(\epsilon(x)) = e^{i\epsilon(x)}$ which may be thought of as an element of the Abelian group $U(1)$. It is possible to generalize this to other continuous groups, called Lie groups, by taking

$$U(\epsilon(x)) = e^{i\epsilon^A(x)T_A}, \tag{2.208}$$

where T_A are the generators of the group. $U[\epsilon(x)]$ is said to provide a representation of the group with ϵ^A the group parameters. Nothing will be lost here by thinking of T_A as a set of matrices, although a more abstract presentation is possible. If the representation of the group is unitary, meaning that $U[\epsilon(x)]$ is a unitary matrix, then the generators T_A are Hermitian: $T_A^\dagger = T_A$. The generators T_A obey the Lie algebra

$$[T_A, T_B] = if_{AB}{}^C T_C, \tag{2.209}$$

where $f_{AB}{}^C = -f_{BA}{}^C$ are called the 'structure constants' of the group.[20] The familiar example is the group of rotations in three-dimensional space, called '$SO(3,\mathbb{R})$', where T_A represent the components of angular momentum, and the parameters ϵ^A are the angles of rotation.[21]

To generalize (2.177) we will consider $\Phi(x)$ to be a set of N complex fields arrayed as a column vector and take

$$\Phi'(x) = U[\epsilon(x)]\Phi(x). \tag{2.210}$$

Because we are not considering the spacetime coordinates as undergoing any transformation, this is an example of what is called an 'internal symmetry'. Our task, as for the local $U(1)$ gauge transformation considered earlier, is to find a Lagrangian density for the fields $\Phi(x)$ which is invariant under the transformation (2.210). To do this we will look at the derivative of Φ and define a gauge-covariant derivative analogous to (2.192) and (2.193).

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[19] For a nice introduction to Lie algebras, aimed at field theory, see Burgess (2002).

[20] Again we emphasize the use of summation convention for the repeated index C in (2.209).

[21] For example, if L_x, L_y, and L_z are the operators representing orbital angular momentum, then $[L_x, L_y] = i\hbar L_z$ is an example of (2.209). See Schiff (1968, p. 199).

Let

$$D_\mu \Phi = \partial_\mu \Phi - iB_\mu \Phi. \tag{2.211}$$

This time because Φ is an N-component vector, we must regard B_μ as an $N \times N$ matrix. We should be able to write B_μ as a linear combination of the generators T_A:

$$B_\mu = B_\mu^A T_A, \tag{2.212}$$

where B_μ^A is a set of vector fields. Since $T_A^\dagger = T_A$ we have $B_\mu^\dagger = B_\mu$. We therefore define (taking the adjoint of (2.211))

$$D_\mu \Phi^\dagger = \partial_\mu \Phi^\dagger + i\Phi^\dagger B_\mu, \tag{2.213}$$

to be the covariant derivative of $\Phi^\dagger$. If Φ is a column vector, then $\Phi^\dagger$ is a row vector. We will now choose the transformation of B_μ to be so that $D_\mu \Phi$ transforms in the same way as Φ under a gauge transformation. We require

$$D'_\mu \Phi' = U D_\mu \Phi. \tag{2.214}$$

Using (2.211) and writing out the gauge-covariant derivatives leads to

$$iB'_\mu U\Phi = iUB_\mu \Phi + (\partial_\mu U)\Phi.$$

Since this must be true for any Φ we must have

$$B'_\mu = UB_\mu U^{-1} - i(\partial_\mu U)U^{-1}. \tag{2.215}$$

Imposing the requirement that B_μ transform in this way ensures that $D_\mu \Phi$ is a gauge-covariant derivative obeying (2.214). We can have a gauge-invariant Lagrangian density

$$\mathcal{L} = (D^\mu \Phi)^\dagger (D_\mu \Phi) - \frac{1}{2} m^2 \Phi^\dagger \Phi - V(\Phi^\dagger \Phi), \tag{2.216}$$

obtained from (2.47) by replacing Φ with a column vector of fields, and the ordinary partial derivative with the covariant derivative.

It is possible to construct a field strength for B_μ analogous to the electromagnetic field strength tensor in (2.198). It is easy to show that (2.198) is not invariant under the transformation for B_μ in (2.215) and therefore must be modified. The appropriate generalization is most simply found by a computation similar to (2.207). A straightforward computation using (2.211) leads to

$$[D_\mu, D_\nu]\Phi = -iF_{\mu\nu}\Phi, \tag{2.217}$$

where

$$F_{\mu\nu} = \partial_\mu B_\nu - \partial_\nu B_\mu - i[B_\mu, B_\nu], \tag{2.218}$$

is the field strength tensor. Unlike the situation for the $U(1)$ gauge theory considered earlier, the field strength tensor is not linear in the vector potential B_μ. It is easily verified that under a local gauge transformation where B_μ obeys (2.215), the field strength tensor transforms like

$$F_{\mu\nu} \to F'_{\mu\nu} = U F_{\mu\nu} U^{-1}. \tag{2.219}$$

The presence of the non-linear commutation term in (2.218) is essential for obtaining a covariant transformation for the field strength.

We can also examine the infinitesimal versions of the above transformations. To first order in $\delta\epsilon^A$ we have from (2.208) that

$$U = I + i\delta\epsilon^A(x) T_A, \tag{2.220}$$
$$U^{-1} = I - i\delta\epsilon^A(x) T_A. \tag{2.221}$$

Working consistently to order $\delta\epsilon^A$ it is easy to show that

$$B'_\mu = B_\mu - i\delta\epsilon^A B_\mu T_A + i\delta\epsilon^A T_A B_\mu + (\partial_\mu \delta\epsilon^A) T_A \tag{2.222}$$

gives the infinitesimal form of the gauge transformation (2.215). If we write B_μ as in (2.212) and use the Lie algebra (2.209), it can be seen that

$$B'^A_\mu = B^A_\mu + f_{BC}{}^A B^B_\mu \delta\epsilon^C + \partial_\mu \delta\epsilon^A \tag{2.223}$$

Unlike the $U(1)$ case, the infinitesimal gauge transformation involves not just the gauge parameters but also the gauge field B^A_μ itself.

In a similar way to (2.212) we can define the components of the field strength $F_{\mu\nu}$ by

$$F_{\mu\nu} = F^A_{\mu\nu} T_A. \tag{2.224}$$

Using (2.212), the definition of $F_{\mu\nu}$ in (2.218), and the Lie algebra (2.209) it is found that

$$F^A_{\mu\nu} = \partial_\mu B^A_\nu - \partial_\nu B^A_\mu + f_{BC}{}^A B^B_\mu B^C_\nu \tag{2.225}$$

gives the components of the field strength. It is easy to verify that the transformation law (2.219) becomes

$$F'^A_{\mu\nu} = F^A_{\mu\nu} + f_{BC}{}^A F^B_{\mu\nu} \delta\epsilon^C, \tag{2.226}$$

in infinitesimal form.

By analogy with electromagnetism we would expect that the action for a non-Abelian gauge theory should involve $F_{\mu\nu} F^{\mu\nu}$. Because $F_{\mu\nu}$ is a matrix, and the Lagrangian density must be a scalar, we can remove the

matrices by taking the trace to get $\mathcal{L} \propto \text{ tr } (F_{\mu\nu}F^{\mu\nu})$. This is Lorentz-invariant, gauge-invariant, and reduces to the Maxwell action in the case of the gauge group $U(1)$. We can choose conventions such that[22]

$$\mathcal{L} = -\frac{1}{4}\delta_{AB}F^A_{\mu\nu}F^{B\mu\nu} \tag{2.227}$$

2.8 Fields of general spin

Relativistic fields of general spin are defined by their transformation properties under Lorentz transformations. In fact we could use the theory of representations of the Lorentz group at this point; however we will adopt a more pedestrian approach.[23]

The inhomogeneous Lorentz transformation is described by the transformation of spacetime coordinates

$$x'^\mu = L^\mu{}_\nu x^\nu + a^\mu, \tag{2.228}$$

where $L^\mu{}_\alpha L^\nu{}_\beta \eta_{\mu\nu} = \eta_{\alpha\beta}$ and a^μ is a constant 4-vector. If we specialize to infinitesimal transformations then

$$L^\mu{}_\nu = \delta^\mu_\nu + \delta\epsilon^\mu{}_\nu, \tag{2.229}$$

$$a^\mu = \delta a^\mu, \tag{2.230}$$

where $\delta\epsilon_{\mu\nu} = -\delta\epsilon_{\nu\mu}$. (We define $\delta\epsilon_{\mu\nu} = \eta_{\mu\lambda}\delta\epsilon^\lambda{}_\nu$.) A scalar field has the transformation property

$$\Phi'(x') = \Phi(x). \tag{2.231}$$

A vector field $A^\mu(x)$ transforms like

$$A'^\mu(x') = L^\mu{}_\nu A^\nu(x), \tag{2.232}$$

under (2.228). More generally we can assume that we have a set of fields $\Psi(x)$ which transforms like

$$\Psi'(x') = D(L,a)\Psi(x), \tag{2.233}$$

for some matrix $D(L,a)$ which depends on the parameters $L^\mu{}_\nu$ and a^μ characterizing the Lorentz transformation. (We will think of Ψ as a column vector of components.) This is similar to the non-Abelian gauge

[22] See Weinberg (1996) for a discussion of this normalization.
[23] See Weinberg (1995) for a more systematic approach.

transformations of Section 2.7 except that here it is the spacetime coordinates that are changing.

We can deduce a number of properties of the matrices $D(L,a)$. First of all if we put ${L^\mu}_\nu = {\delta^\mu}_\nu$ and $a^\mu = 0$, meaning that the spacetime coordinates do not change, then we find

$$\Psi'(x) = D(I,0)\Psi(x).$$

Since $\Psi'(x) = \Psi(x)$ if we do not perform any transformation we must have

$$D(I,0) = I. \tag{2.234}$$

By solving (2.228) for x^μ it is easily seen that the inverse transformation is characterized by parameters $(L^{-1})^\mu{}_\nu$ and $-(L^{-1})^\mu{}_\nu a^\nu$. We can conclude that

$$D^{-1}(L,a) = D(L^{-1}, -L^{-1}a). \tag{2.235}$$

Now consider a sequence of two independent Lorentz transformations. First perform (2.228) followed by the transformation $x'^\mu \to \tilde{x}^\mu$ where

$$\tilde{x}^\mu = \tilde{L}^\mu{}_\nu x'^\nu + \tilde{a}^\mu. \tag{2.236}$$

(We use a tilde to denote that the parameters of the second transformation can differ from those of the first transformation.) By substituting (2.228) into the right-hand side of (2.236) we find

$$\tilde{x}^\mu = \tilde{L}^\mu{}_\nu {L^\nu}_\lambda x^\lambda + \tilde{a}^\mu + \tilde{L}^\mu{}_\nu a^\nu. \tag{2.237}$$

If we perform the same two transformations on the field $\Psi(x)$ we find

$$\begin{aligned}\tilde{\Psi}(\tilde{x}) &= D(\tilde{L},\tilde{a})\Psi'(x') \\ &= D(\tilde{L},\tilde{a})D(L,a)\Psi(x).\end{aligned} \tag{2.238}$$

However we know that performing these two transformations is equivalent to the single transformation (2.237), so we must also have

$$\tilde{\Psi}(\tilde{x}) = D(\tilde{L}L, \tilde{L}a + \tilde{a})\Psi(x). \tag{2.239}$$

Comparing the two expressions (2.238) and (2.239) for $\tilde{\Psi}(\tilde{x})$ allows us to conclude that

$$D(\tilde{L}L, \tilde{L}a + \tilde{a}) = D(\tilde{L},\tilde{a})D(L,a). \tag{2.240}$$

(It is possible to deduce the properties (2.234) and (2.235) from (2.240) by taking $L = I, a = 0$ and $\tilde{L} = L^{-1}, \tilde{a} = -L^{-1}a$ respectively.)

We will now consider the infinitesimal transformations with ${L^\mu}_\nu$ given by (2.229) and $a^\mu = \delta a^\mu$. If $D(L, a)$ is a continuous function of ${L^\mu}_\nu$ and a^μ, as we will assume, then we can expand $D(L, a)$ about ${L^\mu}_\nu = {\delta^\mu}_\nu$ in a Taylor series. The result (2.234) shows that the series begins with the identity matrix. We will write

$$D(I + \delta\epsilon, \delta a) = I + i\delta\epsilon^{\mu\nu}\Sigma_{\mu\nu} + i\delta a^\mu P_\mu, \tag{2.241}$$

to first order in the infinitesimal parameters $\delta\epsilon^{\mu\nu}$ and δa^μ. Here $\Sigma_{\mu\nu}$ and P_μ are some matrices which are called the 'generators of the transformation'. (This is the infinitesimal form of (2.208) specialized to the Lorentz group.) The generators must satisfy certain relations which follow from the properties of $D(L, a)$ and we expect to be able to derive the algebra relations (2.209) for the Lorentz group. Note that because $\delta\epsilon_{\mu\nu} = -\delta\epsilon_{\nu\mu}$ we can take $\Sigma_{\mu\nu}$ to be antisymmetric in its indices μ and ν:

$$\Sigma_{\nu\mu} = -\Sigma_{\mu\nu}. \tag{2.242}$$

It is important to remember that μ and ν do not represent the indices of the matrix here; they are simply labelling different members of a set of matrices.

In order to deduce the properties of the generators we will consider a third transformation in addition to (2.228) and (2.236), from $\tilde{x}^\mu$ to $\bar{x}^\mu$ with

$$\begin{aligned}\bar{x}^\mu &= {\bar{L}^\mu}_\nu \tilde{x}^\nu + \bar{a}^\mu \\ &= {\bar{L}^\mu}_\nu {\tilde{L}^\nu}_\lambda {L^\lambda}_\sigma x^\sigma + {\bar{L}^\mu}_\nu {\tilde{L}^\nu}_\lambda a^\lambda + {\bar{L}^\mu}_\nu \tilde{a}^\nu + \bar{a}^\mu.\end{aligned} \tag{2.243}$$

The second line has followed from substituting (2.236) for $\tilde{x}^\nu$. It is now easy to see that

$$D(\bar{L}\tilde{L}L, \bar{L}\tilde{L}a + \bar{L}\tilde{a} + \bar{a}) = D(\bar{L}, \bar{a})D(\tilde{L}, \tilde{a})D(L, a). \tag{2.244}$$

We specialize to the infinitesimal form $\tilde{L} = I + \delta\tilde{\epsilon}$ and $\tilde{a} = \delta\tilde{a}$, choose $\bar{L} = L^{-1}$ and $\bar{a} = -L^{-1}a$ and work out both sides of (2.244) with this choice. The details involving expansions in the infinitesimal parameters are slightly messy, but the basic idea is straightforward. Working to first order in infinitesimals we find

$$\begin{aligned}\bar{L}\tilde{L}L &= L^{-1}(I + \delta\tilde{\epsilon})L = I + L^{-1}\delta\tilde{\epsilon}L, \\ \bar{L}\tilde{L}a + \bar{L}\tilde{a} + \bar{a} &= L^{-1}\delta\tilde{a} + L^{-1}\delta\tilde{\epsilon}a.\end{aligned}$$

We then find

$$\begin{aligned} D(\bar{L}\tilde{L}L, \bar{L}\tilde{L}a + \bar{L}\tilde{a} + \bar{a}) &= D(I + L^{-1}\delta\tilde{\epsilon}L, L^{-1}\delta\tilde{\epsilon}L + L^{-1}\delta\tilde{a} \\ &\quad + L^{-1}\delta\tilde{a} + L^{-1}\delta\tilde{\epsilon}a) \\ &= I + i(L^{-1})^{\mu}{}_{\lambda}\delta\tilde{\epsilon}^{\lambda}{}_{\sigma}L^{\sigma}{}_{\nu}\Sigma_{\mu}{}^{\nu} \\ &\quad + i(L^{-1})^{\mu}{}_{\nu}\delta\tilde{a}^{\nu}P_{\mu} \\ &\quad + i(L^{-1})^{\mu}{}_{\nu}\delta\epsilon^{\nu}{}_{\lambda}a^{\lambda}P_{\mu}, \end{aligned} \tag{2.245}$$

if we use (2.241) and write out the various matrix multiplications. The right-hand side of (2.244) becomes

$$\begin{aligned} D(\bar{L}, \bar{a})D(\tilde{L}, \tilde{a})D(L, a) &= D^{-1}(L, a)D(I + \delta\tilde{\epsilon}, \delta\tilde{a})D(L, a) \\ &= I + i\delta\tilde{\epsilon}^{\mu\nu}D^{-1}(L, a)\Sigma_{\mu\nu}D(L, a) \\ &\quad + i\delta\tilde{a}^{\mu}D^{-1}(L, a)P_{\mu}D(L, a). \end{aligned} \tag{2.246}$$

Comparing (2.245) with (2.246) shows that

$$\begin{aligned} \delta\tilde{\epsilon}^{\mu\nu}D^{-1}(L, a)\Sigma_{\mu\nu}D(L, a) &= (L^{-1})^{\mu}{}_{\lambda}\delta\tilde{\epsilon}^{\lambda}{}_{\sigma}L^{\sigma}{}_{\nu}\Sigma_{\mu}{}^{\nu} \\ &\quad + (L^{-1})^{\mu}{}_{\nu}\delta\tilde{\epsilon}^{\nu}{}_{\lambda}a^{\lambda}P_{\mu} \end{aligned} \tag{2.247}$$

and

$$\delta\tilde{a}^{\mu}D^{-1}(L, a)P_{\mu}D(L, a) = (L^{-1})^{\mu}{}_{\nu}\delta\tilde{a}^{\nu}P_{\mu}. \tag{2.248}$$

Here we have used the fact that the parameters $\delta\tilde{\epsilon}$ and $\delta\tilde{a}$ are independent of each other so that the terms in each set of parameters much vanish separately. If we use (2.235) we may simplify (2.248) to

$$D(L^{-1}, -L^{-1}a)P_{\mu}D(L, a) = (L^{-1})^{\nu}{}_{\mu}P_{\nu}. \tag{2.249}$$

Removal of the parameters $\delta\tilde{\epsilon}^{\mu\nu}$ from (2.247) is a bit trickier because although the parameters are arbitrary, $\delta\tilde{\epsilon}^{\mu\nu}$ must be antisymmetric in μ and ν. This means that we must be careful to antisymmetrize in μ and ν when cancelling off $\delta\tilde{\epsilon}^{\mu\nu}$. We find

$$\begin{aligned} D(L^{-1}, -L^{-1}a)\Sigma_{\mu\nu}D(L, a) &= \frac{1}{2}(L^{-1})^{\sigma}{}_{\mu}L_{\nu}{}^{\lambda}\Sigma_{\sigma\lambda} - \frac{1}{2}(L^{-1})^{\sigma}{}_{\nu}L_{\mu}{}^{\lambda}\Sigma_{\sigma\lambda} \\ &\quad + \frac{1}{2}(L^{-1})^{\lambda}{}_{\mu}a_{\nu}P_{\lambda} - \frac{1}{2}(L^{-1})^{\lambda}{}_{\nu}a_{\mu}P_{\lambda}. \end{aligned} \tag{2.250}$$

The infinitesimal form for $L^{\mu}{}_{\nu}$ and a^{μ} may be taken in (2.249) and (2.250) with the D matrices expanded to first order in the infinitesimal parameters using (2.241). It is straightforward to show

$$\begin{aligned} D(L^{-1}, -L^{-1}a)P_{\mu}D(L, a) &= D(I - \delta\epsilon, -\delta a)P_{\mu}D(I + \delta\epsilon, \delta a) \\ &= P_{\mu} + i\delta\epsilon^{\alpha\beta}[P_{\mu}, \Sigma_{\alpha\beta}] + i\delta a^{\nu}[P_{\mu}, P_{\nu}]. \end{aligned} \tag{2.251}$$

We also have

$$\begin{aligned}(L^{-1})^{\nu}{}_{\mu}P_{\nu} &= P_{\mu} - \delta\epsilon^{\nu}{}_{\mu}P_{\nu} \\ &= P_{\mu} - \frac{1}{2}\delta\epsilon^{\alpha\beta}(\eta_{\beta\mu}P_{\alpha} - \eta_{\alpha\mu}P_{\beta}),\end{aligned} \tag{2.252}$$

after antisymmetrization on α and β. Using (2.251) and (2.252) in (2.249), along with the independence of the infinitesimal parameters $\delta\epsilon^{\alpha\beta}$ and δa^{μ} results in

$$[P_{\mu}, P_{\nu}] = 0, \tag{2.253}$$

$$[P_{\mu}, \Sigma_{\alpha\beta}] = \frac{i}{2}(\eta_{\beta\mu}P_{\alpha} - \eta_{\alpha\mu}P_{\beta}). \tag{2.254}$$

In a similar way we can use (2.250) to show that

$$[\Sigma_{\mu\nu}, \Sigma_{\alpha\beta}] = \frac{i}{2}(\eta_{\mu\alpha}\Sigma_{\nu\beta} + \eta_{\mu\beta}\Sigma_{\alpha\nu} - \eta_{\alpha\nu}\Sigma_{\mu\beta} - \eta_{\beta\nu}\Sigma_{\alpha\mu}). \tag{2.255}$$

The commutation relations among the generators in (2.253)–(2.255) is called the 'Lie algebra of the inhomogeneous Lorentz group'. The general form of the algebra is as in (2.209) and it is possible to read off the structure constants for the Lie algebra from (2.253) to (2.255). It can be observed that the generators of spacetime translations P_{μ} commute among themselves, but do not commute with $\Sigma_{\mu\nu}$. This can be expected form the composition of two transformations in (2.237). Although the set of inhomogeneous Lorentz transformations has the properties of a group, with the set of translations generated by P_{μ} and the set of transformations generated by $\Sigma_{\mu\nu}$ each forming subgroups, the inhomogeneous Lorentz transformations is not just the direct product of these two subgroups. (It is called a 'semi-direct product'.)

The infinitesimal form of the field transformation (2.233) can also be given. If we use (2.241) we find

$$\Psi'(x + \delta\epsilon\, x + \delta a) = (I + i\delta\epsilon^{\mu\nu}\Sigma_{\mu\nu} + i\delta a^{\mu}P_{\mu})\Psi(x). \tag{2.256}$$

The left-hand side of (2.256) may be expanded in a Taylor series

$$\Psi'(x + \delta\epsilon\, x + \delta a) = \Psi'(x) + \delta\epsilon^{\mu}{}_{\nu}x^{\nu}\partial_{\mu}\Psi'(x) + \delta a^{\mu}\partial_{\mu}\Psi'(x) \tag{2.257}$$

to first order in the infinitesimal parameters $\delta\epsilon^{\mu}{}_{\nu}$ and δa^{μ}. Since $\Psi'(x)$ differs from $\Psi(x)$ only by terms involving $\delta\epsilon$ and δa, if we work only to first order in infinitesimal quantities we may replace $\partial_{\mu}\Psi'$ with $\partial_{\mu}\Psi$ in (2.257). We then find

$$\begin{aligned}\delta\Psi(x) &= \Psi'(x) - \Psi(x) \\ &= i\delta\epsilon^{\mu\nu}\Sigma_{\mu\nu}\Psi(x) - \delta\epsilon^{\mu}{}_{\nu}x^{\nu}\partial_{\mu}\Psi(x) \\ &\quad + i\delta a^{\mu}P_{\mu}\Psi(x) - \delta a^{\mu}\partial_{\mu}\Psi(x). \end{aligned} \tag{2.258}$$

2.9 The Dirac equation

One fundamental difference between the Klein–Gordon equation and the Schrödinger equation is that the Klein–Gordon equation is second order in time derivatives whereas the Schrödinger equation is first order.[24] This motivated Dirac to look for an equation which was relativistically invariant, and which was first order in time derivatives. In order to be relativistically invariant it would be expected to involve only first-order spatial derivatives as well.

Suppose that we write this equation in the form

$$i\frac{\partial}{\partial t}\psi = H_D\psi, \tag{2.259}$$

where

$$H_D = i\vec{\alpha}\cdot\nabla + m\beta. \tag{2.260}$$

Equation (2.259) takes the same form as the Schrödinger equation with H_D the Dirac Hamiltonian. Here m is a constant with units of inverse length (which will be interpreted as the mass), and $\vec{\alpha}$ and β are constant matrices to be determined.[25]

In order that the theory described by (2.259) and (2.260) makes sense physically, $\vec{\alpha}$ and β must satisfy a number of properties. One of these properties follows from the fact that the Hamiltonian H_D must be self-adjoint:

$$\int_{t_1}^{t_2} dt \int_{\Sigma} d\sigma_x \; \psi_1^{\dagger}(H_D\psi_2) = \int_{t_1}^{t_2} dt \int_{\Sigma} d\sigma_x (H_D\psi_1)^{\dagger}\psi_2.$$

It is straightforward to show that this requires $\vec{\alpha}$ and β to be Hermitian matrices:

$$\vec{\alpha}^{\dagger} = \vec{\alpha}, \qquad \beta^{\dagger} = \beta. \tag{2.261}$$

One consequence of relativistic invariance is that the usual relation $E^2 = \mathbf{p}^2 + m^2$ between energy, momentum, and mass must hold. A way to ensure

[24] In addition, the Klein–Gordon equation is invariant under Lorentz transformations, whereas the Schrödinger equation is not.

[25] We will see later that $\vec{\alpha}$ and β cannot simply be a vector and a number.

this is to require all solutions of (2.259) to also satisfy the Klein–Gordon equation. Operating on both sides of (2.259) with $i(\partial/\partial t)$ gives

$$-\frac{\partial^2}{\partial t^2}\psi = i\frac{\partial}{\partial t}(H_D\psi) = H_D\left(i\frac{\partial}{\partial t}\psi\right) = H_D^2\psi.$$

The interchange of $\partial/\partial t$ and H_D is justified because H_D does not have any time dependence. Using $H_D = i\alpha^i\partial_i + \beta m$ we have

$$H_D^2 = -\alpha^i\alpha^j\partial_i\partial_j + im(\alpha^i\beta + \beta\alpha^i)\partial_i + m^2\beta^2.$$

We therefore end up with the requirement that ψ must satisfy

$$\left[\frac{\partial^2}{\partial t^2} - \alpha^i\alpha^j\partial_i\partial_j + im(\alpha^i\beta + \beta\alpha^i)\partial_i + m^2\beta^2\right]\psi = 0.$$

In order that this result gives the Klein–Gordon equation we must have

$$\alpha^i\alpha^j + \alpha^j\alpha^i = 2\delta^{ij}I, \tag{2.262}$$

$$\alpha^i\beta + \beta\alpha^i = 0, \tag{2.263}$$

$$\beta^2 = I, \tag{2.264}$$

where I is the identity matrix. The reasons for (2.263) and (2.264) are obvious, but (2.262) may require some explanation. In order that we end up with the Klein–Gordon equation, we must have $\alpha^i\alpha^j\partial_i\partial_j = I\nabla^2 = I\delta^{ij}\partial_i\partial_j$ where I is the identity matrix. It would be incorrect to deduce from this that $\alpha^i\alpha^j = \delta^{ij}$ because δ^{ij} is symmetric in i and j, whereas we have no reasons to suppose that the product of the two matrices $\alpha^i\alpha^j$ shares this symmetry.[26] Instead we must use the fact that $\partial_i\partial_j = \partial_j\partial_i$ to write $\alpha^i\alpha^j\partial_i\partial_j = (1/2)(\alpha^i\alpha^j + \alpha^j\alpha^i)\partial_i\partial_j$ which makes no unwarranted assumptions about the matrices α^i and α^j. We can now make the equality in (2.262). A final comment concerning (2.262)–(2.264) is that as claimed earlier $\vec{\alpha}$ and β must be matrices; they cannot be a vector and a number, or else (2.264) would imply $\beta = \pm 1$, and (2.263) would imply $\alpha^i = 0$ which does not satisfy (2.262).

Having obtained some requirements that the matrices α^i and β must satisfy, we must now show that there exists matrices with these relevant properties. Let the matrices be $n \times n$. This means that ψ is an n-component field. The matrices are Hermitian, which means that they can be diagonalized and their eigenvalues, appearing down the diagonal, will be real.[27] If we take $i = j$ in (2.262) we can see that $(\alpha^i)^2 = I$.

[26] We would need α^i to commute with α^j for this to be the case.

[27] Note that α^i and β do not commute so that it is not possible to diagonalize them simultaneously.

Including (2.264), we have shown that all $(D+1)$ matrices $\alpha^1, \ldots, \alpha^D, \beta$ square to the identity matrix. This means that the eigenvalues of any of the matrices can be only ± 1.

Now take $i \neq j$ in (2.262). This gives $\alpha^i \alpha^j = -\alpha^j \alpha^i$ for $j \neq i$. Taking the determinant of both sides of this result leads to

$$\det(\alpha^i \alpha^j) = \det(-\alpha^j \alpha^i) = (-1)^n \det(\alpha^i \alpha^j), \tag{2.265}$$

if we use familiar properties of the determinant. Because the eigenvalues of α^i are ± 1, α^i must be a non-singular matrix with a non-zero determinant. This ensures that $\det(\alpha^i \alpha^j) \neq 0$, and for (2.265) to hold, n must be even.

At this stage we can recall the 2×2 Pauli matrices:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{2.266}$$

These three matrices satisfy (2.262). However because the three Pauli matrices along with the identity matrix form a basis for the set of all 2×2 Hermitian matrices, it is impossible to find another 2×2 matrix β which anti-commutes with them. We will try to establish a relation between the dimension of the Dirac matrices α^i and β and the spatial dimension D.

If we have one spatial dimension, $D = 1$, we may choose $\alpha^1 = \sigma_1$ and $\beta = \sigma_3$.[28] In two spatial dimensions, $D = 2$, we can pick $\alpha^1 = \sigma_1, \alpha^2 = \sigma_2$, and $\beta = \sigma_3$. In three or more spatial dimensions, since the dimension of the matrices n must be even, we must have $n \geq 4$. It is possible to construct the matrices in three or more spatial dimensions by taking tensor products of the lower-dimensional matrices, but a more pedestrian approach is simpler. For $D = 3$ we will choose the 4×4 matrix

$$\alpha^1 = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix} \begin{pmatrix} \sigma_1 & 0 \\ 0 & \sigma_1 \end{pmatrix} = \begin{pmatrix} 0 & \sigma_1 \\ \sigma_1 & 0 \end{pmatrix}. \tag{2.267}$$

Similarly,

$$\alpha^2 = \begin{pmatrix} 0 & \sigma_2 \\ \sigma_2 & 0 \end{pmatrix}, \qquad \alpha^3 = \begin{pmatrix} 0 & \sigma_3 \\ \sigma_3 & 0 \end{pmatrix}. \tag{2.268}$$

Finally we pick

$$\beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}. \tag{2.269}$$

The matrices in (2.267)–(2.269) can be shown to be Hermitian and to satisfy the requirements in (2.262)–(2.264). For $D = 4$ we can choose

[28] We could equally well choose $\beta = \sigma_2$.

$\alpha^1, \alpha^2, \alpha^3$ and β to be the same as for $D = 3$, and in addition pick $\alpha^4 = \beta\alpha^1\alpha^2\alpha^3$. Again it is easy to show that this choice satisfies the properties (2.262)–(2.264). The construction just described shows a general feature of the matrices: if we know the matrices in an odd spatial dimension, say $D = 2\delta + 1$, then we can find them in the next even spatial dimension $D = 2\delta + 2$ by taking the extra component of $\vec{\alpha}$ to be proportional to the product of β with all of the lower components $\alpha^1, \ldots, \alpha^{2\delta+1}$. The constant of proportionality can be fixed by the Hermitian property and the requirement that $(\alpha^i)^2 = I$. A corollary of this construction is that the dimension of the matrices in spatial dimensions $D = 2\delta+1$ and $D = 2\delta+2$ must be equal.

All that we now require to complete our construction of the explicit forms for the matrices α^i and β is the knowledge of how to proceed from spatial dimension $2\delta + 2$ to the next higher odd dimension $D = 2\delta + 3$. The first equality in (2.267) contains the key for this step. To see this we will construct the representation for $\vec{\alpha}$ and β in $D = 5$ from our knowledge of the matrices in $D = 4$. Let $\tilde{\alpha}^1, \ldots, \tilde{\alpha}^5$ and $\tilde{\beta}$ be the matrices for $D = 5$ and $\alpha^1, \ldots, \alpha^4$ be those already described for $D = 4$. We then have

$$\tilde{\alpha}^i = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix} \begin{pmatrix} \alpha^i & 0 \\ 0 & \alpha^i \end{pmatrix}, \quad i = 1, \ldots, 4, \tag{2.270}$$

$$\tilde{\alpha}^5 = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix} \begin{pmatrix} \beta & 0 \\ 0 & \beta \end{pmatrix}, \tag{2.271}$$

$$\tilde{\beta} = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \tag{2.272}$$

with I the 4×4 identity matrix. It is straightforward to show that (2.262)–(2.264) are satisfied. Our explicit construction also shows the relationship between the dimension of the matrices n and the spatial dimension D. It is easy to see that $n = 2^{[(D+1)/2]}$ where $[(D + 1)/2]$ is the greatest integer less than or equal to $(D + 1)/2$. The details of the construction are essentially straightforward and will be left as an exercise.

It is conventional to write the Dirac equation in a more symmetrical form. If we take (2.259), multiply both sides by β on the left, and use $\beta^2 = I$, we find

$$i\beta\frac{\partial}{\partial t}\psi = i\beta\alpha^i\partial_i\psi + m\psi.$$

This can be written as

$$(i\gamma^\mu\partial_\mu - m)\psi = 0, \tag{2.273}$$

if we define

$$\gamma^0 = \beta, \tag{2.274}$$
$$\gamma^i = -\beta\alpha^i, \quad i = 1, \ldots, D. \tag{2.275}$$

Because $\vec{\alpha}$ and β are Hermitian we find

$$(\gamma^0)^\dagger = \gamma^0, \tag{2.276}$$
$$(\gamma^i)^\dagger = -\gamma^i. \tag{2.277}$$

These two results may be combined into the single equation

$$(\gamma^\mu)^\dagger = \gamma^0\gamma^\mu\gamma^0. \tag{2.278}$$

It is also easy to show using (2.262)–(2.264) that

$$\gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu = 2\eta^{\mu\nu}I. \tag{2.279}$$

The matrices γ^μ are referred to as the Dirac γ-matrices, or simply as the Dirac matrices if no confusion can arise with $\vec{\alpha}$ and β. An explicit representation for them can be found using the results for $\vec{\alpha}$ and β found above.

If we take the Hermitian conjugate of (2.273) we have

$$0 = i\partial_\mu\psi^\dagger(\gamma^\mu)^\dagger + m\psi.$$

Using (2.278) this may be written as

$$0 = i\partial_\mu\psi^\dagger\gamma^0\gamma^\mu\gamma^0 + m\psi^\dagger.$$

Finally, because $(\gamma^0)^2 = I$, if we multiply both sides of this last result on the right by γ^0 we have

$$0 = i\partial_\mu\bar{\psi}\gamma^\mu + m\bar{\psi}, \tag{2.280}$$

where

$$\bar{\psi} = \psi^\dagger\gamma^0. \tag{2.281}$$

Equation (2.280) is usually called the 'adjoint Dirac equation'.

We now turn to the transformation properties of ψ and $\bar{\psi}$ under Lorentz transformations. The general framework that we need was described in Section 2.8. As in (2.233) we will define

$$\psi'(x') = D(L, a)\psi(x), \tag{2.282}$$

when $x'^{\mu} = L^{\mu}{}_{\nu}x^{\nu} + a^{\mu}$ gives a Lorentz transformation. If we perform the transformation $x^{\mu} \to x'^{\mu}$ on (2.273) we have

$$i\gamma'^{\mu}\partial'_{\mu}\psi'(x') - m\psi'(x') = 0, \tag{2.283}$$

where γ'^{μ} represent the transformed Dirac matrices which must satisfy (2.279). At this stage we note a feature of the algebra of matrices (2.279), namely that any representation we choose for γ^{μ} is only defined up to an arbitrary unitary transformation. If γ^{μ} satisfies (2.279) then so does $U\gamma^{\mu}U^{-1}$ where U is any unitary matrix. This is trivial to show.[29] What is less trivial to show is that all matrices which satisfy (2.279) are related by a unitary transformation.[30] Given that this is the case, we are free to simply take $\gamma'^{\mu} = \gamma^{\mu}$ because the matrices are only defined up to a unitary transformation in any case. Returning to (2.283) we have

$$i\gamma^{\mu}\partial'_{\mu}\psi'(x') - m\psi'(x') = 0. \tag{2.284}$$

It is easy to show

$$\partial'_{\mu} = \frac{\partial}{\partial x'^{\mu}} = \frac{\partial x^{\nu}}{\partial x'^{\mu}}\partial_{\nu} = (L^{-1})^{\nu}{}_{\mu}\partial_{\nu}.$$

From (2.282) we find

$$i\gamma^{\mu}(L^{-1})^{\nu}{}_{\mu}D(L,a)\partial_{\nu}\psi(x) - mD(L,a)\psi(x) = 0.$$

Multiplication on the left by $D^{-1}(L,a)$ results in

$$iD^{-1}(L,a)\gamma^{\mu}(L^{-1})^{\nu}{}_{\mu}D(L,a)\partial_{\nu}\psi(x) - m\psi(x) = 0.$$

Because $\psi(x)$ satisfies (2.273) we must require

$$D^{-1}(L,a)\gamma^{\mu}(L^{-1})^{\nu}{}_{\mu}D(L,a) = \gamma^{\nu}$$

or

$$\gamma^{\mu} = L^{\mu}{}_{\nu}D(L,a)\gamma^{\nu}D^{-1}(L,a). \tag{2.285}$$

If we specialize to homogeneous Lorentz transformations and take the parameters of the transformation to be infinitesimal, so $L^{\mu}{}_{\nu} = \delta^{\mu}_{\nu} + \delta\epsilon^{\mu}{}_{\nu}$, and $D(I + \delta\epsilon, 0) = I + i\delta\epsilon^{\mu\nu}\Sigma_{\mu\nu}$ as in (2.241), then (2.285) becomes

$$\gamma^{\mu} \simeq \gamma^{\mu} - i\delta\epsilon^{\nu\lambda}[\gamma^{\mu}, \Sigma_{\nu\lambda}] + \delta\epsilon^{\mu}{}_{\nu}\gamma^{\nu}, \tag{2.286}$$

[29] U must be unitary to preserve the properties (2.276) and (2.277).
[30] See Good (1955) or the discussion in Schweber (1961) for example.

if we work to first order in $\delta\epsilon$. We therefore have

$$\delta\epsilon^{\mu}{}_{\nu}\gamma^{\nu} = i\delta\epsilon^{\nu\lambda}[\gamma^{\mu}, \Sigma_{\nu\lambda}].$$

If we write

$$\delta\epsilon^{\mu}{}_{\nu}\gamma^{\nu} = \frac{1}{2}(\delta^{\mu}_{\nu}\gamma_{\lambda} - \delta^{\mu}_{\lambda}\gamma_{\nu})\delta\epsilon^{\nu\lambda},$$

(a step which is necessary because $\delta\epsilon^{\nu\lambda}$ is antisymmetric in ν and λ), then we obtain the requirement

$$[\gamma_{\mu}, \Sigma_{\nu\lambda}] = -\frac{i}{2}(\eta_{\mu\nu}\gamma_{\lambda} - \eta_{\mu\lambda}\gamma_{\nu}). \tag{2.287}$$

We would expect $\Sigma_{\nu\lambda}$ to involve the Dirac γ-matrices, and because we require $\Sigma_{\lambda\nu} = -\Sigma_{\nu\lambda}$ a natural choice is

$$\Sigma_{\nu\lambda} = \kappa[\gamma_{\nu}, \gamma_{\lambda}],$$

for some constant κ. By using (2.279) it is easy to show that (2.287) is satisfied if $\kappa = -i/8$. Thus we have

$$\Sigma_{\nu\lambda} = -\frac{i}{8}[\gamma_{\nu}, \gamma_{\lambda}]. \tag{2.288}$$

Straightforward algebra shows that (2.288) satisfies the requirement given in (2.255) for the generators of the Lorentz transformations.

Because of the group property of Lorentz transformations we can build up a finite transformation from repeated infinitesimal ones. This can be illustrated quite simply for rotations which will also demonstrate the spinorial nature of the Dirac field. A rotation of angle θ about the z-axis is characterized by the change of coordinates

$$\begin{aligned} x' &= x\cos\theta + y\sin\theta \\ y' &= -x\sin\theta + y\cos\theta \\ z' &= z \\ t' &= t. \end{aligned} \tag{2.289}$$

If we take the angle $\theta = \delta\theta$ to be infinitesimal, then the non-trivial coordinate transformations obey

$$\begin{aligned} \delta x &= x' - x = \delta\theta\, y \\ \delta y &= y' - y = -\delta\theta\, x. \end{aligned} \tag{2.290}$$

Comparison with the general result $\delta x^\mu = \delta\epsilon^\mu{}_\nu x^\nu$ shows that $\delta\epsilon_{12} = -\delta\epsilon_{21} = -\delta\theta$ are the only non-zero parameters of the rotation. We then have

$$\begin{aligned} D(I+\delta\epsilon,0) &= I + i\delta\epsilon^{\mu\nu}\Sigma_{\mu\nu} \\ &= I + \frac{1}{2}\delta\theta\gamma^2\gamma^1. \end{aligned} \tag{2.291}$$

We may build up a finite transformation by first of all dividing up $\theta = n\delta\theta$, and then taking the limit $n \to \infty$.[31] If we shorten the notation so that $D(\theta)$ represents the result for a finite rotation then

$$D(\theta) = \lim_{n\to\infty}\left(I + \frac{1}{2}\frac{\theta}{n}\gamma^2\gamma^1\right)^n. \tag{2.292}$$

(We have just used (2.291) with $\delta\theta = \theta/n$, and taken n successive transformations.) From the definition of the exponential function, which holds equally well for matrices, we find

$$D(\theta) = \exp\left(\frac{\theta}{2}\gamma^2\gamma^1\right) \tag{2.293}$$

$$= I\cos\left(\frac{\theta}{2}\right) + \gamma^2\gamma^1\sin\left(\frac{\theta}{2}\right). \tag{2.294}$$

(The second line follows by expanding the exponential in its Taylor series and using $(\gamma^2\gamma^1)^{2n} = (-1)^n I$ which comes from (2.279).) The key feature of this result is the presence of half-angles. This means that

$$D(2\pi) = -I = -D(0). \tag{2.295}$$

Since $D(\theta)$ describes what happens to $\psi(x)$ under a rotation of angle θ, this result shows that $\psi(x)$ changes sign under a complete rotation of 2π. Only after a rotation of 4π will $\psi(x)$ return to its original value. This is quite unlike the situation for a scalar or vector field and is the signature of a field with a half-integer spin. $\psi(x)$ is called a spinor field.[32]

If we consider the adjoint spinor in (2.281), under a Lorentz transformation we have

[31] The limit $n \to \infty$ is necessary so that $\delta\theta$ is infinitesimal.

[32] In group theory terms $D(L,a)$ above has provided a representation of the double-covering of the Lorentz group. For a more complete discussion, see Choquet-Bruhat *et al.* (1977).

$$\begin{aligned}\bar{\psi}'(x') &= \psi'^{\dagger}(x')\gamma^0 \\ &= \psi^{\dagger}(x)D^{\dagger}(L,0)\gamma^0 \\ &= \bar{\psi}(x)\gamma^0 D^{\dagger}(L,0)\gamma^0.\end{aligned}$$

From (2.278) and (2.288) it may be shown that

$$\Sigma_{\mu\nu}^{\dagger} = \gamma^0 \Sigma_{\mu\nu}\gamma^0. \tag{2.296}$$

This may be used to show that

$$\gamma^0 D^{\dagger}(L,0)\gamma^0 = D^{\dagger}(L,0),$$

and we find

$$\bar{\psi}'(x') = \bar{\psi}(x)D^{\dagger}(L,0). \tag{2.297}$$

Combining (2.282) with (2.297) it follows that $\bar{\psi}(x)\psi(x)$ is a scalar under Lorentz transformations.

To complete our initial study of the Dirac equation we wish to find a Lagrangian density $\mathcal{L}$ which gives rise to the Dirac equation (2.273) and its adjoint (2.280) under independent variations of $\bar{\psi}(x)$ and $\psi(x)$. It is easy to see that a suitable choice is

$$\begin{aligned}\mathcal{L} &= \frac{1}{2}\bar{\psi}(i\gamma^\mu\partial_\mu - m)\psi - \frac{1}{2}(i\partial_\mu\bar{\psi}\gamma^\mu + m\bar{\psi})\psi \\ &= \frac{i}{2}(\bar{\psi}\gamma^\mu\partial_\mu\psi - \partial_\mu\bar{\psi}\gamma^\mu\psi) - m\bar{\psi}\psi.\end{aligned} \tag{2.298}$$

This has the virtue of being real (as can be seen from the properties (2.278)) and a scalar under Lorentz transformations. The action is

$$\begin{aligned}S[\bar{\psi},\psi] &= \int_{t_1}^{t_2} dt \int_\Sigma d\sigma_x \mathcal{L} \\ &= \int_{t_1}^{t_2} dt \int_\Sigma d\sigma_x \bar{\psi}(i\gamma^\mu\partial_\mu - m)\psi,\end{aligned} \tag{2.299}$$

if we perform an integration by parts and discard a total derivative.

Given the Lagrangian density $\mathcal{L}$ in (2.298) we may find the momentum canonically conjugate to ψ as follows. Write out (2.298) explicitly as (using $\bar{\psi} = \psi^\dagger\gamma^0$)

$$\mathcal{L} = \frac{i}{2}[\psi^\dagger\dot{\psi} + \bar{\psi}\vec{\gamma}\cdot\nabla\psi - \dot{\psi}^\dagger\psi - (\nabla\bar{\psi})\cdot\vec{\gamma}\psi] - m\bar{\psi}\psi.$$

Here $\vec{\gamma}$ has components γ^i. Vary $\mathcal{L}$ with respect to $\dot{\psi}$ to find

$$\pi = \frac{i}{2}\psi^\dagger. \tag{2.300}$$

Vary $\mathcal{L}$ with respect to $\dot{\bar{\psi}}$ to find

$$\bar{\pi} = -\frac{i}{2}\gamma^0\psi = -\frac{i}{2}\bar{\psi}^\dagger. \tag{2.301}$$

The situation here is very similar to that for the Schrödinger field in Section 2.3.3 where the canonical momenta are related to the fields. The reason for this is that in both cases the Lagrangian is linear in time derivatives of the fields.

The Hamiltonian density may also be constructed. We form

$$\begin{aligned}\mathcal{H} &= \pi\dot{\psi} + \dot{\bar{\psi}}\bar{\pi} - \mathcal{L} \\ &= \frac{i}{2}\partial_i\bar{\psi}\gamma^i\psi - \frac{i}{2}\bar{\psi}\gamma^i\partial_i\psi + m\bar{\psi}\psi.\end{aligned} \tag{2.302}$$

If we return to the original matrices $\vec{\alpha}$ and β, and use (2.274) and (2.275) we find

$$\mathcal{H} = \frac{i}{2}\psi^\dagger\vec{\alpha}\cdot\nabla\psi - \frac{i}{2}(\nabla\psi)^\dagger\cdot\vec{\alpha}\psi + m\psi^\dagger\beta\psi. \tag{2.303}$$

The Hamiltonian becomes

$$H = \int_\Sigma d\sigma_x\mathcal{H} = \int_\Sigma d\sigma_x\psi^\dagger(i\vec{\alpha}\cdot\nabla + m\beta)\psi, \tag{2.304}$$

if a total derivative is discarded. The operator occurring in (2.304) is observed to be the Dirac Hamiltonian operator we started with in (2.260). Again the situation is similar to that for the Schrödinger field.

Finally we wish to give the result for a charged Dirac spinor interacting with the electromagnetic field. We can either use the method of the Noether current described in Section 2.7, or else use our previous experience to conclude that we simply need to replace ∂_μ with the gauge-covariant derivative $D_\mu = \partial_\mu - ieA_\mu$. The Dirac equation becomes

$$i\gamma^\mu\partial_\mu\psi + e\gamma^\mu A_\mu\psi - m\psi = 0, \tag{2.305}$$

and its adjoint is

$$i\partial_\mu\bar{\psi}\gamma^\mu - eA_\mu\bar{\psi}\gamma^\mu + m\bar{\psi} = 0. \tag{2.306}$$

The construction of a suitable Lagrangian density for the Dirac field is straightforward and will be left as an exercise.

To finish our discussion of the Dirac equation, we will examine the physically interesting case of $D = 3$ and show that a particle of spin $1/2$ is described. To do this, we will first prove that unless we include spin, the

Dirac equation is not consistent with the conservation of angular momentum. We will concentrate on $L_3 = x_1 p_2 - x_2 p_1$ and evaluate $[L_3, H]$ using $H = \vec{\alpha} \cdot \mathbf{p} + m\beta$. This anticipates the canonical commutation relations between position and momentum $[x_i, p_j] = i\hbar\delta_{ij}$ that we will not establish until the next chapter, but it is expected that the reader has seen them before from a previous encounter with quantum mechanics. (See Schiff (1968) for example.) Since L_3 must be a multiple of the identity matrix, we have

$$\begin{aligned}[L_3, H] &= \alpha^i [L_3, p_i] \\ &= \alpha^i \left\{ [x_1, p_i] p_2 - [x_2, p_i] p_1 \right\} \\ &= i\hbar \left(\alpha^1 p_2 - \alpha^2 p_1 \right). \end{aligned} \tag{2.307}$$

A similar calculation applied to the other components of angular momentum shows that

$$[\mathbf{L}, H] = i\hbar \vec{\alpha} \times \mathbf{p}. \tag{2.308}$$

It therefore follows that $\mathbf{L}$ cannot be a constant of the motion.

This need not be a problem since it can be recalled that the total angular momentum $\mathbf{J} = \mathbf{L} + \mathbf{S}$, and it is the total angular momentum that must be conserved. We therefore can look for an S_3 that we can add to L_3 in order that $[J_3, H] = 0$. A bit of thought shows that if $[S_3, H]$ is to cancel with (2.307), S_3 should be quadratic in the $\vec{\alpha}$ matrices. Furthermore because of the commutation relations (2.262) S_3 need only involve $\alpha^1 \alpha^2$. We will therefore set

$$S_3 = k\alpha^1 \alpha^2 \tag{2.309}$$

for constant k with k chosen such that $[L_3 + S_3, H] = 0$. Because of (2.263) we have $[S_3, \beta] = 0$. Thus,

$$[S_3, H] = k[\alpha^1 \alpha^2, \alpha^i] p_i. \tag{2.310}$$

The commutator on the right-hand side of (2.310) may be evaluated by repeated use of (2.262). The result is

$$[S_3, H] = 2k(\alpha^1 p_2 - \alpha^2 p_1). \tag{2.311}$$

Thus, if we choose $k = -i\hbar/2$ we will have $[L_3 + S_3, H] = 0$. We conclude that

$$S_3 = -\frac{i\hbar}{2} \alpha^1 \alpha^2. \tag{2.312}$$

By symmetry the other components of $\mathbf{S}$ are

$$S_1 = -\frac{i\hbar}{2}\alpha^2\alpha^3, \tag{2.313}$$

$$S_2 = -\frac{i\hbar}{2}\alpha^3\alpha^1. \tag{2.314}$$

If we make use of the explicit representations (2.267, 2.268) for $D = 3$, it is easy to see that

$$\mathbf{S} = \frac{\hbar}{2}\begin{pmatrix} \vec{\sigma} & 0 \\ 0 & \vec{\sigma} \end{pmatrix}. \tag{2.315}$$

This leads to $\mathbf{S} \cdot \mathbf{S} = (3/4)\hbar^2 I$. Comparison with the general result for angular momentum (Schiff, 1968) $\mathbf{S}\cdot\mathbf{S} = s(s+1)\hbar^2 I$ allows us to conclude that $s = 1/2$ and that the Dirac equation describes a particle of spin 1/2.

Notes

The passage from a system of discrete point particles to a continuous system as described in Section 2.1 is well treated by Goldstein (1950). Most quantum field theory books present some of the details of classical field theory. The greatest influences on me have been Wentzel (1949) and Bogoliubov and Shirkov (1959). A newer book that has an interesting approach is Burgess (2002). The treatment of Noether's theorem was influenced by Wentzel (1949) and Hill (1951). I first learned about the approach to gauge invariance described in Section 2.7 from studying supergravity (see van Niewenhuizen (1984) for example). The treatment of non-Abelian gauge symmetry was influenced principally by Abers and Lee (1973). Fields of general spin and their relationship with the representations of the Lorentz group are described in Weinberg (1972, 1995). My main reference for the Dirac equation is Bjorken and Drell (1964, 1965).

3
Action principle in quantum theory

3.1 States and observables

3.1.1 Bras, kets, and operators

There are at least two fundamental assumptions made in classical physics which do not apply in quantum physics. These two assumptions concern the types of measurements we can perform on a given system. The first assumption made is that it is possible, at least in principle, to perform a measurement on a given system in a way in which the interaction between the system being studied and the measuring apparatus can be made as small as we like. Because the act of measurement will disturb the system in some way, it is assumed that we can compensate for this disturbance to minimize the interaction. For example, if we look visually at an object by illuminating it with light, the illumination caused by the light leaving the light source and striking the object before being reflected to our eyes will impart some momentum to the object. Given the wavelength of light used we can always (in classical physics) work out what momentum is imparted, and we can compensate for this change in momentum by applying an appropriate force to the object to counteract this change. The second assumption made in classical physics is that there are no restrictions on what measurements we can make on a system either in type or in accuracy.[1]

Both assumptions can break down when we consider systems which must be described by quantum mechanics. The fact that one type of measurement may limit another is familiar from the Heisenberg uncertainty principle. In addition, the measurement of one property may render our knowledge of previously measured properties of a system useless. It is

[1] We are speaking theoretically here; the practicality of actually doing the compensation for momentum in a real observation is not the point. A similar comment applies to the accuracy.

therefore important to consider the situation for quantum systems most carefully.

Following Dirac (1958) we will speak of possible measurements on a system as observables. Let A_i denote any observable with a_i' a possible outcome of any measurement of this observable. Here $i = 1, 2, \ldots$ label the various observables, and we assume that for every value of i, a_i' is a real number. We can try to extract as much information as possible about a quantum mechanical system at some given instant. In order to do this it must be possible to measure some set of observables $A_1, \ldots, A_n$ without restriction. Such a set of observables is called 'mutually compatible' because the measurement of any observable in the set does not affect the measurement of any of the other observables. We could imagine starting with one observable and adding in a second observable which is mutually compatible with the first. We could then add in a third observable which is mutually compatible with the first two and so on until it is not possible to add any more. This will generate a complete set of mutually compatible observables. The most information we can obtain about our system is a knowledge of the numbers $a_1', \ldots, a_n'$ which are possible values for the complete set of mutually compatible observables. This will be called 'the state of the system'.

Following Dirac (1958) we will associate the state of a system with a vector in a complex vector space V. Since the knowledge of the values for a complete set of mutually compatible observables gives us the maximum information about a state, we can assume that $\{|a'\rangle\}$, the set of all possible states, forms a basis for V. (We have chosen to abbreviate $|a_1', \ldots, a_n'\rangle$ by $|a'\rangle$ here. The states $|a'\rangle$ are called 'kets'.) Strictly speaking a state should really be specified by a ray in V, but as our discussion is not intended to be mathematically rigorous, and because this distinction is not important for our purposes, we will gloss over this point. Similarly we will assume that the limit $n \to \infty$ may be taken without difficulty where necessary.[2]

Associated with any vector space V is the dual space V^* whose elements are called 'bras' in Dirac's terminology. A basis for V^* is denoted by $\{\langle a'|\}$, and is the basis which is dual to $\{|a'\rangle\}$. We assume that

$$\langle a'|a''\rangle = \delta(a', a''), \tag{3.1}$$

where $\delta(a', a'')$ is the Kronecker delta if a' is a discrete set, and the Dirac delta if it is continuous.

[2] For the reader interested in a more careful treatment, a gentle introduction is given by Isham (1989, 1995). For a no-holds barred treatment, see Prugovecki (1982).

The choice of a complete set of mutually compatible observables is not unique. Because we are considering $\{|a'\rangle\}$ to provide a basis for V we can understand this non-uniqueness as a different choice made for the basis vectors of V. Suppose that $\{|b'\rangle\}$ also provides a basis for V relevant to another set of mutually compatible observables $B_1, B_2, \ldots$. The fact that both $\{|a'\rangle\}$ and $\{|b'\rangle\}$ provide bases for V means that it must be possible to express one set of basis vectors in terms of the other. We can write

$$|b'\rangle = \sum_{a'} |a'\rangle\langle a'|b'\rangle, \tag{3.2}$$

where the expansion coefficients $\langle a'|b'\rangle$ are some set of complex numbers. Because of the role played by $\langle a'|b'\rangle$ in affecting a change of basis, $\langle a'|b'\rangle$ will be called the 'transformation function'. As the notation suggests, the transformation function may be identified with the inner product of $|b'\rangle$ with $|a'\rangle$. With this interpretation we may write

$$I = \sum_{a'} |a'\rangle\langle a'|, \tag{3.3}$$

from (3.2) where I is the identity operator. This is often called the 'completeness relation'. The transformation function $\langle a'|b'\rangle$ may be thought of as the elements of a matrix which must be unitary since

$$\delta(b'', b') = \langle b''|b'\rangle = \sum_{a'} \langle b''|a'\rangle\langle a'|b'\rangle, \tag{3.4}$$

if we use (3.1) and (3.2). (The last equality in (3.4) is interpreted as the component form of matrix multiplication in an obvious way.) Thinking of $\langle a'|b'\rangle$ as the components of a unitary matrix leads to

$$\langle b'|a'\rangle^* = \langle a'|b'\rangle, \tag{3.5}$$

from (3.2). If we have a third basis for V provided by $\{|c'\rangle\}$, then it is easy to show from (3.2) written as $|c'\rangle = \sum_{b'} |b'\rangle\langle b'|c'\rangle$ that

$$\langle a'|c'\rangle = \sum_{b'} \langle a'|b'\rangle\langle b'|c'\rangle. \tag{3.6}$$

It is possible to rewrite (3.2) in a matrix form. Let U denote the matrix whose components are the transformation function $\langle a'|b'\rangle$. If we think of $|a'\rangle$ and $|b'\rangle$ as column vectors we can rewrite (3.2) in matrix form as

$$|b'\rangle = U|a'\rangle. \tag{3.7}$$

This should be thought of as applying to each and every member of both sets of bases. The matrix elements of U are $\langle a'|b'\rangle$ with b' labelling the row and a' the column. With this identification (3.7) is identical to (3.2). By changing the notation slightly we can write down the explicit expression for U. Label the bases by $|a(i)\rangle$ and $|b(i)\rangle$ where $i = 1, 2, \ldots$ in place of the usual $|a'\rangle$ and $|b'\rangle$. Then (3.7) becomes

$$|b(i)\rangle = U|a(i)\rangle, \tag{3.8}$$

and we can deduce that

$$U = \sum_i |b(i)\rangle\langle a(i)|. \tag{3.9}$$

It is easy to show from (3.3) that

$$I = U^\dagger U = UU^\dagger, \tag{3.10}$$

proving that U is unitary.

With this vector space description of states we can associate observables with linear operators acting on V which map one vector into another. Since the measurements performed on a system should yield a real number, the natural association is between observables and Hermitian operators because Hermitian operators have real eigenvalues.[3] If A is the Hermitian operator representing some observable, we can write the eigenvalue equation

$$A|a'\rangle = a'|a'\rangle. \tag{3.11}$$

Taking the inner product of (3.11) with $|a''\rangle$ and using (3.1) shows that

$$\langle a''|A|a'\rangle = a'\delta(a'', a'). \tag{3.12}$$

The matrix representation of A is diagonal in the basis specified by its eigenvectors. Under the change of basis (3.7) we have

$$AU^\dagger|b'\rangle = a'U^\dagger|b'\rangle,$$

which we can write as

$$(U\ AU^\dagger)|b'\rangle = a'|b'\rangle. \tag{3.13}$$

(We have used the fact (3.10) that U is unitary here.) If we define

$$\tilde{A} = U\ AU^\dagger, \tag{3.14}$$

[3] See §9 of Dirac (1958), for example.

to be the transformed operator, the result in (3.13) shows that under a unitary transformation the new basis vectors found from (3.9) applied to the original eigenvectors are eigenvectors of the transformed operator $\tilde{A}$ defined in (3.14) with the eigenvalue unchanged. The transformation (3.14) applies to any operator under a change of basis, although (3.12) and (3.14) only apply if the basis $\{|a'\rangle\}$ involves eigenvectors of the operator. Note that the identity operator is singled out as being invariant under a change of basis generated by a unitary transformation.

One final development of the Dirac notation which we will need concerns the representation of an operator. Noting the eigenvalue equation (3.11) it can be seen that we may express A in terms of its eigenvectors as

$$A = \sum_{a'} a'|a'\rangle\langle a'|. \tag{3.15}$$

This obviously implies (3.11) if we use the orthonormality condition (3.1).

3.1.2 Time development

Suppose that at some initial time t_0 the system is described by a quantum state $|\alpha, t_0\rangle$. This state can be assumed to be expressible as a linear combination of the basis kets $|a'\rangle$ corresponding to some set of mutually compatible observables. We wish to know the state at some later time t. Denote the state of the system at time t by $|\alpha, t\rangle$ where $|\alpha, t = t_0\rangle = |\alpha, t_0\rangle$. We will assume that the time evolution of the quantum state occurs by a linear unitary operator which we will call $U(t, t_0)$. We will assume that

$$|\alpha, t\rangle = U(t, t_0)|\alpha, t_0\rangle. \tag{3.16}$$

The condition that $U(t, t_0)$ be a unitary operator preserves the norm of the quantum state under time evolution. The operator $U(t, t_0)$ will be called the 'time evolution', or 'time development', operator.

The time evolution in (3.16) is assumed to be continuous in the time. By taking the limit $t \to t_0$ it is clear that

$$U(t_0, t_0) = \mathrm{I}, \tag{3.17}$$

where I is the identity operator. If we consider a time $t' \geq t$, then the time evolution can be regarded either as occurring in two stages (i.e. from t_0 to t followed by t to t') or directly from t_0 to t'. As a consequence we must have

$$U(t', t_0) = U(t', t)U(t, t_0). \tag{3.18}$$

The time evolution operators form a one parameter group (the parameter being the time).[4] Suppose that we consider the infinitesimal time evolution from time t to time $t+\epsilon$, where ϵ is infinitesimally small. $U(t+\epsilon,t)$ is the operator which describes the evolution. Because the time evolution is assumed to occur continuously in time, and we have (3.17), we must have

$$U(t+\epsilon,t) = \mathrm{I} - \frac{i}{\hbar}\epsilon H(t) \tag{3.19}$$

to first order in ϵ for some Hermitian operator $H(t)$. Using the definition of the partial derivative, we find

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}U(t,t_0) &= i\hbar\lim_{\epsilon\to 0}\frac{1}{\epsilon}[U(t+\epsilon,t_0)-U(t,t_0)] \\ &= i\hbar\lim_{\epsilon\to 0}\frac{1}{\epsilon}[U(t+\epsilon,t)U(t,t_0)-U(t,t_0)] \end{aligned}$$

with the second equality following from the property (3.18). If we now use (3.19), the following result is obtained:

$$i\hbar\frac{\partial}{\partial t}U(t,t_0) = H(t)U(t,t_0). \tag{3.20}$$

We can therefore regard $U(t,t_0)$ as the solution to the first-order differential equation (3.20) which satisfies the boundary condition (3.17). The time-dependent quantum state defined in (3.16) satisfies the differential equation

$$i\hbar\frac{\partial}{\partial t}|\alpha,t\rangle = H(t)|\alpha,t\rangle \tag{3.21}$$

with the boundary condition $|\alpha,t=t_0\rangle = |\alpha,t_0\rangle$.

It now remains to identify the operator $H(t)$ which occurs in the definition (3.19). The operator $H(t)$ is the generator of the time evolution. In classical physics the generator of time evolution is given by the Hamiltonian of the system. (See the discussion in Section 1.4.1 and (1.59).) The simplest possibility is to take $H(t)$ in quantum mechanics to be the operator corresponding to the classical Hamiltonian for the system under consideration. Once this is done, (3.21) may be recognized as the Schrödinger equation for the quantum state.

In the special case where the Hamiltonian $H(t)$ does not have a dependence on the time we may integrate (3.20) directly to give the time evolution operator as

$$U(t,t_0) = \exp\left[-\frac{i}{\hbar}(t-t_0)H\right]. \tag{3.22}$$

[4] The fact that $U(t,t_0)$ is unitary ensures the existence of an inverse operator.

In the case where the Hamiltonian does have a dependence on the time, it is not so easy to solve (3.20) because the operators obtained by evaluating the Hamiltonian at different times may not commute. Instead it is possible to convert (3.20) into an integral equation simply by integrating both sides from time t_0 to t and using (3.17) as the initial condition. This gives

$$U(t,t_0) = \mathrm{I} - \frac{i}{\hbar}\int_{t_0}^{t} dt' H(t')U(t',t_0). \tag{3.23}$$

It is easy to see that this solves (3.20) and the boundary condition (3.17). It is possible to write down a formal solution to (3.23) by an iterative procedure. Write

$$U(t,t_0) = \sum_{n=0}^{\infty} U^{(n)}(t,t_0) \tag{3.24}$$

where $U^{(n)}(t,t_0)$ is of n^{th} order in the Hamiltonian. If we set

$$U^{(0)}(t,t_0) = \mathrm{I}, \tag{3.25}$$

then it is easy to see that

$$U^{(n)}(t,t_0) = \Big(-\frac{i}{\hbar}\Big)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n H(t_1)H(t_2)\cdots H(t_n). \tag{3.26}$$

Because of the limits on the integrals, it is clear that $t \geq t_1 \geq t_2 \geq \cdots \geq t_n \geq t_0$. Although we have not assumed that the Hamiltonian evaluated at different times satisfies any commutation relation, it is observed that the product of factors of the Hamiltonian are ordered in such a way so that the Hamiltonian at an earlier time always appears to the right of the Hamiltonian at a later time. It now proves convenient to introduce Dyson's (Dyson, 1949) chronological, or time ordered, product defined such that

$$\mathrm{T}\Big[H(t_{i_1})\cdots H(t_{i_n})\Big] = H(t_1)\cdots H(t_n), \tag{3.27}$$

for $t_{i_1},\ldots,t_{i_n}$ any ordering of $t_1,\ldots,t_n$ with $t_1 \geq \cdots \geq t_n$. We can now introduce the time-ordering symbol into (3.26) without changing the given expression. However, because of the property of the time-ordering operation defined in (3.27) the order of the operators inside of the time-ordering symbol is irrelevant. This means that $\mathrm{T}\Big[H(t_1)\cdots H(t_n)\Big]$ is a symmetric function of the integration variables $t_1,\ldots,t_n$. It is now easy to convince oneself that

$$\int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n H(t_1) \cdots H(t_n) \tag{3.28}$$

$$= \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \cdots \int_{t_0}^{t_{n-1}} dt_n \mathrm{T}\Big[H(t_1) \cdots H(t_n)\Big]$$

$$= \frac{1}{n!} \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \cdots \int_{t_0}^{t} dt_n \mathrm{T}\Big[H(t_1) \cdots H(t_n)\Big]. \tag{3.29}$$

The factor of $1/n!$ comes from the $n!$ possible permutations of the time variables inside of the time-ordering symbol. A formal proof of (3.29) can be given by induction. The expression for the time evolution operator now becomes

$$U(t, t_0) = \sum_{n=0}^{\infty} \frac{1}{n!} \Big(-\frac{i}{\hbar}\Big)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \cdots \int_{t_0}^{t} dt_n \mathrm{T}\Big[H(t_1) \cdots H(t_n)\Big]. \tag{3.30}$$

It is customary to write this last result in the convenient shorthand notation as

$$U(t, t_0) = \mathrm{T} \exp\left[-\frac{i}{\hbar} \int_{t_0}^{t} dt' H(t')\right]. \tag{3.31}$$

In the special case where the Hamiltonian operator has no explicit time dependence, the result of (3.22) is regained. However, in the general case no such simple solution is possible.

3.1.3 Heisenberg and Schrödinger pictures

In the previous section we considered the time development of the system to be through the state vector describing the system. This is called the 'Schrödinger picture'. An alternate approach is to take the state vector to be constant in time and to allow the observables to be time dependent. This is called the 'Heisenberg picture'. If $|\alpha, t\rangle_S$ represents the state vector in the Schrödinger picture, and $|\alpha, t\rangle_H$ represents the state vector in the Heisenberg picture, then we will define

$$|\alpha, t\rangle_H = |\alpha, t_0\rangle \tag{3.32}$$

where the initial state $|\alpha, t_0\rangle$ is independent of the picture adopted. (In other words, we choose the two pictures to be the same at the initial time t_0.) In the Heisenberg picture, the state vector remains frozen at its initial value for all time and does not evolve.

If A_S represents an observable in the Schrödinger picture, we will let $A_H(t)$ represent the same observable in the Heisenberg picture. Because

the states have a different time evolution in the two pictures, the operators will also evolve differently. However, the expectation value of a given observable should be independent of which picture is employed since expectation values are associated with measurable quantities. This gives the relation

$$ {}_S\langle \alpha, t|A_S|\alpha, t\rangle_S = {}_H\langle \alpha, t|A_H|\alpha, t\rangle_H. \tag{3.33} $$

Using (3.16) on the left-hand side, and (3.32) on the right-hand side, we find

$$ \langle \alpha, t_0|U^\dagger(t, t_0)A_S U(t, t_0)|\alpha, t_0\rangle = \langle \alpha, t_0|A_H(t)|\alpha, t_0\rangle, $$

from which we can conclude that the operators in the two pictures are related by

$$ A_H(t) = U^\dagger(t, t_0)A_S U(t, t_0). \tag{3.34} $$

Because of (3.33), operators in the two pictures are seen to coincide at the initial time t_0. We have not written any time argument for the Schrödinger picture operators; however, operators in the Schrödinger picture may have an explicit time dependence. An example is the Hamiltonian for a charged particle in a time-dependent electromagnetic field. In the Schrödinger picture the Hamiltonian is time dependent due to the explicit time dependence of the magnetic field. We wish to include this possibility in what follows.

In the Heisenberg picture, the time evolution of the system is expressed through the operators since the state vector is constant in time. We can find the equation which governs the behaviour of an operator in the Heisenberg picture by differentiating (3.34). If we use the differential equation (3.20) satisfied by the time evolution operator along with the adjoint of the equation which governs $U^\dagger(t, t_0)$, we find

$$ \begin{aligned} i\hbar\frac{d}{dt}A_H(t) = &- U^\dagger(t, t_0)H_S A_S U(t, t_0) + U^\dagger(t, t_0)A_S H_S U(t, t_0) \\ &+ i\hbar U^\dagger(t, t_0)\frac{\partial A_S}{\partial t}U(t, t_0). \end{aligned} $$

The Hamiltonian which enters the right hand-side follows from (3.20) and is therefore in the Schrödinger picture. We have also allowed for the possibility that the Schrödinger picture operators may have an explicit time dependence as mentioned earlier. The right-hand side of this last result may be rewritten in terms of the Heisenberg picture operator using (3.34). This gives

$$ \begin{aligned} i\hbar\frac{d}{dt}A_H(t) = &A_H(t)U^\dagger(t, t_0)H_S U(t, t_0) - U^\dagger(t, t_0)H_S U(t, t_0)A_H(t) \\ &+ i\hbar U^\dagger(t, t_0)\frac{\partial A_S}{\partial t}U(t, t_0). \end{aligned} $$

As should be evident from the previous section, there is no reason to suppose that H_S commutes with $U(t, t_0)$ in general. Equation (3.34) applies equally well to the Hamiltonian

$$H_H(t) = U^\dagger(t, t_0) H_S U(t, t_0) \tag{3.35}$$

which may be different in the two pictures. Finally, we will define

$$\frac{\partial}{\partial t} A_H(t) = U^\dagger(t, t_0) \frac{\partial A_S}{\partial t} U(t, t_0) \tag{3.36}$$

which may be understood as the transformation of $\partial A_S/\partial t$ from the Schrödinger picture to the Heisenberg picture. The Heisenberg picture operator satisfies

$$i\hbar \frac{d}{dt} A_H(t) = [A_H(t), H_H(t)] + i\hbar \frac{\partial}{\partial t} A_H(t). \tag{3.37}$$

We emphasize that the last term on the right-hand side is given meaning via (3.36), and is absent in the case where the Schrödinger picture operator has no explicit time dependence. This result should be compared with (1.30) found in classical mechanics. The results are the same if we replace dynamical variables with operator observables, take the Hamiltonian to be an operator, and replace the Poisson bracket with the quantum mechanical commutator divided by $i\hbar$.

In the special case where $[H_S, U(t, t_0)] = 0$, it is easily seen from (3.35) that $H_H(t) = H_S$. In this case the Hamiltonian is independent of the picture. This is always the case for time-independent Hamiltonians. It is also the case for time-dependent Hamiltonians provided that the Hamiltonians obtained at different times commute with each other. It is only in this case that the time-ordering operation in (3.31) is redundant.

A possible source of confusion concerns the time dependence of the base kets corresponding to some observable in the two pictures. Naively, one would expect the base kets to have the same time dependence as the state vector of the system; namely, that they would evolve with time in the Schrödinger picture according to the Schrödinger equation, and that in the Heisenberg picture they would be independent of time. However, a bit of thought will show that this is not the case.

Suppose that we have the eigenvalue equation

$$A|a'\rangle = a'|a'\rangle \tag{3.38}$$

for some observable A. If we consider the Schrödinger picture first, then the operator A does not evolve with time, so neither can the eigenvalue a' nor the eigenvectors $|a'\rangle$. Thus in the Schrödinger picture the base kets

of an observable do not evolve with time. We consider the operator and eigenvector in (3.38) to be in the Schrödinger picture.

Now consider the same situation using the Heisenberg picture. The relation between the Heisenberg and the Schrödinger picture operators was given in (3.34). If we invert (3.34) and use (3.38) we find

$$U(t,t_0)A_H(t)U^\dagger(t,t_0)|a'\rangle = a'|a'\rangle.$$

This can be written as the eigenvalue equation

$$A_H(t)U^\dagger(t,t_0)|a'\rangle = a'U^\dagger(t,t_0)|a'\rangle \tag{3.39}$$

where the eigenvalues are unchanged from (3.38), but where the eigenvectors are now given by $U^\dagger(t,t_0)|a'\rangle$. We will define

$$|a',t\rangle_H = U^\dagger(t,t_0)|a'\rangle \tag{3.40}$$

to be the base kets in the Heisenberg picture. They are seen to be time dependent, but the time dependence is different from that of the state vector in the Schrödinger picture. Taking the adjoint, or Hermitian conjugate, of (3.20) it is easily seen from (3.40) that

$$i\hbar\frac{\partial}{\partial t}|a',t\rangle_H = -H_H(t)|a',t\rangle_H. \tag{3.41}$$

This shows that $|a',t\rangle_H$ develops backwards in time when compared with the Schrödinger picture state vector in (3.21).

There is an analogy between the two pictures in quantum mechanics and the treatment of classical mechanics in a rotating frame which might make things a bit clearer. A vector in a rotating frame can be considered from two points of view. We may either consider the vector to be rotating with respect to a set of fixed axes (analogous to the Schrödinger picture with the state vector evolving in time but with the base kets fixed) or consider the vector to be fixed but take the coordinate axes to be rotating (analogous to the Heisenberg picture with the state vector fixed). In order that these two different views describe exactly the same physics, in the second case the axes must rotate in the opposite direction to that of the vector in the first case.

If we write the Schrödinger picture operator A as in (3.15), then (3.34) gives us

$$\begin{aligned} A_H(t) &= U^\dagger(t,t_0)\sum_{a'} a'|a'\rangle\langle a'|U(t,t_0) \\ &= \sum_{a'} a'|a',t\rangle_H{}_H\langle a',t| \end{aligned} \tag{3.42}$$

if we use (3.40). This shows that (3.15) applies equally well to the Heisenberg picture provided that the Heisenberg picture base kets (3.40) are used.

3.2 Schwinger action principle

Schwinger's action principle is based around the transformation function. We had in (3.6) that

$$\sum_{b'} \langle a'|b'\rangle\langle b'|c'\rangle = \langle a'|c'\rangle. \tag{3.43}$$

From (3.5) we had

$$\langle b'|a'\rangle^* = \langle a'|b'\rangle. \tag{3.44}$$

These are the two basic properties of the transformation function. Suppose that we subject the transformation function to, in Schwinger's words, any conceivable infinitesimal variation. Then by performing an arbitrary variation of (3.43) we must have

$$\delta\langle a'|c'\rangle = \sum_{b'} \Big[\left(\delta\langle a'|b'\rangle\right) \langle b'|c'\rangle + \langle a'|b'\rangle \left(\delta\langle b'|c'\rangle\right) \Big], \tag{3.45}$$

and from (3.44) we must have

$$\delta\langle b'|a'\rangle^* = \delta\langle a'|b'\rangle. \tag{3.46}$$

Define an operator δW_{ab} by the requirement

$$\delta\langle a'|b'\rangle = \frac{i}{\hbar}\langle a'|\delta W_{ab}|b'\rangle. \tag{3.47}$$

(The presence of $\hbar$ on the right-hand side of this definition for δW_{ab} is so that δW_{ab} will have the correct dimensions of action; namely energy times time.)

If we use (3.47) in (3.45) we see that

$$\begin{aligned}\langle a'|\delta W_{ac}|c'\rangle &= \sum_{b'} \Big[\langle a'|\delta W_{ab}|b'\rangle\langle b'|c'\rangle + \langle a'|b'\rangle\langle b'|\delta W_{bc}|c'\rangle\Big] \\ &= \langle a'|(\delta W_{ab} + \delta W_{bc})|c'\rangle\end{aligned}$$

if we use the completeness relation $\sum_{b'} |b'\rangle\langle b'| = \mathrm{I}$. This last result implies that

$$\delta W_{ac} = \delta W_{ab} + \delta W_{bc}. \tag{3.48}$$

If we identify the b and a descriptions in (3.47) and use $\delta\langle a'|a''\rangle = 0$, that is true by varying both sides of (3.1), then we conclude

$$\delta W_{aa} = 0. \tag{3.49}$$

Identification of the a and c descriptions in (3.48) and use of (3.49) results in

$$\delta W_{ba} = -\delta W_{ab}. \tag{3.50}$$

If we take the complex conjugate of (3.47) with the a and b descriptions reversed and use the result in (3.46) we find that

$$-\frac{i}{\hbar}\langle b'|\delta W_{ba}|a'\rangle^* = \frac{i}{\hbar}\langle a'|\delta W_{ab}|b'\rangle,$$

giving

$$-\langle a'|\delta W_{ba}^\dagger|b'\rangle = \langle a'|\delta W_{ab}|b'\rangle.$$

If we use (3.50), it follows that

$$\delta W_{ab}^\dagger = \delta W_{ab}. \tag{3.51}$$

(The factor of i on the right-hand side of (3.47) was to ensure that δW_{ab} was a Hermitian operator.) The properties (3.48)–(3.51) satisfied by δW_{ab} are a consequence of the basic properties satisfied by the transformation function.

In the previous section we considered the theory of quantum dynamics. In the Heisenberg picture the base kets become time dependent, and the general transformation function relates states which are eigenstates of different complete sets of commuting observables at different times. We will consider $\langle a_2', t_2|a_1', t_1\rangle$ where the subscripts 1 and 2 will denote different complete sets of commuting observables. This replaces our previous notation which used different letters for different sets. We can write

$$\delta\langle a_2', t_2|a_1', t_1\rangle = \frac{i}{\hbar}\langle a_2', t_2|\delta W_{21}|a_1', t_1\rangle \tag{3.52}$$

in place of (3.47). The fundamental assumption of Schwinger's approach is that the infinitesimal operator δW_{21} defined in (3.52) is obtained from the variation of a single operator W_{21} which we will call the action operator. For consistency with (3.48)–(3.51) we will require

$$W_{31} = W_{32} + W_{21}, \tag{3.53}$$

$$W_{11} = 0, \tag{3.54}$$

$$W_{21} = -W_{12} = W_{21}^\dagger. \tag{3.55}$$

If the evolution from the state $|a_1', t_1\rangle$ to the state $|a_2', t_2\rangle$ at the later time t_2 is regarded as occurring continuously in time, then we may write

$$W_{21} = \int_{t_1}^{t_2} dt\, L(t), \tag{3.56}$$

where $L(t)$ will be called the 'Lagrangian operator'. Provided that

$$L^\dagger(t) = L(t), \tag{3.57}$$

properties (3.53)–(3.55) will hold.

We can now be more explicit about the possible variations considered in (3.52). It is usual that the Lagrangian operator will depend on some set of Hermitian variables. For example, the Lagrangian may depend on the positions and velocities of a set of particles. It will also involve the masses and some coupling constants, and possibly some external fields, such as an applied electromagnetic field. The variation denoted by δ in (3.52) can then refer to

- the initial time t_1 or the final time t_2;
- variables occurring in $L(t)$;
- the structure of $L(t)$ (e.g. masses, coupling constants, external fields).

We will have occasion to consider a variety of variations in the following sections. We will refer to (3.52) with (3.56) and (3.57) as the Schwinger action principle in what follows.

3.3 Equations of motion and canonical commutation relations

As we have already seen in Chapter 1, in classical mechanics the principle of stationary action can be used to derive the classical equations of motion. Here we wish to consider the analogue for the Schwinger action principle.

Suppose that the members of the complete set of commuting observables A_1 whose eigenvectors are denoted by $|a_1', t_1\rangle$ in the Heisenberg picture are altered in some way at time t_1. We will take the alteration in the observables to correspond to a unitary transformation $A \to U^\dagger A U$ with $U^\dagger = U^{-1}$. The corresponding states must transform like $|a'\rangle \to U^\dagger|a'\rangle$ to remain eigenstates of the transformed operator. (See the discussion in Section 3.1.3.) For an infinitesimal transformation we may take $U = \mathrm{I} + (i/\hbar)G$ where G is Hermitian. We will therefore define

$$\delta|a_1', t_1\rangle = -\frac{i}{\hbar} G_1 |a_1', t_1\rangle, \tag{3.58}$$

for some Hermitian operator G_1 which depends only on the observables A_1 at time t_1. In a similar way, if we alter the observables A_2 at time t_2, we will have

$$\delta\langle a_2, t_2| = \frac{i}{\hbar}\langle a_2', t_2|G_2, \tag{3.59}$$

where G_2 depends only on the observables A_2 at the time t_2. If both sets of observables A_1 and A_2 are altered infinitesimally, then the change in the transformation function is

$$\delta\langle a_2', t_2|a_1', t_1\rangle = \frac{i}{\hbar}\langle a_2', t_2|(G_2 - G_1)|a_1', t_1\rangle. \tag{3.60}$$

Comparison of (3.60) with (3.52) shows that

$$\delta W_{21} = G_2 - G_1. \tag{3.61}$$

An important consequence of (3.61) is that if the dynamical variables which enter $L(t)$ are altered in an arbitrary infinitesimal way between the times t_1 and t_2, but are not changed at the times t_1 and t_2, then

$$\delta W_{21} = 0. \tag{3.62}$$

This result contains the operator equations of motion.[5]

In classical mechanics canonical transformations may be considered as transformations of the generalized coordinates and momenta which change the Lagrangian by a total time derivative as discussed in Chapter 1. If we consider altering the quantum Lagrangian in (3.56) by a total time derivative

$$\bar{L}(t) = L(t) - \frac{d}{dt}F, \tag{3.63}$$

for some function F, then it is clear that

$$\bar{W}_{21} = \int_{t_1}^{t_2} dt\, \bar{L}(t) = W_{21} - F_2 + F_1, \tag{3.64}$$

where F_1 and F_2 denote F evaluated at the times t_1 and t_2 respectively. Variation of both sides of (3.64) results in

$$\delta\bar{W}_{21} = \delta W_{21} - \delta F_2 + \delta F_1. \tag{3.65}$$

[5] Note that (3.62) follows because if the dynamical variables are not altered at times t_1 and t_2, then the observables, which can be regarded as some functions of the dynamical variables, will not be altered; hence, $G_1 = G_2 = 0$ in this case.

Defining

$$\delta \bar{W}_{21} = \bar{G}_2 - \bar{G}_1, \tag{3.66}$$

as in (3.61), it can be seen that

$$\bar{G}_{1,2} = G_{1,2} - \delta F_{1,2}. \tag{3.67}$$

The operator equations of motion are not altered by (3.63), but an infinitesimal unitary transformation of the base eigenstates is induced at the initial and final times. Thus the analogue of a canonical transformation in classical mechanics is a unitary transformation on the observables.

The usual form for the operator Lagrangian is

$$L(t) = \frac{1}{2}(p_i \dot{x}^i + \dot{x}^i p_i) - H(x, p, t), \tag{3.68}$$

where the first term has been symmetrized to make $L(t)$ Hermitian. Had we simply adopted $p_i \dot{x}^i$ for the first term of $L(t)$ as in classical mechanics the result obtained for $L(t)$ would not have been Hermitian because the operators p_i and $\dot{x}^i$ do not commute. The Hamiltonian operator $H(x, p, t)$ is assumed to be Hermitian. We are using the summation convention in (3.68) where the index i is summed over all degrees of freedom. The action operator is given by (3.56). We now wish to compute the variation δW_{21}. Because we want the freedom to vary the endpoints t_1 and t_2, we will follow Schwinger and change the variable of integration from t to τ where $t = t(\tau)$. This allows us to vary the functional dependence of t on τ with the variable of integration τ held fixed. With this change of integration variable we have

$$W_{21} = \int_{\tau_1}^{\tau_2} d\tau \left[\frac{1}{2}\Big(\tilde{p}_i \frac{d\tilde{x}^i}{d\tau} + \frac{d\tilde{x}^i}{d\tau} \tilde{p}_i \Big) - \tilde{H}(\tilde{x}, \tilde{p}, \tau) \frac{dt}{d\tau} \right], \tag{3.69}$$

where

$$\tilde{H}(\tilde{x}, \tilde{p}, \tau) = H(x, p, t), \tag{3.70}$$

with $\tilde{x}^i(\tau) = x^i(t)$ and $\tilde{p}_i(\tau) = p_i(t)$ when $t = t(\tau)$ is used.[6] Performing the infinitesimal variation of (3.69) we have

$$\begin{aligned} \delta W_{21} = \int_{\tau_1}^{\tau_2} d\tau \Bigg[& \frac{1}{2} \delta \tilde{p}_i \frac{d\tilde{x}^i}{d\tau} + \frac{1}{2} \tilde{p}_i \delta \Big(\frac{d\tilde{x}^i}{d\tau} \Big) + \frac{1}{2} \delta \Big(\frac{d\tilde{x}^i}{d\tau} \Big) \tilde{p}_i \\ & + \frac{1}{2} \frac{d\tilde{x}^i}{d\tau} \delta \tilde{p}_i - \delta \tilde{H} \frac{dt}{d\tau} - \tilde{H} \delta \Big(\frac{dt}{d\tau} \Big) \Bigg]. \end{aligned}$$

[6] It would be an abuse of notation to retain the same symbols under the change of variable $t = t(\tau)$, although this is common practice in physics.

(We wish to emphasize that the arbitrary parameter τ is held fixed under the variation, but the dependence of t on τ is allowed to vary.) Using the relation

$$\delta\left[\frac{df(\tau)}{d\tau}\right] = \frac{d}{d\tau}\delta f(\tau),$$

we have

$$\delta W_{21} = \int_{\tau_1}^{\tau_2} d\tau \Big\{ \frac{1}{2}\Big(\delta\tilde{p}_i \frac{d\tilde{x}^i}{d\tau} + \frac{d\tilde{x}^i}{d\tau}\delta\tilde{p}_i - \frac{d\tilde{p}_i}{d\tau}\delta\tilde{x}^i - \delta\tilde{x}^i\frac{d\tilde{p}_i}{d\tau}\Big) - \delta\tilde{H}\frac{dt}{d\tau} + \frac{d\tilde{H}}{d\tau}\delta t + \frac{d}{d\tau}\Big[\frac{1}{2}(\tilde{p}_i\delta\tilde{x}^i + \delta\tilde{x}^i\tilde{p}_i) - \tilde{H}\delta t\Big]\Big\}. \tag{3.71}$$

So far we have been careful not to make any assumptions concerning the commutation properties of the variations $\delta\tilde{x}^i$ and $\delta\tilde{p}_i$ with the dynamical variables. At this stage we will assume that the variations are multiples of the identity operator which commute with everything. More general possibilities will be considered later (see Section 7.6). This leads to some simplifications in (3.71). After changing the variable of integration back to t, we find

$$\delta W_{21} = \int_{t_1}^{t_2} dt \left(\delta p_i \dot{x}^i - \dot{p}_i \delta x^i + \frac{dH}{dt}\delta t - \delta H\right) + G_2 - G_1, \tag{3.72}$$

where G_1 and G_2 denote

$$G = p_i \delta x^i - H\delta t \tag{3.73}$$

evaluated at $t = t_1$ and $t = t_2$ respectively. Equation (3.72) can be written as

$$\delta W_{21} = \int_{t_1}^{t_2} dt \left[\delta p_i\Big(\dot{x}^i - \frac{\partial H}{\partial p_i}\Big) - \delta x^i\Big(\dot{p}_i + \frac{\partial H}{\partial x^i}\Big) + \Big(\frac{dH}{dt} - \frac{\partial H}{\partial t}\Big)\delta t\right] + G_2 - G_1, \tag{3.74}$$

if we define

$$\delta H = \delta x^i \frac{\partial H}{\partial x^i} + \delta p_i \frac{\partial H}{\partial p_i} + \delta t \frac{\partial H}{\partial t}. \tag{3.75}$$

If the variations are taken with fixed endpoints, so that $G_1 = G_2 = 0$, then the operator equations of motion which follow from (3.74) are

$$\dot{x}^i = \frac{\partial H}{\partial p_i}, \tag{3.76}$$

$$\dot{p}_i = -\frac{\partial H}{\partial x^i}, \tag{3.77}$$

$$\frac{dH}{dt} = \frac{\partial H}{\partial t}. \tag{3.78}$$

These results are identical to the classical Hamiltonian equations of motion. The derivatives which occur in (3.76) and (3.77) are with respect to operators, and can be given meaning by (3.75).[7]

There is another way of using the action principle to obtain the operator equations of motion. Let B represent any observable, and consider the matrix element $\langle a'|B|a''\rangle$. Suppose that the observables A are subjected to a unitary transformation $A \to \bar{A} = UAU^\dagger$ with U unitary. Then the eigenstates of $\bar{A}$ are $\overline{|a'\rangle} = U|a'\rangle$ which have the eigenvalue a'. We can define

$$\bar{B} = UBU^\dagger \tag{3.79}$$

so that

$$\overline{\langle a'|}\bar{B}\overline{|a''\rangle} = \langle a'|B|a''\rangle, \tag{3.80}$$

If we define the infinitesimal unitary transformation by

$$U = \mathrm{I} - \frac{i}{\hbar}G_a, \tag{3.81}$$

where G_a is Hermitian and can depend on the observables A, then

$$\delta_{G_a}|a'\rangle = \overline{|a'\rangle} - |a'\rangle = -\frac{i}{\hbar}G_a|a'\rangle, \tag{3.82}$$

and

$$\bar{B} = B - \frac{i}{\hbar}[G_a, B]. \tag{3.83}$$

We will use the symbol δ_{G_a} to denote the change caused by the canonical transformation whose infinitesimal generator is G_a. This is to distinguish it from the more general type of variation we have been considering earlier in this section which is not necessarily generated by a unitary transformation.

We can now consider the change in the matrix element $\langle a'|B|a''\rangle$ from two points of view. The first way is to consider the change in the matrix

[7] For example, if H contains a term $H_1 = p_i f^i(x)$, then $\delta H_1 = \delta p_i f^i(x) + p_i \delta f^i(x)$. With $\delta f^i(x) = [(\partial/\partial x^j) f^i(x)]\delta x^j$, we see that $\partial H_1/\partial x^i = p_j(\partial/\partial x^j)f^j(x)$ and $\partial H_1/\partial p_i = f^i(x)$. The property that the infinitesimal variation δx^i commutes with everything has been used here. Other examples can be evaluated in a similar manner.

element as entirely due to the change in the state, with the operator B held fixed.[8] This gives

$$\begin{aligned}\delta_{G_a}\langle a'|B|a''\rangle &= \overline{\langle a'|}B\overline{|a''\rangle} - \langle a'|B|a''\rangle \\ &= \langle a'|\frac{i}{\hbar}[G_a, B]|a''\rangle \end{aligned} \tag{3.84}$$

to first order in G_a. The second point of view is to take the change in $\langle a'|B|a''\rangle$ as due to a change in the operator B with the states held fixed.[9] We will define the change in B as $\delta_{G_a}B$ where [10]

$$\delta_{G_a}\langle a'|B|a''\rangle = \langle a'|\delta_{G_a}B|a''\rangle. \tag{3.85}$$

Because the result for the change in $\langle a'|B|a''\rangle$ should not depend on which of the two viewpoints is adopted, equating (3.84) with (3.85) leads to

$$\delta_{G_a}B = \frac{i}{\hbar}[G_a, B]. \tag{3.86}$$

Note from (3.83) that with this definition of $\delta_{G_a}B$ we have

$$\bar{B} = B - \delta_{G_a}B, \tag{3.87}$$

if $\bar{B}$ is defined by (3.79).

Suppose that we now consider the change in the operators A at times t_1 and t_2 as due to a change in the time $t \to t + \delta t$, with x^i fixed at times t_1 and t_2. The generator of this transformation follows from (3.73) as $G(t) = -H(t)\delta t$ where $t = t_1$ or t_2. From (3.86) it follows that

$$\delta_{G_a}B = \frac{i}{\hbar}[B, H]\delta t \tag{3.88}$$

where B and H are evaluated at the same time. If B has an explicit dependence on the time we must take care when evaluating δB, defined in (3.87), because the change there refers to that coming only from a change in the complete set of commuting observables defining the quantum state. It is only the change in B resulting from a change in the operators which is to be considered here. Specifically, if $B = B[A(t), t]$, then $\bar{B} = B[A(t + \delta t), t]$, and from (3.87) we find

$$\delta B = -\delta t\Big(\frac{dB}{dt} - \frac{\partial B}{\partial t}\Big). \tag{3.89}$$

[8] This is similar to the Schrödinger picture when the time development was considered.

[9] This is analogous to the Heisenberg picture when the time development was considered earlier.

[10] Note that in general we should regard B as some function of the operators A, so that a unitary change of A will affect B.

The term in $\partial B/\partial t$ is subtracted off in (3.89) because the change in the explicit dependence on t in B does not result from an operator transformation. The minus sign in (3.89) is due to that in (3.87). If we now use (3.89) in (3.88) we find

$$\frac{dB}{dt} = \frac{\partial B}{\partial t} + \frac{i}{\hbar}[H, B]. \tag{3.90}$$

This result is in complete agreement with the Heisenberg picture equation of motion (3.48). Note that by taking $B = H$, the result in (3.78) is regained. By taking $B = x^i$ we have

$$\dot{x}^i = \frac{i}{\hbar}[H, x^i], \tag{3.91}$$

and by taking $B = p_i$ we have

$$\dot{p_i} = \frac{i}{\hbar}[H, p_i]. \tag{3.92}$$

These last two results must be consistent with (3.76) and (3.77).

It is possible to use the action principle to derive the canonical commutation relations. We will reconsider this from a more general standpoint later when we come to quantum field theory. For now, suppose that we fix δt at times t_1 and t_2 but allow δx^i to vary. From (3.73) the generator of this transformation is [11]

$$G_x = p_i \delta x^i. \tag{3.93}$$

Equations (3.86) and (3.87) still hold for any operator B. In this case

$$\delta B = \frac{i}{\hbar}\delta x^i [p_i, B]. \tag{3.94}$$

Taking $B = x^i$ in (3.94) gives

$$[x^i, p_j] = i\hbar \delta^i{}_j. \tag{3.95}$$

Taking $B = p_j$ in (3.94) and noting that δp_i and δx^i are independent variations leads to

$$[p_i, p_j] = 0. \tag{3.96}$$

More generally, if B in (3.87) has a dependence on x, then from $\delta B = B[x(t)] - B[x(t) - \delta x(t)]$ we find

$$[p_i, B] = -i\hbar \frac{\partial}{\partial x^i} B. \tag{3.97}$$

[11] We do not indicate explicitly the time dependence in G_x.

Again we emphasize that $\bar{B}$ in (3.87) is $B(x-\delta x)$ rather than $B(x+\delta x)$ since (3.87) applies equally well to the operator $x(t)$.

Equations (3.95) and (3.96) give part of the complete set of canonical commutation relations. In order to deduce $[x^i, x^j]$ we can use the freedom of altering the Lagrangian operator by the addition of a total time derivative as in (3.63). If we choose

$$F = \frac{1}{2}(p_i x^i + x^i p_i), \tag{3.98}$$

so that $F^\dagger = F$, then

$$\delta F = \delta p_i x^i + p_i \delta x^i, \tag{3.99}$$

and

$$\bar{G} = G - \delta F = -\delta p_i x^i - H\delta t. \tag{3.100}$$

Taking $\delta t = 0$, and defining

$$G_p = -\delta p_i x^i, \tag{3.101}$$

we have

$$\delta B = -\frac{i}{\hbar}\delta p_i [x^i, B] \tag{3.102}$$

for any operator B. By taking $B = p_j$ the result (3.95) is regained. If we take $B = x^j$ and again use the independence of δx^i and δp_i, (3.102) gives

$$[x^i, x^j] = 0. \tag{3.103}$$

This demonstrates how the canonical commutation relations follow from the action principle.

3.4 Position and momentum eigenstates

So far we have considered observables having discrete eigenvalues, and ignored any subtleties associated with having an infinite number of them. However, there are important classes of observables whose eigenvalues are continuous. One example of such an observable is position. Another is momentum. The Dirac bra-ket formalism we have developed up to this stage can be extended to operators with continuous spectra provided that the Kronecker delta symbol is understood to be the Dirac delta distribution, and the sum over eigenvalues $\sum_{a'}$ that has occurred in the formalism is understood to be an integral if a' is a continuous variable. For example, if a' and b' are both continuous, then $|b'\rangle = \sum_{a'} C_{a'}|a'\rangle$ is written as

$$|b'\rangle = \int da' C(a')|a'\rangle \tag{3.104}$$

where $C(a')$ is some continuous function. An expression like

$$|b'\rangle = \sum_{a'} |a'\rangle\langle a'|b'\rangle$$

becomes

$$|b'\rangle = \int da'|a'\rangle\langle a'|b'\rangle \tag{3.105}$$

in the continuous case. $\delta(a', a'')$ represents the Dirac δ-distribution defined by

$$\int da''\delta(a', a'')f(a'') = f(a') \tag{3.106}$$

for an arbitrary test function $f(a')$. This cursory treatment of continuous spectra glosses over a large number of important mathematical points. The interested reader should consult Prugovecki (1982) for example. In this section we will continue in a heuristic manner to establish a number of results for the position and momentum operators and show consistency with the commutation relations established in Section 3.3.

If x is the operator representing the position of a particle in one spatial dimension, we can write the eigenvector of x as $|x'\rangle$ where

$$x|x'\rangle = x'|x'\rangle. \tag{3.107}$$

In more than one spatial dimension the generalization of (3.107) is

$$\mathbf{x}|\mathbf{x}'\rangle = \mathbf{x}'|\mathbf{x}'\rangle. \tag{3.108}$$

Note that it is assumed that the operators representing different components of the position commute so that the different components of position can be simultaneously specified. This follows from the canonical commutation relations established in (3.103). The set $\{|\mathbf{x}'\rangle\}$ is assumed to be complete, meaning that any state $|\alpha\rangle$ can be expanded as

$$|\alpha\rangle = \int d^D x'|\mathbf{x}'\rangle\langle\mathbf{x}'|\alpha\rangle, \tag{3.109}$$

where D is the spatial dimension.

In order to define the operator representing the momentum we will identify it with the generator of spatial translations. This is a natural association in view of the connection between invariance under translations and conservation of momentum established in Section 1.5.2. Let $T(\epsilon)$ be the unitary operator representing a translation of the position by an amount ϵ. This means that for any state $|\alpha\rangle$, $T(\epsilon)|\alpha\rangle$ is the state which

has the eigenvalue $\mathbf{x}'$ of the position operator $\mathbf{x}$ replaced with $\mathbf{x}' + \epsilon$.[12] If we apply the translation operator to the ket $|\mathbf{x}'\rangle$ we obtain the ket $|\mathbf{x}' + \epsilon\rangle$. Because $T(\epsilon)$ is unitary, it must be possible to express it as

$$T(\epsilon) = \exp\Big(-\frac{i}{\hbar}\epsilon \cdot \mathbf{p}\Big) \tag{3.110}$$

for some Hermitian operator $\mathbf{p}$. The factor of $\hbar$ is included in the argument of the exponential so that the operator $\mathbf{p}$ has the right dimensions to be associated with momentum. It is straightforward to show using the definition of $T(\epsilon)|\mathbf{x}'\rangle = |\mathbf{x}' + \epsilon\rangle$ that

$$\big[x^i, T(\epsilon)\big]\,|\mathbf{x}'\rangle = \epsilon^i |\mathbf{x}' + \epsilon\rangle, \tag{3.111}$$

where $i = 1, \ldots, D$ labels the spatial components of the D-dimensional vectors $\mathbf{x}$ and ϵ. Since ϵ is continuously variable, we may differentiate both sides of (3.111) with respect to ϵ^i and then set $\epsilon^i = 0$. From (3.110) we find

$$\frac{\partial}{\partial \epsilon^i} T(\epsilon)\bigg|_{\epsilon=\mathbf{0}} = -\frac{i}{\hbar} p_i. \tag{3.112}$$

It now follows quite simply that

$$[x^i, p_j] = i\hbar \delta^i{}_j, \tag{3.113}$$

in complete agreement with (3.95). Note that $\mathbf{x} \cdot \mathbf{p} = x^i p_i$ with the usual index summation convention. In the limit $\hbar \to 0$, the position and momentum operators are seen to commute; therefore, although there is no impediment in classical physics to simultaneously specifying both the position and the momentum of a particle with arbitrary accuracy, it is not possible to do so in quantum mechanics.

It is straightforward to show that

$$[p_i, p_j] = 0 \tag{3.114}$$

as a consequence of the fact that the operators corresponding to two independent spatial translations commute. This recovers what we established in a different way in (3.96). The result means that it is possible to simultaneously specify the different components of momentum, just as we can for position.

[12] It can be noted that the set of all spatial translations forms an Abelian group.

It is possible to obtain a direct result for the matrix element of the momentum operator in the basis specified by the basis kets $\{|\mathbf{x}'\rangle\}$. If we take the matrix element of the operator $T(\epsilon)$ we have

$$\langle \mathbf{x}'|T(\epsilon)|\mathbf{x}''\rangle = \langle \mathbf{x}'|\mathbf{x}'' + \epsilon\rangle \tag{3.115}$$

$$= \delta(\mathbf{x}', \mathbf{x}'' + \epsilon) \tag{3.116}$$

where the first equality has followed from the definition of $T(\epsilon)$ as the generator of spatial translations, and the second equality has followed from the assumption that the position eigenstates form a complete set in the sense of (3.109). If we now differentiate (3.116) with respect to ϵ^i and then set $\epsilon^i = 0$ we find, using (3.112), that

$$\langle \mathbf{x}'|p_i|\mathbf{x}''\rangle = i\hbar \frac{\partial}{\partial x''^i}\delta(\mathbf{x}', \mathbf{x}''). \tag{3.117}$$

An equivalent expression can be obtained by first noting that $\langle \mathbf{x}'|T(\epsilon) = [T^\dagger(\epsilon)|\mathbf{x}'\rangle]^\dagger$ and the fact that $T^\dagger(\epsilon) = T^{-1}(\epsilon) = T(-\epsilon)$. In place of (3.115) and (3.116) we obtain

$$\langle \mathbf{x}'|T(\epsilon)|\mathbf{x}''\rangle = \langle \mathbf{x}' - \epsilon|\mathbf{x}''\rangle \tag{3.118}$$

$$= \delta(\mathbf{x}' - \epsilon, \mathbf{x}''). \tag{3.119}$$

Differentiation with respect to ϵ followed by setting $\epsilon = \mathbf{0}$ now results in

$$\langle \mathbf{x}'|p_i|\mathbf{x}''\rangle = -i\hbar \frac{\partial}{\partial x'^i}\delta(\mathbf{x}', \mathbf{x}''). \tag{3.120}$$

This result may be obtained more simply from (3.117) by making use of the property

$$\frac{\partial}{\partial x'^i}\delta(\mathbf{x}', \mathbf{x}'') = -\frac{\partial}{\partial x''^i}\delta(\mathbf{x}', \mathbf{x}'') \tag{3.121}$$

of the Dirac δ-distribution. The property of the Dirac δ-distribution in (3.121) may also be shown to follow directly from the basic definition (3.106) by integrating both sides of (3.121) with a suitable test function.

We can define a set of basis kets appropriate to the momentum operator by

$$\mathbf{p}|\mathbf{p}'\rangle = \mathbf{p}'|\mathbf{p}'\rangle. \tag{3.122}$$

It is possible to find the transformation function $\langle \mathbf{x}'|\mathbf{p}'\rangle$ which relates the position and momentum eigenkets as follows. We have from (3.122) that

$$\langle \mathbf{x}'|\mathbf{p}|\mathbf{p}'\rangle = \mathbf{p}'\langle \mathbf{x}'|\mathbf{p}'\rangle. \tag{3.123}$$

The left-hand side may be rewritten as

$$\begin{aligned}\langle \mathbf{x}'|\mathbf{p}|\mathbf{p}'\rangle &= \int d^D x'' \langle \mathbf{x}'|\mathbf{p}|\mathbf{x}''\rangle\langle \mathbf{x}''|\mathbf{p}'\rangle \\ &= -i\hbar\nabla'\langle \mathbf{x}'|\mathbf{p}'\rangle \end{aligned} \tag{3.124}$$

if we use (3.120). If we compare (3.123) and (3.124) we find the simple partial differential equation

$$-i\hbar\nabla'\langle \mathbf{x}'|\mathbf{p}'\rangle = \mathbf{p}'\langle \mathbf{x}'|\mathbf{p}'\rangle, \tag{3.125}$$

for the transformation function $\langle \mathbf{x}'|\mathbf{p}'\rangle$ whose solution is

$$\langle \mathbf{x}'|\mathbf{p}'\rangle = N \exp\Big(\frac{i}{\hbar}\mathbf{p}'\cdot\mathbf{x}'\Big). \tag{3.126}$$

Here N is an arbitrary constant of integration that can be determined using

$$\langle \mathbf{x}'|\mathbf{x}''\rangle = \int d^D p' \langle \mathbf{x}'|\mathbf{p}'\rangle\langle \mathbf{p}'|\mathbf{x}''\rangle. \tag{3.127}$$

Substitution of (3.126) and its complex conjugate on the right-hand side of (3.127) and using the completeness relation for the position eigenstates on the left-hand side results in

$$\delta(\mathbf{x}', \mathbf{x}'') = |N|^2 \int d^D p' \exp\left[\frac{i}{\hbar}\mathbf{p}'\cdot(\mathbf{x}' - \mathbf{x}'')\right].$$

In order that the right-hand side of this result corresponds to a representation of the Dirac δ-distribution as in (2.76), we must have

$$|N|^2 = (2\pi\hbar)^{-D}.$$

We will choose N to be real and positive, without any loss of generality, and therefore (3.126) becomes

$$\langle \mathbf{x}'|\mathbf{p}'\rangle = (2\pi\hbar)^{-D/2} \exp\Big(\frac{i}{\hbar}\mathbf{p}'\cdot\mathbf{x}'\Big). \tag{3.128}$$

3.5 Simple harmonic oscillator

The simple harmonic oscillator is by far the most important model in theoretical physics. It forms the basis for many models in condensed matter physics, quantum statistical mechanics, and quantum field theory. A thorough understanding of the simple harmonic oscillator is essential.

The classical Hamiltonian is

$$H = \frac{1}{2m}p^2 + \frac{1}{2}m\omega^2 x^2 \tag{3.129}$$

where m is the mass and ω is the classical frequency of oscillation.[13] The quantum Hamiltonian operator will be chosen to have the same form as (3.129) but where p and x are regarded as operators with

$$[x, p] = i\hbar. \tag{3.130}$$

We will work in the Schrödinger picture initially.

Instead of working with x and p, it is more advantageous to introduce two new operators a and $a^\dagger$ defined by

$$a = \left(\frac{m\omega}{2\hbar}\right)^{1/2}\left(x + \frac{i}{m\omega}p\right), \tag{3.131}$$

$$a^\dagger = \left(\frac{m\omega}{2\hbar}\right)^{1/2}\left(x - \frac{i}{m\omega}p\right). \tag{3.132}$$

Equivalently,

$$x = \left(\frac{\hbar}{2m\omega}\right)^{1/2}\left(a + a^\dagger\right), \tag{3.133}$$

$$p = i\left(\frac{m\omega\hbar}{2}\right)^{1/2}\left(a^\dagger - a\right). \tag{3.134}$$

It is easy to show that

$$[a, a^\dagger] = 1, \tag{3.135}$$

and that

$$aa^\dagger + a^\dagger a = \frac{m\omega}{\hbar}\left(x^2 + \frac{p^2}{m^2\omega^2}\right). \tag{3.136}$$

Using (3.136) it is possible to rewrite the Hamiltonian in (3.129) in terms of a and $a^\dagger$. The result is

$$H = \frac{1}{2}\hbar\omega(aa^\dagger + a^\dagger a). \tag{3.137}$$

The result can also be written as

$$H = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right), \tag{3.138}$$

if it is noted that $aa^\dagger = 1 + a^\dagger a$ which follows from (3.135).

[13] We will deal only with the one-dimensional oscillator here.

The result in (3.138) shows that

$$[H, a^\dagger a] = 0. \tag{3.139}$$

A consequence of this is that H and $a^\dagger a$ have simultaneous eigenvectors. We will define

$$a^\dagger a|n'\rangle = n'|n'\rangle \tag{3.140}$$

for some number n' to be determined. If

$$H|n'\rangle = E_{n'}|n'\rangle \tag{3.141}$$

it follows from (3.138) and (3.140) that

$$E_{n'} = \left(n' + \frac{1}{2}\right)\hbar\omega. \tag{3.142}$$

The number n' defined in (3.140) can be found as follows. If we take the inner product of (3.140) with $|n'\rangle$, the result is

$$\langle n'|a^\dagger a|n'\rangle = n'\langle n'|n'\rangle. \tag{3.143}$$

The left-hand side of (3.143) may be recognized as the norm of the ket $a|n'\rangle$ which must be non-negative. It follows that $n' \geq 0$ with $n' = 0$ if and only if $a|n'\rangle = 0$. We will denote[14] the state with the zero eigenvalue by $|0\rangle$:

$$a|0\rangle = 0. \tag{3.144}$$

We will next show that the state $|0\rangle$ must be one of the eigenvectors of $a^\dagger a$. In order to do this, operate on both sides of (3.140) with the operator a. This gives

$$aa^\dagger a|n'\rangle = n'a|n'\rangle.$$

We can use (3.135) to write $aa^\dagger a = (1 + a^\dagger a)a$ giving

$$(a^\dagger a)a|n'\rangle = (n' - 1)a|n'\rangle. \tag{3.145}$$

This shows that $a|n'\rangle$ is an eigenvector of $a^\dagger a$ with eigenvalue $(n' - 1)$. By operating on (3.145) with a it is easy to show that $a^2|n'\rangle$ is an eigenvector of $a^\dagger a$ with eigenvalue $(n' - 2)$. Generally, as can be shown by induction, $a^k|n'\rangle$ is an eigenvector of $a^\dagger a$ with eigenvalue $(n' - k)$ for any integer k. Eventually we will obtain an eigenvector of $a^\dagger a$ with an

[14] No confusion should arise here over the omission of the prime on 0 in $|0\rangle$.

eigenvalue between 0 and 1. Unless 0 is the smallest eigenvalue of $a^\dagger a$, a further application of the operator a to $a^k|n'\rangle$ will result in an eigenvector with a negative eigenvalue. However, we know that this is impossible, as discussed above, if the norm of the associated eigenvector is to be non-negative. Thus, $n' = 0$ must be the smallest eigenvalue, and the state denoted by $|0\rangle$ in (3.144) is the associated eigenstate.

In order that the process we have just described in the preceding paragraph result ultimately in $n' = 0$, it should be obvious that n' must be an integer. Another way to see this is to consider the state $(a^\dagger)^k|0\rangle$ where k is any non-negative integer. Using (3.135) it follows that

$$\begin{aligned} a^\dagger a(a^\dagger)^k|0\rangle &= a^\dagger a a^\dagger (a^\dagger)^{k-1}|0\rangle \\ &= a^\dagger(1 + a^\dagger a)(a^\dagger)^{k-1}|0\rangle \\ &= (a^\dagger)^k|0\rangle + a^\dagger(a^\dagger a)(a^\dagger)^{k-1}|0\rangle. \end{aligned}$$

If we define

$$a^\dagger a(a^\dagger)^k|0\rangle = \lambda_k(a^\dagger)^k|0\rangle,$$

then the previous line shows that

$$\lambda_k = \lambda_{k-1} + 1.$$

We know from (3.144) that $\lambda_0 = 0$. It then follows that $\lambda_k = k$.

We can now write

$$|n'\rangle = C_{n'}(a^\dagger)^{n'}|0\rangle \tag{3.146}$$

for some normalization constant $C_{n'}$ which is chosen so that

$$\langle n''|n'\rangle = \delta_{n''n'}.$$

We know from above that $a|n'\rangle$ is an eigenvector of $a^\dagger a$ with eigenvalue $n' - 1$. Thus, it must be that

$$a|n'\rangle = B_{n'}|n' - 1\rangle \tag{3.147}$$

for some constant $B_{n'}$. If we take the norm of the state in (3.147) we find

$$\begin{aligned} |B_{n'}|^2 &= \langle n'|a^\dagger a|n'\rangle \\ &= n' \end{aligned} \tag{3.148}$$

since the states are assumed to be normalized, and we have $a^\dagger a|n'\rangle = n'|n'\rangle$. It therefore follows from (3.147) and (3.148) that

$$a|n'\rangle = \sqrt{n'}\,|n' - 1\rangle, \tag{3.149}$$

with a choice of phase making $B_{n'}$ real. Because of its role in (3.149), the operator a is called the 'annihilation (or destruction or lowering) operator'.

The normalization constant in (3.146) can now be evaluated. If we use (3.146) in the left-hand side of (3.149) we have

$$C_{n'} a(a^\dagger)^{n'}|0\rangle = \sqrt{n'}\,|n'-1\rangle. \tag{3.150}$$

The left-hand side of this last equation can be rewritten using (3.135) to give

$$\begin{aligned} a(a^\dagger)^{n'}|0\rangle &= aa^\dagger(a^\dagger)^{n'-1}|0\rangle \\ &= (1+a^\dagger a)(a^\dagger)^{n'-1}|0\rangle \\ &= (a^\dagger)^{n'-1}|0\rangle + (a^\dagger a)(a^\dagger)^{n'-1}|0\rangle. \end{aligned}$$

The right-hand side of this result can be rewritten in terms of $|n'-1\rangle$ if we use (3.146) with n' replaced with $n'-1$. This yields

$$\begin{aligned} a(a^\dagger)^{n'}|0\rangle &= \frac{1}{C_{n'-1}}|n'-1\rangle + \frac{1}{C_{n'-1}}a^\dagger a|n'-1\rangle \\ &= \frac{n'}{C_{n'-1}}|n'-1\rangle \end{aligned}$$

if we note that $a^\dagger a|n'-1\rangle = (n'-1)|n'-1\rangle$. It now follows from (3.150) that

$$n'\frac{C_{n'}}{C_{n'-1}} = \sqrt{n'},$$

whence

$$C_{n'} = \frac{C_{1'}}{\sqrt{n'!}}. \tag{3.151}$$

$C_{1'}$ can be fixed very simply from taking the norm of the state with $n'=1$ in (3.146):

$$\begin{aligned} 1 &= |C_{1'}|^2\langle 0|aa^\dagger|0\rangle \\ &= |C_{1'}|^2 \end{aligned}$$

where the last line has followed upon use of the commutation relation (3.135), the definition of the state $|0\rangle$ in (3.144), and the assumption $\langle 0|0\rangle = 1$. We therefore have

$$|n'\rangle = \frac{1}{\sqrt{n'!}}(a^\dagger)^{n'}|0\rangle. \tag{3.152}$$

The orthogonality of $|n'\rangle$ and $|n''\rangle$ if $n' \neq n''$ can be shown as follows. We have

$$a^\dagger a|n'\rangle = n'|n'\rangle, \tag{3.153}$$
$$a^\dagger a|n''\rangle = n''|n''\rangle. \tag{3.154}$$

If we take the inner product of (3.153) with $|n''\rangle$, and the inner product of (3.154) with $|n'\rangle$ we find

$$\langle n''|a^\dagger a|n'\rangle = n'\langle n''|n'\rangle,$$
$$\langle n'|a^\dagger a|n''\rangle = n''\langle n'|n''\rangle.$$

Taking the complex conjugate of the second equation and comparing the result with the first equation leads to

$$(n'' - n')\langle n''|n'\rangle = 0,$$

proving that $\langle n''|n'\rangle = 0$ if $n'' \neq n'$.

By applying $a^\dagger$ to (3.152) it is easily seen that

$$a^\dagger|n'\rangle = \sqrt{n'+1}\,|n'+1\rangle. \tag{3.155}$$

This result can be contrasted with (3.149). Because of the role of $a^\dagger$ in (3.155), $a^\dagger$ is called the 'creation (or raising) operator'.

Because of the special role played by $a^\dagger a$ in the analysis, we will define

$$n = a^\dagger a \tag{3.156}$$

and call n the number operator. We have $n|n'\rangle = n'|n'\rangle$. Because of (3.142) the state $|n'\rangle$ having energy $E_{n'} = (n'+1/2)\hbar\omega$ can be thought of as a state with n' quanta, where each of the quanta has an energy of $\hbar\omega$. The special state $|0\rangle$ having no quanta is called the 'ground (or vacuum) state'. It is observed that even the state with no quanta has an energy of $\hbar\omega/2$ associated with it. This energy is called the 'zero point energy', and we will return to it again when we discuss quantum field theory.

To finish this section, we will look at the time development using the Heisenberg picture. Using (3.37) for the operator a and the Hamiltonian in (3.138) we find[15]

$$\begin{aligned} i\hbar\dot{a}_H(t) &= [a_H(t), H] \\ &= \hbar\omega[a_H(t), a_H^\dagger(t)a_H(t)] \\ &= \hbar\omega a_H(t). \end{aligned} \tag{3.157}$$

[15] Note that because H is time independent, it can be written directly in terms of the Heisenberg picture creation and annihilation operators.

The solution to (3.157) is

$$a_H(t) = \exp\Big[-i\omega(t-t_0)\Big]a(t_0) \tag{3.158}$$

where $a(t_0)$ can be taken in either the Schrödinger or the Heisenberg picture since the two pictures coincide at the initial time t_0. The adjoint of (3.158) gives

$$a_H^\dagger(t) = \exp\Big[i\omega(t-t_0)\Big]a^\dagger(t_0). \tag{3.159}$$

This last result can also be found directly by solving the Heisenberg equation of motion for $a^\dagger$ just as we did for a.

The position operator can now be found using (3.133) along with the solutions we have just obtained for $a_H(t)$ and $a_H^\dagger(t)$ to be

$$x_H(t) = \cos\omega(t-t_0)\; x(t_0) + \sin\omega(t-t_0)\;\frac{p(t_0)}{m\omega}. \tag{3.160}$$

In a similar way, the momentum operator is found from (3.134) to be

$$p_H(t) = \cos\omega(t-t_0)\; p(t_0) - m\omega\sin\omega(t-t_0)\; x(t_0). \tag{3.161}$$

The solutions in (3.160) and (3.161) are the same as those found for the classical simple harmonic oscillator if the operators are replaced with their classical counterparts.

Instead of solving the Heisenberg equations of motion directly, we can use the formal solution (3.34) with the time development operator

$$U(t,t_0) = \exp\Big[-i(t-t_0)H/\hbar\Big].$$

In order to evaluate $U^\dagger(t,t_0)a(t_0)U(t,t_0)$ we will consider a general operator identity that we will also use later. Define

$$F(\beta) = e^{-\beta H}Ae^{\beta H}, \tag{3.162}$$

where β is a parameter and A is any operator which obeys

$$[H,A] = -\lambda A, \tag{3.163}$$

for some number λ. In the case of immediate interest, we have $A = a(t_0)$ and the commutator $[H,A]$ has already been worked out in (3.157) giving $\lambda = \hbar\omega$. Differentiating $F(\beta)$ with respect to β results in

$$F'(\beta) = -[H,F(\beta)]. \tag{3.164}$$

By differentiating repeatedly and using $F(\beta = 0) = A$ along with (3.163) it follows that

$$\left.\frac{d^n F(\beta)}{d\beta^n}\right|_{\beta=0} = \lambda^n A.$$

From the Taylor series expansion of $F(\beta)$ about $\beta = 0$, we find

$$\begin{aligned} F(\beta) &= \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \left.\frac{d^n F(\beta)}{d\beta^n}\right|_{\beta=0} \\ &= \sum_{n=0}^{\infty} \frac{(\beta\lambda)^n}{n!} A \\ &= e^{\beta\lambda} A. \end{aligned}$$

We have therefore proven that if an operator A satisfies (3.163), then it obeys

$$e^{-\beta H} A e^{\beta H} = e^{\beta\lambda} A. \tag{3.165}$$

Setting $\beta = -i(t - t_0)/\hbar$ and $\lambda = \hbar\omega$ with $A = a(t_0)$ we find

$$a_H(t) = e^{-i\omega(t-t_0)} a(t_0),$$

as in (3.158).

Finally we note from (3.40) that the energy eigenstates in the Heisenberg picture are

$$\begin{aligned} |n', t\rangle_H &= \exp\left[\frac{i}{\hbar}(t - t_0)H\right] |n'\rangle_S \\ &= \exp\left[i\omega(t - t_0)\left(n' + \frac{1}{2}\right)\right] |n'\rangle_S, \end{aligned} \tag{3.166}$$

if we use (3.142). We can verify that $a_H(t)$ and $a_H^\dagger(t)$ have the raising and lowering properties like the Schrödinger picture operators had in (3.149) and (3.155). For example,

$$\begin{aligned} a_H(t)|n', t\rangle_H &= e^{[-i\omega(t-t_0)]} a(t_0) \exp\left[i(t - t_0)\omega\left(n' + \frac{1}{2}\right)\right] |n'\rangle_S \\ &= \exp\left[i\omega(t - t_0)\left(n' - \frac{1}{2}\right)\right] \sqrt{n'}\, |n' - 1\rangle_S \\ &= \sqrt{n'}\, |n' - 1, t\rangle_H. \end{aligned}$$

3.6 Real scalar field

In quantum mechanics the position and momentum of a point particle are viewed as operators. These operators satisfy canonical commutation relations which can be obtained from the classical Poisson brackets by the replacement $\{\ ,\ \} \to (1/i)[\ ,\ ]$. (We will take $\hbar = 1$ in the following.) In Section 3.3, we showed how the canonical commutation relations could be derived from the Schwinger action principle. In Section 2.4 we discussed how classical field theory could thought of in relation to point particle mechanics. It is therefore natural to replace the classical field $\varphi(x)$ which describes a real scalar field and the canonical momentum $\pi(x)$ with field operators which satisfy

$$[\varphi(t,\mathbf{x}),\varphi(t,\mathbf{x}')] = 0, \tag{3.167}$$

$$[\pi(t,\mathbf{x}),\pi(t,\mathbf{x}')] = 0, \tag{3.168}$$

$$[\varphi(t,\mathbf{x}),\pi(t,\mathbf{x}')] = i\delta(\mathbf{x},\mathbf{x}') \tag{3.169}$$

The analogous results for classical field theory expressed in terms of Poisson brackets are (2.98) and (2.99). These relations can also be derived by a repetition of the analysis presented in Section 3.3 suitably modified for field theory. The basic Schwinger action principle described in Section 3.2 only used the notion of quantum states. We begin with the action functional for a real scalar field

$$S[\varphi] = \int_{t_1}^{t_2} dt \int_\Sigma d\sigma_x \left[\frac{1}{2}\partial^\mu\varphi\partial_\mu\varphi - \frac{1}{2}m^2\varphi^2 - U(\varphi)\right]. \tag{3.170}$$

(The potential term $U(\varphi)$ can be omitted if desired because it plays no role in the derivation of the field commutation relations.) φ is to be regarded as an operator here. We subject $S[\varphi]$ to an arbitrary variation $\varphi \to \varphi + \delta\varphi$, where $\delta\varphi$ is a multiple of the identity operator and therefore commutes with everything. After an integration by parts we find

$$\delta S[\varphi] = \int_{t_1}^{t_2} dt \int_\Sigma d\sigma_x \delta\varphi \left[-\Box\varphi - m^2\varphi - U'(\varphi)\right] + G_\varphi(t_2) - G_\varphi(t_1),$$

where

$$\begin{aligned} G_\varphi(t) &= \int_\Sigma d\sigma_x \delta\varphi(t,\mathbf{x})\dot{\varphi}(t,\mathbf{x}) \\ &= \int_\Sigma d\sigma_x \delta\varphi(t,\mathbf{x})\pi(t,\mathbf{x})\ . \end{aligned}$$

We have identified $\dot{\varphi}$ as the field momentum π in the last line (see Section 2.3.1). From (3.86) with $B = \varphi(t, \mathbf{x})$ we have ($\hbar$=1)

$$\delta\varphi(t, \mathbf{x}) = i \int_\Sigma d\sigma_{x'} \delta\varphi(t, \mathbf{x}')[\pi(t, \mathbf{x}'), \varphi(t, \mathbf{x})].$$

With $B = \pi(t, \mathbf{x})$, since G_φ generates a unitary transformation where only φ is varied, we have

$$\delta\pi(t, \mathbf{x}) = 0 = i \int_\Sigma d\sigma_{x'} \delta\varphi(t, \mathbf{x}')[\pi(t, \mathbf{x}'), \pi(t, \mathbf{x})].$$

In this way we deduce (3.168) and (3.169).

To deduce (3.167) we must find the unitary operator which corresponds to a variation of π with φ held fixed. This can be done as in Section 3.3 by using the freedom to add a total time derivative to the Lagrangian $L(t)$ as in (3.63). We will choose

$$F(t) = \frac{1}{2} \int_\Sigma d\sigma_x \left(\varphi(t, \mathbf{x})\pi(t, \mathbf{x}) + \pi(t, \mathbf{x})\varphi(t, \mathbf{x})\right),$$

as the analogue of (3.98). It is not difficult to show that this leads to

$$G_\pi(t) = -\int_\Sigma d\sigma_x \delta\pi(t, \mathbf{x})\varphi(t, \mathbf{x}).$$

Use of (3.86) with $B = \varphi(t, \mathbf{x})$ recovers (3.167).

There is a sense in which we can think of the free (i.e. $U(\varphi) = 0$) real scalar field as being made up of an infinite set of non-interacting simple harmonic oscillators. This interpretation is useful because we already know quite a lot about the simple harmonic oscillator. We will discuss this in a more general setting than flat Minkowski space here. Take Σ to be a D-dimensional Riemannian manifold without boundary.[16] The usual procedure in flat space consists of Fourier expanding the field operator in terms of plane waves. Our first task will be to generalize this to the space Σ.

Consider the Laplacian $-\nabla^2$ defined on Σ. Suppose that we let $\{f_n(\mathbf{x})\}$ denote a complete set of eigenfunctions of $-\nabla^2$ with σ_n the eigenvalue. We will write

$$-\nabla^2 f_n(\mathbf{x}) = \sigma_n f_n(\mathbf{x}), \tag{3.171}$$

[16] More loosely we can think of the space Σ as a D-dimensional closed space of finite volume with no edges, such as a sphere or a torus. As always, the reader not interested in this generality can think of Σ as flat space with periodic boundary conditions imposed with the infinite volume limit taken at the end.

$$\int_\Sigma d\sigma_x f_n^*(\mathbf{x}) f_{n'}(\mathbf{x}) = \delta_{nn'}. \tag{3.172}$$

In general we will assume that $f_n(\mathbf{x})$ is complex as in the case of plane waves where we have $e^{i\mathbf{k}\cdot\mathbf{x}}$ in place of $f_n(\mathbf{x})$. We will use n to be a collective index which labels the different solutions. For plane waves in flat space we would use $\mathbf{k}$. One of the advantages of assuming that Σ is compact is that the solutions will be labelled by a set of integers n rather than a continuous label as for plane waves.

We will first prove that the eigenvalues σ_n in (3.171) are all real and non-negative. To do this multiply both sides of (3.171) by $f_n^*(\mathbf{x})$ and integrate over Σ. Using the normalization (3.172) we find

$$\begin{aligned} \sigma_n &= \int_\Sigma d\sigma_x f_n^*(\mathbf{x}) \left[-\nabla^2 f_n(\mathbf{x})\right], \\ &= \int_\Sigma d\sigma_x \left|\nabla f_n(\mathbf{x})\right|^2, \end{aligned} \tag{3.173}$$

where the last line has used integration by parts. This last equality allows us to deduce that σ_n is real with $\sigma_n \geq 0$. Furthermore we can see that $\sigma_n = 0$ if and only if f_n is constant. The normalization (3.172) fixes any constant eigenfunction to be $f_n = V^{-1/2}$ where V is the finite volume of the space Σ. It may be that the boundary conditions prohibit constant eigenfunctions.[17] In this case all of the eigenvalues of the Laplacian must be positive.

We have assumed that $\{f_n(\mathbf{x})\}$ provides a complete set of functions. This means that it must be possible to express $f_n^*(\mathbf{x})$ as a linear combination of the $f_n(\mathbf{x})$. We can write

$$f_n^*(\mathbf{x}) = \sum_{n'} C_{nn'} f_{n'}(\mathbf{x}), \tag{3.174}$$

for some expansion coefficients $C_{nn'}$. From (3.172) we have

$$C_{nn'} = \int_\Sigma d\sigma_x f_n^*(\mathbf{x}) f_{n'}^*(\mathbf{x}), \tag{3.175}$$

and by taking the complex conjugate of this result,

$$C_{nn'}^* = \int_\Sigma d\sigma_x f_n(\mathbf{x}) f_{n'}(\mathbf{x}). \tag{3.176}$$

From (3.175) we can see that $C_{nn'} = C_{n'n}$.

[17] A simple case is provided by imposing antiperiodic boundary conditions on the walls of a box in flat space.

Because σ_n is real, by taking the complex conjugate of (3.171) we have

$$-\nabla^2 f_n^*(\mathbf{x}) = \sigma_n f_n^*(\mathbf{x}). \tag{3.177}$$

If we operate with $-\nabla^2$ on both sides of (3.174) and use (3.171) and (3.177) we find

$$\sigma_n f_n^*(\mathbf{x}) = \sum_{n'} C_{nn'} \sigma_{n'} f_{n'}(\mathbf{x}).$$

The expansion (3.174) may be used for $f_n^*(\mathbf{x})$ to rewrite this last result as

$$\sum_{n'} (\sigma_n - \sigma_{n'}) C_{nn'} f_{n'}(\mathbf{x}) = 0.$$

Finally, the assumption that $\{f_n(\mathbf{x})\}$ is a complete orthonormal set allows the conclusion

$$0 = (\sigma_n - \sigma_{n'}) C_{nn'}, \tag{3.178}$$

for all n and n'.

If it is the case that for $n \neq n'$ we have $\sigma_n \neq \sigma_{n'}$, then from (3.178) we can deduce that $C_{nn'} = 0$. However, this may not be the case. For example, for plane waves in flat space we could choose $f_{\mathbf{k}}(\mathbf{x}) \propto e^{i\mathbf{k}\cdot\mathbf{x}}$ resulting in $\sigma_{\mathbf{k}} = |\mathbf{k}|^2$. In this case we have $f_{\mathbf{k}}^*(\mathbf{x}) = f_{-\mathbf{k}}(\mathbf{x})$ and note that $\sigma_{-\mathbf{k}} = \sigma_{\mathbf{k}}$. The labels $-\mathbf{k}$ and $\mathbf{k}$ on the eigenfunctions correspond to the same eigenvalue. This is an example of degeneracy; in this case a rather simple example. A less trivial example occurs for $\Sigma = S^2$ where the eigenfunctions of the Laplacian are the spherical harmonics: $f_{l,m} \propto Y_{l,m}(\theta, \phi)$ if polar coordinates are used. We have $f_{l,m}^* \propto Y_{l,m}^* = Y_{l,-m}$ and $\sigma_{lm} = l(l+1)$. Here σ_{lm} has no explicit dependence on the label m, and because $m = -l, -l+1, \ldots, l-1, l$, the eigenvalues are $(2l+1)$-fold degenerate. It would therefore be incorrect to assume generally that $\sigma_n \neq \sigma_{n'}$ if $n \neq n'$. Therefore it does not follow that $C_{nn'}$ vanishes for $n \neq n'$. Fortunately the property derived in (3.178) is the crucial feature that we require. It is straightforward to generalize (3.178) to any function of $-\nabla^2$, say $F(-\nabla^2)$, which can be expanded in a Taylor series:

$$F(\sigma_n) C_{nn'} = F(\sigma_{n'}) C_{nn'}. \tag{3.179}$$

A final property of the expansion coefficients $C_{nn'}$ defined in (3.174) may be found if we use (3.172). Substitution of (3.174) into (3.172) gives

$$\begin{aligned} \delta_{nn'} &= \int_\Sigma d\sigma_x \left[\sum_{n''} C_{nn''} f_{n''}(\mathbf{x}) \right] f_{n'}(\mathbf{x}) \\ &= \sum_{n''} C_{nn''} C^*_{n''n'}, \end{aligned} \tag{3.180}$$

if we use (3.175) in the second line. Because $C_{nn'}$ is symmetric in n and n', this shows that if the $C_{nn'}$ are regarded as the matrix elements of a matrix C, then this matrix is unitary.

We can now return to the real scalar field $\varphi(t, \mathbf{x})$. Because $\{f_n(\mathbf{x})\}$ is a complete set of functions, we can expand

$$\varphi(t, \mathbf{x}) = \sum_n \varphi_n(t) f_n(\mathbf{x}), \tag{3.181}$$

for some $\varphi_n(t)$. If $\varphi(t, \mathbf{x})$ is an operator, then $\varphi_n(t)$ must also be an operator since $f_n(\mathbf{x})$ is just an ordinary function. The field operator should satisfy the Klein–Gordon equation

$$0 = (\Box + m^2)\varphi(t, \mathbf{x}),$$

where $\Box = (\partial^2/\partial t) - \nabla^2$. Use of the expansion (3.181) and the fact that $f_n(\mathbf{x})$ is an eigenfunction of $-\nabla^2$ with eigenvalue σ_n shows that

$$0 = \sum_n \left[\ddot{\varphi}_n(t) + \sigma_n \varphi_n(t) + m^2 \varphi_n(t)\right] f_n(\mathbf{x}).$$

The linear independence of the $f_n(\mathbf{x})$ leads to the conclusion that

$$0 = \ddot{\varphi}_n(t) + [\sigma_n + m^2]\varphi(t). \tag{3.182}$$

We know that $\sigma_n \geq 0$, so that the general solution to (3.182) is

$$\varphi_n(t) = \varphi_n^{(+)}(t) + \varphi_n^{(-)}(t), \tag{3.183}$$

where

$$\varphi_n^{(\pm)}(t) = e^{\mp i E_n t} \varphi_n^{(\pm)}. \tag{3.184}$$

Here

$$E_n = \sqrt{\sigma_n + m^2}, \tag{3.185}$$

and $\varphi_n^{(\pm)}$ in (3.184) denote constant operators. It is more conventional to write

$$\varphi(t, \mathbf{x}) = \sum_n \left[f_n(\mathbf{x}) e^{-i E_n t} \varphi_n^{(+)} + f_n^*(\mathbf{x}) e^{i E_n t} \varphi_n^{(-)}\right], \tag{3.186}$$

which is possible using (3.174) and redefining $\varphi_n^{(-)}$. If $\varphi(t, \mathbf{x})$ is real, meaning $\varphi^\dagger(t, \mathbf{x}) = \varphi(t, \mathbf{x})$, we must have $\varphi_n^{(-)} = \varphi_n^{(+)\dagger}$. Finally it is advantageous to rescale $\varphi_n^{(+)}$ and write (3.186) as

$$\varphi(t, \mathbf{x}) = \sum_n (2E_n)^{-1/2} \left[f_n(\mathbf{x}) e^{-i E_n t} a_n + f_n^*(\mathbf{x}) e^{i E_n t} a_n^\dagger\right], \tag{3.187}$$

for constant operators a_n and $a_n^\dagger$. Since $\pi(t,\mathbf{x}) = \dot{\varphi}(t,\mathbf{x})$, the canonical field momentum operator is

$$\pi(t,\mathbf{x}) = \sum_n i\left(\frac{E_n}{2}\right)^{1/2}\left[f_n^*(\mathbf{x})e^{iE_nt}a_n^\dagger - f_n(\mathbf{x})e^{-iE_nt}a_n\right]. \qquad (3.188)$$

We can solve (3.187) and (3.188) for a_n and $a_n^\dagger$. From (3.187), using (3.172) and (3.175), it is easy to show that

$$\int_\Sigma d\sigma_x f_n^*(\mathbf{x})\varphi(t,\mathbf{x}) = (2E_n)^{-1/2}e^{-iE_nt}a_n + \sum_{n'}(2E_{n'})^{-1/2}e^{iE_{n'}t}C_{nn'}a_{n'}^\dagger. \qquad (3.189)$$

Since $E_{n'} = \sqrt{\sigma_{n'} + m^2}$ we can use (3.179) to obtain

$$\int_\Sigma d\sigma_x f_n^*(\mathbf{x})\varphi(t,\mathbf{x}) = (2E_n)^{-1/2}e^{-iE_nt}a_n + (2E_n)^{-1/2}e^{iE_nt}\sum_{n'}C_{nn'}a_{n'}^\dagger. \qquad (3.190)$$

A similar calculation based around (3.188) gives

$$\int_\Sigma d\sigma_x f_n^*(\mathbf{x})\pi(t,\mathbf{x}) = -i\left(\frac{E_n}{2}\right)^{1/2}e^{-iE_nt}a_n + i\left(\frac{E_n}{2}\right)^{1/2}e^{iE_nt}\sum_{n'}C_{nn'}a_{n'}^\dagger. \qquad (3.191)$$

We can solve (3.190) and (3.191) to find

$$a_n = \left(\frac{E_n}{2}\right)^{1/2}e^{iE_nt}\int_\Sigma d\sigma_x f_n^*(\mathbf{x})\left(\varphi(t,\mathbf{x}) + \frac{i}{E_n}\pi(t,\mathbf{x})\right). \qquad (3.192)$$

At no stage has it been necessary to know the explicit form of $C_{nn'}$; the basic property (3.179) was sufficient. To obtain $a_n^\dagger$ we simply take the Hermitian conjugate of (3.192) to find[18]

$$a_n^\dagger = \left(\frac{E_n}{2}\right)^{1/2}e^{-iE_nt}\int_\Sigma d\sigma_x f_n(\mathbf{x})\left(\varphi(t,\mathbf{x}) - \frac{i}{E_n}\pi(t,\mathbf{x})\right). \qquad (3.193)$$

[18] Both the field and the canonical momentum are Hermitian.

We are now in a position to use (3.167)–(3.169) to evaluate the commutation relations among a_n and $a_n^\dagger$. First of all we have using (3.192)

$$\begin{aligned}
[a_n, a_{n'}] &= \frac{1}{2}(E_n E_{n'})^{1/2} e^{i(E_n+E_{n'})t} \int_\Sigma d\sigma_x f_n^*(\mathbf{x}) \int_\Sigma d\sigma_{x'} f_{n'}^*(\mathbf{x}') \\
&\quad \times [\varphi(t,\mathbf{x}) + \frac{i}{E_n}\pi(t,\mathbf{x}), \varphi(t,\mathbf{x}') + \frac{i}{E_{n'}}\pi(t,\mathbf{x}')] \\
&= \frac{1}{2}(E_n E_{n'})^{1/2} e^{i(E_n+E_{n'})t} \int_\Sigma d\sigma_x f_n^*(\mathbf{x}) f_{n'}^*(\mathbf{x}) \left(\frac{1}{E_n} - \frac{1}{E_{n'}}\right) \\
&= \frac{1}{2}(E_n E_{n'})^{1/2} e^{i(E_n+E_{n'})t} \left(\frac{1}{E_n} - \frac{1}{E_{n'}}\right) C_{nn'} \\
&= 0. \qquad (3.194)
\end{aligned}$$

The second equality above has arisen from evaluating the field commutators using (3.167)–(3.169) and integrating over $\mathbf{x}'$ using the property (2.72) of the Dirac delta distribution. The third line has used (3.175), and the final line has used the basic property (3.179). Hermitian conjugation of (3.194) yields

$$[a_n^\dagger, a_{n'}^\dagger] = 0. \qquad (3.195)$$

Finally we use (3.192) and (3.193) to evaluate

$$\begin{aligned}
[a_n, a_{n'}^\dagger] &= \frac{1}{2}(E_n E_{n'})^{1/2} e^{i(E_n-E_{n'})t} \int_\Sigma d\sigma_x f_n^*(\mathbf{x}) \int_\Sigma d\sigma_{x'} f_{n'}(\mathbf{x}') \\
&\quad \times [\varphi(t,\mathbf{x}) + \frac{i}{E_n}\pi(t,\mathbf{x}), \varphi(t,\mathbf{x}') - \frac{i}{E_{n'}}\pi(t,\mathbf{x}')] \\
&= \frac{1}{2}(E_n E_{n'})^{1/2} e^{i(E_n-E_{n'})t} \int_\Sigma d\sigma_x f_n^*(\mathbf{x}) f_{n'}(\mathbf{x}) \left(\frac{1}{E_n} + \frac{1}{E_{n'}}\right) \\
&= \delta_{nn'}. \qquad (3.196)
\end{aligned}$$

Again we use (3.167)–(3.169) to evaluate the field commutators, and integrate the resulting Dirac delta functions over $\mathbf{x}'$. The integral in the second line of the above equality may be done using (3.172). The results in (3.194)–(3.196) show that the operators a_n and $a_n^\dagger$ obey the same commutation relations as a set of non-interacting simple harmonic oscillators. This is the reason for our rescaling of $\varphi_n^{(\pm)}$ above.

In order to proceed further we will evaluate the Hamiltonian operator

$$H = \int_\Sigma d\sigma_x \left(\frac{1}{2}\pi^2(t,\mathbf{x}) + \frac{1}{2}|\nabla\varphi(t,\mathbf{x})|^2 + \frac{1}{2}m^2\varphi^2(t,\mathbf{x})\right), \qquad (3.197)$$

in terms of a_n and $a_n^\dagger$. The aim will be to show that H can be written as a sum with each term in the sum representing the Hamiltonian for the

simple harmonic oscillator. First of all use (3.188) for $\pi(t,\mathbf{x})$ and perform the integration over $\mathbf{x}$ using the orthonormality property (3.172) and the results (3.175) and (3.176). The result can be simplified using (3.179) to obtain

$$\int_\Sigma d\sigma_x \pi^2(t,\mathbf{x}) = \sum_n \frac{1}{2}E_n\left(a_n^\dagger a_n + a_n a_n^\dagger\right) - \sum_{n,n'}\frac{1}{2}E_n\Bigg(C_{nn'}e^{2iE_nt}a_n^\dagger a_{n'}^\dagger + C_{nn'}^* e^{-2iE_nt}a_n a_{n'}\Bigg). \tag{3.198}$$

A similar calculation using (3.187) shows that

$$\int_\Sigma d\sigma_x \varphi^2(t,\mathbf{x}) = \sum_n \frac{1}{2E_n}\left(a_n^\dagger a_n + a_n a_n^\dagger\right) + \sum_{n,n'}\frac{1}{2E_n}\Bigg(C_{nn'}e^{2iE_nt}a_n^\dagger a_{n'}^\dagger + C_{nn'}^* e^{-2iE_nt}a_n a_{n'}\Bigg). \tag{3.199}$$

In order to evaluate $\int_\Sigma d\sigma_x|\nabla\varphi|^2$ we first integrate by parts to obtain

$$\begin{aligned}\int_\Sigma d\sigma_x|\nabla\varphi(t,\mathbf{x})|^2 &= \int_\Sigma d\sigma_x \varphi(t,\mathbf{x})\left[-\nabla^2\varphi(t,\mathbf{x})\right]\\ &= \sum_n \frac{\sigma_n}{(2E_n)}\left(a_n a_n^\dagger + a_n^\dagger a_n\right) + \sum_{n,n'}\frac{\sigma_n}{(2E_n)}\\ &\quad\times\left(C_{nn'}e^{2iE_nt}a_n^\dagger a_{n'}^\dagger + C_{nn'}^* e^{-2iE_nt}a_n a_{n'}\right).\end{aligned} \tag{3.200}$$

(After integrating by parts we substitute (3.187) for the field operator φ.) Substitution of (3.198)–(3.200) into (3.197) results in

$$\begin{aligned}H &= \sum_n\left(\frac{1}{4}E_n + \frac{\sigma_n}{4E_n} + \frac{m^2}{4E_n}\right)\left(a_n a_n^\dagger + a_n^\dagger a_n\right)\\ &\quad + \sum_{n.n'}\left(-\frac{1}{4}E_n + \frac{\sigma_n}{4E_n} + \frac{m^2}{4E_n}\right)\\ &\quad\times\left(C_{nn'}e^{2iE_nt}a_n^\dagger a_{n'}^\dagger + C_{nn'}^* e^{-2iE_nt}a_n a_{n'}\right).\end{aligned} \tag{3.201}$$

From (3.185) we have $E_n^2 = \sigma_n + m^2$. As a consequence, the last set of terms in (3.201) involving $C_{nn'}$ vanish. In addition the coefficient of the first term simplifies to give

$$H = \frac{1}{2}\sum_n E_n(a_n a_n^\dagger + a_n^\dagger a_n). \tag{3.202}$$

Each term in this last result has the form of a simple harmonic oscillator Hamiltonian as promised earlier.

Quantization of the real scalar field can therefore proceed, at least formally, exactly as if we had an infinite collection of non-interacting simple harmonic oscillators. If we define the vacuum state $|0\rangle$ by $a_n|0\rangle = 0$, then we can build up the excited states by repeated application of $a_n^\dagger$ to $|0\rangle$. The only complication is that unlike the situation for ordinary quantum mechanics, we have an infinite collection of oscillators. This means that in place of finite sums, we have infinite sums which may not converge. As an example, suppose that we ask for the energy of the vacuum state. Taking the expectation value of the Hamiltonian H in (3.202) we find

$$\langle 0|H|0\rangle = \frac{1}{2}\sum_n E_n, \tag{3.203}$$

which is the infinite sum of zero-point energies. If we consider the case where Σ is three-dimensional Euclidean space, then we know that $E_{\mathbf{k}} = \sqrt{\mathbf{k}^2 + m^2}$ and the sum on n becomes an integral over $\mathbf{k}$. This integral is clearly divergent. We will postpone the discussion of how this can be dealt with until the next chapter.

3.7 Complex scalar field

The complex scalar field can be quantized using our knowledge of the real scalar field found in Section 3.6. If $\Phi(t, \mathbf{x})$ is the complex scalar field, we can always express it in terms of its real and imaginary parts as

$$\Phi(t, \mathbf{x}) = \frac{1}{\sqrt{2}}\Big\{\varphi_1(t, \mathbf{x}) + i\varphi_2(t, \mathbf{x})\Big\}, \tag{3.204}$$

where φ_1 and φ_2 are real scalar fields. This makes the quantization of the theory straightforward. From (3.187) we may expand

$$\varphi_1(t, \mathbf{x}) = \sum_n (2E_n)^{-1/2}\Big\{f_n(\mathbf{x})e^{-iE_n t}a_n + f_n^*(\mathbf{x})e^{iE_n t}a_n^\dagger\Big\}, \tag{3.205}$$

$$\varphi_2(t, \mathbf{x}) = \sum_n (2E_n)^{-1/2}\Big\{f_n(\mathbf{x})e^{-iE_n t}b_n + f_n^*(\mathbf{x})e^{iE_n t}b_n^\dagger\Big\}, \tag{3.206}$$

since both φ_1 and φ_2 satisfy the Klein–Gordon equation. The functions $f_n(\mathbf{x})$ obey the same relations as in Section 3.6. E_n is still given by (3.185). Because the fields φ_1 and φ_2 are independent of each other the operators a_n and b_n which appear in (3.205) and (3.206) are distinct and must commute with each other. We have

$$[a_n, a_{n'}^\dagger] = \delta_{nn'} = [b_n, b_{n'}^\dagger], \tag{3.207}$$

with

$$0 = [a_n, b_{n'}] = [a_n, b^\dagger_{n'}] = [a_n, a_{n'}] = [b_n, b_{n'}]. \tag{3.208}$$

It is easy to show by substituting (3.205) and (3.206) into (3.204) that the complex scalar field $\Phi(t, \mathbf{x})$ may be expressed as

$$\Phi(t, \mathbf{x}) = \sum_n (2E_n)^{-1/2} \Big\{ f_n(\mathbf{x}) e^{-iE_n t} A_n + f^*_n(\mathbf{x}) e^{iE_n t} B^\dagger_n \Big\}, \tag{3.209}$$

where we have defined

$$A_n = \frac{1}{\sqrt{2}}(a_n + ib_n), \qquad B_n = \frac{1}{\sqrt{2}}(a_n - ib_n). \tag{3.210}$$

The commutation relations (3.207) and (3.208) may be used to show

$$[A_n, A^\dagger_{n'}] = \delta_{nn'} = [B_n, B^\dagger_{n'}], \tag{3.211}$$

$$0 = [A_n, B_{n'}] = [A_n, B^\dagger_{n'}] = [A_n, A_{n'}] = [B_n, B_{n'}]. \tag{3.212}$$

The Hamiltonian operator H will be the sum of two terms, one representing the Hamiltonian for the real scalar field φ_1 and the other that for φ_2. From (3.202) we have

$$H = \frac{1}{2} \sum_n E_n (a_n a^\dagger_n + a^\dagger_n a_n + b_n b^\dagger_n + b^\dagger_n b_n). \tag{3.213}$$

If we solve (3.210) for a_n and b_n we find

$$a_n = \frac{1}{\sqrt{2}}(A_n + B_n), \qquad b_n = \frac{i}{\sqrt{2}}(B_n - A_n). \tag{3.214}$$

We can now write H directly in terms of A_n and B_n as

$$H = \frac{1}{2} \sum_n E_n (A^\dagger_n A_n + B_n B^\dagger_n + A_n A^\dagger_n + B^\dagger_n B_n). \tag{3.215}$$

This expression can be written in alternate ways if we use the commutation relations (3.211) obeyed by the operators. For example, we can write H in the shorter form

$$H = \sum_n E_n (A^\dagger_n A_n + B_n B^\dagger_n). \tag{3.216}$$

A new feature which arises for the charged scalar field is the invariance under a rigid gauge transformation.[19] If we extend this rigid gauge invariance to local gauge invariance, then as discussed in Sections 2.5 and 2.7 we have a conserved current arising from Noether's theorem which can be associated with the charge of the field. The formalism of Section 2.5 was set up to deal with real fields so we will deal with Φ written in terms of φ_1 and φ_2. The Lagrangian density is (see Section 2.3.2)

$$\mathcal{L} = \frac{1}{2}\partial^\mu\varphi_1\partial_\mu\varphi_1 + \frac{1}{2}\partial^\mu\varphi_2\partial_\mu\varphi_2 - \frac{1}{2}m^2(\varphi_1^2 + \varphi_2^2). \tag{3.217}$$

Take the infinitesimal form of the gauge transformation to be (see (2.179) and (2.180) for the Schrödinger field and set $\delta\epsilon = -e\delta\theta$)

$$\delta\Phi = -ie\delta\theta\Phi, \qquad \delta\Phi^\dagger = ie\delta\theta\Phi^\dagger. \tag{3.218}$$

Since $\Phi = (1/\sqrt{2})(\varphi_1 + i\varphi_2)$ we find

$$\delta\varphi_1 = e\delta\theta\varphi_2, \qquad \delta\varphi_2 = -e\delta\theta\varphi_1. \tag{3.219}$$

Because this transformation does not involve a transformation of the space–time coordinates, if we refer back to (2.124) we may set $\lambda_A^\mu = 0$ (see (2.100)) there and conclude that

$$\begin{aligned} J^\mu &= e\varphi_2\frac{\partial\mathcal{L}}{\partial(\partial_\mu\varphi_1)} - e\varphi_1\frac{\partial\mathcal{L}}{\partial(\partial_\mu\varphi_2)} \\ &= e\varphi_2\partial^\mu\varphi_1 - e\varphi_1\partial^\mu\varphi_2 \end{aligned} \tag{3.220}$$

is the conserved Noether current.[20] The conserved charge is

$$Q = \int_\Sigma d\sigma_x J^0 = e\int_\Sigma d\sigma_x(\varphi_2\dot{\varphi}_1 - \varphi_1\dot{\varphi}_2). \tag{3.221}$$

The charge can now be written back in terms of the complex field Φ and its Hermitian conjugate $\Phi^\dagger$ using (3.204)

$$Q = ie\int_\Sigma d\sigma_x(\Phi^\dagger\dot{\Phi} - \Phi\dot{\Phi}^\dagger). \tag{3.222}$$

In our derivation of J^μ and Q we have treated the fields as classical fields so that the order of $\Phi^\dagger$ and $\dot{\Phi}$ does not matter; however, if we now regard Φ as an operator, since the charge is an observable it must be a

[19] Equivalently, if we use the description in terms of real fields φ_1 and φ_2 there is an invariance under a rotation of the two-dimensional vector formed with components φ_1 and φ_2.

[20] In fact, it is straightforward to show directly from (3.220) and using the Klein–Gordon equation that $\partial_\mu J^\mu = 0$ without any application of Noether's theorem.

Hermitian operator. This will be the case if we define the charge operator to be

$$Q = ie \int_\Sigma d\sigma_x (\Phi^\dagger \dot{\Phi} - \dot{\Phi}^\dagger \Phi). \tag{3.223}$$

We can now express Q in terms of A_n and B_n using (3.209). After a short calculation we find

$$Q = e \sum_n (A_n^\dagger A_n - B_n B_n^\dagger). \tag{3.224}$$

If we take the expectation value of the charge operator Q given in (3.224) with the ground state $|0\rangle$, we find that we encounter the same difficulty as we had for the expectation value of the Hamiltonian for the real scalar field at the end of Section 3.6; namely, an infinite expression is found. We would expect that the ground state being devoid of particles should have no net charge, and therefore expect that we should have $\langle 0|Q|0\rangle = 0$. Although the terms in (3.224) with $A_n^\dagger A_n$ give no contribution to the expectation value of Q, we have $\langle 0|B_n B_n^\dagger|0\rangle = 1$, and it is this which leads to the infinite expression for $\langle 0|Q|0\rangle$. If we want to demand that $\langle 0|Q|0\rangle = 0$, then the order of B_n and $B_n^\dagger$ in (3.224) must be switched and we must define

$$: Q := e \sum_n (A_n^\dagger A_n - B_n^\dagger B_n). \tag{3.225}$$

This re-ordered operator has the property that $\langle 0| : Q : |0\rangle = 0$. The operator $: Q :$ differs from Q by a constant; albeit an infinite one. This is a simple example of the process of renormalization and is done on physical grounds to ensure that the ground state has no charge. $: Q :$ is called the 'normal-ordered form of Q'. Generally the normal ordered form of any product of creation and annihilation operators is obtained by moving all annihilation operators to the right of all creation operators. The colons denote that the operator has been normal ordered. It is conventional in most field theory books to also normal order the Hamiltonian operator so that the ground state expectation value vanishes. We will discuss why we do not wish to do this in the next chapter.

Consider the 1-particle state defined by $|n\rangle_A = A_n^\dagger|0\rangle$. Because A_n and $A_n^\dagger$ commute with B_n and $B_n^\dagger$ we will have

$$\begin{aligned} : Q : |n\rangle_A &= e \sum_{n'} A_{n'}^\dagger A_{n'} A_n^\dagger |0\rangle \\ &= e \sum_{n'} A_{n'}^\dagger (\delta_{nn'} + A_n^\dagger A_{n'})|0\rangle \\ &= e|n\rangle_A. \end{aligned} \tag{3.226}$$

The 1-particle state $A_n^\dagger|0\rangle$ has energy E_n and charge e. Now consider the 1-particle state $|n\rangle_B = B_n^\dagger|0\rangle$. This time we find

$$:Q:|n\rangle_B = -e|n\rangle_B. \tag{3.227}$$

The 1-particle state $B_n^\dagger|0\rangle$ has energy E_n and charge $-e$. If we identify the 1-particle state $A_n^\dagger|0\rangle$ with a particle, then the state $B_n^\dagger|0\rangle$ can be identified in a natural way with an anti-particle. We may interpret the operators A_n as associated with particles and B_n as associated with anti-particles. The theory of the quantized complex scalar field therefore contains both particles and anti-particles.

3.8 Schrödinger field

The Schrödinger field Ψ must obey (with $\hbar = 1$ as usual)

$$-\frac{1}{2m}\nabla^2\Psi + V\Psi = i\frac{\partial}{\partial t}\Psi. \tag{3.228}$$

Assume for simplicity that the potential $V = V(\mathbf{x})$ has no time dependence. Let

$$\left(-\frac{1}{2m}\nabla^2 + V\right) f_n(\mathbf{x}) = E_n f_n(\mathbf{x}), \tag{3.229}$$

with

$$\int_\Sigma d\sigma_x f_n^*(\mathbf{x}) f_{n'}(\mathbf{x}) = \delta_{nn'}. \tag{3.230}$$

The functions $f_n(\mathbf{x})$ may be recognized as solutions to the time-independent Schrödinger equation. We will assume that they form a complete set. The Schrödinger field operator may be expanded in terms of the $f_n(\mathbf{x})$ as

$$\Psi(t,\mathbf{x}) = \sum_n f_n(\mathbf{x}) e^{-iE_n t} A_n, \tag{3.231}$$

for some constant operators A_n. It is clear that this expansion satisfies (3.228). The main difference between the non-relativistic case considered here, and the complex relativistic scalar field is that here there are no negative energy solutions to the field equations. Given the association between negative energy solutions and anti-particles, we can say that there are no anti-particles present in non-relativistic field theory.

We are now faced with the task of determining the commutation relations among A_n. To do this note that the canonical field momentum for Ψ was found in Section 2.3.3 to be

$$\begin{aligned}\Pi(t,\mathbf{x}) &= \frac{i}{2}\Psi^\dagger(t,\mathbf{x}) \\ &= \frac{i}{2}\sum_n f_n^*(\mathbf{x})e^{iE_nt}A_n^\dagger. \end{aligned} \tag{3.232}$$

If we use the orthonormality property (3.230) it is easy to see from (3.231) and (3.232) that

$$A_n = e^{iE_nt}\int_\Sigma d\sigma_x f_n^*(\mathbf{x})\Psi(t,\mathbf{x}), \tag{3.233}$$

$$A_n^\dagger = -2ie^{-iE_nt}\int_\Sigma d\sigma_x f_n(\mathbf{x})\Pi(t,\mathbf{x}). \tag{3.234}$$

The question now arises as to the commutation relations for the field operators. A simple way to deduce them is as follows. Since $\Psi(t,\mathbf{x})$ is a field operator in the Heisenberg picture it should obey the Heisenberg equation of motion

$$i\frac{\partial}{\partial t}\Psi(t,\mathbf{x}) = [\Psi(t,\mathbf{x}), H(t)]. \tag{3.235}$$

The Hamiltonian was given in (2.58) for the classical field theory. If we replace the classical fields in $H(t)$ with field operators we find

$$i\tfrac{\partial}{\partial t}\Psi(t,\mathbf{x}) = \textstyle\int_\Sigma d\sigma_{x'}\left[\Psi(t,\mathbf{x}), \Psi^\dagger(t,\mathbf{x}')\left(-\frac{1}{2m}\nabla'^2 + V(\mathbf{x}')\right)\Psi(t,\mathbf{x}')\right]. \tag{3.236}$$

The commutator appearing in (3.236) can be simplified using the easily proven operator identity (simply write out both sides to see that they agree)

$$[A,BC] = [A,B]C + B[A,C]\,. \tag{3.237}$$

We may now show that (3.236) evaluates to

$$\begin{aligned} i\frac{\partial}{\partial t}\Psi(t,\mathbf{x}) = &\int_\Sigma d\sigma_{x'}[\Psi(t,\mathbf{x}), \Psi^\dagger(t,\mathbf{x}')]\left(-\frac{1}{2m}\nabla'^2 + V(\mathbf{x}')\right)\Psi(t,\mathbf{x}') \\ &+ \int_\Sigma d\sigma_{x'}\Psi^\dagger(t,\mathbf{x}')\left(-\frac{1}{2m}\nabla'^2 + V(\mathbf{x}')\right) \\ &\times[\Psi(t,\mathbf{x}), \Psi(t,\mathbf{x}')]. \end{aligned} \tag{3.238}$$

The equation of motion in the Heisenberg picture should be equivalent to the equation of motion (3.228). The simplest way to achieve equality of (3.238) with (3.228) is if we impose

$$[\Psi(t,\mathbf{x}),\Psi^\dagger(t,\mathbf{x}')]=\delta(\mathbf{x},\mathbf{x}'), \tag{3.239}$$

$$[\Psi(t,\mathbf{x}),\Psi(t,\mathbf{x}')]=0. \tag{3.240}$$

Hermitian conjugation of this last result yields

$$[\Psi^\dagger(t,\mathbf{x}),\Psi^\dagger(t,\mathbf{x}')]=0. \tag{3.241}$$

When written in terms of $\Pi(t,\mathbf{x})$, the first result (3.239) becomes

$$[\Psi(t,\mathbf{x}),\Pi(t,\mathbf{x}')]=\frac{i}{2}\delta(\mathbf{x},\mathbf{x}'). \tag{3.242}$$

The crucial thing to notice is the factor of $1/2$ on the right-hand side of (3.242) which would have been missed if we were not careful. The origin of this is because $\mathcal{L}$ for the Schrödinger field involves only first-order derivatives in the time, rather than the second-order ones present in the relativistic theory. If we use (3.240)–(3.242) along with (3.233) and (3.234), we find

$$[A_n,A_{n'}]=0=[A_n^\dagger,A_{n'}^\dagger], \tag{3.243}$$

$$[A_n,A_{n'}^\dagger]=\delta_{nn'}. \tag{3.244}$$

The vacuum state is defined in the usual way by $A_n|0\rangle=0$, and the excited states built up by repeated application of $A_n^\dagger$ to $|0\rangle$. If we form the state $|n_1,n_2\rangle = A_{n_1}^\dagger A_{n_2}^\dagger|0\rangle$, it can be interpreted as a state with two particles, one of energy E_{n_1} and the other of energy E_{n_2}. Because $[A_n^\dagger,A_{n'}^\dagger]=0$, this two-particle state is symmetric under the interchange of the two particles; that is $|n_1,n_2\rangle = |n_2,n_1\rangle$. This is consistent with particles that obey Bose–Einstein statistics. If we are interested in a system of fermions, then they must obey Fermi–Dirac statistics. If $\Psi(t,\mathbf{x})$ is to describe fermions, in order that the two-particle state $|n_1,n_2\rangle$ be anti-symmetric under particle interchange, and hence describe particles which obey Fermi–Dirac statistics, it is necessary to have $A_{n_1}^\dagger A_{n_2}^\dagger = -A_{n_2}^\dagger A_{n_1}^\dagger$, and by conjugation $A_{n_1}A_{n_2} = -A_{n_2}A_{n_1}$. This can be deduced as a consistent choice from the Heisenberg equation of motion for the field operator as well if in place of (3.237) we use instead the identity

$$[A,BC]=[A,B]_+C-B[A,C]_+, \tag{3.245}$$

where we have defined the anti-commutator bracket

$$[A,B]_+=AB+BA. \tag{3.246}$$

It is now easy to show from (3.236) that

$$[\Psi(t,\mathbf{x}),\Psi^\dagger(t,\mathbf{x}')]_+ = \delta(\mathbf{x},\mathbf{x}'), \tag{3.247}$$

$$[\Psi(t,\mathbf{x}),\Psi(t,\mathbf{x}')]_+ = 0 = [\Psi^\dagger(t,\mathbf{x}),\Psi^\dagger(t,\mathbf{x}')]_+. \tag{3.248}$$

Substitution of the field expansion (3.231) leads to

$$[A_n, A_{n'}]_+ = 0 = [A_n^\dagger, A_{n'}^\dagger]_+, \tag{3.249}$$

$$[A_n, A_{n'}^\dagger]_+ = \delta_{nn'}. \tag{3.250}$$

We are therefore free to impose anti-commutation relations on the field operator in place of commutation relations, and this will lead to consistency with Fermi–Dirac statistics. We note that for Fermi–Dirac statistics the field operators at a given time anti-commute with one another, rather than commute. In order to be simultaneously measurable, according to the basic principles of quantum mechanics, the operators should commute. This means that the field operator for fermions does not represent a measurable quantity. Another way to see this is to consider what happens in the classical limit. In this limit we cannot describe $\Psi(t,\mathbf{x})$ for a fermion by an ordinary complex function because we must have the property $\Psi(t,\mathbf{x})\Psi(t,\mathbf{x}') = -\Psi(t,\mathbf{x}')\Psi(t,\mathbf{x})$. Instead we must introduce $\Psi(t,\mathbf{x})$ as a new type of object called an 'anti-commuting complex number'. If z_1 and z_2 are anti-commuting complex numbers, then $z_1 z_2 = -z_2 z_1$. More mathematically, such numbers are said to lie in the odd sector of a Grassmann algebra. Finally we can see that in order to have a measurable quantity formed from Fermi–Dirac fields it must be at least quadratic in the fields, such as $\Psi^\dagger(t,\mathbf{x})\Psi(t,\mathbf{x})$.

It is also instructive to see how the Schwinger action principle can be used to derive the basic commutation or anti-commutation relations for the Schrödinger field. The action functional is

$$S = \int_{t_1}^{t_2} dt \int_\Sigma d\sigma_x \left\{ \frac{i}{2}(\Psi^\dagger\dot{\Psi} - \dot{\Psi}^\dagger\Psi) - \frac{1}{2m}\nabla^i\Psi^\dagger\nabla_i\Psi \right\}.$$

If we vary S treating Ψ and $\Psi^\dagger$ as independent it is straightforward to show that

$$\delta S = \int_{t_1}^{t_2} dt \int_\Sigma d\sigma_x \left\{ \delta\Psi^\dagger \left(i\dot{\Psi} + \frac{1}{2m}\nabla^2\Psi \right) + \left(-i\dot{\Psi}^\dagger + \frac{1}{2m}\nabla^2\Psi^\dagger \right)\delta\Psi \right\} + G(t_2) - G(t_1), \tag{3.251}$$

where

$$G(t) = \frac{i}{2}\int_\Sigma d\sigma_x(\Psi^\dagger\delta\Psi - \delta\Psi^\dagger\Psi). \tag{3.252}$$

The terms in the first line of (3.251) lead to the equations of motion for the field operators Ψ and $\Psi^\dagger$. In order to use $G(t)$ to derive the field commutators in an unambiguous way, it is advantageous to have an expression in which only $\delta\Psi$ or $\delta\Psi^\dagger$ occurs. We can obtain such an expression by adding a total time derivative to the Lagrangian just as we did for the point particle in Section 3.3. Let

$$\Lambda_\kappa(t) = \frac{i\kappa}{2}\int_\Sigma d\sigma_x \Psi^\dagger(t,\mathbf{x})\Psi(t,\mathbf{x}), \tag{3.253}$$

where κ is a constant, and define

$$L_\kappa(t) = L(t) + \frac{d}{dt}\Lambda_\kappa(t). \tag{3.254}$$

This will not change the equations of motion for the field, but it is easy to show that $G(t)$ in (3.252) is altered to $G_\kappa(t)$ where

$$\begin{aligned} G_\kappa(t) &= G(t) + \delta\Lambda_\kappa(t) \\ &= \frac{i}{2}\int_\Sigma d\sigma_x \Big\{(\kappa+1)\Psi^\dagger\delta\Psi + (\kappa-1)\delta\Psi^\dagger\Psi\Big\}. \end{aligned} \tag{3.255}$$

Thus by choosing $\kappa = 1$ we obtain

$$G_+(t) = i\int_\Sigma d\sigma_x \Psi^\dagger\delta\Psi, \tag{3.256}$$

involving only the variation $\delta\Psi$, and by choosing $\kappa = -1$ we obtain

$$G_-(t) = -i\int_\Sigma d\sigma_x \delta\Psi^\dagger\Psi, \tag{3.257}$$

involving only the variation $\delta\Psi^\dagger$. We may now use the general result in (3.86) to find the change in any operator under the unitary transformation generated by $G_\pm(t)$. Because $G_+(t)$ generates a transformation in which only Ψ is changed ($\Psi^\dagger$ is not altered) we have

$$\delta\Psi(t,\mathbf{x}) = i[G_+(t), \Psi(t,\mathbf{x})], \tag{3.258}$$

$$\delta\Psi^\dagger(t,\mathbf{x}) = 0 = i[G_+(t), \Psi^\dagger(t,\mathbf{x})]. \tag{3.259}$$

Similarly, because $G_-(t)$ generates a transformation in which $\Psi^\dagger$ is altered with Ψ fixed we have

$$\delta\Psi(t,\mathbf{x}) = 0 = i[G_-(t), \Psi(t,\mathbf{x})], \tag{3.260}$$

$$\delta\Psi^\dagger(t,\mathbf{x}) = i[G_-(t), \Psi^\dagger(t,\mathbf{x})]. \tag{3.261}$$

Up to this stage we have not made any assumptions concerning the commutation properties of $\delta\Psi$ and $\delta\Psi^\dagger$ with Ψ and $\Psi^\dagger$. If we wish to have the field describe bosons, then the natural assumption to make is that the infinitesimal variations commute with the fields. This allows (3.258)–(3.261) to be simplified to

$$\begin{aligned}
\delta\Psi(t,\mathbf{x}) &= -\int_\Sigma d\sigma_{x'}[\Psi^\dagger(t,\mathbf{x}'), \Psi(t,\mathbf{x})]\delta\Psi(t,\mathbf{x}'),\\
0 &= -\int_\Sigma d\sigma_{x'}[\Psi^\dagger(t,\mathbf{x}'), \Psi^\dagger(t,\mathbf{x})]\delta\Psi(t,\mathbf{x}'),\\
0 &= \int_\Sigma d\sigma_{x'}\delta\Psi^\dagger(t,\mathbf{x}')[\Psi(t,\mathbf{x}'), \Psi(t,\mathbf{x})],\\
\delta\Psi^\dagger(t,\mathbf{x}) &= \int_\Sigma d\sigma_{x'}\delta\Psi^\dagger(t,\mathbf{x}')[\Psi(t,\mathbf{x}'), \Psi^\dagger(t,\mathbf{x})].
\end{aligned}$$

We therefore recover the commutation relations in (3.239)–(3.241).

If we wish to describe fermions with our Schrödinger field then it is natural to assume that the infinitesimal variations $\delta\Psi$ and $\delta\Psi^\dagger$ anti-commute with the fields Ψ and $\Psi^\dagger$. This results in

$$\begin{aligned}
\delta\Psi(t,\mathbf{x}) &= \int_\Sigma d\sigma_{x'}[\Psi^\dagger(t,\mathbf{x}'), \Psi(t,\mathbf{x})]_+\delta\Psi(t,\mathbf{x}'),\\
0 &= \int_\Sigma d\sigma_{x'}[\Psi^\dagger(t,\mathbf{x}'), \Psi^\dagger(t,\mathbf{x})]_+\delta\Psi(t,\mathbf{x}'),\\
0 &= \int_\Sigma d\sigma_{x'}\delta\Psi^\dagger(t,\mathbf{x}')[\Psi(t,\mathbf{x}'), \Psi(t,\mathbf{x})]_+,\\
\delta\Psi^\dagger(t,\mathbf{x}) &= \int_\Sigma d\sigma_{x'}\delta\Psi^\dagger(t,\mathbf{x}')[\Psi(t,\mathbf{x}'), \Psi^\dagger(t,\mathbf{x})]_+.
\end{aligned}$$

We now recover the anti-commutation relations (3.247) and (3.248).

A comment regarding the application of the Schwinger action principle to deduce the field commutation or anti-commutation relations is in order. Unless sufficient care is exercised it is easy to deduce erroneous relations among the field operators. (This point was made originally by Schwinger (1953c) in response to a paper by Burton and Touschek (1953).) If we simply took $B = \Pi$ or $\Psi^\dagger$ in (3.86) using $G(t)$ as given in (3.252), we would obtain results which differed from those found above (which we know are correct because they are consistent with the Heisenberg equations of motion) by a factor of 2. More seriously, if we used $G_\kappa(t)$ in (3.255) without specifying κ as we did, then the field commutators would involve the

arbitrary parameter κ, and hence be ambiguous. The arbitrary constant κ does not change the equations of motion for the field. The mistake in this is that we have not been careful about how Ψ and $\Psi^\dagger$ change under the transformation generated by $G_\kappa(t)$. The only safe way to proceed is to choose κ so that only Ψ or $\Psi^\dagger$ changes on its own, corresponding to the transformation $\Psi \to \Psi + \delta\Psi$ with $\Psi^\dagger$ fixed, or else $\Psi^\dagger \to \Psi^\dagger + \delta\Psi$ with Ψ fixed as we did above. In this way we can now see that

$$G_\kappa(t) = \frac{1}{2}(\kappa+1)G_+(t) + \frac{1}{2}(\kappa-1)G_-(t) \tag{3.262}$$

corresponds to the change $\Psi \to \Psi + (1/2)(\kappa+1)\delta\Psi$ and $\Psi^\dagger \to \Psi^\dagger + (1/2)(\kappa-1)\delta\Psi^\dagger$. With this correct interpretation the commutation or anti-commutation relations are unambiguous. The original result for $G(t)$ in (3.252) corresponded to $\kappa = 0$.

There is another way to confirm this interpretation for $G(t)$ in (3.252) if Ψ is a charged field. In this case we have invariance under the local gauge transformation

$$\delta\Psi(t,\mathbf{x}) = ie\delta\theta(t,\mathbf{x})\Psi(t,\mathbf{x}), \tag{3.263}$$

$$\delta\Psi^\dagger(t,\mathbf{x}) = -ie\delta\theta(t,\mathbf{x})\Psi^\dagger(t,\mathbf{x}), \tag{3.264}$$

for arbitrary $\delta\theta(t,\mathbf{x})$. This requires the addition of the gauge field as described in Section 2.7. $G(t)$ in (3.252) becomes

$$G(t) = -e\int_\Sigma d\sigma_x \delta\theta(t,\mathbf{x})\Psi^\dagger(t,\mathbf{x})\Psi(t,\mathbf{x}), \tag{3.265}$$

and is interpreted as the generator of the transformation in (3.263) and (3.264). We therefore have

$$\begin{aligned} ie\delta\theta(t,\mathbf{x})\Psi(t,\mathbf{x}) &= -ie\int_\Sigma d\sigma_{x'}\delta\theta(t,\mathbf{x}') \\ &\quad\times[\Psi^\dagger(t,\mathbf{x}')\Psi(t,\mathbf{x}'),\Psi(t,\mathbf{x})], \end{aligned} \tag{3.266}$$

$$\begin{aligned} -ie\delta\theta(t,\mathbf{x})\Psi^\dagger(t,\mathbf{x}) &= -ie\int_\Sigma d\sigma_{x'}\delta\theta(t,\mathbf{x}') \\ &\quad\times[\Psi^\dagger(t,\mathbf{x}')\Psi(t,\mathbf{x}'),\Psi^\dagger(t,\mathbf{x})], \end{aligned} \tag{3.267}$$

if we use (3.86). These results require

$$[\Psi^\dagger(t,\mathbf{x}')\Psi(t,\mathbf{x}'),\Psi(t,\mathbf{x})] = -\Psi(t,\mathbf{x})\delta(\mathbf{x},\mathbf{x}'), \tag{3.268}$$

$$[\Psi^\dagger(t,\mathbf{x}')\Psi(t,\mathbf{x}'),\Psi^\dagger(t,\mathbf{x})] = \Psi^\dagger(t,\mathbf{x})\delta(\mathbf{x},\mathbf{x}'), \tag{3.269}$$

which are consistent with either the commutation relations or the anti-commutation relations found above. Because the last results (3.268) and (3.269) are independent of the charge of the field they should also be true for the free field.

To conclude this section we write the Hamiltonian operator H and the charge operator Q in terms of creation and annihilation operators. We have

$$H = \int_\Sigma d\sigma_x \Psi^\dagger(t,\mathbf{x}) \left(-\frac{1}{2m}\nabla^2 + V \right) \Psi(t,\mathbf{x}) \tag{3.270}$$

and

$$Q = e \int_\Sigma d\sigma_x \Psi^\dagger(t,\mathbf{x}) \Psi(t,\mathbf{x}). \tag{3.271}$$

Substitution of the field expansion (3.231) into (3.270) and (3.271) results in

$$H = \sum_n E_n A_n^\dagger A_n, \tag{3.272}$$

$$Q = e \sum_n A_n^\dagger A_n. \tag{3.273}$$

The Hamiltonian is seen to consist of a sum of simple harmonic oscillator Hamiltonians with the zero-point energy removed. We will return to discuss this in more detail in Section 5.5.

3.9 Dirac field

The action for the Dirac field is

$$S = \int_{t_1}^{t_2} dt \int_\Sigma d\sigma_x \left\{ \frac{i}{2} \left(\Psi^\dagger \dot{\Psi} - \dot{\Psi}^\dagger \Psi + \bar{\Psi}\gamma^i \nabla_i \Psi - \nabla_i \bar{\Psi} \gamma^i \Psi \right) - m\bar{\Psi}\Psi \right\}. \tag{3.274}$$

Here $\bar{\Psi} = \Psi^\dagger \gamma^0$ and the repeated index i is summed over the number of spatial dimensions. Because Ψ is to describe the electron which obeys Fermi–Dirac statistics we expect the field to obey anti-commutation, instead of commutation, relations. The aim will be to use the Schwinger action principle to derive the anti-commutation relations. Ψ is a spinor field with $2^{[(D+1)/2]}$ components. We will use $\Psi^I(t,\mathbf{x})$ to denote the components of $\Psi(t,\mathbf{x})$ and $\Psi_I^\dagger(t,\mathbf{x})$ to denote those of $\Psi^\dagger(t,\mathbf{x})$. The variations $\delta\Psi^I(t,\mathbf{x})$ and $\delta\Psi_I^\dagger(t,\mathbf{x})$ will be treated as independent and anti-commuting with Ψ and $\Psi^\dagger$. Apart from the fact that Ψ is a spinor field with a number of components the analysis will be very similar to that of

the Schrödinger field in the previous section. The important part of the action for the application of the Schwinger action principle is that which involves time derivatives, and comparison of the actions for the two fields shows that the time-dependent parts are the same.

Performing the variation of the action functional in (3.274) with respect to Ψ and $\Psi^\dagger$ leads to (after integration by parts)

$$\begin{aligned}\delta S = \int_{t_1}^{t_2} dt \int_\Sigma d\sigma_x \Big\{ & \delta\Psi^\dagger \left(i\dot{\Psi} + i\gamma^0\gamma^i\nabla_i\Psi - m\gamma^0\Psi \right) \\ & + \left(-i\dot{\Psi}^\dagger - i\nabla_i\bar{\Psi}\gamma^i - m\bar{\Psi} \right) \delta\Psi \Big\} \\ & + G(t_2) - G(t_1), \end{aligned} \tag{3.275}$$

with

$$G(t) = \frac{i}{2}\int_\Sigma d\sigma_x \left(\Psi^\dagger\delta\Psi - \delta\Psi^\dagger\Psi \right). \tag{3.276}$$

The terms in the first two lines of (3.275) lead to the equations of motion for the Dirac field and its adjoint. The expression for $G(t)$ is the same as that we found in (3.252) for the Schrödinger field, apart from the fact that Ψ is now a spinor. As explained above this similarity is because the Schrödinger field action and Dirac action have the same time dependence. We can use what we learned about the interpretation of $G(t)$ for the Schrödinger field at the end of the last section to interpret $G(t)$ in (3.276) as the generator of the transformation $\Psi \to \Psi + (1/2)\delta\Psi$ and $\Psi^\dagger \to \Psi^\dagger + (1/2)\delta\Psi^\dagger$. (Alternatively we could repeat the analysis given in Section 3.8 by adding on the total time derivative of Λ_κ given in (3.253).) It now follows from the general result (3.86) that

$$\frac{1}{2}\delta\Psi^I(t,\mathbf{x}) = \frac{i}{\hbar}[G(t), \Psi^I(t,\mathbf{x})], \tag{3.277}$$

$$\frac{1}{2}\delta\Psi^\dagger_I(t,\mathbf{x}) = \frac{i}{\hbar}[G(t), \Psi^\dagger_I(t,\mathbf{x})]. \tag{3.278}$$

Assuming that $\delta\Psi$ and $\delta\Psi^\dagger$ anti-commute with Ψ and $\Psi^\dagger$ results in

$$\begin{aligned}\frac{1}{2}\delta\Psi^I(t,\mathbf{x}) = \frac{1}{2\hbar}\int_\Sigma d\sigma_{x'} \Big\{ & \Big[\Psi^\dagger_J(t,\mathbf{x}'), \Psi^I(t,\mathbf{x})\Big]_+ \delta\Psi^J(t,\mathbf{x}') \\ & + \delta\Psi^\dagger_J(t,\mathbf{x}')\Big[\Psi^J(t,\mathbf{x}'), \Psi^I(t,\mathbf{x})\Big]_+ \Big\}, \\ \frac{1}{2}\delta\Psi^\dagger_I(t,\mathbf{x}) = \frac{1}{2\hbar}\int_\Sigma d\sigma_{x'} \Big\{ & \Big[\Psi^\dagger_J(t,\mathbf{x}'), \Psi^\dagger_I(t,\mathbf{x})\Big]_+ \delta\Psi^J(t,\mathbf{x}') \\ & + \delta\Psi^\dagger_J(t,\mathbf{x}')\Big[\Psi^J(t,\mathbf{x}'), \Psi^\dagger_I(t,\mathbf{x})\Big]_+ \Big\}. \end{aligned}$$

We can conclude that

$$[\Psi^I(t,\mathbf{x}),\Psi^\dagger_J(t,\mathbf{x}')]_+ = \hbar\delta^I{}_J\delta(\mathbf{x},\mathbf{x}'), \tag{3.279}$$

$$[\Psi^I(t,\mathbf{x}),\Psi^J(t,\mathbf{x}')]_+ = 0 = [\Psi^\dagger_I(t,\mathbf{x}),\Psi^\dagger_J(t,\mathbf{x}')]_+. \tag{3.280}$$

These are the basic field anti-commutators.

We now wish to write down the field expansions for the Dirac field and its adjoint in terms of creation and annihilation operators as we have done for other fields. In order to make this as clear as possible we will specialize to the case of $D = 3$, to avoid dealing with the complications of the Dirac matrices in arbitrary dimensions, and to Σ flat, to avoid the additional complications present for curved space. We will allow Σ to have an arbitrary boundary with the Dirac field satisfying some specified boundary conditions.

Because the Dirac field also satisfies the Klein–Gordon equation (as we showed in Section 2.9) we expect that the Dirac equation should have both positive and negative energy solutions. Ψ satisfies

$$i\frac{\partial}{\partial t}\Psi = H_D\Psi, \tag{3.281}$$

where $H_D = i\alpha^i\partial_i + m\beta$ is the Dirac Hamiltonian (see Section 2.9). Define

$$\Psi^{(+)}_n(t,\mathbf{x}) = e^{-iE_nt}\psi^{(+)}_n(\mathbf{x}), \tag{3.282}$$

to be a positive energy solution. Then $\psi^{(+)}_n(\mathbf{x})$ must satisfy

$$E_n\psi^{(+)}_n(\mathbf{x}) = (i\alpha^i\partial_i + m\beta)\psi^{(+)}_n(\mathbf{x}). \tag{3.283}$$

Using the representation (2.267)–(2.269) for α^i and β we find

$$E_n\psi^{(+)}_n(\mathbf{x}) = \begin{pmatrix} m & i\sigma^i\partial_i \\ i\sigma^i\partial_i & -m \end{pmatrix}\psi^{(+)}_n(\mathbf{x}). \tag{3.284}$$

Here $\psi^{(+)}_n(\mathbf{x})$ is a 4-component spinor. The form of (3.284) suggests writing

$$\psi^{(+)}_n(\mathbf{x}) = \begin{pmatrix} f_n(\mathbf{x}) \\ g_n(\mathbf{x}) \end{pmatrix}, \tag{3.285}$$

where $f_n(\mathbf{x})$ and $g_n(\mathbf{x})$ are 2-component spinors. We find the set of coupled equations,

$$i\sigma^i\partial_i g_n(\mathbf{x}) + mf_n(\mathbf{x}) = E_nf_n(\mathbf{x}), \tag{3.286}$$

$$i\sigma^i\partial_i f_n(\mathbf{x}) - mg_n(\mathbf{x}) = E_ng_n(\mathbf{x}). \tag{3.287}$$

Assuming that $E_n \geq 0$, we can solve (3.287) for

$$g_n(\mathbf{x}) = \frac{i\sigma^i \partial_i f_n(\mathbf{x})}{(E_n + m)}. \tag{3.288}$$

This means that if we know $f_n(\mathbf{x})$ in (3.285), then $g_n(\mathbf{x})$ is completely determined. Only half of the components of $\psi_n^{(+)}(\mathbf{x})$ are independent.

We will require $f_n(\mathbf{x})$ to satisfy the eigenvalue equation

$$i\sigma^i \partial_i f_n(\mathbf{x}) = \lambda_n f_n(\mathbf{x}). \tag{3.289}$$

This can be regarded as a system of two equations for the two components of $f_n(\mathbf{x})$. It is easy to see that

$$E_n = \sqrt{\lambda_n^2 + m^2}, \tag{3.290}$$

if we use (3.288) and (3.289) in (3.286). Because the two components of $f_n(\mathbf{x})$ are linearly independent there will be two linearly independent solutions to (3.289). We will label the two independent solutions $f_{n\lambda}(\mathbf{x})$, where $\lambda = 1, 2$. We therefore have two independent positive energy solutions given from (3.282) with

$$\psi_{n\lambda}^{(+)}(\mathbf{x}) = \begin{pmatrix} f_{n\lambda}(\mathbf{x}) \\ \frac{\lambda_n}{E_n + m} f_{n\lambda}(\mathbf{x}) \end{pmatrix}. \tag{3.291}$$

Suppose that we now turn to the negative energy solutions defined analogously to (3.282) by

$$\Psi_n^{(-)}(\mathbf{x}) = e^{iE_n t} \psi_n^{(-)}(\mathbf{x}). \tag{3.292}$$

$\psi_n^{(-)}(\mathbf{x})$ satisfies

$$-E_n \psi_n^{(-)}(\mathbf{x}) = (i\alpha^i \partial_i + m\beta)\psi_n^{(-)}(\mathbf{x}). \tag{3.293}$$

This is the same as the equation satisfied by $\psi_n^{(+)}(\mathbf{x})$ except that the sign of E_n is different. An equivalent way to view the similarity between (3.282) and (3.293) is that $\psi_n^{(-)}(\mathbf{x})$ satisfies the same equation as $\psi_n^{(+)}(\mathbf{x})$ but with α^i replaced with $-\alpha^i$ and β replaced with $-\beta$. This last observation allows us to obtain $\psi_n^{(-)}(\mathbf{x})$ from $\psi_n^{(+)}(\mathbf{x})$ in a simple way. First of all because $-\alpha^i$ and $-\beta$ satisfy the same relations (2.262)–(2.264) as α^i and β we can deduce that $-\alpha^i$ and $-\beta$ must be related to α^i and β by a unitary transformation.[21] We can write

[21] This is because any representation for the matrices which satisfies the properties in (2.262)–(2.264) is only defined up to a unitary transformation.

$$-\alpha^i = S^{-1}\alpha^i S, \tag{3.294}$$

$$-\beta = S^{-1}\beta S, \tag{3.295}$$

for some unitary matrix S.[22] It then follows that $S\psi_n^{(-)}(\mathbf{x})$ satisfies the same equation as $\psi_n^{(+)}(\mathbf{x})$, so that we may write

$$\psi_n^{(-)}(\mathbf{x}) = S^\dagger \psi_n^{(+)}(\mathbf{x}). \tag{3.296}$$

With the representation (2.267)–(2.269) for α^i and β it is easy to show that we may take

$$S = \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix}, \tag{3.297}$$

satisfying (3.294) and (3.295). We therefore have

$$\psi_{n\lambda}^{(-)}(\mathbf{x}) = \begin{pmatrix} -\frac{\lambda_n}{E_n+m} f_{n\lambda}(\mathbf{x}) \\ f_{n\lambda}(\mathbf{x}) \end{pmatrix}. \tag{3.298}$$

The normalization of the solutions $f_{n\lambda}(\mathbf{x})$ to (3.289) may be chosen to be

$$\int_\Sigma d\sigma_x f_{n\lambda}^\dagger(\mathbf{x}) f_{n'\lambda'}(\mathbf{x}) = \delta_{nn'}\delta_{\lambda\lambda'}, \tag{3.299}$$

and we will assume that $\{f_{n\lambda}(\mathbf{x})\}$ provides a complete set of solutions. It is straightforward to show that

$$\int_\Sigma d\sigma_x \psi_{n\lambda}^{(\pm)\dagger}(\mathbf{x}) \psi_{n'\lambda'}^{(\pm)}(\mathbf{x}) = \frac{2E_n}{E_n+m}\,\delta_{nn'}\delta_{\lambda\lambda'}, \tag{3.300}$$

$$\int_\Sigma d\sigma_x \psi_{n\lambda}^{(\pm)\dagger}(\mathbf{x}) \psi_{n'\lambda'}^{(\mp)}(\mathbf{x}) = 0. \tag{3.301}$$

The Dirac field operator may be expanded in terms of the positive and the negative energy parts as

$$\Psi(t,\mathbf{x}) = \sum_{n,\lambda} \left(\frac{E_n+m}{2E_n}\right)^{1/2} \left\{ e^{-iE_n t}\psi_{n\lambda}^{(+)}(\mathbf{x}) a_{n\lambda} + e^{iE_n t}\psi_{n\lambda}^{(-)}(\mathbf{x}) b_{n\lambda}^\dagger \right\}, \tag{3.302}$$

where $a_{n\lambda}$ and $b_{n\lambda}^\dagger$ are constant operators. The normalization factor of $[(E_n+m)/(2E_n)]^{1/2}$ is to facilitate the comparison of the quantized Dirac

[22] i.e. $S^{-1} = S^\dagger$.

field with the simple harmonic oscillator. Apart from the different normalization and the spinor nature of $\psi^{(\pm)}_{n\lambda}(\mathbf{x})$, this expansion is the same as that for the complex scalar field in Section 3.7.

If we use the properties (3.300) and (3.301) we can solve for

$$a_{n\lambda} = \left(\frac{E_n + m}{2E_n}\right)^{1/2} e^{iE_n t} \int_\Sigma d\sigma_x \psi^{(+)\dagger}_{n\lambda}(\mathbf{x})\Psi(t,\mathbf{x}), \tag{3.303}$$

$$b_{n\lambda} = \left(\frac{E_n + m}{2E_n}\right)^{1/2} e^{iE_n t} \int_\Sigma d\sigma_x \Psi^\dagger(t,\mathbf{x})\psi^{(-)}_{n\lambda}(\mathbf{x}), \tag{3.304}$$

along with their Hermitian conjugates. The anti-commutation relations given in (3.279) and (3.280) may now be used to show that

$$[a_{n\lambda}, a^\dagger_{n'\lambda'}]_+ = \delta_{nn'}\delta_{\lambda\lambda'} = [b_{n\lambda}, b^\dagger_{n'\lambda'}]_+, \tag{3.305}$$

$$0 = [a_{n\lambda}, a_{n'\lambda'}]_+ = [a_{n\lambda}, b_{n'\lambda'}]_+ = [a_{n\lambda}, b^\dagger_{n'\lambda'}]_+ = [b_{n\lambda}, b_{n'\lambda'}]_+, \tag{3.306}$$

along with the Hermitian conjugates of the last set of equations. Based on our experience with the quantization of the Schrödinger field, we can interpret $a_{n\lambda}$ and $b_{n\lambda}$ and their adjoints as sets of independent creation and annihilation operators for fermions.

It is possible to write the Hamiltonian in terms of $a_{n\lambda}$ and $b_{n\lambda}$ as usual. We have

$$H(t) = \int_\Sigma d\sigma_x \left\{ \frac{i}{2}(\partial_i \bar{\Psi}\gamma^i\Psi - \bar{\Psi}\gamma^i\partial_i\Psi) + m\bar{\Psi}\Psi \right\}, \tag{3.307}$$

from (2.302) and (2.303). Rather than substitute the expansion (3.302) for Ψ directly into this expression for $H(t)$ it is easier to first simplify the expression by using the equation of motion for Ψ and $\bar{\Psi}$ to write

$$H(t) = \frac{i}{2}\int_\Sigma d\sigma_x(\Psi^\dagger\dot{\Psi} - \dot{\Psi}^\dagger\Psi). \tag{3.308}$$

It is now simple to show that

$$H(t) = \sum_{n,\lambda} E_n(a^\dagger_{n\lambda}a_{n\lambda} - b_{n\lambda}b^\dagger_{n\lambda}), \tag{3.309}$$

if (3.302) and the orthogonality results (3.300) and (3.301) are used. If we use the anti-commutation relations (3.305) for $b_{n\lambda}$ and $b^\dagger_{n\lambda}$, this last result for the Hamiltonian may be written as

$$H(t) = \sum_{n,\lambda} E_n(a^\dagger_{n\lambda}a_{n\lambda} + b_{n\lambda}b^\dagger_{n\lambda} - 1). \tag{3.310}$$

At this point it is possible to understand why the Dirac field must be quantized using anti-commutation rather than commutation relations. Had we used commutation relations for $b_{n\lambda}$ and $b^\dagger_{n\lambda}$, apart from violating the Pauli exclusion principle, we would have found the coefficient of $b^\dagger_{n\lambda} b_{n\lambda}$ in (3.310) to be negative rather than positive. This would have resulted in a Hamiltonian operator which did not have a lower bound on its eigenvalues. With the energy not bounded from below it would not be possible to identify a stable ground state. This problem is avoided with the use of anti-commutation relations.

Defining the ground state in the usual way by imposing

$$a_{n\lambda}|0\rangle = b_{n\lambda}|0\rangle = 0, \tag{3.311}$$

the ground state energy is seen to be

$$\langle 0|H|0\rangle = -\sum_{n,\lambda} E_n = -2\sum_n E_n, \tag{3.312}$$

since λ has two possible values. The zero-point energy for the Dirac field is seen to be negative in contrast to the value found for the scalar field. Apart from the sign change, the result for $\langle 0|H|0\rangle$ is that for the complex scalar field. This factor can be understood as due to the two possible spin states for the Dirac field.

Although our results have assumed $D = 3$, it is possible to show that for general D similar results hold if we change the dimension of the spinor Ψ from 4 to $2^{[(D+1)/2]}$. The split into positive and negative energy parts now involves $(1/2)2^{[(D+1)/2]}$ independent components. The expansion for Ψ in terms of $a_{n\lambda}$ and $b^\dagger_{n\lambda}$ in (3.302) is unchanged if λ is understood to run over $(1/2)2^{[(D+1)/2]}$ possible values. The zero-point energy is accordingly

$$\langle 0|H|0\rangle = -\frac{1}{2}2^{[\frac{(D+1)}{2}]}\sum_n E_n. \tag{3.313}$$

3.10 Electromagnetic field

The Lagrangian density which gave rise to the Maxwell equations was[23]

$$\mathcal{L} = -\frac{1}{4}F_{\mu\nu}F^{\mu\nu}, \tag{3.314}$$

where

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu. \tag{3.315}$$

[23] See (2.69) with $J_\mu = 0$.

The first step in quantizing the theory is to identify the canonical field momentum $\Pi_\mu(t, \mathbf{x})$ defined by

$$\Pi_\mu(t, \mathbf{x}) = \frac{\delta L(t)}{\delta \dot{A}^\mu(t, \mathbf{x})}, \tag{3.316}$$

with

$$L(t) = \int_\Sigma d\sigma_x \mathcal{L}, \tag{3.317}$$

the Lagrangian. By writing out the time derivatives of A_μ in (3.314) explicitly it can be seen that

$$L(t) = \int_\Sigma d\sigma_x \left(-\frac{1}{2}\dot{A}_i\dot{A}^i + \dot{A}^i\partial_i A_0 - \frac{1}{2}\partial^i A_0 \partial_i A_0 - \frac{1}{4}F_{ij}F^{ij} \right). \tag{3.318}$$

Since $\dot{A}^0$ does not appear in (3.318), it follows from (3.316) that $\Pi_0 = 0$. There is a problem with a straightforward application of the Hamiltonian analysis to the electromagnetic field since A_0 has no canonical momentum. The reason we obtained $\Pi_0 = 0$ was because $L(t)$ in (3.318) did not contain any dependence on $\dot{A}_0$. We should therefore not view A_0 as a true dynamical variable in the theory. This suggests trying to define only the field momenta canonically conjugate to A^i. There is no problem in obtaining

$$\Pi_i = -\dot{A}_i + \partial_i A_0 = -F_{0i}. \tag{3.319}$$

From (2.66), Π_i can be recognized as the electric field.

Because A_0 is not a true dynamical degree of freedom we can try to simply impose the canonical commutation relations on the spatial components $A^i(t, \mathbf{x})$ and $\Pi_i(t, \mathbf{x})$. We would expect to have

$$[A^i(t, \mathbf{x}), \Pi_j(t, \mathbf{x}')] = i\hbar\delta^i{}_j\delta(\mathbf{x}, \mathbf{x}'), \tag{3.320}$$

on the basis of our experience with scalar fields. However, there is a problem with imposing this relation since it is not consistent with the Maxwell equation $\nabla \cdot \mathbf{E} = 0$.[24] Taking the divergence of both sides of (3.320) leads to an obvious inconsistency. We must conclude that a straightforward application of the usual canonical quantization procedure must be modified in some way.

[24] This equation follows from variation of the Lagrangian with respect to A_0 which we have stated is not a true dynamical variable. A_0 plays the role of a Lagrange multiplier which enforces $\nabla \cdot \mathbf{E} = 0$. The equation $\nabla \cdot \mathbf{E} = 0$ is called a 'constraint equation'.

There is another way to see that (3.320) must be incorrect. The spatial components of the vector potential $A^i(t, \mathbf{x})$ cannot represent an observable (unlike $\Pi(t, \mathbf{x})$ which represents the electric field). The reason for this is that $L(t)$ is invariant under the gauge transformation $A_i(t, \mathbf{x}) \to A_i(t, \mathbf{x}) + \partial_i \theta(\mathbf{x})$ for arbitrary $\theta(\mathbf{x})$. Observables must be independent of the arbitrary parameters of a gauge transformation. The root cause of the failure of the standard canonical quantization procedure lies in the gauge invariance of the Maxwell theory.

There are many possible ways to approach the quantization of the Maxwell theory. One way is to remove the gauge invariance of the theory by modification of the original Lagrangian by adding on a term, usually chosen to be proportional to $(\partial_\mu A^\mu)^2$, called the 'gauge breaking term'. It is then necessary to show how the Maxwell theory is recovered from this modified theory.[25] Another possibility is to relax the constraint $\nabla \cdot \mathbf{\Pi} = 0$ as an operator equation and to just impose it on the quantum states to restrict the Hilbert space. The full application of this approach is called the 'Gupta–Bleuler formalism' and is described in Heitler (1984), Schweber (1961) and Jauch and Rohrlich (1980) for example. A widely used (perhaps overused!) method to deal with theories with constraints is to apply the general theory developed by Dirac (1964). This method is described in Sundermeyer (1982), for example. Another very simple approach is to modify the canonical commutation relation (3.320) so that the constraint $\nabla \cdot \mathbf{\Pi} = 0$ can be imposed consistently. This is described by Schiff (1968), Bjorken and Drell (1965) and involves the introduction of the 'transverse delta function' in place of $\delta^i{}_j \delta(\mathbf{x}, \mathbf{x}')$ on the right-hand side of (3.320). This is by no means a complete list of the possible approaches.

The method we will use utilizes the Schwinger action principle, and was presented in Schwinger (1953a) with characteristic simplicity and elegance. The canonical commutation relations are obtained in a clear and unambiguous manner without any modifications to the basic action principle. Instead of starting from (3.314) with (3.315) imposed, we will begin with

$$\mathcal{L} = \frac{1}{4} F_{\mu\nu} F^{\mu\nu} - \frac{1}{4} F^{\mu\nu} (\partial_\mu A_\nu - \partial_\nu A_\mu) - \frac{1}{4} (\partial_\mu A_\nu - \partial_\nu A_\mu) F^{\mu\nu}, \quad (3.321)$$

where $F_{\mu\nu}$ and A_μ are treated independently (i.e. we do not assume the relation (3.315) between them). The last two terms of $\mathcal{L}$ have been written in a symmetrized form so that $\mathcal{L}$ is Hermitian. This Lagrangian density is invariant under the transformation

[25] See Wentzel (1949) for a very clear discussion of this method.

$$A_\mu \to A_\mu + \partial_\mu \theta, \tag{3.322}$$

$$F_{\mu\nu} \to F_{\mu\nu}, \tag{3.323}$$

for arbitrary θ. This means that when we vary $\mathcal{L}$ to find the equations of motion, not all of the variables will be independent. A simple calculation, assuming the variations δA_μ and $\delta F_{\mu\nu}$ to commute with the field operators, leads to

$$\delta\mathcal{L} = \frac{1}{2}\delta F^{\mu\nu}(F_{\mu\nu} - \partial_\mu A_\nu + \partial_\nu A_\mu) + \nabla_\mu F^{\mu\nu}\delta A_\nu - \nabla_\mu(F^{\mu\nu}\delta A_\nu). \tag{3.324}$$

To obtain the equations of motion we take the variations δA_ν to vanish on the spacetime boundary, and we find

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu, \tag{3.325}$$

$$\nabla_\mu F^{\mu\nu} = 0. \tag{3.326}$$

These results are equivalent to the vacuum Maxwell equations. Note also that if we substitute (3.325) back into (3.321) we recover the usual form (3.314) for the Lagrangian density.

Imposing the equations of motion (3.325) and (3.326) and allowing the variations δA_ν to be arbitrary at times t_1 and t_2 results in the change in the action

$$\begin{aligned}\delta S &= -\int_{t_1}^{t_2} dt \int_\Sigma d\sigma_x \nabla_\mu (F^{\mu\nu}\delta A_\nu) \\ &= G(t_2) - G(t_1),\end{aligned} \tag{3.327}$$

where

$$G(t) = -\int_\Sigma d\sigma_x F^{0i}(t,\mathbf{x})\delta A_i(t,\mathbf{x}). \tag{3.328}$$

We have performed an integration by parts and assumed the variations vanish on the boundary of Σ or else that Σ has no boundary. Because (3.319) still holds for $\mathcal{L}$ in the form (3.321) we can write $G(t)$ as

$$G(t) = \int_\Sigma d\sigma_x \Pi_i(t,\mathbf{x})\delta A^i(t,\mathbf{x}). \tag{3.329}$$

This is the direct counterpart of (3.93) for field theory. The basic result in (3.86) expressing the change in any observable under a unitary transformation generated by $G(t)$ still applies.

In obtaining the canonical commutation relations in quantum mechanics, as well as in other field theory models, we used the freedom to add a total time derivative to the Lagrangian which does not change the

equations of motion. (See the steps leading up to (3.101) for quantum mechanics.) In the present case we may define

$$\tilde{\mathcal{L}} = \mathcal{L} + \nabla_\mu (F^{\mu\nu} A_\nu). \tag{3.330}$$

The variation of $\tilde{\mathcal{L}}$ is

$$\delta\tilde{\mathcal{L}} = \frac{1}{2}\delta F^{\mu\nu}(F_{\mu\nu} - \partial_\mu A_\nu + \partial_\nu A_\mu) + \delta A_\nu \nabla_\mu F^{\mu\nu} + \nabla_\mu(\delta F^{\mu\nu} A_\nu). \tag{3.331}$$

$\tilde{\mathcal{L}}$ leads to the same field equations (3.325) and (3.326) as $\mathcal{L}$, but in place of (3.327) we find

$$\delta S = \tilde{G}(t_2) - \tilde{G}(t_1),$$

where

$$\begin{aligned}\tilde{G}(t) &= \int_\Sigma d\sigma_x \delta F^{0i}(t,\mathbf{x}) A_i(t,\mathbf{x}) \\ &= -\int_\Sigma d\sigma_x \delta\Pi_i(t,\mathbf{x}) A^i(t,\mathbf{x}).\end{aligned} \tag{3.332}$$

$\tilde{G}(t)$ is the direct counterpart of G_p in (3.101).

The new feature which arises at this stage is that we must be careful about the lack of independence of the variations δA^i in (3.329) and $\delta\Pi_i$ in (3.332). Because Π_i is constrained to satisfy $\nabla^i \Pi_i = 0$, it follows that $\delta\Pi_i$ must also satisfy $\nabla^i \delta\Pi_i = 0$. This means that only $(D-1)$ components of the D-dimensional vector $\delta\Pi_i$ are independent. This must be taken into account when using (3.332). In (3.329) it can be seen that δA^0 does not appear. As noted earlier, A_0 should not be regarded as a true dynamical degree of freedom, so this should not be surprising. Because of the constraint $\nabla^i \Pi_i = 0$ satisfied by Π_i, it is clear that $G(t)$ in (3.329) will be unaffected by the addition of a term $\nabla^i \lambda$ to δA^i. The variations δA^i are only independent up to the addition of the gradient of a scalar. Thus there are only $(D-1)$ independent variations δA^i. We can conclude that the physical content of Maxwell electrodynamics is specified by $(D-1)$ independent degrees of freedom. For $D = 3$ the classical analogue of these degrees of freedom correspond to the two possible polarizations of an electromagnetic wave.

There are two possible ways of applying the Schwinger action principle. The first is to keep all of the variations δA^i and $\delta\Pi_i$, but to incorporate the non-uniqueness discussed above. Provided that we focus on observables which must be gauge-invariant operators consistent with the constraint $\nabla^i \Pi_i = 0$ we can be certain of obtaining correct results. The second way is to select out only the $(D-1)$ physical degrees of freedom. This is done

by the imposition of a gauge condition. We will discuss both approaches here, as did Schwinger (1953a).

The change in any operator representing an observable under a unitary transformation generated by $G(t)$ was given in (3.86).[26] With $G(t)$ given by (3.329) we find

$$\delta B(t) = \frac{i}{\hbar}\int_\Sigma d\sigma_x \,[\Pi_i(t,\mathbf{x}), B(t)]\,\delta A^i(t,\mathbf{x}). \tag{3.333}$$

Taking $B(t) = \Pi_j(t,\mathbf{x}')$, and using the independence of the variations $\delta\Pi_i$ and δA^i, we conclude that

$$[\Pi_i(t,\mathbf{x}), \Pi_j(t,\mathbf{x}')] = 0. \tag{3.334}$$

This result is clearly consistent with the constraint $\nabla^i\Pi_i = 0$. The next obvious choice is to consider $B(t) = A^j(t,\mathbf{x}')$; however, as we have discussed this choice does not correspond to an observable, since A^j is gauge dependent. Instead we may take $B(t) = F_{jk}(t,\mathbf{x}') = \partial'_j A_k(t,\mathbf{x}') - \partial'_k A_j(t,\mathbf{x}')$ which is gauge-invariant and does represent an observable. (It is the magnetic field as seen in (2.66).) From (3.333) we find

$$\partial'_j A_k(t,\mathbf{x}') - \partial'_k A_j(t,\mathbf{x}') = \frac{i}{\hbar}\int_\Sigma d\sigma_x \,[\Pi_i(t,\mathbf{x}), F_{jk}(t,\mathbf{x}')]\,\delta A^i(t,\mathbf{x}),$$

which leads to

$$\frac{i}{\hbar}\,[\Pi_i(t,\mathbf{x}), F_{jk}(t,\mathbf{x}')] = g_{ik}(\mathbf{x})\partial'_j\delta(\mathbf{x}',\mathbf{x}) - g_{ij}(\mathbf{x})\partial'_k\delta(\mathbf{x}',\mathbf{x}) \tag{3.335}$$

$$= g_{ij}(\mathbf{x})\partial_k\delta(\mathbf{x},\mathbf{x}') - g_{ik}(\mathbf{x})\partial_j\delta(\mathbf{x},\mathbf{x}') \tag{3.336}$$

where we have used the properties of the Dirac delta distribution in the second line. This result is also consistent with the $\nabla^i\Pi_i = 0$ constraint. Note that (3.335) or (3.336) tells us the commutation relation between the components of the electric and the magnetic fields. Here $g_{ij}(\mathbf{x})$ is the metric tensor on Σ; for flat space in Cartesian coordinates we can choose $g_{ij} = \delta_{ij}$.

To obtain the remaining independent commutation relations we must use (3.86) with $\tilde{G}(t)$ given in (3.332) in place of $G(t)$. We must be careful to note that the variation $\delta\Pi_i$ satisfies $\nabla^i\Pi_i = 0$. At this stage Schwinger (1953a) uses a clever trick by setting

$$\delta\Pi_i = \nabla^j\delta Z_{ji}, \tag{3.337}$$

[26] Equally well we could use $\tilde{G}(t)$ in place of $G(t)$.

where $Z_{ji} = -Z_{ij}$ ensures that $\nabla^i \delta\Pi_i = 0$.[27] Using (3.337) in (3.332) and performing an integration by parts leads to

$$\begin{aligned}\tilde{G}(t) &= \int_\Sigma d\sigma_x \delta Z^{ij}(t,\mathbf{x}) \nabla_j A_i(t,\mathbf{x}) \\ &= -\frac{1}{2}\int_\Sigma d\sigma_x \delta Z^{ij}(t,\mathbf{x}) F_{ij}(t,\mathbf{x}).\end{aligned} \tag{3.338}$$

This gives

$$\delta B(t) = -\frac{i}{2\hbar}\int_\Sigma d\sigma_x \delta Z^{ij}(t,\mathbf{x}) \left[F_{ij}(t,\mathbf{x}), B(t)\right]. \tag{3.339}$$

If we consider $B(t) = F_{kl}(t,\mathbf{x}')$, because no variation of A_i appears in the right-hand side of the resulting expression, we must have

$$[F_{ij}(t,\mathbf{x}), F_{kl}(t,\mathbf{x}')] = 0. \tag{3.340}$$

The other gauge-invariant choice $B(t) = \Pi_k(t,\mathbf{x}')$ leads to (3.335) and (3.336) again.

We have therefore found the canonical commutation relations for the field strength components which represent observables. In some sense this should be good enough; however, it is often convenient to have commutation relations which involve the vector potential directly. Because A^i cannot represent an observable due to its gauge arbitrariness we will pick a gauge to select out the physical degrees of freedom.

In three spatial dimensions Helmholtz's theorem of vector calculus (Arfken, 1970), tells us that any vector field $\mathbf{A}$ can always be written as $\mathbf{A} = \mathbf{A}^\perp + \nabla\Theta$, where $\nabla \cdot A = 0$ and Θ is a scalar field. For general Σ the same result holds true as a consequence of the Hodge–de Rham theorem (Choquet-Bruhat *et al.*, 1977) (apart from the addition of a harmonic term which is of no relevance to us here). Under a gauge transformation $\mathbf{A} \to \mathbf{A} + \nabla\lambda$, so that $\mathbf{A}^\perp$ is unaffected and $\Theta \to \Theta + \lambda$. This suggests that the physical content of $\mathbf{A}$ is contained in $\mathbf{A}^\perp$. In fact if we perform the gauge transformation with $\lambda = -\Theta$ we can force $\mathbf{A}$ to satisfy

$$\nabla \cdot \mathbf{A} = 0 = \nabla_i A^i. \tag{3.341}$$

The constraint equation $\nabla_i F^{i0} = 0$ becomes $\nabla^2 A^0 = 0$ in this gauge. We can solve the constraint by

$$A^0 = 0. \tag{3.342}$$

[27] This follows simply from the anti-symmetry of Z_{ij} under a relabelling of the indices.

The gauge specified by (3.341)and (3.342) is called the 'radiation gauge'. The condition (3.341) provides one constraint on the D components of $\mathbf{A}$ leaving us with $(D-1)$ physical degrees of freedom. Variation of (3.341) shows that the variations δA^i must satisfy

$$\nabla_i \delta A^i = 0 \tag{3.343}$$

in the radiation gauge.

If we return to (3.333), except with δA^i restricted by (3.343), choosing $B(t) = \Pi_j(t, \mathbf{x}')$ recovers (3.334). Because the gauge arbitrariness has been fixed by specification of a gauge condition, we can take $B(t) = A^j(t, \mathbf{x}')$ and find

$$\delta A^j(t, \mathbf{x}') = \frac{i}{\hbar} \int_\Sigma d\sigma_x \delta A^i(t, \mathbf{x}) \left[\Pi_i(t, \mathbf{x}), A^j(t, \mathbf{x}')\right]. \tag{3.344}$$

Since δA^i obeys (3.343) the commutator appearing on the right-hand side of (3.344) is only determined up to an additive term:

$$\frac{i}{\hbar} \left[\Pi_i(t, \mathbf{x}), A^j(t, \mathbf{x}')\right] = \delta^i{}_j \delta(\mathbf{x}', \mathbf{x}) + \nabla_i \lambda^j(\mathbf{x}', \mathbf{x}), \tag{3.345}$$

with $\lambda^j(\mathbf{x}', \mathbf{x})$ as an arbitrary distribution. It is easy to see that the term in λ^j is not fixed by the basic result in (3.344). However, λ^j can be fixed by requiring that the result (3.345) be consistent with the constraint $\nabla^i \Pi_i = 0$. By operating on both sides of (3.345) with ∇^i we find

$$\nabla^i \nabla_i \lambda^j(\mathbf{x}', \mathbf{x}) = -\nabla^j \delta(\mathbf{x}', \mathbf{x}). \tag{3.346}$$

If we define $G(\mathbf{x}, \mathbf{x}')$ to be the Green function for the scalar Laplacian,

$$\nabla^i \nabla_i G(\mathbf{x}, \mathbf{x}') = -\nabla^2 G(\mathbf{x}, \mathbf{x}') = \delta(\mathbf{x}, \mathbf{x}'), \tag{3.347}$$

then the solution to (3.346) is

$$\lambda^j(\mathbf{x}', \mathbf{x}) = \nabla'^j G(\mathbf{x}, \mathbf{x}'). \tag{3.348}$$

We therefore find

$$\frac{i}{\hbar} \left[\Pi_i(t, \mathbf{x}), A^j(t, \mathbf{x}')\right] = \delta^i{}_j \delta(\mathbf{x}', \mathbf{x}) + \nabla_i \nabla'^j G(\mathbf{x}, \mathbf{x}'). \tag{3.349}$$

This result is also consistent with the constraint (3.341). In flat space, the distribution appearing on the right-hand side of (3.349) can be seen to be the 'transverse delta function' introduced by Bjorken and Drell (1965). The Schwinger action principle shows how this modification of the naive

canonical commutation relations in (3.320) is a necessary consequence of the formalism.

Finally we turn to the use of $\tilde{G}(t)$ in (3.86). If we take $B(t) = A^j(t, \mathbf{x}')$ it is easy to see that

$$[A^i(t, \mathbf{x}), A^j(t, \mathbf{x}')] = 0. \tag{3.350}$$

This is consistent with (3.341) and completes our evaluation of the electromagnetic field commutators.

An interesting feature of (3.349) is that for $\mathbf{x}' \neq \mathbf{x}$ $\Pi_i(t, \mathbf{x})$ does not commute with $A^j(t, \mathbf{x}')$ since the Green function $G(\mathbf{x}, \mathbf{x}')$ will not vanish in general. This means that it is not possible to measure $A^j(t, \mathbf{x}')$ and $\Pi_i(t, \mathbf{x})$ simultaneously. However, this should cause no concern because the electric and magnetic field operators do commute for $\mathbf{x}' \neq \mathbf{x}$, and it is these fields that are measurable. It is straightforward to show that (3.335) and (3.336) are recovered from (3.349), the terms in the Green function cancelling out when the field strength is computed.

We now wish to expand the field operators in terms of creation and annihilation operators. This is easiest if we adopt the radiation gauge. Let $\mathbf{f}_n(\mathbf{x})$ be a vector field that satisfies

$$-\nabla^2 \mathbf{f}_n(\mathbf{x}) = \sigma_n \mathbf{f}_n(\mathbf{x}), \tag{3.351}$$

for some eigenvalue σ_n. If $\mathbf{f}_n(\mathbf{x})$ is to serve as an expansion function for $\mathbf{A}(t, \mathbf{x})$, then it must satisfy the gauge condition (3.341),

$$\nabla \cdot \mathbf{f}_n(\mathbf{x}) = 0. \tag{3.352}$$

Because of the constraint (3.352) on the solutions to (3.351) only $(D-1)$ linearly independent solutions will exist. We will label them by $\mathbf{f}_{n\lambda}(\mathbf{x})$ where λ has $(D-1)$ possible values, and assume the orthonormality condition

$$\int_\Sigma d\sigma_x \mathbf{f}^*_{n\lambda}(\mathbf{x}) \cdot \mathbf{f}_{n'\lambda'}(\mathbf{x}) = \delta_{nn'}\delta_{\lambda\lambda'}. \tag{3.353}$$

It is worth remembering that $\mathbf{A} \cdot \mathbf{B} = A^1 B^1 + \cdots = -A^1 B_1 + \cdots = -A^i B_i$ here with our choice for the metric signature. Thus (3.353) can be written as

$$\int_\Sigma d\sigma_x f^*_{n\lambda i}(\mathbf{x}) f_{n'\lambda'}{}^i(\mathbf{x}) = -\delta_{nn'}\delta_{\lambda\lambda'} \tag{3.354}$$

in terms of the components $f_{n\lambda}{}^i(\mathbf{x})$ of $\mathbf{f}_{n\lambda}(\mathbf{x})$. We will also assume that $\{\mathbf{f}_{n\lambda}(\mathbf{x})\}$ is complete in the sense that any solution to (3.351) which obeys

the radiation gauge condition (3.341) can be expanded in terms of the $\mathbf{f}_{n\lambda}(\mathbf{x})$. It is easy to see that the completeness relation becomes

$$\sum_{n\lambda} f_{n\lambda}{}^{i}(\mathbf{x}) f^{*}_{n\lambda j}(\mathbf{x}') = -\left[\delta^{i}{}_{j}\delta(\mathbf{x},\mathbf{x}') + \nabla^{i}\nabla'_{j}G(\mathbf{x},\mathbf{x}')\right], \tag{3.355}$$

with $G(\mathbf{x},\mathbf{x}')$ satisfying (3.347).

As for the real scalar field in Section 3.6, it is convenient to regard the eigenfunctions of the Laplacian $\mathbf{f}_{n\lambda}(\mathbf{x})$ as complex. We should have, analogously to (3.174) for scalar fields,

$$\mathbf{f}^{*}_{n\lambda}(\mathbf{x}) = \sum_{n'\lambda'} C_{n\lambda n'\lambda'}\mathbf{f}_{n'\lambda'}(\mathbf{x}), \tag{3.356}$$

for some coefficients $C_{n\lambda n'\lambda'}$. Using (3.353) shows that[28]

$$C_{n\lambda n'\lambda'} = \int_{\Sigma} d\sigma_{x}\mathbf{f}^{*}_{n\lambda}(\mathbf{x})\cdot\mathbf{f}^{*}_{n'\lambda'}(\mathbf{x}). \tag{3.357}$$

Because the eigenvalues in (3.351) are real, it is easy to repeat the steps which led up to (3.179) in the scalar field case, and prove that

$$F(\sigma_{n})C_{n\lambda n'\lambda'} = F(\sigma_{n'})C_{n\lambda n'\lambda'}. \tag{3.358}$$

We now expand

$$\mathbf{A}(t,\mathbf{x}) = \sum_{n\lambda}(2E_{n})^{-1/2}\left\{\mathbf{f}_{n\lambda}(\mathbf{x})e^{-iE_{n}t}a_{n\lambda} + \mathbf{f}^{*}_{n\lambda}(\mathbf{x})e^{iE_{n}t}a^{\dagger}_{n\lambda}\right\}, \tag{3.359}$$

for some constant operators $a_{n\lambda}$ and their Hermitian conjugates $a^{\dagger}_{n\lambda}$. In the radiation gauge (3.319) becomes $\mathbf{\Pi}(t,\mathbf{x}) = -\dot{\mathbf{A}}(t,\mathbf{x})$, and (3.359) gives

$$\mathbf{\Pi}(t,\mathbf{x}) = i\sum_{n\lambda}\left(\frac{E_{n}}{2}\right)^{1/2}\left\{\mathbf{f}_{n\lambda}(\mathbf{x})e^{-iE_{n}t}a_{n\lambda} - \mathbf{f}^{*}_{n\lambda}(\mathbf{x})e^{iE_{n}t}a^{\dagger}_{n\lambda}\right\}. \tag{3.360}$$

The field equation for $\mathbf{A}$ follows from (3.326) as

$$\frac{\partial^{2}}{\partial t^{2}}\mathbf{A} - \nabla^{2}\mathbf{A} = 0. \tag{3.361}$$

[28] Compare with (3.175) for the scalar field.

This leads to

$$E_n = \sqrt{\sigma_n}, \tag{3.362}$$

with σ_n defined in (3.351).

We may solve for $a_{n\lambda}$ and $a^\dagger_{n\lambda}$ in terms of $\mathbf{A}(t,\mathbf{x})$ and $\mathbf{\Pi}(t,\mathbf{x})$ exactly as we did for the scalar field. From (3.359) using (3.353), (3.357) and (3.358) leads to

$$a_{n\lambda} = e^{iE_n t}\int_\Sigma d\sigma_x \mathbf{f}^*_{n\lambda}(\mathbf{x})\cdot\left\{\left(\frac{E_n}{2}\right)^{1/2}\mathbf{A}(t,\mathbf{x}) - \frac{i}{(2E_n)^{1/2}}\mathbf{\Pi}(t,\mathbf{x})\right\}, \tag{3.363}$$

$$a^\dagger_{n\lambda} = e^{-iE_n t}\int_\Sigma d\sigma_x \mathbf{f}_{n\lambda}(\mathbf{x})\cdot\left\{\left(\frac{E_n}{2}\right)^{1/2}\mathbf{A}(t,\mathbf{x}) + \frac{i}{(2E_n)^{1/2}}\mathbf{\Pi}(t,\mathbf{x})\right\}. \tag{3.364}$$

It is now straightforward to show using (3.334), (3.349), and (3.350) that

$$[a_{n\lambda}, a_{n'\lambda'}] = 0 = [a^\dagger_{n\lambda}, a^\dagger_{n'\lambda'}], \tag{3.365}$$

$$[a_{n\lambda}, a^\dagger_{n'\lambda'}] = \delta_{nn'}\delta_{\lambda\lambda'}. \tag{3.366}$$

The term in $G(\mathbf{x},\mathbf{x}')$ in (3.349) makes no contribution to (3.366) because of the constraint (3.352).

Finally we can evaluate the Hamiltonian operator in the radiation gauge. We have

$$\begin{aligned} H(t) &= \int_\Sigma d\sigma_x \Pi_i(t,\mathbf{x})\dot{A}^i(t,\mathbf{x}) - L(t) \\ &= \int_\Sigma d\sigma_x \left(-\frac{1}{2}\Pi_i\Pi^i + \frac{1}{4}F_{ij}F^{ij}\right), \end{aligned} \tag{3.367}$$

if we use (3.318) specialized to the radiation gauge. It is now a straightforward matter of substituting the field expansions (3.359) and (3.360) to find

$$H(t) = \sum_{n\lambda}\frac{1}{2}E_n(a_{n\lambda}a^\dagger_{n\lambda} + a^\dagger_{n\lambda}a_{n\lambda}). \tag{3.368}$$

This shows that we can consider the quantized electromagnetic field as a collection of $(D-1)$ uncoupled simple harmonic oscillators. Defining the ground state in the usual way by $a_{n\lambda}|0\rangle = 0$, the energy of the ground state is

$$\langle 0|H|0\rangle = \frac{1}{2}\sum_{n\lambda}E_n = \frac{1}{2}(D-1)\sum_n E_n. \tag{3.369}$$

Notes

The material presented here is not to be viewed as a first introduction to quantum mechanics; rather, it is a review of the basics and an establishment of notation. Suggested references are Powell and Craseman (1961), Sakurai (1994), and Schiff (1968) for the traditional approach, and Isham (1995) for something different. Dirac (1958) is still worth reading for the fundamentals. A classic discussion of the physical basis of quantum mechanics is Heisenberg (1930). A careful treatment of the intricacies involved in the case of operators with continuous spectra may be found in Prugovecki (1982). My main references for the Schwinger action principle were Schwinger's original papers Schwinger (1951b, 1953a,b,c) and his book Schwinger (1970). After a draft of this book had been completed, I became aware of an edition of Schwinger's lectures on quantum mechanics that had been published posthumously (Schwinger, 2001) that mainly concentrates on Schwinger's approach to quantum theory, based on selective quantum measurements. The treatment of field theory that we offer in the present chapter differs from that found in other books in as much as we do not assume flat space with its accompanying momentum space expansions. By keeping the volume of space finite from the start some of the results look a bit cleaner. The idea of using what are now called 'Grassmann variables' was first used by Schwinger in the field theory context (see Schwinger (1953c) for example).

4
The effective action

4.1 Introduction

The development of relativistic quantum field theory was stimulated by the need to deal with scattering processes in high energy physics. A successful implementation of quantum electrodynamics was given in the late 1940s and early 1950s. The applications of this theory are described in the classic textbooks and a history of the subject is given in Schweber (1994). Similar methods may be applied to the more modern standard model which deals with the weak and electromagnetic interactions of quarks and leptons.[1] It is perfectly possible to extend the start we have made in Chapter 3 to make contact with this approach which concentrates on the calculation of scattering amplitudes and cross-sections. Instead of pursuing this more traditional path we will adopt an alternate approach which is useful for understanding symmetry breaking and phase transitions in physics. The principal aim of this chapter will be to develop the effective action method in a very simple way and apply it to a number of problems. It is not necessary to use the full formalism of the effective action to follow simple applications, and we will postpone the full development until Chapter 8.

In the last chapter we saw how quantum field theory was obtained from classical field theory by replacing the classical field variables with appropriate operators. In this chapter we wish to go back to dealing with ordinary field variables again, but with ones that somehow include quantum corrections to the classical theory. We will call this field the mean field to distinguish it from the classical field variable. If $\bar{\varphi}$ is this mean field we now wish to require that its equation of motion follow from a principle of stationary action. The action functional which leads to the

[1] See Halzen and Martin (1984) for a pedagogical introduction.

equation of motion for $\bar{\varphi}$ is called the 'effective action' and is denoted by $\Gamma[\bar{\varphi}]$. Because the field equation for $\bar{\varphi}$ must include quantum corrections to the classical field equation, we can think of $\Gamma[\bar{\varphi}]$ as being comprised of the classical action plus all of its quantum corrections. In this chapter we will be concerned with only the first-order quantum corrections to the classical theory. In Chapter 8 we will consider the effective action in much greater generality and justify the approach used in the present chapter as the first-order term in a systematic expansion of the effective action.

Given an expression for the effective action $\Gamma[\bar{\varphi}]$ we can define an effective Lagrangian density $\mathcal{L}_{\text{eff}}$ in an obvious way by

$$\Gamma[\bar{\varphi}] = \int_{t_1}^{t_2} dt \int_{\Sigma} d\sigma_x \, \mathcal{L}_{\text{eff}}(t, \mathbf{x}). \tag{4.1}$$

The principle of stationary action may be stated as

$$\Gamma\left[\bar{\varphi} + \delta\bar{\varphi}\right] = \Gamma[\bar{\varphi}], \tag{4.2}$$

to first order in $\delta\bar{\varphi}$. Just as in classical field theory this will give rise to an equation of motion, except that this time it will be for the mean field $\bar{\varphi}$. Because the Lagrangian density is just the difference between the kinetic energy density and the potential energy density, we can define the effective potential energy density by taking the mean field to be such that the kinetic energy density vanishes. If we think of the real or complex scalar fields, for example, this will occur if the mean fields are independent of time. We can write

$$\Gamma[\bar{\varphi}] = -(t_2 - t_1) \int_{\Sigma} d\sigma_x \, V_{\text{eff}}, \tag{4.3}$$

in this case. We will be concerned with time-independent situations for this chapter and the subsequent one, so that we can use (4.3). By complete analogy with classical mechanics we can define naturally the ground state to correspond to the value of the mean field which minimizes the potential energy. It may be the case that the ground state also corresponds to a mean field which has no dependence on position. This would be expected to hold if our space Σ was a homogeneous and isotropic space such as infinite flat space, or the surface of a sphere since the mean field would be expected to share the symmetries of the space. If this is the case, then we have the even simpler result that

$$\Gamma[\bar{\varphi}] = -(t_2 - t_1) V_{\Sigma} V_{\text{eff}}, \tag{4.4}$$

where V_{Σ} is the volume of the space Σ. The equation for the mean field $\bar{\varphi}$ becomes simply $(\partial/\partial\bar{\varphi})V_{\text{eff}} = 0$ in cases where (4.4) applies. This will be

the case in many of our examples, and is the case in almost all of particle physics where Σ corresponds to flat infinite Euclidean space.

We are in the position now where if we know $\Gamma[\bar{\varphi}]$ or V_{eff} we can obtain the equation of motion for the mean field representing the ground state of the system. We now need to discuss how to obtain an expression for V_{eff}. Because V_{eff} can be thought of as the classical potential energy density plus the quantum corrections to the classical result, if we only work to first order in quantum corrections to the classical theory we can write

$$V_{\text{eff}} = V_{\text{eff}}^{(0)} + V_{\text{eff}}^{(1)} + \cdots, \tag{4.5}$$

where $V_{\text{eff}}^{(0)}$ is the classical contribution and $V_{\text{eff}}^{(1)}$ is the first-order correction to the classical result which arises from quantization of the theory. We can read off $V_{\text{eff}}^{(0)}$ from the classical Lagrangian for the theory. To obtain $V_{\text{eff}}^{(1)}$ we can note that we are regarding the theory as an infinite collection of simple harmonic oscillators. Therefore to get the ground state energy we merely need to sum the zero-point energies. This will be our recipe for obtaining the lowest-order effective potential. A full justification of this recipe, and a prescription for obtaining higher-order terms in the perturbative expansion will be considered in Chapter 8.

Suppose that we have a real scalar field described by the classical action functional

$$S[\varphi] = \int_{t_1}^{t_2} dt \int_{\Sigma} d\sigma_x \left[\frac{1}{2} \partial^{\mu} \varphi \partial_{\mu} \varphi - \frac{1}{2} m^2 \varphi^2 - U(\varphi) \right]. \tag{4.6}$$

In the previous chapter we discussed the free-field case where we took $U(\varphi) = 0$. Here we will allow an arbitrary potential term for the field which can represent a self-interaction or interaction with some externally applied fields. Setting the variation of $S[\varphi]$ with respect to φ to zero results in

$$\Box \varphi + m^2 \varphi + U'(\varphi) = 0. \tag{4.7}$$

In order to obtain the zero-point energy in this case we will set

$$\varphi = \bar{\varphi} + \psi, \tag{4.8}$$

where ψ represents the quantum fluctuation about the mean field $\bar{\varphi}$ and linearize (4.7) in ψ. This gives the equation

$$\Box \psi + m^2 \psi + U''(\bar{\varphi}) \psi = 0. \tag{4.9}$$

Note that we do not claim that $\bar{\varphi}$ satisfies the zeroth-order equation resulting from the substitution of (4.8) into (4.7); rather we have defined

$\bar{\varphi}$ to be the solution which minimizes the effective potential. However, since ψ will be of necessity first order at least in quantum corrections, the equation satisfied by ψ (4.9) is correct to lowest order in the quantum corrections. (That is quantum corrections to the classical action can only affect ψ at second order.)

We can take as our basic solutions to (4.9) the normal modes

$$\psi_n(t, \mathbf{x}) = e^{-iE_n t} f_n(\mathbf{x}), \tag{4.10}$$

where $f_n(\mathbf{x})$ satisfies

$$\left[-\nabla^2 + U''(\bar{\varphi})\right] f_n(\mathbf{x}) = \sigma_n f_n(\mathbf{x}), \tag{4.11}$$

and

$$E_n = \sqrt{\sigma_n + m^2}. \tag{4.12}$$

This is a straightforward generalization of what we did in the free-field case in Chapter 3. Our assumption that $\bar{\varphi}$ is independent of time has been used in an important way here; otherwise the time dependence of the solutions will not be simple exponentials. We will assume that $\{f_n(\mathbf{x})\}$ is a complete set of orthonormal solutions to (4.10). If we do not assume that $\bar{\varphi}$ is constant, then it will be impossible to solve (4.10) for $f_n(\mathbf{x})$ in general, and hence we cannot know the eigenvalues σ_n explicitly in this general situation.

We can now write down the formal expression for the terms in the expansion of the effective action arising from the potential given in (4.5). We have

$$\Gamma[\bar{\varphi}] = \Gamma^{(0)}[\bar{\varphi}] + \Gamma^{(1)}[\bar{\varphi}] + \cdots, \tag{4.13}$$

$$\Gamma^{(0)} = -(t_2 - t_1) \int_\Sigma d\sigma_x \left[\frac{1}{2}\partial^i \bar{\varphi} \partial_i \bar{\varphi} + \frac{1}{2} m^2 \bar{\varphi}^2 + U(\bar{\varphi})\right], \tag{4.14}$$

$$\Gamma^{(1)} = -(t_2 - t_1) \sum_n \frac{\hbar}{2} E_n. \tag{4.15}$$

$\Gamma^{(0)}$ is the same as the classical action with the field replaced with the time independent mean field. The mean field satisfies the equation resulting from making $\Gamma[\bar{\varphi}]$ in (4.13) stationary. It proves convenient to introduce $\hbar$ in (4.15) to signify that the result is first order in quantum corrections.

We must now face the problem of evaluating the infinite sum of zero-point energies if we are to evaluate $\Gamma^{(1)}$. If we take the simplest case of a free scalar field theory in flat space, then $E_n \sim \sqrt{n^2 + m^2}$ and the sum over n in (4.15) involves the evaluation of $\int d^D n \sqrt{n^2 + m^2}$, which is infinite. This forces us to introduce a regularization method to try

to deal with such an infinite expression. One elegant way for doing this is to use ζ-function regularization. The basic idea of the method is to define the divergent sum over zero-point energies in (4.15) by the analytic continuation of a convergent sum. We will define the energy ζ-function $E(s)$ by

$$E(s) = \sum_n E_n (\ell E_n)^{-s}. \tag{4.16}$$

Here s is a complex variable and ℓ is a constant with units of length, called the 'renormalization length', introduced to keep ℓE_n dimensionless. This ensures that $E(s)$ has dimensions of energy for all values of s. Because the origin of the infinite result of the sum in (4.15) was due to the fact that $E_n \to \infty$ as $n \to \infty$, we can turn this problem into a virtue. By taking s to be complex with[2] $\mathcal{R}(s)$ sufficiently large we can make the energy ζ-function in (4.16) converge. We can then analytically continue the result for $E(s)$ back into the region of the complex s-plane where the expression for $E(s)$ as the sum in (4.16) no longer applies. In particular, we can try to define the sum over zero-point energies by $E(s = 0)$. Thus we can take

$$\Gamma^{(1)}[\bar{\varphi}] = -(t_2 - t_1)\frac{\hbar}{2}E(0), \tag{4.17}$$

as our definition for $\Gamma^{(1)}$. It may be that $E(s)$ has a singularity at $s = 0$. In this case we will understand (4.17) to mean the analytic continuation of $E(s)$ to a small neighbourhood of $s = 0$. The essential part of our method is therefore an evaluation of the energy ζ-function.

In some cases we may wish to obtain an expression for the effective potential energy density for the ground state directly. In this case $\langle 0|\mathcal{H}|0\rangle$ should give us the quantum correction to the ground state energy density, where $\mathcal{H}$ is the Hamiltonian density.[3] From the expansion of the scalar field in terms of creation and annihilation operators given in (3.187) it is easily seen that

$$\varphi(t, \mathbf{x})|0\rangle = \sum_n (2E_n)^{-1/2} e^{iE_n t} f_n^*(\mathbf{x}) a_n^\dagger |0\rangle \tag{4.18}$$

if we use $a_n|0\rangle = 0$. A similar expression follows from (3.188) for the canonical momentum. It is then possible to evaluate $\langle 0|\mathcal{H}|0\rangle$ with $\mathcal{H}$, the integrand of the Hamiltonian given in (3.197). It is easy to show, using

[2] Here $\mathcal{R}(s)$ denotes the real part of the complex number s.

[3] It is also possible to consider the more general expression $\langle 0|T_{\mu\nu}|0\rangle$ where $T_{\mu\nu}$ is the stress–energy–momentum operator.

the canonical commutation relations $[a_n, a^\dagger_{n'}] = \delta_{nn'}$, that[4]

$$\langle 0|\mathcal{H}|0\rangle = \frac{\hbar}{2}\sum_n E_n |f_n(\mathbf{x})|^2. \tag{4.19}$$

The effective potential density $V^{(1)}_{\rm eff}$ will be defined to be

$$V^{(1)}_{\rm eff} = \frac{\hbar}{2}\sum_n E_n |f_n(\mathbf{x})|^2. \tag{4.20}$$

If $|f_n(\mathbf{x})|^2$ is constant, then the normalization condition on $f_n(\mathbf{x})$ restricts $|f_n(\mathbf{x})| = V_\Sigma^{-1/2}$ and we obtain

$$V^{(1)}_{\rm eff} = \hbar\frac{E(0)}{2V_\Sigma} \tag{4.21}$$

if we define the sum over energy levels in terms of the energy ζ-function. If $|f_n(\mathbf{x})|$ is not constant, then use of (4.21) rather than (4.20) will give us an effective potential averaged over Σ rather than a local expression. If we really want to obtain the energy density, then (4.20) must be used. We can, however, still use (4.21) to obtain the total energy due to quantum effects. An example illustrating the use of and regularization of (4.20) will be given in Section 4.7.

4.2 Free scalar field in Minkowski spacetime

As our first example we will study the free scalar field in the case where Σ approaches flat Euclidean space in the infinite volume limit. To do this we will choose Σ to be a D-dimensional rectangular box and impose periodic boundary conditions on the walls of the box. Let $L_1, \ldots, L_D$ be the sides of the box. Ultimately we will let $L_1, \ldots, L_D$ all become infinitely large.

We need the energy eigenvalues E_n defined in (4.12). Because of the choice of periodic boundary conditions on the walls of the box we can pick

$$f_{\mathbf{n}}(\mathbf{x}) = V_\Sigma^{-1/2} \exp\left\{\sum_{j=1}^{D}\left(\frac{2\pi i n_j}{L_j}x^j\right)\right\}, \tag{4.22}$$

with $\mathbf{x} = (x^1, \ldots, x^D)$ the usual Cartesian coordinates and $\mathbf{n}$ standing for the D-tuple of integers $\mathbf{n} = (n_1, \ldots, n_D)$. Here $n_i = 0, \pm1, \pm2, \ldots$ for each $i = 1, \ldots, D$. The eigenvalues of the Laplacian are

[4] A spatial total derivative has been discarded to get this.

$$\sigma_{\mathbf{n}} = \sum_{j=1}^{D} \left(\frac{2\pi n_j}{L_j} \right)^2 , \tag{4.23}$$

and the energy eigenvalues are just as in (4.12). The energy ζ-function (4.16) reads

$$E(s) = \sum_{n_1=-\infty}^{\infty} \cdots \sum_{n_D=-\infty}^{\infty} \ell^{-s} (\sigma_{\mathbf{n}} + m^2)^{(1-s)/2}. \tag{4.24}$$

The case we are interested in corresponds to the limit $L_1, \ldots, L_D \to \infty$. In this case we can approximate the sums that occur in (4.24) over the integers $n_1, \ldots, n_D$ with integrals. (Later on we will examine this procedure more closely.) This leads to

$$E(s) = \int \frac{d^D p}{(2\pi)^D} \; \ell^{-s} \left[\sum_{j=1}^{D} \left(\frac{2\pi n_j}{L_j} \right)^2 + m^2 \right]^{(1-s)/2} . \tag{4.25}$$

With the change of variable $n_j \to L_j p_j/(2\pi)$ we find

$$E(s) = \ell^{-s} V_\Sigma \int \frac{d^D p}{(2\pi)^D} \, (\mathbf{p}^2 + m^2)^{(1-s)/2}. \tag{4.26}$$

This integral is of a type we will encounter many times, so it is worth going through its evaluation in detail.

First of all we use the identity

$$a^{-z} = \frac{1}{\Gamma(z)} \int_0^\infty dt \, t^{z-1} e^{-at}, \tag{4.27}$$

which holds for $\mathcal{R}(z) > 0$ and $\mathcal{R}(a) > 0$. This is just the definition of the Γ-function (see (A1.1) in Appendix 1). With $a = \mathbf{p}^2 + m^2$ and $z = (s-1)/2$ we find

$$E(s) = \frac{\ell^{-s} V_\Sigma}{\Gamma[(s-1)/2]} \int \frac{d^D p}{(2\pi)^D} \int_0^\infty dt \, t^{(s-3)/2} e^{-(\mathbf{p}^2 + m^2)t}. \tag{4.28}$$

The integration over $\mathbf{p}$ now involves simple Gaussians, and we have

$$\int \frac{d^D p}{(2\pi)^D} \; e^{-t\mathbf{p}^2} = \left(\int_{-\infty}^{\infty} \frac{dp}{2\pi} e^{-tp^2} \right)^D = (4\pi t)^{-D/2}. \tag{4.29}$$

Using this result back in (4.29) results in

$$E(s) = \ell^{-s} V_\Sigma \frac{1}{\Gamma[(s-1)/2]} (4\pi)^{-D/2} \int_0^\infty dt\, t^{(s-3-D)/2} e^{-m^2 t}$$
$$= \frac{V_\Sigma}{(4\pi)^{D/2}} \frac{\Gamma\left[(s-1-D)/2\right]}{\Gamma\left[(s-1)/2\right]} (m^2)^{(D+1)/2} (m^2\ell^2)^{-s/2}, \quad (4.30)$$

if we use (4.27) again. In order that this last step be justified we must assume $\mathcal{R}(s) > D+1$; however, the result in (4.30) may now be analytically continued throughout the complex s-plane using properties of the Γ-function.

We now need to evaluate $E(s=0)$. Whether or not the result in (4.30) is analytic at $s=0$ is determined by the properties of the Γ-functions occurring. The basic properties we need are summarized in Section A1.1. $\Gamma(z)$ is analytic if $\mathcal{R}(z) > 0$ and has simple poles on the real axis at $z = 0, -1, -2, \ldots$. The Laurent expansion about the poles is given in (A1.5), (A1.8), (A1.12), and (A1.16). In (4.30) the only poles at $s=0$ can come from $\Gamma[(s-1-D)/2]$, and these can only occur if D is odd. If D is even we can conclude that $E(s)$ is analytic at $s=0$ with the result

$$E(0) = \frac{V_\Sigma}{(4\pi)^{D/2}} \frac{\Gamma\left[-(D+1)/2\right]}{\Gamma\left[-(1/2)\right]} (m^2)^{(D+1)/2}$$
$$= V_\Sigma \left(-\frac{1}{\pi}\right)^{D/2} \frac{(D/2)!}{(D+1)!} (m^2)^{(D+1)/2}, \quad (4.31)$$

if we use (A1.20) to simplify the expressions in the Γ-functions. The quantum correction to the effective potential therefore contains

$$V_{\text{eff}}^{(1)} = \frac{\hbar}{2} \left(-\frac{1}{\pi}\right)^{D/2} \frac{(D/2)!}{(D+1)!} (m^2)^{(D+1)/2}, \quad (4.32)$$

if the spatial dimension D is even. (Note from (4.22) that $|f_n(\mathbf{x})|^2 = 1/V_\Sigma$ is constant so (4.21) can be used.)

When D is odd $\Gamma[(s-1-D)/2]$ has a simple pole at $s=0$. If we expand about the pole we find

$$E(0) = -\frac{V_\Sigma}{[(D+1)/2]!} \left(-\frac{m^2}{4\pi}\right)^{(D+1)/2} \Big[\frac{2}{s} - 1 + \frac{1}{2} + \frac{1}{3} + \ldots$$
$$+ \frac{2}{D+1} - \ln\Big(\frac{\ell^2 m^2}{4}\Big)\Big]. \quad (4.33)$$

The quantum part of the effective potential is therefore

$$V_{\text{eff}}^{(1)} = -\frac{\hbar}{2\,[(D+1)/2]!}\left(-\frac{m^2}{4\pi}\right)^{(D+1)/2}\Big[\,\frac{2}{s} - 1 + \frac{1}{2} + \frac{1}{3} + \cdots + \frac{2}{D+1} - \ln\Big(\frac{\ell^2 m^2}{4}\Big)\Big], \quad (4.34)$$

in the case where the spatial dimension D is odd.

There are two obvious differences between the results found for even and odd D. In the case where D is odd, $V_{\text{eff}}^{(1)}$ has a simple pole at $s = 0$ and in addition depends on the arbitrary length scale ℓ. For even D the effective potential $V_{\text{eff}}^{(1)}$ is finite at $s = 0$ and has no dependence on ℓ. As we will discuss later the presence of the pole term in $1/s$ as $s \to 0$ and the dependence on ℓ are linked.

In either case we get the complete effective potential by combining $V_{\text{eff}}^{(1)}$ with $V^{(0)}$, where $V^{(0)}$ comes from the classical Lagrangian. We have taken $U'(\varphi) = 0$ in (4.7) so that we have a free field theory. This means that $U(\varphi)$ is a constant independent of φ. We can write

$$V_{\text{eff}}^{(0)} = \frac{1}{2}m^2\bar{\varphi}^2 + c + \frac{1}{2}|\nabla\bar{\varphi}|^2, \quad (4.35)$$

where c is an arbitrary constant. At this stage we can introduce the concept of renormalization. Because our example is so simple, $V_{\text{eff}}^{(1)}$ has no dependence on the background field $\bar{\varphi}$ in this case. The only effect of quantum corrections to the classical theory was to alter the value of the constant term in the potential. Generally what we wish to do is to try and identify terms in the effective action with physically measurable quantities. As a step in this direction we will impose renormalization conditions on the effective action. In our simple example above, this entails only a condition on the constant term in the potential. Because we are considering flat Minkowski spacetime here the natural condition to impose is that the ground state energy vanishes. This is natural because any non-zero value for the ground state energy would lead to a curvature of spacetime using the Einstein equations of general relativity. (The argument often given is that only energy differences have any physical meaning, therefore the absolute value of the energy scale can be set to zero.) We therefore impose a renormalization condition

$$V_{\text{eff}}(\bar{\varphi} = 0) = 0, \quad (4.36)$$

which fixes

$$0 = c + V_{\text{eff}}^{(1)}. \quad (4.37)$$

This leaves us with simply

$$V_{\text{eff}} = \frac{1}{2}m^2\bar{\varphi}^2 + \frac{1}{2}|\nabla\bar{\varphi}|^2, \tag{4.38}$$

in this case. The quantum correction to the classical potential energy makes no contribution for this simple example. We will return to this process of renormalization with a less trivial example in subsequent sections.

At this stage we can reconsider the process of normal ordering the Hamiltonian. Had we normal ordered H we would have obtained exactly the same conclusion as in (4.38) without doing any work at all. However, if we do normal order H we will always obtain $\langle 0|H|0\rangle = 0$ for any choice of Σ. As we will show, this is not the correct thing to do. If we are only interested in field theory in flat Minkowski spacetime, then normal ordering H is completely equivalent to imposing the renormalization condition (4.36).

4.3 Casimir effect

A more interesting example of the evaluation of the effective potential occurs if instead of regarding Σ as infinite space, we introduce some boundaries. A prototype for this calculation is the Casimir effect (Casimir (1948)) which is concerned with vacuum fluctuations in the electromagnetic field between two uncharged parallel conducting plates. In this section we will consider the scalar field analogue of this. We will take a massive real scalar field which satisfies Dirichlet boundary conditions at $x^1 = 0$ and $x^1 = L_1$ but is unconfined in the remaining directions.[5] We will deal with the directions where the field is not confined by again imposing periodic boundary conditions on the field in these directions and then taking the infinite volume limit. The mode functions, which are normalized eigenfunctions of the Laplacian, are

$$f_{\mathbf{n}}(\mathbf{x}) = \left(\frac{2}{V_\Sigma}\right)^{1/2} \sin\left(\frac{\pi n_1 x^1}{L_1}\right) \prod_{j=2}^{D} e^{\left(2\pi i n_j x^j/L_j\right)}, \tag{4.39}$$

where $n_1 = 1, 2, \ldots$ and $n_j = 0, \pm 1, \pm 2, \ldots$ for $j = 2, \ldots, D$.[6] It is easy to see that

$$\sigma_{\mathbf{n}} = \left(\frac{\pi n_1}{L_1}\right)^2 + \sum_{j=2}^{D}\left(\frac{2\pi n_j}{L_j}\right)^2. \tag{4.40}$$

[5] Dirichlet boundary conditions means that the field vanishes at $x^1 = 0$ and $x^1 = L_1$.

[6] Note that $n_1 = 0$ is not allowed because it leads to $f_n(\mathbf{x}) = 0$ which is not a normalizable eigenfunction.

The energy ζ-function becomes

$$E(s) = \sum_{n_1=1}^{\infty} \sum_{n_2=-\infty}^{\infty} \cdots \sum_{n_D=-\infty}^{\infty} \ell^{-s} (\sigma_{\mathbf{n}} + m^2)^{(1-s)/2}$$
$$= \ell^{-s} L_2 \cdots L_D \sum_{n_1=1}^{\infty} \int \frac{d^{D-1}p}{(2\pi)^{D-1}} \left[\left(\frac{\pi n_1}{L_1} \right)^2 + \mathbf{p}^2 + m^2 \right]^{(1-s)/2} \tag{4.41}$$

if we take $L_2, \ldots, L_D$ very large and replace the sums over $n_2, \ldots, n_D$ with integrals. The integration over $\mathbf{p}$ is performed exactly as described in the previous section with the result

$$E(s) = \ell^{-s} \frac{L_2 \cdots L_D}{(4\pi)^{(D-1)/2}} \frac{\Gamma\left[(s-D)/2\right]}{\Gamma\left[(s-1)/2\right]} \sum_{n_1=1}^{\infty} \left[\left(\frac{\pi n_1}{L_1} \right)^2 + m^2 \right]^{(D-s)/2} . \tag{4.42}$$

If we wish to keep L_1 finite we cannot just replace the sum over n_1 in (4.42) with an integral as we have done up to now. We will first proceed more heuristically and examine the limit where $mL_1 << 1$. Later we will return to the exact result.

Physically the limit $mL_1 << 1$ corresponds to the Compton wavelength of the scalar field much larger than the separation between the two idealized parallel plates located at the boundaries $x^1 = 0$ and $x^1 = L_1$ of Σ. This limit is of interest if we also wish to examine the massless limit of the theory. For $mL_1 << 1$, we may expand the argument of the sum in (4.42) in powers of mL_1 using the binomial expansion. We will specialize to the case $D = 3$ here since this is of most direct physical interest. (We will give the result for general D later when we evaluate the exact expression.) If we keep only the first few terms in the expansion we find

$$E(s) = \frac{L_2 L_3}{4\pi \ell^s} \left(\frac{2}{s-3} \right) \left(\frac{\pi}{L_1} \right)^{3-s} \sum_{n_1=1}^{\infty} n_1^{3-s} \left[1 + \left(\frac{3-s}{2} \right) \left(\frac{mL_1}{\pi n_1} \right)^2 \right.$$
$$\left. + \frac{1}{2} \left(\frac{3-s}{2} \right) \left(\frac{1-s}{2} \right) \left(\frac{mL_1}{\pi n_1} \right)^4 \right]$$
$$= \frac{L_2 L_3}{4\pi \ell^s} \left(\frac{\pi}{L_1} \right)^{3-s} \left[\frac{2}{(s-3)} \zeta(s-3) - \left(\frac{mL_1}{\pi} \right)^2 \zeta(s-1) \right.$$
$$\left. - \frac{1}{4}(1-s) \left(\frac{mL_1}{\pi} \right)^4 \zeta(s+1) \right] . \tag{4.43}$$

The definition of the Riemann ζ-function $\zeta(s) = \sum_{n=1}^{\infty} n^{-s}$ for $\mathcal{R}(s) > 1$ has been used here. (See Appendix A1.2 for a brief summary of the properties of the Riemann ζ-function.) Using results given in Sections A1.1 and A1.2, and noting that $V_\Sigma = L_1 L_2 L_3$, we find

$$V_{\text{eff}}^{(1)} = \frac{\hbar\pi^2}{8L_1^4}\left\{-\frac{1}{180} + \frac{1}{12}\left(\frac{mL_1}{\pi}\right)^2 - \frac{1}{4}\left(\frac{mL_1}{\pi}\right)^4\left[\frac{1}{s} + \gamma - \ln\left(\frac{\pi\ell}{L_1}\right)\right]\right\}. \tag{4.44}$$

If we compare the result (4.44) with (4.34) where $D = 3$ is used, it can be observed that the pole parts of both expressions are the same (i.e., both expressions have the same coefficients of $1/s$). The divergent part of the effective potential is not sensitive to whether Σ is infinite space or a semi-infinite space with two parallel plane boundaries. A consequence of this is that a natural procedure to adopt is to fix the constant c which occurs in the classical potential to be the same as it was in infinite flat space. If we do this then we are guaranteed that as we let $L_1 \to \infty$ the energy associated with the ground state will vanish. The renormalized effective potential becomes (to the order of mL_1 that we are working)

$$\begin{aligned} V_{\text{eff}} = \frac{1}{2}|\nabla\bar{\varphi}|^2 + \frac{1}{2}m^2\bar{\varphi}^2 - \frac{\pi^2\hbar}{1440L_1^4}\left[1 - 15\left(\frac{mL_1}{\pi}\right)^2\right] \\ - \frac{\hbar m^4}{32\pi^2}\left[\frac{1}{4} + \gamma + \frac{1}{2}\ln\left(\frac{m^2L_1^2}{4\pi^2}\right)\right]. \end{aligned} \tag{4.45}$$

In this case there is a non-zero energy associated with the vacuum state. If we take the limit of a massless theory by letting $m \to 0$, we are left with simply

$$V_{\text{eff}} = \frac{1}{2}|\nabla\bar{\varphi}|^2 - \frac{\pi^2\hbar}{1440L_1^4}. \tag{4.46}$$

This result is exact.

The result in (4.46) has an immediate physical consequence. We may first set $\bar{\varphi} = 0$ since this should represent the ground state of the theory. If we take the planes $x^1 = 0$ and $x^1 = L_1$ to represent physical boundaries, such as a pair of parallel uncharged conducting plates whose area $A = L_2 L_3$ is very large in comparison to their separation L_1, then (4.46) tells us that the total energy associated with the vacuum is

$$E_{\text{vac}} = -\frac{\hbar\pi^2 A}{1440L_1^3}. \tag{4.47}$$

This is observed to be negative and is solely a consequence of quantum effects. It is half of the result found originally by Casimir (1948). The reason for the factor of one-half between our result and that of Casimir is easily understood as a consequence of the fact that for the electromagnetic field there are two possible polarizations; the scalar field having spin 0 has only one possible spin state. What this negative energy means physically is that work must be done to keep the two parallel plates apart. Thus the two plates will attract each other. If we move the plates from separation L_1 to $L_1 + \delta L_1$, the force we must apply is F_{app} given by

$$F_{\text{app}} \delta L_1 = \delta E_{\text{vac}}, \tag{4.48}$$

where δE_{vac} represents the change in the vacuum energy. The attractive force between the plates is just the negative of the applied force, so that

$$F = -\frac{\partial E_{\text{vac}}}{\partial L_1} = -\frac{\hbar \pi^2 A}{240 L_1^4} \tag{4.49}$$

represents the force between the plates. The force between them varies as L_1^{-4} where L_1 is the separation. This was first looked for by Sparnaay (1958), and later demonstrated in subsequent experiments (see Lamoreaux (1999) for example). The real experiment pertains to the electromagnetic field, so that the result should be twice as big as (4.49).

4.4 Constant gauge field background

Suppose that we consider a complex scalar field Φ coupled to an electromagnetic gauge field A_μ. The classical action functional for the scalar field is

$$S_{\text{scalar}} = \int_{t_1}^{t_2} dt \int_\Sigma d\sigma_x \left[(D_\mu \Phi)^\dagger (D^\mu \Phi) - m^2 \Phi^\dagger \Phi + c \right], \tag{4.50}$$

if we do not include scalar self-interactions. Here

$$D_\mu \Phi = \partial_\mu \Phi - ieA_\mu \tag{4.51}$$

is the gauge covariant derivative and c is an arbitrary constant that we expect to be needed to renormalize the vacuum energy. If we take

$$\Phi'(t, \mathbf{x}) = e^{ie\theta(t,\mathbf{x})} \Phi(t, \mathbf{x}) \tag{4.52}$$

as our local gauge transformation, then

$$A'_\mu(t, \mathbf{x}) = A_\mu(t, \mathbf{x}) + \partial_\mu \theta(t, \mathbf{x}), \tag{4.53}$$

for the theory to have local gauge invariance. To the scalar field action (4.50) we must add the action for the electromagnetic field which is

$$S_{\rm em} = -\frac{1}{4}\int_{t_1}^{t_2} dt \int_\Sigma d\sigma_x \; F_{\mu\nu}F^{\mu\nu}, \tag{4.54}$$

to obtain the total action ($F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$). The field equations which follow from varying (4.50) and (4.54) with respect to $\Phi^\dagger$ and A_μ are

$$D^\mu D_\mu \Phi + m^2\Phi = 0, \tag{4.55}$$

$$\partial_\nu F^{\mu\nu} = ie(\Phi^\dagger\partial^\mu\Phi - \partial^\mu\Phi^\dagger\Phi) + 2e^2A^\mu\Phi^\dagger\Phi. \tag{4.56}$$

The last equation can be recognized as the Maxwell equations with a current source derived from the scalar field. The current source corresponds to the Noether current arising from local gauge symmetry. There is also another equation which is simply the Hermitian conjugate of (4.55). We are free to impose a gauge condition on A_μ.

In this example instead of working out the effective action for the scalar field as we have done before, we will look at the effective action for the electromagnetic field. We will therefore set the value of the background scalar field to zero and write

$$A_\mu = \bar{A}_\mu + a_\mu, \tag{4.57}$$

where $\bar{A}_\mu$ represents the background vector potential, and a_μ represents the fluctuation about the background. If we linearize the equations of motion (4.55) and (4.56) in the fluctuations about the background fields, we find

$$\bar{D}_\mu\bar{D}^\mu\Phi + m^2\Phi = 0, \tag{4.58}$$

$$\partial_\nu f^{\mu\nu} = 0, \tag{4.59}$$

where $f_{\mu\nu} = \partial_\mu a_\nu - \partial_\nu a_\mu$, and $\bar{D}_\mu$ is like D_μ in (4.51) but with A_μ replaced with the background field $\bar{A}_\mu$. The linearized Maxwell equation (4.59) has no dependence on the background field $\bar{A}_\mu$. If we are only interested in the contribution to the effective action which has a dependence on $\bar{A}_\mu$, we can ignore the zero-point energy from the vector field since, although it will not vanish, it can have no background field dependence. This would no longer be true if we included scalar field self-interactions with a non-zero background scalar field. Written out in detail (4.58) becomes[7]

$$0 = \Box\Phi - ie(\partial_\mu\bar{A}^\mu)\Phi - 2ie\bar{A}^\mu\partial_\mu\Phi - e^2\bar{A}^\mu\bar{A}_\mu\Phi + m^2\Phi. \tag{4.60}$$

[7] There is also the Hermitian conjugate of this equation.

Suppose that we take $\Sigma = \mathbb{R}^{D-1} \times \mathbb{S}^1$ where the x coordinate obeys $0 \leq x \leq L$ with $x = 0$ and $x = L$ identified to give the topology of a circle.[8] As before we can deal with the $D-1$ non-compact dimensions by imposing box normalization and taking the large box limit. The space here is like that for the Casimir effect in the last example, except that instead of adopting Dirichlet (vanishing) boundary conditions in the x-direction we choose periodic ones. The background electromagnetic field classically must satisfy $\partial_\nu \bar{F}^{\mu\nu} = 0$. An obvious solution to this is $\bar{F}^{\mu\nu} = 0$, corresponding to no electromagnetic field present. This would be expected to describe the ground state. If we impose the radiation gauge condition

$$\bar{A}_0 = 0, \qquad \nabla \cdot \bar{\mathbf{A}} = 0, \tag{4.61}$$

then a solution to $\bar{F}^{\mu\nu} = 0$ is $\bar{\mathbf{A}} = \vec{\alpha}$ where $\vec{\alpha}$ is an arbitrary constant vector. Normally by performing the gauge transformation $\bar{\mathbf{A}}' = \bar{\mathbf{A}} + \nabla\theta$ and choosing $\theta = -\vec{\alpha} \cdot \mathbf{x}$, we can see that without loss of generality we can choose $\bar{\mathbf{A}}' = 0$. However, if the space Σ is not simply connected there is a problem with this. Because we have identified $x = 0$ with $x = L$ to give a circle, the gauge transformation required to set $\alpha_x = 0$ (where α_x is the x-component of $\vec{\alpha}$) is not single-valued: $\theta(x = L) = -\alpha_x L + \theta(x = 0)$. This means that if our original scalar field Φ satisfies periodic boundary conditions on the circle, when we perform the gauge transformation (4.52), we end up with a field Φ' which is no longer periodic; the boundary conditions are changed by the gauge transformation because it is not single-valued. There are two equivalent ways we can deal with this. The first is to restrict ourselves to single-valued gauge transformations. This allows us to regard the boundary conditions imposed on the fields as fixed. However, we must then take $\bar{\mathbf{A}} = \vec{\alpha}$ to be non-zero since we are not allowed to perform the gauge transformation required to set it to zero. The second viewpoint is to allow gauge transformations that are not single-valued. In this case we are allowed to set $\bar{\mathbf{A}} = 0$. However, we can no longer fix the boundary conditions on the scalar fields. The boundary conditions must be allowed to vary in a way which depends on the arbitrary constant vector $\vec{\alpha}$.

In the case of $\Sigma = \mathbb{R}^{D-1} \times \mathbb{S}^1$, we may set all components of $\bar{\mathbf{A}}$ to zero except for the x-component chosen as

$$\bar{A}_x = \alpha. \tag{4.62}$$

Take the scalar field Φ to be periodic around the circle: $\Phi(x = L) = \Phi(x = 0)$. If we allow gauge transformations which are not single-valued,

[8] In other words, we impose periodic boundary conditions in one of the spatial directions.

then by choosing $\theta = -\alpha x$ the gauge transformed field Φ' in (4.52) will obey

$$\Phi'(x = L) = e^{-ie\alpha L}\Phi'(x = 0). \tag{4.63}$$

The gauge transformed field changes by a phase. We now have $\bar{\mathbf{A}}' = 0$ so that (4.60) becomes

$$0 = \Box\Phi' + m^2\Phi'. \tag{4.64}$$

We wish to solve (4.64) with the boundary condition (4.63). Write

$$f_n(\mathbf{x}) = e^{i\kappa x}\prod_{j=2}^{D} e^{(2\pi i n_j x^j/L_j)}. \tag{4.65}$$

where the constant κ is chosen so that (4.63) holds. It is easy to see that

$$E_n = \left[\kappa^2 + \sum_{j\,=\,2}^{D}\left(\frac{2\pi n_j}{L_j}\right)^2 + m^2\right]^{1/2}. \tag{4.66}$$

Demanding that $f_n(\mathbf{x})$ satisfies (4.63) results in

$$e^{i\kappa L} = e^{-ie\alpha L}. \tag{4.67}$$

This is satisfied if $\kappa L = -e\alpha L + 2\pi n_1$, for $n_1 = 0, \pm1, \pm2, \ldots$. We then find E_n in (4.66) to be

$$E_n = \left[\left(\frac{2\pi n_1}{L} - e\alpha\right)^2 + \sum_{j\,=\,2}^{D}\left(\frac{2\pi n_j}{L_j}\right)^2 + m^2\right]^{1/2}. \tag{4.68}$$

The quantum part of the effective potential is

$$V_{\text{eff}}^{(1)} = \frac{\hbar}{V_\Sigma}E(0), \tag{4.69}$$

where $E(s)$ is the energy ζ-function defined in (4.16). This differs by a factor of 2 from the expression given in (4.21) because we have a complex scalar field with two real degrees of freedom here. Taking the large box limit for the $D-1$ non-compact dimensions and proceeding as in our previous examples, we find

$$\begin{aligned} E(s) = {} & \frac{L_2\cdots L_D}{(4\pi)^{(D-1)/2}}\ell^{-s}\frac{\Gamma\left[(s-D)/2\right]}{\Gamma\left[(s-1)/2\right]} \\ & \times \sum_{n_1=-\infty}^{\infty}\left[\left(\frac{2\pi n_1}{L} - e\alpha\right)^2 + m^2\right]^{(D-s)/2}. \end{aligned} \tag{4.70}$$

The remaining sum is similar to that we encountered for the Casimir effect in Section 4.3. A method to evaluate it is given in Section A1.3. Using the notation of Section A1.3, we find

$$E(s) = \frac{V_\Sigma}{(4\pi)^{D/2}}\ell^{-s}\frac{\Gamma\left[(s-D-1)/2\right]}{\Gamma\left[(s-1)/2\right]}m^{D+1-s} + \frac{4V_\Sigma}{(4\pi)^{(D-1)/2}L}\ell^{-s}\left(\frac{2\pi}{L}\right)^{D-s}\frac{f_{(s-D)/2}\left(e\alpha L/2\pi, mL/2\pi\right)}{\Gamma\left[(s-1)/2\right]\Gamma\left[1+(D-s)/2\right]}. \tag{4.71}$$

$f_\lambda(a,b)$ is the integral given in (A1.65).

The first term on the right-hand side of the energy ζ-function may be seen to be identical to that found in (4.30). As $s \to 0$ this term is finite for even D and has a simple pole for odd D. All of the physical consequences of the non-trivial topology of the circle are contained in the second term of (4.71). If we impose the renormalization condition that $V_{\text{eff}} = 0$ as $L \to \infty$, we are left with

$$V_{\text{eff}} = -\frac{4\hbar\pi^{1+D/2}}{L^D\Gamma\left[1+(D/2)\right]}f_{-D/2}\left(\frac{e\alpha L}{2\pi}, \frac{mL}{2\pi}\right). \tag{4.72}$$

as the renormalized effective potential. The background gauge field enters through the constant α. We can now look at the stationary points of V_{eff} to find the ground state, since for α constant the minima of V_{eff} should give the effective field equations.[9]

Minimizing V_{eff} entails knowing the stationary points of $f_{-D/2}(a,b)$. If we assume a and b to be real here, then

$$\frac{\partial}{\partial a}f_{-D/2}(a,b) = -2\pi\Im\int_b^\infty (x^2-b^2)^{D/2}\frac{e^{2\pi(x+ia)}}{\left[e^{2\pi(x+ia)}-1\right]^2}dx, \tag{4.73}$$

where $\Im$ denotes the imaginary part. It is obvious that the integrand in (4.73) will have a non-vanishing imaginary part unless $e^{2\pi ia}$ is real. We therefore have $(\partial/\partial a)f_{-D/2}(a,b) = 0$, when a is an integer or a half-integer: $a = k/2$ for $k = 0, \pm 1, \ldots$. To see if $a = k/2$ corresponds to a maximum or a minimum we simply need to compute the sign of the second derivative of $f_{-D/2}(a,b)$ with respect to a evaluated at $a = k/2$. A straightforward calculation shows that

$$\text{sign}\left[\frac{\partial^2}{\partial a^2}f_{-D/2}(a,b)\right]\Bigg|_{a=k/2} = (-1)^k. \tag{4.74}$$

[9] Even if we adopt a different renormalization prescription the first term in (4.71) is independent of α and therefore will not contribute to the effective field equations.

Thus $f_{-D/2}(a,b)$ has a minimum when k is an even integer and a maximum when k is an odd integer. Because of the overall minus sign in (4.72) we conclude that the effective potential has a minimum when $e\alpha L = 2\pi l + \pi$ for $k = 0, \pm 1, \ldots$, and a maximum when $e\alpha L = 2\pi k$ for $k = 0, \pm 1, \ldots$. It is interesting to note that if we had chosen $\alpha = 0$ we would not have found the ground state. To express this another way, the gauge potential $\bar{A}_\mu = 0$ is not a stable solution to the Maxwell equations.[10] The ground state is determined by

$$e\alpha = \frac{\pi}{L}(2k+1), \tag{4.75}$$

for $k = 0, \pm 1, \ldots$. This ground state has been found from the quantum part of the effective potential. Classically the value of α can be any real number and the ground state is continuously degenerate. Quantum effects result in a discrete set of possible values for α which lifts the ground state degeneracy from a continuum to be denumerable. Finally we note that the value of the ground state fixes the boundary conditions on the scalar field to be anti-periodic, as is evident from using (4.75) in (4.63).

4.5 Constant magnetic field

We now consider a complex scalar field in a constant background magnetic field. The eigenfunctions $f_n(\mathbf{x})$ must satisfy

$$-\mathbf{D}^2 f_n(\mathbf{x}) = \sigma_n f_n(\mathbf{x}), \tag{4.76}$$

where $\mathbf{D} = \nabla - ie\mathbf{A}$. $\mathbf{A}$ is the vector potential which gives rise to the constant magnetic field. We are free to fix a gauge condition on $\mathbf{A}$ and we choose the radiation gauge $A^0 = 0$ with $\nabla \cdot \mathbf{A} = 0$. Take Σ to be a box with sides $L_1, \ldots, L_D$ with boundary conditions on the walls of the box to be specified. We will only take $F_{12} = -F_{21} = B$ to be non-zero, corresponding to a constant magnetic field in the z-direction. With the radiation gauge condition imposed, we may pick

$$A_1 = \alpha y + a_1, \qquad A_2 = (B+\alpha)x + a_2, \tag{4.77}$$

where α, a_1, a_2 are arbitrary constants. We have labelled $x^1 = x$ and $x^2 = y$ for simplicity of notation here. The constant α can be freely chosen to be what we like (popular choices are $\alpha = 0$ or $-B/2$), but as we saw in Section 4.4 it will not be possible to remove the constants a_1 and a_2

[10] This conclusion was first observed by Ford (1980).

with a single-valued gauge transformation in general. We must therefore solve

$$-\Big\{\Big(\frac{\partial}{\partial x}-ie\alpha y-iea_1\Big)^2+\Big(\frac{\partial}{\partial y}-ie(B+\alpha)x-iea_2\Big)^2 +\sum_{j=3}^{D}\frac{\partial^2}{\partial {x^j}^2}\Big\}f_n(\mathbf{x})=\sigma_n f_n(\mathbf{x}). \tag{4.78}$$

The boundary conditions on $f_n(\mathbf{x})$ remain to be specified. It is tempting to simply demand that $f_n(\mathbf{x})$ satisfy periodic boundary conditions on the walls of the box, but there is a problem with this. Unlike the cases we have considered up until now, the operator in (4.78) is not periodic in the spatial coordinates. There is no problem with imposing periodic boundary conditions in the coordinates $x^3,\ldots,x^D$, but the operator is not periodic in x and y. If we translate $x\to x+L_1$, we see from (4.77) that $A_2\to A_2+(B+\alpha)L_1$. Similarly if we translate $y\to y+L_2$, we see that $A_1\to A_1+\alpha L_2$. There is no choice of α we can make to eliminate both changes in the vector potential simultaneously. The key to dealing with this is to regard the transformations of $\mathbf{A}$ arising from spatial translations as gauge transformations. We can then obtain covariance of the eigenvalue equation (4.78) by performing a gauge transformation on $f_n(\mathbf{x})$ at the same time as we translate the coordinates x and y. Let

$$f_n(x+L_1,y)=e^{i\theta_x}f_n(x,y), \tag{4.79}$$

$$f_n(x,y+L_2)=e^{i\theta_y}f_n(x,y), \tag{4.80}$$

for some functions θ_x and θ_y. We will fix θ_x and θ_y by requiring that when $x\to x+L_1$,

$$D_2f_n(x,y)\to e^{i\theta_y}f_n(x,y), \tag{4.81}$$

and when $y\to y+L_2$ we have[11]

$$D_1f_n(x,y)\to e^{i\theta_x}f_n(x,y). \tag{4.82}$$

To summarize, we demand that on the walls of the box the eigenfunctions $f_n(\mathbf{x})$ (and hence the scalar field) are only periodic up to a phase factor (or gauge transformation).

It is easy to find θ_x and θ_y using (4.81) and (4.82). We can choose

$$\theta_x=e(B+\alpha)L_1y, \tag{4.83}$$

$$\theta_y=e\alpha L_2x. \tag{4.84}$$

[11] Here $D_1=(\partial/\partial x)-ieA_1$ with a similar expression for D_2.

Because θ_x and θ_y involve the coordinates x and y it is not clear that the boundary conditions we have chosen may be imposed in a consistent manner. Because the order that we perform translations in the x and y directions should not matter we must require that a translation $x \to x + L_1$ followed by $y \to y + L_2$ has the same result on $f_n(\mathbf{x})$ as the translation $y \to y + L_2$ followed by $x \to x + L_1$, since both result in $f_n(x + L_1, y + L_2)$. Using (4.79) with (4.83) we find

$$f_n(x + L_1, y) = e^{ie(B+\alpha)L_1 y} f_n(x, y).$$

Performing the translation in the y-direction using (4.80) with (4.84) now results in

$$f_n(x + L_1, y + L_2) = e^{ie(B+\alpha)L_1(y+L_2)+ie\alpha L_2 x} f_n(x, y). \tag{4.85}$$

If we translate first in the y-direction using (4.80) with (4.84), we find

$$f_n(x, y + L_2) = e^{ie\alpha L_2 x} f_n(x, y).$$

Translation of this in the x-direction gives

$$f_n(x + L_1, y + L_2) = e^{ie\alpha L_2(x+L_1)+ie(B+\alpha)L_1 y} f_n(x, y). \tag{4.86}$$

Demanding equality of the two expressions (4.85) and (4.86) results in

$$e^{ieBL_1L_2} = 1. \tag{4.87}$$

This requires

$$eBL_1L_2 = 2\pi k. \tag{4.88}$$

for some integer k. This consistency condition is independent of the arbitrary gauge parameter α as well as the constants a_1 and a_2. The physical interpretation of (4.88) is that the magnetic flux through the sides of the box must be quantized for the theory to be consistent.

The next task is to solve for the eigenvalues σ_n in (4.78). Because of the boundary conditions (4.79) and (4.80) on the eigenfunctions, this is not so straightforward. First of all define

$$\tilde{f}_n(x, y) = e^{-ie\alpha xy} f_n(x, y), \tag{4.89}$$

where the factor of $e^{-ie\alpha xy}$ is chosen so that

$$\tilde{f}_n(x, y + L_2) = \tilde{f}_n(x, y). \tag{4.90}$$

The boundary condition in the x-direction is

$$\tilde{f}_n(x + L_1, y) = e^{ieBL_1 y} \tilde{f}_n(x, y). \tag{4.91}$$

We can substitute for $\tilde{f}_n(\mathbf{x})$ in (4.78) to find

$$-\Big[\Big(\frac{\partial}{\partial x}-iea_1\Big)^2+\Big(\frac{\partial}{\partial y}-ieBx-iea_2\Big)^2+\sum_{j=3}^{D}\frac{\partial}{\partial x^{j\,2}}\Big]\tilde{f}_n(\mathbf{x})=\sigma_n\tilde{f}_n(\mathbf{x}). \tag{4.92}$$

In addition to simplifying the boundary condition in the y-direction, the transformation (4.89) shows that the gauge parameter α has cancelled out of the equation and therefore does not affect the eigenvalues, as would be expected.

Because $\tilde{f}_n(x,y,x^3,\ldots,x^D)$ is periodic in x^j, where $j=3,\ldots,D$ with period L_j we can Fourier expand it as

$$\tilde{f}_n(x,y,x^3,\ldots,x^D)=(L_3\cdots L_D)^{-1/2}\exp\left(2\pi i\sum_{j=3}^{D}\frac{n_jx^j}{L_j}\right)\varphi_n(x,y). \tag{4.93}$$

Here $n_j=0,\pm1,\pm2,\ldots$ and $\varphi_n(x,y)$ satisfies

$$\left[-\left(\frac{\partial}{\partial x}-iea_1\right)^2-\left(\frac{\partial}{\partial y}-ieBx-iea_2\right)^2+\sum_{j=3}^{D}\left(\frac{2\pi n_j}{L_j}\right)^2\right]\varphi_n =\sigma_n\varphi_n, \tag{4.94}$$

with the boundary conditions (4.91) and $\varphi_n(x,y+L_2)=\varphi_n(x,y)$. Because $\varphi_n(x,y)$ is periodic in y, we can Fourier expand it as[12]

$$\varphi_n(x,y)=L_2^{-1/2}\sum_{l=-\infty}^{\infty}c_l(x)e^{(2\pi ily/L_2)}. \tag{4.95}$$

Substitution into (4.94) leads to

$$\left[-\left(\frac{\partial}{\partial x}-iea_1\right)^2-\left(\frac{2\pi l}{L_2}-eBx-ea_2\right)^2+\sum_{j=3}^{D}\left(\frac{2\pi n_j}{L_j}\right)^2\right]c_l(x) =\sigma_nc_l(x). \tag{4.96}$$

[12] For simplicity of notation we will suppress the label n on $c_l(x)$.

The remaining boundary condition (4.91) turns into a condition on $c_l(x)$. We have

$$L_2^{-1/2}\sum_{l=-\infty}^{\infty} c_l(x+L_1)e^{2\pi ily/L_2} = e^{ieBL_1y}L_2^{-1/2}\sum_{l=-\infty}^{\infty} c_l(x)e^{2\pi ily/L_2}, \tag{4.97}$$

if we use (4.95). However, $eBL_1 = 2\pi k/L_2$ from (4.88). This allows us to simplify (4.97):

$$\begin{aligned}\sum_{l=-\infty}^{\infty} c_l(x+L_1)e^{2\pi ily/L_2} &= \sum_{l=-\infty}^{\infty} c_l(x)e^{(2\pi i/L_2)(k+l)y} \\ &= \sum_{l=-\infty}^{\infty} c_{l-k}(x)e^{2\pi ily/L_2},\end{aligned}$$

where the second line has followed by relabelling the summation index. It therefore follows that we must solve (4.96) with $c_l(x)$ obeying the condition

$$c_l(x+L_1) = c_{l-k}(x). \tag{4.98}$$

The solution to (4.96) proceeds as in the case of the simple harmonic oscillator. Define

$$D_\pm = i\frac{\partial}{\partial x} + ea_1 \pm i\left(\frac{2\pi l}{L_2} - ea_2 - eBx\right). \tag{4.99}$$

It is easy to show that these two operators obey

$$[D_+, D_-] = -2eB, \tag{4.100}$$

and that (4.96) may be written as

$$[D_+D_- + eB]c_l(x) = \tilde{\sigma}_n c_l(x), \tag{4.101}$$

with

$$\tilde{\sigma}_n = \sigma_n - \sum_{j=3}^{D}\left(\frac{2\pi n_j}{L_j}\right)^2. \tag{4.102}$$

Because of (4.100) we have

$$[D_+D_-, D_+] = 2eBD_+, \tag{4.103}$$

$$[D_+D_-, D_-] = -2eBD_-. \tag{4.104}$$

Comparison of these results with those found for the simple harmonic oscillator in Section 3.5 shows that we may interpret D_+ as a raising

operator and D_- as a lowering operator. The argument given for the existence of a state of lowest energy may be repeated here to conclude that there must exist an eigenvector $c_l^{(0)}$ satisfying

$$D_- c_l^{(0)}(x) = 0. \tag{4.105}$$

It is easily seen that

$$\tilde{\sigma}_0 = eB \tag{4.106}$$

is the corresponding eigenvalue. Because D_+ acts like a raising operator, we expect that $c_l^{(m)} \propto D_+^m c_l^{(0)}$ with eigenvalue

$$\tilde{\sigma}_m = (2m+1)eB, \tag{4.107}$$

since each application of D_+ will increase the eigenvalue by $2eB$.[13] The eigenvalues in (4.96) are therefore given by

$$\sigma_n = (2m+1)eB + \sum_{j=3}^{D} \left(\frac{2\pi n_j}{L_j} \right)^2, \tag{4.108}$$

where $m = 0, 1, 2, \ldots$. It can be noted that the arbitrary phases a_1 and a_2 do not enter the eigenvalue. Because the eigenvalue depends only on $(D-1)$ quantum numbers (m and n_j for $j = 3, \ldots, D$), it must have a degeneracy that we need to determine. This can be done from studying the eigenfunctions corresponding to the eigenvalues (4.108).

The determination of the eigenfunctions is more complicated than in the case of the simple harmonic oscillator because of the need to satisfy the condition (4.98). However, if we can find the eigenfunction corresponding to the lowest eigenvalue, all of the rest are determined by repeated application of D_+. The eigenfunction of lowest eigenvalue satisfies (4.105). Using the result for D_- in (4.99) it is easy to show that

$$c_l^{(0)}(x) = e^{-(1/2)eBx^2 + iea_1 x - ea_2 x + (2\pi l/L_2)x} c_l^{(0)}, \tag{4.109}$$

where $c_l^{(0)}$ on the right-hand side is a constant. This solution must obey the condition (4.98) following from the requirement that the constant $c_l^{(0)}$ must obey

$$c_{l-k}^{(0)} = e^{-(1/2)eBL_1^2 + iea_1 L_1 - ea_2 L_1 + (2\pi l L_1/L_2)} c_l^{(0)}. \tag{4.110}$$

[13] This can be seen from (4.103).

Because of the quadratic dependence on L_1, this suggests that we try a solution to (4.110) of the form

$$c_l^{(0)} = e^{-\alpha l^2 - \beta l}, \tag{4.111}$$

for some appropriately chosen values of α and β. A straightforward substitution of (4.111) into (4.110) shows that

$$e^{-(1/2)eBL_1^2 + (2\pi l L_1/L_2) + (iea_1 - ea_2)L_1} = e^{\alpha k(2l-k) + \beta k}.$$

The integer k is given in (4.88) and it is easily seen that

$$-\frac{1}{2}eBL_1^2 + \frac{2\pi l L_1}{L_2} = \frac{\pi L_1}{L_2}(2l - k).$$

If we choose

$$\alpha = \frac{\pi L_1}{kL_2} = \frac{2\pi^2}{eBL_2^2}, \tag{4.112}$$

$$\beta = \frac{2\pi i}{BL_2}(a_1 + ia_2), \tag{4.113}$$

this gives us the solution for $c_l^{(0)}$ and hence determines the eigenfunctions. Because of the relation (4.110) between $c_{l-k}^{(0)}$ and $c_l^{(0)}$, there are exactly k undetermined values for $c_l^{(0)}$. Thus the ground state is k-fold degenerate where $k = eBL_1L_2/2\pi$. Because the excited states follow from a mechanical application of D_+ to the ground state, they will also be k-fold degenerate. For a more heuristic and physical interpretation of this degeneracy, see Landau and Lifshitz (1958). The treatment here has been based on that in Laughlin (1989).

Now that we have the energy eigenvalues and their degeneracy we can proceed with the calculation of the effective action by evaluating the energy ζ-function. We have

$$E(s) = \hbar \frac{eBL_1L_2}{2\pi\ell^s} \sum_{n=0}^{\infty} \sum_{n_3=-\infty}^{\infty} \cdots \sum_{n_D=-\infty}^{\infty} \left[(2n+1)eB + \sum_{j=3}^{D} \left(\frac{2\pi n_j}{L_j} \right)^2 + m^2 \right]^{(1-s)/2}. \tag{4.114}$$

Taking the large box limit, and turning the sums over $n_3, \ldots, n_D$ into integrals, we find

$$
\begin{aligned}
E(s) &= \frac{\hbar e B V_\Sigma}{2\pi\ell^s}(4\pi)^{1-D/2}\frac{\Gamma\left[(s-D+1)/2\right]}{\Gamma\left[(s-1)/2\right]} \\
&\quad \sum_{n=0}^{\infty}\left[(2n+1)eB+m^2\right]^{(D-s-1)/2} \\
&= \frac{\hbar e B V_\Sigma}{2\pi\ell^s}(4\pi)^{1-D/2}\frac{\Gamma\left[(s-D+1)/2\right]}{\Gamma\left[(s-1)/2\right]}(2eB)^{(D-s-1)/2} \\
&\quad \times\zeta\left(\frac{s-D+1}{2},\frac{m^2+eB}{2eB}\right),
\end{aligned}
\tag{4.115}
$$

where $\zeta(z,a)$ is the Hurwitz ζ-function defined in Section A1.2.

The expression given in (4.115) is sufficient for obtaining the energy for general spatial dimension D. To obtain a more explicit expression, we must expand about $s=0$ using properties of the Γ- and ζ-functions, and again even and odd D must be considered separately. By making use of the results of Sections A1.1 and A1.2 it is possible to obtain an expression valid for arbitrary D; however, in order to illustrate a simpler alternative, we will only look at $D=3$. Putting $D=3$ in (4.115) we find

$$
E(s) = \hbar V_\Sigma \frac{e^2B^2}{2\pi^{3/2}}(2eB\ell^2)^{-s/2}\frac{\Gamma(s/2-1)}{\Gamma\left[(s-1)/2\right]}\zeta\left(\frac{s}{2}-1,\frac{1}{2}+\frac{m^2}{2eB}\right).
\tag{4.116}
$$

The most straightforward way to proceed is to make use of the various properties of the Γ- and ζ-functions, and expand about $s=0$ in an obvious way. If we proceed in this manner, because of the pole in $\Gamma(s/2-1)$ at $s=0$, we will encounter $(d/dz)\zeta(z,a)|_{z=-1}$ from the expansion of the Hurwitz ζ-function, and it is not easy to obtain a simple representation for this quantity. Instead we will proceed differently by first of all noting from (4.116) that we really only require the combination $\Gamma(z)\zeta\ [z,(1/2)+\alpha]$ near $z=-1$, with the definition

$$
\alpha = \frac{m^2}{2eB}.
\tag{4.117}
$$

Using the integral representation (A1.29), we find

$$
\Gamma(s/2-1)\zeta\left(\frac{s}{2}-1,\frac{1}{2}+\alpha\right) = \int_0^\infty dt\, t^{s/2-2}e^{-[(1/2)+\alpha]t}(1-e^{-t})^{-1},
\tag{4.118}
$$

valid for $\mathcal{R}(s)>4$. Our aim is to perform an analytic continuation to $s=0$. If we simply set $s=0$ in (4.118) the integral diverges, since as

$t \to 0$ the integrand behaves like t^{-3}. However, by adding and subtracting terms to the integrand in a suitable way we can end up with an expression that can be analytically continued to $s = 0$. Noting the expansion (A1.30), we will define

$$F(t) = e^{-t/2}(1 - e^{-t})^{-1} - \frac{1}{t} + \frac{t}{24}, \tag{4.119}$$

so that as $t \to 0$, $F(t)$ behaves like t^3. By adding and subtracting the last two terms of (4.119) to the integrand in (4.118) we obtain

$$\begin{aligned}\Gamma(s/2-1)\zeta\left(\frac{s}{2}-1, \frac{1}{2}+\alpha\right) &= \int_0^\infty dt\, t^{s/2-2}e^{-\alpha t}F(t) \\ &\quad + \int_0^\infty dt\, t^{s/2-2}e^{-\alpha t}\left(t^{s/2-3} - \frac{1}{24}t^{s/2-1}\right) \\ &= \int_0^\infty dt\, t^{s/2-2}e^{-\alpha t}F(t) \\ &\quad + \Gamma(s/2-2)\alpha^{2-s/2} - \frac{1}{24}\Gamma(s/2)\alpha^{-s/2}.\end{aligned} \tag{4.120}$$

We have used the integral representation of the Γ-function in (A1.1) here, which we are allowed to do because we are assuming that $\mathcal{R}(s) > 4$. The expression in (4.120) may now be analytically continued to a neighbourhood of $s = 0$ using the known behaviour of the Γ-function, and the fact that the integral is finite at $s = 0$. (We know that $t^{-2}F(t)$ behaves like t as $t \to 0$ ensuring convergence of the integral at its lower limit, and the exponential factor ensures convergence at the upper limit since we assume that $\alpha > 0$.) It is now easy to expand about $s = 0$.

To evaluate $E(s)$ we also need

$$\frac{(2eB\ell^2)^{-s/2}}{\Gamma\left[(s-1/2)\right]} = -\frac{1}{2\pi^{1/2}}\left\{1 + s\left[\frac{1}{2}\gamma - 1 - \frac{1}{2}\ln\left(\frac{eB\ell^2}{2}\right)\right] + \cdots\right\}. \tag{4.121}$$

After a bit of calculation we find

$$\begin{aligned}E(s) = -\hbar\frac{V_\Sigma}{4\pi^2}\Bigg\{&\left(\frac{m^4}{4} - \frac{e^2B^2}{12}\right)\left[\frac{1}{s} - \frac{1}{2}\ln\left(\frac{m^2\ell^2}{4}\right)\right] \\ &-\frac{m^4}{16} + \frac{e^2B^2}{12} + e^2B^2 I\left(\frac{m^2}{2eB}\right)\Bigg\}\end{aligned} \tag{4.122}$$

where

$$I(\alpha) = \int_0^\infty dt\, t^{-2}e^{-\alpha t}F(t) \tag{4.123}$$

is the integral appearing in (4.120).

We can see that the pole term of (4.122) involves m^4, familiar from our earlier discussion of the free scalar field, and in addition a new term proportional to B^2. We can deal with the m^4 pole by a renormalization of the vacuum energy as before. To deal with the pole proportional to B^2, we will first of all consider the classical energy density for a magnetic field, which is $(1/2)B^2$. If we regard the field B which appears here as a bare field strength which gets renormalized, then we will be able to absorb the pole term in (4.122) proportional to B^2. The classical energy density is

$$V^{(0)} = c_B + \frac{1}{2}B_B^2, \tag{4.124}$$

where c_B is the bare vacuum energy density, and B_B is the bare magnetic field which gets renormalized. Write

$$B_B = Z_B^{1/2} B, \tag{4.125}$$

where Z_B is the magnetic field renormalization factor, and B on the right-hand side is the renormalized magnetic field strength. We can express

$$Z_B = 1 + \hbar\, \delta Z_B^{(1)} + \cdots, \tag{4.126}$$

if we work to order $\hbar$. Choosing the renormalized value of the constant c to vanish, we have

$$c_B = \hbar\, \delta c^{(1)} + \cdots. \tag{4.127}$$

The classical potential becomes

$$V^{(0)} = \frac{1}{2}B^2 + \hbar\, \delta c^{(1)} + \frac{1}{2}\hbar\, \delta Z_B^{(1)} B^2, \tag{4.128}$$

if we work to order $\hbar$. The complete effective potential density then follows from (4.122) and (4.128) as[14]

$$\begin{aligned} V_{\text{eff}} = {} & \frac{1}{2}B^2 + \hbar\, \delta c^{(1)} + \frac{1}{2}\hbar\, \delta Z_B^{(1)} B^2 \\ & + \frac{\hbar}{4\pi^2}\left(\frac{e^2B^2}{12} - \frac{m^4}{4}\right)\left[\frac{1}{s} - \frac{1}{2}\ln\left(\frac{m^2\ell^2}{4}\right)\right] \\ & + \hbar\frac{m^4}{64\pi^2} - \hbar\frac{e^2B^2}{48\pi^2} - \hbar\frac{e^2B^2}{4\pi^2} I\left(\frac{m^2}{2eB}\right). \end{aligned} \tag{4.129}$$

[14] As in our earlier discussions of renormalization, to order $\hbar$ we can regard all of the parameters coming from $E(s)$ as renormalized.

We will choose renormalization conditions so that

$$V_{\text{eff}}(B=0)=0, \tag{4.130}$$

$$\frac{\partial}{\partial B^2}V_{\text{eff}}(B)\bigg|_{B=0}=\frac{1}{2}, \tag{4.131}$$

to agree with the classical potential. The last term of (4.129) makes no contribution to either of the renormalization conditions, and we find

$$\begin{aligned}\delta c^{(1)}&=\frac{m^4}{16\pi^2}\left[\frac{1}{s}-\frac{1}{2}\ln\left(\frac{m^2\ell^2}{4}\right)-\frac{1}{4}\right],\\ \delta Z_B^{(1)}&=-\frac{e^2}{24\pi^2}\left[\frac{1}{s}-\frac{1}{2}\ln\left(\frac{m^2\ell^2}{4}\right)-1\right],\end{aligned} \tag{4.132}$$

for the renormalization counterterms. The renormalized effective potential follows as

$$V_{\text{eff}}=\frac{1}{2}B^2-\frac{\hbar}{4\pi^2}\,e^2B^2\,I\left(\frac{m^2}{2eB}\right). \tag{4.133}$$

The quantum corrections to the classical theory are therefore embodied in the second term on the right-hand side of (4.133) and will result in a non-linear modification of Maxwell's laws.

For small values of the magnetic field, specifically for $eB << m^2$, the integral $I(\alpha)$ may be approximated as follows. Because the exponential factor $e^{-\alpha t}$ in the integrand falls off very rapidly for large α as t increases, the dominant contribution to the integral should come from small values of t. If we expand $t^{-2}F(t)$ about $t=0$, it can be shown that

$$I(\alpha)\simeq\frac{7}{5760}\alpha^{-2}-\frac{31}{161\,280}\alpha^{-4}+\mathcal{O}(\alpha^{-6}),$$

give the leading terms for large α. Using this in our expression (4.133) for the effective potential results in the expansion

$$V_{\text{eff}}\simeq\frac{1}{2}B^2-\frac{7\hbar\,e^4B^4}{5760\pi^2m^4}+\frac{31\hbar\,e^6B^6}{40\,320\pi^2m^8}+\cdots. \tag{4.134}$$

This result can be shown to agree with that found by Schwinger (1951a).

4.6 Self-interacting scalar field

Up to now we have been considering only fields interacting with background fields that can be treated classically. Here we wish to consider a field with a self-interaction. We will choose the space Σ to be flat

D-dimensional space. Because Σ is isotropic and homogeneous the background field $\bar{\varphi}$ representing the ground state would be expected to be constant. We will assume this in what follows. The eigenfunctions and eigenvalues are determined by (4.9)–(4.12).

At this stage we note the simplicity arising from assuming $\bar{\varphi}$ to be constant. Although the potential term in (4.9) can be non-trivial, it must be constant. Thus the only change from the free-field case is that we replace m^2 in our free-field results with $m^2 + U''(\bar{\varphi})$. We find immediately from (4.32) that for the spatial dimension D even,

$$V_{\text{eff}}^{(1)} = \frac{\hbar}{2}\left(-\frac{1}{\pi}\right)^{D/2} \frac{(D/2)!}{(D+1)!}[m^2 + U''(\bar{\varphi})]^{(D+1)/2}. \tag{4.135}$$

There is no pole term in the energy ζ-function in this case. For D odd we use (4.34) to obtain

$$V_{\text{eff}}^{(1)} = -\frac{\hbar}{2\,[(D+1)/2]!}\left[-\frac{m^2 + U''(\bar{\varphi})}{4\pi}\right]^{(D+1)/2}\left(\frac{2}{s} - 1 + \frac{1}{2} + \frac{1}{3} + \cdots + \frac{2}{D+1} - \ln\left\{\frac{\ell^2}{4}[m^2 + U''(\bar{\varphi})]\right\}\right). \tag{4.136}$$

In either case the total effective potential is

$$V_{\text{eff}}(\bar{\varphi}) = \frac{1}{2}m^2\bar{\varphi}^2 + U(\bar{\varphi}) + V_{\text{eff}}^{(1)}. \tag{4.137}$$

The renormalization procedure is not quite so simple as it was for the free field theory. We will look at the case[15] where the potential $U(\varphi)$ is a polynomial in φ of degree N,

$$U(\varphi) = \sum_{n=3}^{N} \frac{\lambda_n}{n!}\varphi^n + c. \tag{4.138}$$

The basic idea of renormalization theory is that the pole terms in (4.136) should be removable by a renormalization of the coupling constants c, m^2, λ_n appearing in the classical theory. We will write

$$c = c_R + \delta c, \tag{4.139}$$

$$m^2 = m_R^2 + \delta m^2, \tag{4.140}$$

$$\lambda_n = \lambda_{nR} + \delta\lambda_n, \tag{4.141}$$

[15] Because the mass term is already quadratic in the field, we will start the potential off at cubic order.

where the subscript 'R' denotes a renormalized value for the relevant quantity.[16] The terms in $\delta c, \delta m^2$, and $\delta\lambda_n$ are called 'counterterms'. Because we do not need to perform any renormalization in the classical theory these counterterms are at least of order $\hbar$. It is these counterterms that will absorb any divergences which might be present. Right away we can see that there is a problem with (4.136). The pole term contains

$$\left[m^2 + \sum_{n=3}^{N} \frac{\lambda_n}{(n-2)!}\bar{\varphi}^{n-2}\right]^{(D+1)/2}.$$

The highest power of $\bar{\varphi}$ occurring is $\bar{\varphi}^{(N-2)(D+1)/2}$, and if we are to renormalize V_{eff} using the counterterms above, we must have $(N-2)(D+1)/2 \leq N$ or $N \leq (2D+2)/(D-1)$ (assuming $D > 1$). (For $D = 1$, corresponding to a theory in two spacetime dimensions, there is no restriction on the potential.) If we put $D = 3$ we must have $N \leq 4$. For $D = 5$ we require $N \leq 3$. For $D \geq 7$ we must have $N < 3$ meaning that the self-interacting theory is not renormalizable with any interaction of the form (4.138). For D even, since there is no pole term, we do not need to perform any infinite renormalizations; however, it must be remembered that we are only working to lowest order in perturbation theory with a single real scalar field. At higher orders in perturbation theory the upper limit of $D = 5$ still holds for a potential of the form (4.138) to lead to a renormalizable theory. Requiring renormalizability leads to a restriction on the types of interactions allowed.

Suppose that we do not require the theory to be renormalizable. For concreteness, take $U \propto \bar{\varphi}^6$ and $D = 3$. Then (4.136) requires us to add on a counterterm proportional to $\bar{\varphi}^8$. This entails adding on the bare term $\lambda_8\bar{\varphi}^8$ to $U(\bar{\varphi})$. Unless we have some good reason for demanding the renormalized value of λ_8 to vanish, we will end up with a pole term proportional to $\bar{\varphi}^{12}$ in $V_{\text{eff}}^{(1)}$. This requires us to add on the term $\lambda_{12}\bar{\varphi}^{12}$ to $U(\bar{\varphi})$ and so on. Allowing a non-renormalizable interaction results in a theory with an infinite number of coupling constants. These parameters must ultimately be fixed by experiment, so there is no predictive power in such a theory. If, on the other hand, we have only a finite number of coupling constants to fix by comparing our theory with experiment, then once these parameters have been fixed we can then use the theory to calculate and predict the results of other experiments. This is the basic

[16] In general, we would also have to renormalize $\bar{\varphi}$, but this proves to not be required if we only work to order $\hbar$. This will be shown in Chapter 8.

reason for insisting on renormalizability as a criterion, and the requirement of renormalizability permeates the classic texts on quantum field theory.

However, over about the past 20 years, a new way of thinking about quantum field theory has emerged. This makes a break with the older tradition of regarding our field theories as providing a fundamental and ultimate description of the physical world. Rather, because we only compare our theories with experiments at low energies, all that we can describe with any confidence is the low energy effective field theory. If E_{max} is some energy scale, then when $E > E_{max}$ we do not necessarily trust the results of our low energy effective field theory. Instead of energy we can talk equally well about length scales. If L_{min} is some minimum length scale, then the effective field theory is good for lengths which are greater than L_{min}. In order to see how this applies to renormalizable versus non-renormalizable theories, suppose that we consider the dimensions of λ_n in (4.138). We know that $m^2\varphi^2$ has dimensions of energy density, which is mass/volume in units with the speed of light $c = 1$. We have also set $\hbar = 1$ so that mass has units of inverse length.[17] Thus $m^2\varphi^2$ has dimensions of $L^{-(D+1)}$ where L is an arbitrary length scale. Since m^2 has dimensions of L^{-2} we find the dimensions of φ to be $L^{(1-D)/2}$. This means that λ_n has dimensions $L^{(D-1)n/2-D-1}$. If $D = 1$, we find that λ_n has dimensions of L^{-2} for any value of n. If $D > 1$, we can write $\dim(\lambda_n) = L^{[(D-1)/2]\{n-[2(D+1)/(D-1)]\}}$. The requirement of renormalizability therefore translates into the requirement that $\dim(\lambda_n) = L^{-\alpha}$ where $\alpha \geq 0$. Non-renormalizable interactions are characterized by $\alpha < 0$.

We can broaden our interpretation of an acceptable field theory by adopting the effective field theory point of view. We will look at the theory at length scales $L >> L_{min}$ with L_{min} some minimum length scale. We do not ask what happens when $L < L_{min}$. The natural length scale in the theory is L_{min}. Non-renormalizable interactions will lead to results proportional to $(L_{min}/L)^\beta$ for $\beta > 0$ at length scale L. Thus for $L >> L_{min}$ the effects of non-renormalizable interactions are suppressed relative to renormalizable ones. The effective theory at large distances is determined to high accuracy by the renormalizable part. From the effective field theory viewpoint, this is why we can focus on renormalizable theories. Although the motivation is different from the older viewpoint, the net result is that at large distances (or low energies) the important physics is determined by a renormalizable field theory.

[17] Think about the Compton wavelength of a particle of mass m which is $\hbar/mc$ in conventional units.

As a concrete application of the renormalization process in action, suppose that we take $D = 3$, and

$$U(\phi) = c + \frac{\lambda}{4!}\phi^4. \tag{4.142}$$

In this case we have

$$V_{\text{eff}}^{(1)} = -\frac{\hbar}{64\pi^2}\left(m^2 + \frac{\lambda}{2}\bar{\varphi}^2\right)^2 \left\{\frac{2}{s} - \frac{1}{2} - \ln\left[\frac{\ell^2}{4}\left(m^2 + \frac{\lambda}{2}\bar{\varphi}^2\right)\right]\right\}. \tag{4.143}$$

In order to deal with the pole term at $s = 0$ we now use the expressions (4.139)–(4.141) for the coupling constants expressed in terms of renormalized values and counterterms. If the counterterms are of order $\hbar$, which they must be if they are to absorb the $1/s$ pole in $V_{\text{eff}}^{(1)}$, then we may take m^2 and λ in $V_{\text{eff}}^{(1)}$ to be renormalized values if we work only to $O(\hbar)$. We then have (from (4.137))

$$\begin{aligned} V_{\text{eff}}(\bar{\varphi}) = {} & c_R + \delta c + \frac{1}{2}(m_R^2 + \delta m^2)\bar{\varphi}^2 + \frac{(\lambda_R + \delta\lambda)}{4!}\bar{\varphi}^4 \\ & - \frac{\hbar}{64\pi^2}\left(m_R^2 + \frac{\lambda_R}{2}\bar{\varphi}^2\right)^2 \left\{\frac{2}{s} - \frac{1}{2} - \ln\left[\frac{\ell^2}{4}\left(m_R^2 + \frac{\lambda_R}{2}\bar{\varphi}^2\right)\right]\right\}. \end{aligned} \tag{4.144}$$

In order to fully fix the counterterms we will adopt a set of renormalization conditions

$$V_{\text{eff}}(\bar{\varphi} = 0) = c_R, \tag{4.145}$$

$$\frac{\partial^2}{\partial\bar{\varphi}^2} V_{\text{eff}}\bigg|_{\bar{\varphi}=0} = m_R^2, \tag{4.146}$$

$$\frac{\partial^4}{\partial\bar{\varphi}^4} V_R\bigg|_{\bar{\varphi}=0} = \lambda_R. \tag{4.147}$$

The values on the right-hand side are chosen to agree with what is found for the classical potential. A straightforward exercise in differentiation leads to

$$\delta c = \frac{\hbar}{64\pi^2} m_R^4 \left[\frac{2}{s} - \frac{1}{2} - \ln\left(\frac{\ell^2}{4} m_R^2\right)\right], \tag{4.148}$$

$$\delta m^2 = \frac{\hbar}{32\pi^2} \lambda_R m_R^2 \left[\frac{2}{s} - 1 - \ln\left(\frac{\ell^2}{4} m_R^2\right)\right], \tag{4.149}$$

$$\delta\lambda = \frac{3\hbar}{32\pi^2} \lambda_R^2 \left[\frac{2}{s} - 2 - \ln\left(\frac{\ell^2}{4} m_R^2\right)\right]. \tag{4.150}$$

The renormalized effective potential is therefore

$$V_{\text{eff}}(\bar{\varphi}) = c_R + \frac{1}{2}m_R^2\bar{\varphi}^2 + \frac{\lambda_R}{4!}\bar{\varphi}^4 - \frac{\hbar\lambda_R}{128\pi^2}m_R^2\bar{\varphi}^2 - \frac{3\hbar\lambda_R^2}{512\pi^2}\bar{\varphi}^4 + \frac{\hbar}{64\pi^2}\left(m_R^2 + \frac{\lambda_R}{2}\bar{\varphi}^2\right)^2 \ln\left(1 + \frac{\lambda_R\bar{\varphi}^2}{2m_R^2}\right). \tag{4.151}$$

The terms of zeroth order in $\hbar$ agree with the classical potential with renormalized coupling constants appearing.

The expression (4.151) has no explicit dependence on the renormalization length ℓ. Like the pole term in $1/s$, the renormalization length has disappeared into the counterterms. Because the renormalization length is introduced through the process of regularization and renormalization, we can assume that ℓ does not enter the unrenormalized, or bare, coupling constants. So[18]

$$\ell\frac{d}{d\ell}c = 0, \tag{4.152}$$

$$\ell\frac{d}{d\ell}m^2 = 0, \tag{4.153}$$

$$\ell\frac{d}{d\ell}\lambda = 0. \tag{4.154}$$

If we use (4.139)–(4.141) along with the counterterms given in (4.148)–(4.141) we find (to order $\hbar$)

$$\ell\frac{d}{d\ell}c_R = \frac{\hbar}{32\pi^2}m_R^4, \tag{4.155}$$

$$\ell\frac{d}{d\ell}m_R^2 = \frac{\hbar}{16\pi^2}\lambda_R m_R^2, \tag{4.156}$$

$$\ell\frac{d}{d\ell}\lambda_R = \frac{3\hbar}{16\pi^2}\lambda_R^2. \tag{4.157}$$

These differential equations tell us how the renormalized coupling constants depend on the arbitrary renormalization length ℓ. If we decide to change the renormalization length ℓ, then we must change the renormalized coupling constants in the manner determined by (4.155)–(4.157). These equations are usually called the 'renormalization group equations'. Note that the terms appearing on the right-hand side of (4.155)–(4.157)

[18] We take $\ell(d/d\ell)$ so that the differential operator is dimensionless.

are the $1/s$ pole terms appearing in the counterterms. This is not a coincidence.

Suppose that we had a massless theory. If we try to let $m_R^2 \to 0$ in (4.151) there is a problem in the last term. This is due to our choice for $\delta\lambda$ in (4.150) which is seen to diverge as $m_R^2 \to 0$. The behaviour of $\delta\lambda$ is due in turn to our choice of renormalization condition (4.147). Recall from the discussion at the start of this section that the theory is like a free massive theory with $m^2 \to m^2 + (\lambda/2)\bar{\varphi}^2$. If we set $m^2 = 0$, then the theory is like a free massive theory with $(\lambda/2)\bar{\varphi}^2$ playing the role of the mass. By imposing the renormalization conditions at $\bar{\varphi} = 0$ we are encountering infra-red divergences due to the fact that the energy ζ-function will not remain finite if $E_n \to 0$.[19] The resolution of this problem is simple if we note that the choice of imposing the renormalization conditions (4.145)–(4.147) at $\bar{\varphi} = 0$ was an arbitrary decision. We could instead choose

$$\left.\frac{\partial^4 V_{\text{eff}}}{\partial\bar{\varphi}^4}\right|_{\bar{\varphi}=M} = \lambda_R, \tag{4.158}$$

where M is arbitrary. If we take $m_R^2 \to 0$ in (4.144) we have

$$\begin{aligned} V_{\text{eff}}(\bar{\varphi}) = c_R \; &+\delta c + \frac{1}{2}\delta m^2\bar{\varphi}^2 + \frac{(\lambda_R + \delta\lambda)}{4!}\bar{\varphi}^4 \\ &-\frac{\hbar}{128\pi^2}\lambda_R^2\bar{\varphi}^4\left[\frac{2}{s} - \frac{1}{2} - \ln\left(\frac{\ell^2\lambda_R}{8}\bar{\varphi}^2\right)\right]. \end{aligned} \tag{4.159}$$

For the massless theory we see that the only pole term is proportional to $\bar{\varphi}^4$; thus, there is no need for any δc or δm^2 counterterms. This is consistent with the massless limit of (4.148) and (4.149). If we impose (4.158), we find

$$\delta\lambda = \frac{\hbar\lambda_R^2}{16\pi^2}\left[\frac{3}{s} - 7 - \frac{3}{2}\ln\left(\frac{\lambda_R\ell^2M^2}{8}\right)\right]. \tag{4.160}$$

This leads to the result

$$V_{\text{eff}}(\bar{\varphi}) = c_R + \frac{\lambda_R}{4!}\bar{\varphi}^4 + \frac{\hbar\lambda_R^2}{256\pi^2}\bar{\varphi}^4\left[\ln\left(\frac{\bar{\varphi}^2}{M^2}\right) - \frac{25}{6}\right], \tag{4.161}$$

first given by Coleman and Weinberg (1973).

The fact that this result appears to depend on the arbitrary parameter M might seem to present a problem. However, renormalization theory

[19] The divergences we have met up to now have corresponded to the divergence of the energy ζ-function as $E_n \to \infty$. These are called 'ultraviolet divergences'.

turns this problem into a virtue. Just as we discussed earlier when considering the dependence on the renormalization length ℓ, the bare coupling constant λ should not depend on M:

$$M\frac{d\lambda}{dM} = 0. \tag{4.162}$$

A consequence of this is that the renormalized value of λ, namely λ_R, must depend on M, and it is simple to see that

$$M\frac{d\lambda_R}{dM} = \frac{3\hbar\lambda_R^2}{16\pi^2}. \tag{4.163}$$

This is the same as (4.157) if we replace $\ell \to M^{-1}$.[20] Now suppose that we compute $M(d/dM)V_{\text{eff}}$ working for consistency to order $\hbar$. Because the last term of (4.161) is already of order $\hbar$, we can regard λ_R in this term as fixed. However, the $(\lambda_R/4!)\bar{\varphi}^4$ term is of zeroth order in $\hbar$ so we must use (4.163) to evaluate its change. We find

$$\begin{aligned} M\frac{d}{dM}V_{\text{eff}} &= \frac{\bar{\varphi}^4}{4!}M\frac{d\lambda_R}{dM} - \frac{\hbar\lambda_R^2}{128\pi^2}\bar{\varphi}^4 \\ &= 0. \end{aligned} \tag{4.164}$$

Thus the apparent dependence on M in (4.161) is an illusion.

4.7 Local Casimir effect

Suppose that we are interested in the energy density, as opposed to the total energy. We mentioned at the beginning of this section that the energy density can differ from the constant value of E/V where E is the total energy. Consider the case of a real scalar field whose Hamiltonian density is given in (2.45) as

$$\begin{aligned} \mathcal{H} &= \frac{1}{2}\dot{\varphi}^2 + \frac{1}{2}|\nabla\varphi|^2 + \frac{1}{2}m^2\varphi^2 \\ &= \frac{1}{2}\dot{\varphi}^2 + \frac{1}{2}\varphi(-\nabla^2)\varphi + \frac{1}{2}m^2\varphi^2 + \cdots, \end{aligned} \tag{4.165}$$

where $\cdots$ denotes a total derivative term. The expansion of the field operator φ in terms of creation and annihilation operators was given in (3.187) as

$$\varphi(t,\mathbf{x}) = \sum_n (2E_n)^{-1/2}\left[e^{-iE_nt}f_n(\mathbf{x})a_n + e^{iE_nt}f_n^*(\mathbf{x})a_n^\dagger\right]. \tag{4.166}$$

[20] Note that M has dimensions of mass or inverse length.

Operating with $\varphi(t,\mathbf{x})$ on the vacuum state results in

$$\varphi(t,\mathbf{x})|0\rangle = \sum_n (2E_n)^{-1/2} e^{iE_n t} f_n^*(\mathbf{x}) a_n^\dagger |0\rangle. \tag{4.167}$$

If we discard the total derivative in $\mathcal{H}$, we find

$$\langle 0|\mathcal{H}|0\rangle = \frac{1}{2}\sum_n E_n |f_n(\mathbf{x})|^2. \tag{4.168}$$

Integration over all space produces the result of Section 4.3 for the zero-point energy, since $\int_\Sigma d\sigma_x |f_n(\mathbf{x})|^{1/2} = 1$.

As a generalization of the ζ-function method we have been considering, define

$$\rho(s;\mathbf{x},\mathbf{x}') = \sum_n E_n (\ell^2 E_n)^{-s} f_n(\mathbf{x}) f_n^*(\mathbf{x}'). \tag{4.169}$$

It is obvious that the energy ζ-function is given in terms of $\rho(s;\mathbf{x},\mathbf{x}')$ by

$$E(s) = \int_\Sigma d\sigma_x \rho(s;\mathbf{x},\mathbf{x}). \tag{4.170}$$

We can call $\rho(s;\mathbf{x},\mathbf{x}')$ the local energy ζ-function. The regularised zero-point energy density will be defined as

$$\langle 0|\mathcal{H}|0\rangle = \frac{1}{2}\rho(0;\mathbf{x},\mathbf{x}). \tag{4.171}$$

As with our previous method, the right-hand side is defined by analytic continuation to $s = 0$.

For the Casimir effect in Section 4.3 we had $f_n(\mathbf{x})$ given in (4.39) with σ_n in (4.40). It follows from (4.169) that

$$\begin{aligned}\rho(s;\mathbf{x},\mathbf{x}) = {} & \frac{2}{\ell^{2s} L_1} \sum_{n=1}^{\infty} \int \frac{d^{D-1}k}{(2\pi)^{D-1}} \sin^2\left(\frac{\pi n x}{L_1}\right) \\ & \times \left[\left(\frac{\pi n}{L_1}\right)^2 + k^2 + m^2\right]^{(1-s)/2}\end{aligned} \tag{4.172}$$

where we have taken $L_2,\ldots,L_D$ to be very large and replaced sums with integrals as usual. This is very similar to what we had in our energy ζ-function in Section 4.3 except for the presence of $\sin^2(\pi n\mathbf{x}/L_1)$. If we integrate (4.172) over space, we recover exactly the energy ζ-function we

had earlier. The momentum integral in (4.172) can be performed as in Section 4.2 to give

$$\rho(s;\mathbf{x},\mathbf{x}) = \frac{2}{L_1}\ell^{-2s}(4\pi)^{-(D-1)/2}\frac{\Gamma\left[(s-D)/2\right]}{\Gamma\left[(s-1)/2\right]} \times \sum_{n=1}^{\infty}\sin^2\left(\frac{\pi n x}{L_1}\right)\left[\left(\frac{\pi n}{L_1}\right)^2 + m^2\right]^{(D-s)/2}. \quad (4.173)$$

It is possible to derive an integral representation for the sum in (4.173) using the method described in Section A1.3. However, for simplicity we will only consider the massless limit here. In this limit, (4.173) becomes

$$\rho(s;\mathbf{x},\mathbf{x}) = \frac{2}{L_1}(4\pi)^{(D-1)/2}\ell^{-2s}\frac{\Gamma\left[(s-D)/2\right]}{\Gamma\left[(s-1)/2\right]}\left(\frac{\pi}{L_1}\right)^{D-s} \times \sum_{n=1}^{\infty} n^{D-s}\sin^2\left(\frac{\pi n x}{L_1}\right). \quad (4.174)$$

The remaining sum can be done a simple way as follows. Note that

$$\sum_{n=1}^{\infty} n^{-z}\sin^2(an) = \frac{1}{2}\sum_{n=1}^{\infty} n^{-z}(1-\cos 2an) = \frac{1}{2}\zeta(z) - \frac{1}{2}g(z,2a) \quad (4.175)$$

where

$$g(z,b) = \sum_{n=1}^{\infty} n^{-z}\cos\, bn. \quad (4.176)$$

We have

$$\rho(s;\mathbf{x},\mathbf{x}) = \frac{1}{L_1}(4\pi)^{-(D-1)/2}\ell^{-2s}\frac{\Gamma\left[(s-D)/2\right]}{\Gamma\left[(s-1)/2\right]}\left(\frac{\pi}{L_1}\right)^{D-s} \times \left[\zeta(s-D) - g\left(s-D, \frac{2\pi x}{L_1}\right)\right]. \quad (4.177)$$

All we need is the evaluation of $g(z,b)$ to complete the analysis. There are many ways to deal with this, but a quick method begins by differentiating (4.176) twice,

$$\frac{\partial^2}{\partial b^2}g(z,b) = -g(z-2,b). \quad (4.178)$$

Also, by taking $z = 1$ in (4.176), we have

$$\begin{aligned} g(1,b) &= \sum_{n=1}^{\infty} \frac{\cos\, bn}{n} \\ &= \mathcal{R} \sum_{n=1}^{\infty} \frac{e^{ibn}}{n} \\ &= \mathcal{R}\left[-\ln\left(1-e^{ib}\right)\right] \\ &= -\ln|2\sin\frac{b}{2}| \end{aligned} \tag{4.179}$$

if we assume $0 < b < 2\pi$. If $b = 0$ or 2π we must use

$$g(z,0) = g(z,2\pi) = \zeta(z) \tag{4.180}$$

which follows from (4.176) for $\mathcal{R}(z) > 1$, and for all other values of z by analytic continuation. We can use (4.178) with (4.179) to find[21]

$$\begin{aligned} g(-1,b) &= -\frac{\partial^2}{\partial b^2} g(1,b) \\ &= -\frac{1}{4\sin^2(b/2)}, \end{aligned} \tag{4.181}$$

and

$$\begin{aligned} g(-3,b) &= -\frac{\partial^2}{\partial b^2} g(-1,b) \\ &= \frac{3-2\sin^2(b/2)}{8\sin^4(b/2)}. \end{aligned} \tag{4.182}$$

If we set $D = 3$ in (4.177) and analytically continue s to $s = 0$ we have[22]

$$\rho(0;\mathbf{x},\mathbf{x}) = -\frac{\pi^2}{48L_1^4}\left[\frac{1}{15} - \frac{3-2\sin^2(\pi x/L_1)}{\sin^4(\pi x/L_1)}\right]. \tag{4.183}$$

The regularized energy density follows from (4.171) as

$$\langle 0|\mathcal{H}|0\rangle = -\frac{\pi^2}{96L_1^4}\left[\frac{1}{15} - \frac{3-2\sin^2(\pi x/L_1)}{\sin^4(\pi x/L_1)}\right] \tag{4.184}$$

[21] Take $z = 1$ and $z = -1$ respectively in (4.178).
[22] We have used $\zeta(-3) = 1/120$ here. See Section A1.2.

if we assume $0 < x < L_1$. If we let $x \to 0$ in (4.184) it can be seen that $\langle 0|\mathcal{H}|0\rangle$ diverges. Expanding (4.184) about $x = 0$ results in

$$\langle 0|\mathcal{H}|0\rangle = \frac{1}{32\pi^2 x^4} + \frac{\pi^2}{1512 L_1^6} x^2 + \cdots . \tag{4.185}$$

A similar behaviour is easily found for $x \to L_1$. This divergent behaviour is linked to the boundary conditions that we have adopted. In the case of the electromagnetic field with real conducting plates, the electromagnetic field would be expected to penetrate the plates in a way determined by the skin depth of the conducting material. This must be taken into account in any realistic model of a conductor.[23]

It is also worth pointing out how an erroneous conclusion about the divergent behaviour of the energy density could have been obtained. The mode functions (4.39) vanish on the boundaries at $x = 0$ and $x = L_1$. If we naively take $x = 0$ or $x = L_1$ in (4.174), then we deduce that the local energy ζ-function will vanish at these values of x, rather than diverge leading to the behaviour that we found in (4.184). The resolution to this contradiction results from noticing that taking $x \to 0$ in (4.174) interchanges the orders of limit and sum. The sum is not uniformly convergent vitiating this exchange of order.

Notes

The effective action was first introduced by Schwinger (see the comments by DeWitt (1996)) and developed extensively by DeWitt (1965). Many other people contributed to the method and related functional methods that we consider in Chapter 8. The simple approach described in the present chapter was given in Toms (1997). The regularization method is an adaptation of the method of generalized ζ-function regularization used in quantum field theory by Hawking (1977) and Dowker and Critchley (1976). It is related to the analytic regularization method of Bollini *et al.* (1964). For a more complete discussion of effective field theories, see Weinberg (1996). The extension of the calculation described in Section 4.4 was given originally by Hosotani (1983) and Toms (1983). A more complete treatment of the Casimir effect can be found in Milton (2001) or Bordag *et al.* (2005).

[23] See Sopova and Ford (2002) for example.

5
Quantum statistical mechanics

5.1 Introduction

In our treatment of quantum mechanics we discussed the notion of the state of a given system. The state was specified by giving the eigenvalues of a maximal set of mutually commuting observables. This represented the most information we could have about a given system in principle. In practice, of course, we do not really have all of the necessary information about the eigenvalues available. No experimentalist sets out with the primary intention of obtaining results which correspond to a maximal set of mutually compatible observables for any macroscopic system, such as a gas. Even a very small volume of gas contains an enormous number of particles. The quantum mechanical state would require us to know a great deal of information about the internal states of the electrons and nuclei of the gas molecules. The experimentalist may only be concerned with gross properties such as the pressure, internal energy, or specific heat for example. Most of the detailed information about the detailed state of the system is neither observed, nor of direct interest. Instead we must content ourselves with a description of the average, or most likely, behaviour of the system in the probabilistic sense. The usual technique for doing this consists of the introduction of an ensemble, meaning a very large collection of systems whose measured macroscopic properties are the same as those for the system we are interested in, but whose unobserved properties can vary. The details of this is the subject of statistical mechanics and is discussed in some detail in any good textbook (Tolman, 1938; ter Haar, 1958; Pathria, 1972; Huang, 1987). We will assume that the reader is familiar with the basic principles of statistical mechanics, and will briefly review only the basic necessities here.

We will assume that each member of our statistical ensemble has the same Hamiltonian H, and we will assume that H is time-independent. We

will let $H|n\rangle = E_n|n\rangle$ define the energy eigenstates $|n\rangle$ with energy eigenvalues E_n. As usual it is assumed that $\{|n\rangle\}$ is a complete orthonormal set.[1] Let P_n denote the probability that a given member of the ensemble has an energy E_n. The statistical, or ensemble, average of any observable A is defined by

$$\langle A\rangle = \sum_n P_n \langle n|A|n\rangle. \tag{5.1}$$

It proves convenient to define the density operator ρ by

$$\rho = \sum_n P_n |n\rangle\langle n|. \tag{5.2}$$

Since P_n is real and must satisfy $\sum_n P_n = 1$, it is easy to see that ρ is Hermitian (i.e. $\rho^\dagger = \rho$) with

$$\mathrm{tr}\rho = \sum_n \langle n|\rho|n\rangle = 1. \tag{5.3}$$

If the system under investigation is to be in equilibrium, P_n should be independent of time. It is easy to deduce from (5.2) that ρ satisfies the equation of motion

$$i\dot{\rho} = [H, \rho]\ . \tag{5.4}$$

ρ may be thought of as the quantum mechanical generalization of the classical phase space density, and (5.4) as the generalization of Liouville's theorem.

If we note from (5.2) that

$$\rho|n\rangle = P_n|n\rangle, \tag{5.5}$$

then we can write

$$\begin{aligned}\langle A\rangle &= \sum_n \langle n|A\rho|n\rangle \\ &= \mathrm{tr}(A\rho)\end{aligned} \tag{5.6}$$

from (5.1). Although we have chosen to adopt the basis vectors specified by the energy eigenstates, because the trace is invariant under any unitary transformation of basis, the statistical average in (5.6) is also independent of the choice of basis. The use of the energy basis is convenient because (5.5) shows that $\langle m|\rho|n\rangle = 0$ if $m \neq n$, and $\langle n|\rho|n\rangle = P_n$.

[1] We will not put the usual prime on the eigenvalues since we do not need to distinguish operators from eigenvalues here.

For a system in equilibrium it is natural to assume that $\dot{\rho} = 0$ since this guarantees $\dot{P}_n = 0$. In this case (5.4) shows that $[H, \rho] = 0$, so that ρ must depend only on constants of the motion. The choice for ρ is dictated by the nature of the ensemble. We will be concerned with the grand canonical ensemble here that allows our system to exchange energy and particles (or charge) with its surroundings. This is the most physically relevant in many cases of interest, and can be viewed as a smaller subsystem of a much larger isolated system (Tolman, 1938; ter Haar, 1958). For non-relativistic systems it is conventional to speak about the number of particles, although strictly speaking the particle number is not really conserved, but is only approximately conserved. In relativistic systems we can create both particles and antiparticles, that have opposite charges, so it is really the difference between the number of particles and the number of antiparticles that is conserved (Haber and Weldon, 1982). For particles of rest mass m, when $kT << mc^2$, we would expect the creation of particles and antiparticles to be highly suppressed. This is the case for molecules or atoms of a gas under normal experimental temperatures, and because we normally have matter, as opposed to antimatter, we are justified to a very good approximation in ignoring the creation of particles and may speak about the particle number as if it was conserved. Of course there may be situations, such as the early universe, where $kT >> mc^2$, in which case we must be more careful. It should be clear from the nature of the system under consideration whether or not we need to consider the distinction between particle number and charge conservation.[2]

Let $\mathcal{N}_i$ be a set of operators corresponding to a set of conserved quantities.[3] The density operator for the grand canonical ensemble is defined to be

$$\rho = e^{-q-\beta\bar{H}}, \tag{5.7}$$

where

$$\bar{H} = H - \mu \cdot \mathcal{N}. \tag{5.8}$$

We use $\mu \cdot \mathcal{N} = \sum_i \mu_i \mathcal{N}_i$ here. β is a constant given in terms of the temperature T by

$$\beta = (kT)^{-1} \tag{5.9}$$

[2] We will discuss the non-relativistic limit of the relativistic theory in more detail later in this chapter.

[3] For non-relativistic systems we could have $\mathcal{N}_i$ as the number operators for different species of particles. For relativistic systems we could have $\mathcal{N}_i$ as the charge operators for different particle species.

with k the Boltzmann constant. We will choose units in which $k = 1$ so that β becomes just the inverse temperature. q is a constant called the 'q-potential' (ter Haar, 1958; Pathria, 1972) which is fixed by the condition (5.3) to be

$$q = \ln \operatorname{tr} e^{-\beta \bar{H}}. \tag{5.10}$$

The grand partition function $\mathfrak{Z}$ is often defined by

$$\mathfrak{Z} = \operatorname{tr} e^{-\beta \bar{H}}, \tag{5.11}$$

so that we have

$$q = \ln \mathfrak{Z}. \tag{5.12}$$

The physical meaning of the grand canonical ensemble is that it represents a system which is weakly coupled to a much larger reservoir with which it can exchange energy and particle number (or charge). There will be fluctuations in both energy and particle number about their average values.

In order to establish the connection between statistical mechanics and thermodynamics it is useful to consider a variation of q when parameters which enter the grand canonical ensemble are changed (ter Haar, 1958). Under a general variation it is easy to show from (5.11) and (5.12) that

$$\delta q = -\langle \delta(\beta \bar{H}) \rangle, \tag{5.13}$$

if we use the definition of the statistical average (5.6). From this result it follows quite simply that

$$\frac{1}{\beta} \delta[q + \langle \beta \bar{H} \rangle] = \delta \langle \bar{H} \rangle - \langle \delta \bar{H} \rangle. \tag{5.14}$$

It is this relation which allows us to make the connection with macroscopic thermodynamics (ter Haar, 1958). By thinking of $\bar{H}$ as a generalized Hamiltonian, $\langle \delta \bar{H} \rangle$ represents the work done on the system, and $\delta \langle \bar{H} \rangle$ represents the change in the internal energy. The right-hand side of (5.14) can therefore be thought of as the heat added to the system which leads to the identification

$$\frac{1}{\beta} \delta[q + \langle \beta \bar{H} \rangle] = T \delta S \tag{5.15}$$

with S the entropy. Given that $\beta = 1/T$, we find

$$S = q + \beta(E - \mu \cdot \mathbf{N}), \tag{5.16}$$

with

$$E = \langle H \rangle, \tag{5.17}$$

$$\mathbf{N} = \langle \mathcal{N} \rangle. \tag{5.18}$$

We can now invoke standard results from thermodynamics. Of special importance is the Helmholtz free energy

$$F = E - TS \tag{5.19}$$

$$= -\frac{q}{\beta} + \mu \cdot \mathbf{N}. \tag{5.20}$$

Various other thermodynamic functions can be easily defined.

An explicit evaluation of δq in (5.13) leads to

$$\delta q = -\delta\beta E + \delta(\beta\mu) \cdot \mathbf{N} - \beta\langle \delta H \rangle + \beta\mu \cdot \langle \delta\mathcal{N} \rangle. \tag{5.21}$$

We can therefore conclude that

$$E = -\left(\frac{\partial q}{\partial \beta}\right)\Big|_{\beta\mu_i,\ldots} \tag{5.22}$$

$$N_i = -\left[\frac{\partial q}{\partial(\beta\mu_i)}\right]\Big|_{\beta,\ldots} \tag{5.23}$$

where ... represents whatever needs to be held constant for the last two terms of (5.21) to vanish. Generally we will hold the volume of the system and the fields fixed as discussed in the examples to follow.

The importance of the Helmholtz free energy resides in the fact that for a fixed $T, V, \mathbf{N}$ it is a minimum for a system in thermodynamic equilibrium (Guggenheim, 1959). The fact that F is stationary follows immediately from (5.19) and the first law of thermodynamics (Guggenheim, 1959) which reads (with P the pressure)

$$dE = TdS - PdV + \mu \cdot d\mathbf{N}. \tag{5.24}$$

We find

$$dF = -SdT - PdV + \mu \cdot d\mathbf{N}. \tag{5.25}$$

Another useful definition is the thermodynamic potential Ω given by

$$\Omega = -\frac{q}{\beta} = F - \mu \cdot \mathbf{N}. \tag{5.26}$$

Ω is the generalization of the effective action to finite temperature. Because Ω and F differ by only a Legendre transformation we can freely

use Ω in place of F whenever convenient. Minimizing F at fixed $T, V, \mathbf{N}$ is completely equivalent to minimizing Ω at fixed T, V, μ. We have

$$d\Omega = -SdT - PdV - d\mu \cdot \mathbf{N}. \tag{5.27}$$

This shows that

$$S = -\left(\frac{\partial \Omega}{\partial T}\right)\Big|_{V,\mu}, \tag{5.28}$$

$$P = -\left(\frac{\partial \Omega}{\partial V}\right)\Big|_{T,\mu}, \tag{5.29}$$

$$N_i = -\left(\frac{\partial \Omega}{\partial \mu_i}\right)\Big|_{T,V}, \tag{5.30}$$

In most cases we will be interested in the limit in which the volume V becomes very large. We will find that $\Omega \propto V$ just as we did for the effective action at zero temperature in Chapter 3.

5.2 Simple harmonic oscillator

We will begin with the one-dimensional simple harmonic oscillator whose quantum mechanics was described in Section 3.5. The energy levels are $E_n = [n + (1/2)]\omega$ (with $\hbar = 1$) and n is the eigenvalue of the number operator.[4] According to (5.8) and (5.10) we have (since $\mathcal{N}$ is the number operator with eigenvalue n)

$$\begin{aligned} q &= \ln \operatorname{tr} e^{-\beta(H-\mu\mathcal{N})} \\ &= \ln \sum_{n=0}^{\infty} e^{-\beta\{[n+(1/2)]\omega - \mu n\}} \\ &= \ln \left\{ e^{-(1/2)\beta\omega} \left[1 - e^{-\beta(\omega-\mu)}\right] \right\}^{-1} \qquad (5.31) \\ &= -\frac{1}{2}\beta\omega - \ln\left[1 - e^{-\beta(\omega-\mu)}\right]. \qquad (5.32) \end{aligned}$$

The grand partition function is just the argument of the logarithm in (5.31) according to the definition (5.12). In obtaining (5.31) from the previous line we have just summed the geometric series.

From (5.22) we find the internal energy to be

$$E = \frac{1}{2}\omega + \omega[e^{\beta(\omega-\mu)} - 1]^{-1}. \tag{5.33}$$

[4] We drop the primes on the eigenvalues here.

From (5.23) the average particle number is

$$N = [e^{\beta(\omega-\mu)} - 1]^{-1}. \tag{5.34}$$

Using (5.34) in (5.33) results in

$$E = \frac{1}{2}\omega + \omega N. \tag{5.35}$$

The thermodynamic potential follows from (5.26) and (5.32) as

$$\Omega = \frac{1}{2}\omega + \frac{1}{\beta}\ln\left[1 - e^{-\beta(\omega-\mu)}\right]. \tag{5.36}$$

If we let $T \to 0$, or $\beta \to \infty$, then $N \to 0$ and the internal energy is comprised of just the zero-point energy, and the thermodynamic potential becomes $\Omega \to (1/2)\omega = E$. This was what we used in the previous chapter to evaluate the effective potential. At non-zero temperature it is clear from (5.33) that we must include the thermal contribution.

The generalization of the simple harmonic oscillator to more than three spatial dimensions is straightforward. We can define

$$E_n = \sum_{j=1}^{D}\left(n_j + \frac{1}{2}\right)\omega_j \tag{5.37}$$

as the energy levels where $n_j = 0, 1, 2, \ldots$ with ω_j the classical oscillator frequency in the jth direction. Because $[\bar{H}_j, \bar{H}_{j'}] = 0$, where $\bar{H} = \sum_{j=1}^{D}\bar{H}_j$ with $\bar{H}_j$ the one-dimensional Hamiltonian for the jth direction, we have

$$\Omega = \frac{1}{2}\sum_{j=1}^{D}\omega_j + \frac{1}{\beta}\sum_{j=1}^{D}\ln[1 - e^{-\beta(\omega_j-\mu)}]. \tag{5.38}$$

The internal energy is

$$E = \frac{1}{2}\sum_{j=1}^{D}\omega_j + \sum_{j=1}^{D}\omega_j[e^{\beta(\omega_j-\mu)} - 1]^{-1}. \tag{5.39}$$

The average particle number is

$$N = \sum_{j=1}^{D}[e^{\beta(\omega_j-\mu)} - 1]^{-1}. \tag{5.40}$$

It is also instructive to approach the evaluation of $\langle A \rangle$ for observable A from a different point of view that will prove useful later. We know that the Hamiltonian operator for a simple harmonic oscillator in D dimensions, which is equivalent to a system of D one-dimensional oscillators, is

$$H = \sum_{j=1}^{D} \left(a_j^\dagger a_j + \frac{1}{2} \right) \omega_j, \tag{5.41}$$

where a_j and $a_j^\dagger$ are the annihilation and creation operators (see the definitions in Section 3.5). The operator for the total number of particles is

$$\mathcal{N} = \sum_{j=1}^{D} a_j^\dagger a_j. \tag{5.42}$$

Thus

$$\bar{H} = H - \mu \mathcal{N} = \sum_{j=1}^{D} \frac{1}{2} \omega_j + \sum_{j=1}^{D} (\omega_j - \mu) a_j^\dagger a_j. \tag{5.43}$$

We now wish to compute $\langle A \rangle = \mathfrak{Z}^{-1} \mathrm{tr}(\rho A)$ where $\rho = e^{-\beta \bar{H}}$. To do this we can use the identity (3.165) with λ defined in (3.163) if we replace H with $\bar{H}$. If A is such that

$$[\bar{H}, A] = -\lambda A \tag{5.44}$$

then

$$\begin{aligned} \langle A \rangle &= \frac{1}{\mathfrak{Z}} \mathrm{tr}(e^{-\beta \bar{H}} A) \\ &= \frac{1}{\mathfrak{Z}} \mathrm{tr}(e^{-\beta \bar{H}} A e^{\beta \bar{H}} e^{-\beta \bar{H}}) \\ &= \frac{1}{\mathfrak{Z}} \mathrm{tr}(e^{\lambda \beta} A e^{-\beta \bar{H}}) \\ &= e^{\lambda \beta} \langle A \rangle. \end{aligned} \tag{5.45}$$

This is sufficient to show that unless $\lambda = 0$, so that the observable A commutes with $\bar{H}$, we must have $\langle A \rangle = 0$. Note that we have not shown that $\langle A \rangle = 0$ unless $[\bar{H}, A] = 0$ for all operators A; rather we have only shown this for special operators which satisfy the relation (5.44) for some constant λ.

An important class of operators of interest to us are those which can be expressed in terms of the creation and annihilation operators. Suppose that we take $A = a_j$. Then

$$[\bar{H}, A] = -\omega_j a_j \tag{5.46}$$

satisfies (5.44) with $\lambda = \omega_j$. We can conclude immediately from (5.45) that

$$\langle a_j \rangle = 0. \tag{5.47}$$

In a similar way it can be shown that

$$\langle a_j^\dagger \rangle = 0. \tag{5.48}$$

The next simplest possibility for A occurs if A is the product of two of the a_j or $a_j^\dagger$. Consider first $A = a_j a_{j'}$. Then

$$[\bar{H}, a_j a_{j'}] = -(\omega_j + \omega_{j'}) a_j a_{j'},$$

and we again conclude from (5.45) that

$$\langle a_j a_{j'} \rangle = 0, \tag{5.49}$$

with the similar result $\langle a_j^\dagger a_{j'}^\dagger \rangle = 0$. If we take $A = a_j^\dagger a_{j'}$, we find

$$[\bar{H}, a_j^\dagger a_{j'}] = (\omega_j - \omega_{j'}) a_j^\dagger a_{j'}. \tag{5.50}$$

We can conclude

$$\langle a_j^\dagger a_{j'} \rangle = 0 \text{ for } j \neq j'. \tag{5.51}$$

However, if $j = j'$ we cannot conclude anything about the average of $a_j^\dagger a_j$. In fact $a_j^\dagger a_j$ may be recognized as the number operator for the jth oscillator and we would not expect its statistical average to vanish.

To evaluate $\langle a_j^\dagger a_j \rangle$ we can go back and note that

$$e^{-\beta \bar{H}} a_j^\dagger = e^{-\beta \omega_j} a_j^\dagger e^{-\beta \bar{H}} \tag{5.52}$$

from (3.165). We then have

$$\begin{aligned} \langle a_j^\dagger a_{j'} \rangle &= \mathfrak{Z}^{-1} \mathrm{tr}[e^{-\beta \bar{H}} a_j^\dagger a_{j'}] \\ &= e^{-\beta \omega_j} \mathfrak{Z}^{-1} \mathrm{tr}[a_j^\dagger e^{-\beta \bar{H}} a_{j'}] \\ &= e^{-\beta \omega_j} \langle a_{j'} a_j^\dagger \rangle \end{aligned} \tag{5.53}$$

where in the last line we have used the cyclic property of the trace (i.e. $\mathrm{tr}(AB) = \mathrm{tr}(BA)$). We also know that the creation and annihilation operators satisfy the canonical commutation relations $a_{j'} a_j^\dagger - a_j^\dagger a_{j'} = \delta_{jj'}$, so by taking the statistical average we have

$$\langle a_{j'} a_j^\dagger \rangle = \delta_{jj'} + \langle a_j^\dagger a_{j'} \rangle. \tag{5.54}$$

If we now use (5.54) in (5.53), we find

$$\langle a_j^\dagger a_{j'} \rangle = e^{\beta(\omega_j - \mu)} [e^{\beta(\omega_j - \mu)} - 1]^{-1} \delta_{jj'}, \tag{5.55}$$

$$\langle a_{j'} a_j^\dagger \rangle = [e^{\beta(\omega_j - \mu)} - 1]^{-1} \delta_{jj'}. \tag{5.56}$$

The previous results (5.39) and (5.40) now follow easily from the average of (5.41) and (5.42).

We can also work out the q-potential if we note that[5]

$$a_j^\dagger a_j = \frac{\partial \bar{H}}{\partial \omega_j} - \frac{1}{2}\,.$$

Taking the statistical average of this last result gives

$$\begin{aligned} \langle a_j^\dagger a_j \rangle &= \left\langle \frac{\partial \bar{H}}{\partial \omega_j} \right\rangle - \frac{1}{2} \\ &= \mathfrak{Z}^{-1} \mathrm{tr} \left(e^{-\beta \bar{H}} \frac{\partial \bar{H}}{\partial \omega_j} \right) - \frac{1}{2} \\ &= -\frac{1}{\beta} \frac{\partial}{\partial \omega_j} \ln \mathfrak{Z} - \frac{1}{2} \\ &= -\frac{1}{\beta} \frac{\partial q}{\partial \omega_j} - \frac{1}{2}. \end{aligned} \tag{5.57}$$

An integration of this result using (5.55) with $j = j'$ on the left-hand side recovers (5.38) up to a constant of integration.

5.3 Real scalar field

Having discussed the simple harmonic oscillator in the previous section we can move on to field theory. As noted in Section 3.6, the real scalar field is just an infinite collection of simple harmonic oscillators, so we can proceed immediately to field theory at finite temperature using the results of the previous section. The Hamiltonian operator was given in Section 3.6 as

$$H = \frac{1}{2} \sum_n E_n (a_n^\dagger a_n + a_n a_n^\dagger),$$

with E_n given in (3.185) as $E_n = \sqrt{\sigma_n + m^2}$ with σ_n the eigenvalues of the Laplacian $-\nabla^2$. When we use the canonical commutation relations to write $a_n a_n^\dagger = 1 + a_n^\dagger a_n$, we see that H is given as in (5.41) but with

[5] We treat all of the frequencies as independent.

the oscillators labelled with the index n. Since particle numbers are not conserved in a relativistic theory with interactions present (which we will consider later), and the real scalar field is uncharged, we will set $\mu = 0$. The thermodynamic potential follows from (5.38) as

$$\Omega = \frac{1}{2}\sum_n E_n + \frac{1}{\beta}\sum_n \ln(1 - e^{-\beta E_n}). \tag{5.58}$$

In the zero temperature limit, only the fist term survives, and this is exactly the expression used for the effective action in the previous chapter. The statistical aspects of the theory at finite temperature lead to an additive correction to the $T = 0$ theory.

The actual evaluation of the finite temperature part of (5.58) even in the simplest case of flat space proves difficult. We will define

$$\Omega_{T\neq 0} = \frac{1}{\beta}\sum_n \ln(1 - e^{-\beta E_n}), \tag{5.59}$$

and interpret this as the finite temperature contribution to the thermodynamic potential.[6] The eigenvalues of the Laplacian are given by (4.23) if we use box normalization. Taking the infinite volume limit results in

$$\Omega_{T\neq 0} = \frac{V}{\beta}\int \frac{d^D p}{(2\pi)^D} \ln\left(1 - e^{-\beta\sqrt{\mathbf{p}^2+m^2}}\right). \tag{5.60}$$

It is not possible to obtain a result for this in a simple form. There are a number of ways to proceed and obtain expansions. We will describe one method here which will prove useful in other examples, and is successful in evaluating the thermodynamic potential at high temperature.

We begin by expanding the logarithm in (5.60) in terms of its Taylor series. This gives

$$\Omega_{T\neq 0} = -\frac{V}{\beta}\sum_{k=1}^{\infty}\frac{1}{k}\int \frac{d^D p}{(2\pi)^D} e^{-k\beta\sqrt{\mathbf{p}^2+m^2}}. \tag{5.61}$$

Although it is possible to evaluate the integral in terms of Bessel functions, we will not do this. Instead we will use the Mellin–Barnes representation for the exponential function which reads

$$e^{-x} = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} d\alpha \Gamma(\alpha) x^{-\alpha}, \tag{5.62}$$

[6] The zero temperature contribution was discussed in Section 4.2.

where $c \in \mathbb{R}$ with $c > 0$ chosen so that the integration contour lies to the right of the poles of the Γ-function. The proof of (5.62) is simple. Close the contour in the left-hand side of the complex α-plane. From Section A1.1 we note that $\Gamma(\alpha)$ has simple poles at $\alpha = -n$ for $n = 0, 1, 2, \ldots$ with residue $(-1)^n/n!$. The residue theorem gives

$$\frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} d\alpha \Gamma(\alpha) x^{-\alpha} = \sum_{n=0}^{\infty} \frac{(-x)^n}{n!} = e^{-x},$$

as claimed. If we use (5.62) for the exponential in (5.61) it is found that

$$\Omega_{T\neq 0} = -\frac{V}{\beta}\sum_{k=1}^{\infty}\int \frac{d^D p}{(2\pi)^D}\frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} d\alpha \Gamma(\alpha) k^{-\alpha}\beta^{-\alpha}(\mathbf{p}^2 + m^2)^{-\alpha/2}. \tag{5.63}$$

If the order of the integrations over $\mathbf{p}$ and α is interchanged, we may compute the integral over $\mathbf{p}$ exactly as we did in Section 4.2 to be

$$\int \frac{d^D p}{(2\pi)^D}(\mathbf{p}^2 + m^2)^{-\alpha/2} = (4\pi)^{-D/2}\frac{\Gamma\left[(\alpha - D)/2\right]}{\Gamma(\alpha/2)}(m^2)^{(D-\alpha)/2}. \tag{5.64}$$

This assumes $\mathcal{R}(\alpha) > D$ and $c > D$. The sum over k in (5.63) just involves the Riemann ζ-function (see Section A1.2). We end up with a contour integral expression for the thermodynamic potential

$$\begin{aligned}\Omega_{T\neq 0} =& -\frac{V}{\beta}\left(\frac{m^2}{4\pi}\right)^{D/2}\frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} d\alpha \frac{\Gamma(\alpha)\Gamma\left[(\alpha - D)/2\right]}{\Gamma(\alpha/2)}\zeta_R(1+\alpha)(\beta m)^{-\alpha} \\ =& -\frac{V}{\beta\sqrt{4\pi}}\left(\frac{m^2}{4\pi}\right)^{D/2}\frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} d\alpha \Gamma\left(\frac{\alpha+1}{2}\right)\Gamma\left(\frac{\alpha - D}{2}\right) \\ & \times \zeta_R(1+\alpha)\left(\frac{\beta m}{2}\right)^{-\alpha}\end{aligned} \tag{5.65}$$

if we use the duplication formula (A1.21) for the Γ-function in the second line to simplify the expression.

If we close the contour in the left-hand side of the complex plane we encounter three sources of poles. $\Gamma\left[(\alpha+1)/2\right]$ has simple poles at $\alpha = -1-2n$ for $n = 0, 1, 2, \ldots$; $\Gamma\left[(\alpha - d)/2\right]$ has simple poles at $\alpha = D-2n$ for $n = 0, 1, 2, \ldots$; $\zeta_R(1+\alpha)$ has a simple pole at $\alpha = 0$. Because $\zeta_R(-2n) = 0$ for $n = 1, 2, \ldots$ it follows that $\Gamma\left[(\alpha+1)/2\right]\zeta_R(\alpha+1)$ has simple poles only at $\alpha = 0, -1$. It is easy to show that when D is even, the integrand of (5.65) has a double pole at $\alpha = 0$, and when D is odd, there is a double pole at $\alpha = -1$. In either case all remaining poles are simple ones. It is

therefore expedient to examine the cases of even and odd D separately again.

For even D it is straightforward to show using the residue theorem that

$$\begin{aligned}\Omega_{T\neq 0} = &- \frac{V}{\pi^{(D+1)/2}\beta^{D+1}} \sum_{n=0, n\neq D/2}^{\infty} \frac{1}{n!}\Gamma\left(\frac{D+1}{2}-n\right) \\ &\times \zeta_R(D+1-2n)\left(-\frac{1}{4}\beta^2 m^2\right)^n \\ &- \frac{V}{2\beta}\left(-\frac{m^2}{4\pi}\right)^{D/2} \frac{1}{(D/2)!}\left[\sum_{k=1}^{D/2}\frac{1}{k} - \ln(\beta^2 m^2)\right] \\ &+ \frac{1}{2}V\left(\frac{m^2}{4\pi}\right)^{(D+1)/2}\Gamma\left(\frac{-1-D}{2}\right). \end{aligned} \tag{5.66}$$

For odd D

$$\begin{aligned}\frac{\Omega_{T\neq 0}}{V} = &- \pi^{-(D+1)/2}\beta^{-D-1} \sum_{n=0}^{(D-1)/2} \frac{(-1)^n}{n!}\Gamma\left(\frac{D+1}{2}-n\right) \\ &\times \zeta_R(D+1-2n)\left(\frac{\beta m}{2}\right)^{2n} \\ &- \frac{1}{2}\left(-\frac{m^2}{4\pi}\right)^{(D+1)/2} \frac{1}{[(D+1)/2]!}\left[2\gamma - \sum_{k=1}^{(D+1)/2} + 2\ln\left(\frac{\beta m}{4\pi}\right)\right] \\ &- \frac{1}{2}\beta^{-1}\left(\frac{m^2}{4\pi}\right)^{D/2}\Gamma\left(-\frac{D}{2}\right) - \pi^{-(D+1)/2}\beta^{-D-1} \\ &\times \sum_{n=(D+3)/2}^{\infty} \frac{(-1)^n}{n!}(-\pi^2)^{n+1+(D+1)/2}\frac{\zeta_R(D-2n)}{\Gamma(2-D/2)}\left(\frac{\beta m}{2}\right)^{2n}. \end{aligned} \tag{5.67}$$

It is possible to simplify the result using properties of the Γ- and ζ-functions (see Sections A1.1 and A1.2). In the physically interesting case of $D = 3$, we find

$$\begin{aligned}\frac{\Omega_{T\neq 0}}{V} = &- \frac{\pi^2}{90}\beta^{-4} + \frac{1}{24}\beta^{-2}m^2 - \frac{1}{12\pi}\beta^{-1}m^3 \\ &- \frac{m^4}{64\pi^2}\left[2\gamma - \frac{3}{2} + 2\ln\left(\frac{\beta m}{4\pi}\right)\right] \\ &- \frac{1}{2}\pi^{-7/2}\beta^{-4}\sum_{n=3}^{\infty}\frac{B_{n-1}}{(n-1)n!}\left(-\frac{\pi^2}{4}\beta^2 m^2\right)^n. \end{aligned} \tag{5.68}$$

B_n are the Bernoulli numbers.

5.4 Charged scalar field

As a field theory example with a non-zero chemical potential we will examine the charged scalar field. From Section 3.7 we have the Hamiltonian operator

$$H = \sum_n E_n (A_n^\dagger A_n + B_n B_n^\dagger) \tag{5.69}$$

and the charge operator

$$Q = e \sum_n (A_n^\dagger A_n - B_n^\dagger B_n). \tag{5.70}$$

The charge operator has been normal ordered. We form

$$\bar{H} = H - \mu Q = \sum_n [E_n + (E_n - e\mu) A_n^\dagger A_n + (E_n + e\mu) B_n^\dagger B_n], \tag{5.71}$$

if we use the commutation relations for B_n and $B_n^\dagger$. The first term represents the sum of the two zero-point energies of $(1/2)\sum_n E_n$, one for the particle and one for the antiparticle. We will define

$$\bar{H}_A = \sum_n (E_n - e\mu) A_n^\dagger A_n, \tag{5.72}$$

$$\bar{H}_B = \sum_n (E_n + e\mu) B_n^\dagger B_n. \tag{5.73}$$

Because A_n and $A_n^\dagger$ commute with B_n and $B_n^\dagger$, we have $[\bar{H}_A, \bar{H}_B] = 0$. The grand partition function is

$$\begin{aligned} \mathfrak{Z} &= \mathrm{tr}(e^{-\beta \bar{H}}) \\ &= e^{-\beta \sum_n E_n} \mathrm{tr}(e^{-\beta \bar{H}_A} e^{-\beta \bar{H}_B}), \end{aligned}$$

if we use (5.71)–(5.73).[7] Furthermore we can write

$$\mathfrak{Z}_A = \mathrm{tr}(e^{-\beta \bar{H}_A}) \tag{5.74}$$

$$\mathfrak{Z}_B = \mathrm{tr}(e^{-\beta \bar{H}_B}) \tag{5.75}$$

and

$$\mathfrak{Z} = e^{-\beta \sum_n E_n} \mathfrak{Z}_A \mathfrak{Z}_B \tag{5.76}$$

because a general energy eigenstate is the product of the states corresponding to the particles and antiparticles. (The states for particles are

[7] Note that because $[\bar{H}_A, \bar{H}_B] = 0$ we can use $e^{-\beta(\bar{H}_A + \bar{H}_B)} = e^{-\beta \bar{H}_A} e^{-\beta \bar{H}_B}$.

built up by acting with $A_n^\dagger$ on the vacuum state $|0\rangle$. Because B_n and $B_n^\dagger$ commute with $A_n^\dagger$ they will annihilate the particle states and vice versa. This means that $e^{-\beta \bar{H}_B}$ acts like the identity operator on particle states, and $e^{-\beta \bar{H}_A}$ acts like the identity operator on antiparticle states.)

We can compute $\mathfrak{Z}_A$ and $\mathfrak{Z}_B$ exactly as we did for the simple harmonic oscillator or the real scalar field. For $\mathfrak{Z}_A$ we write

$$\mathfrak{Z}_A = \mathrm{tr}\left[\prod_n e^{-\beta \bar{H}_A^{(n)}}\right] \tag{5.77}$$

where $\bar{H}_A^{(n)} = (E_n - e\mu)A_n^\dagger A_n$. Using the same procedure as we did in Section 5.3 for the real scalar field we have

$$\mathfrak{Z}_A = \prod_n \mathfrak{Z}_A^{(n)} \tag{5.78}$$

where

$$\begin{aligned}\mathfrak{Z}_A^{(n)} &= \mathrm{tr} e^{-\beta \bar{H}_A^{(n)}} \\ &= \sum_{n'=0}^{\infty} {}_A\langle n'|e^{-\beta \bar{H}_A^{(n)}}|n'\rangle_A\end{aligned}$$

with $A_n^\dagger A_n |n'\rangle_A = n'|n'\rangle_A$. We end up with

$$\begin{aligned}\mathfrak{Z}_A^{(n)} &= \sum_{n'=0}^{\infty} e^{-\beta(E_n - e\mu)n'} \\ &= \left[1 - e^{-\beta(E_n - e\mu)}\right]^{-1}.\end{aligned} \tag{5.79}$$

Thus if we use (5.80) in (5.78) we find

$$\mathfrak{Z}_A = \prod_n \left[1 - e^{-\beta(E_n - e\mu)}\right]^{-1}. \tag{5.80}$$

A similar calculation leads to[8]

$$\mathfrak{Z}_B = \prod_n \left[1 - e^{-\beta(E_n + e\mu)}\right]^{-1}. \tag{5.81}$$

Defining the thermodynamic potential by combining (5.12) and (5.26) to give $\Omega = -\beta^{-1} \ln \mathfrak{Z}$, and using (5.76), (5.80), and (5.81) to obtain $\mathfrak{Z}$, we have

[8] The only difference between $\mathfrak{Z}_A$ and $\mathfrak{Z}_B$ in (5.74) and (5.75) is in the sign of $e\mu$.

$$\Omega = \sum_n E_n + \frac{1}{\beta}\sum_n \left\{ \ln\left[1 - e^{-\beta(E_n - e\mu)}\right] + \ln\left[1 - e^{-\beta(E_n + e\mu)}\right] \right\}. \tag{5.82}$$

We can also compute the statistical average of products of creation and annihilation operators. By following the same procedure as for the real scalar field in Section 5.3 it is not difficult to show that

$$\langle A_n^\dagger A_{n'} \rangle = [e^{\beta(E_n - e\mu)} - 1]^{-1}\delta_{nn'}, \tag{5.83}$$

$$\langle B_n^\dagger B_{n'} \rangle = [e^{\beta(E_n + e\mu)} - 1]^{-1}\delta_{nn'}. \tag{5.84}$$

The average value of the charge follows from (5.70) as

$$\langle Q \rangle = e\sum_n \left\{ [e^{\beta(E_n - e\mu)} - 1]^{-1} - [e^{\beta(E_n + e\mu)} - 1]^{-1} \right\}. \tag{5.85}$$

This result is consistent with what is obtained using the fundamental relation (5.30) along with our result (5.82) for the thermodynamic potential.

We can now study the evaluation of Ω in the high temperature limit and see what complications occur when the chemical potential is present beyond what we found for the real scalar field. If we think of $[e^{\beta(E_n - e\mu)} - 1]^{-1}$ as the number of particles and $[e^{\beta(E_n + e\mu)} - 1]^{-1}$ as the number of antiparticles present with energy E_n, it is clear that because both of these expressions must be positive

$$|e\mu| \leq E_0. \tag{5.86}$$

Here $E_0 = \sqrt{\sigma_0 + m^2}$ is the lowest energy eigenvalue. In flat empty space we have $\sigma_0 = 0$ so that the restriction (5.86) becomes $|e\mu| \leq m$. We will return to a more detailed study of what happens when $|e\mu| = m$ in the next chapter.

If we define $\Omega_{T\neq 0}$ by

$$\Omega_{T\neq 0} = \frac{1}{\beta}\sum_n \left\{ \ln\left[1 - e^{-\beta(E_n - e\mu)}\right] + \ln\left[1 - e^{-\beta(E_n + e\mu)}\right] \right\},$$

(so that $\Omega_{T\neq 0}$ again represents just the finite temperature correction to the zero temperature result) by expanding the logarithms in their Taylor series we find

$$\Omega_{T\neq 0} = -\frac{2}{\beta}\sum_{k=1}^{\infty}\sum_n e^{-k\beta E_n}\frac{\cosh(k\beta e\mu)}{k}. \tag{5.87}$$

In the last section we used the Mellin–Barnes integral representation for the exponential function $e^{-k\beta E_n}$ to obtain the high temperature expansion for $\Omega_{T\neq 0}$. If we try to do this here we run into a problem because of the presence of $\cosh(k\beta e\mu)$ that involves exponentials of both positive and negative arguments. This factor leads to a divergence in the sum over k if $\mu \neq 0$. Instead we must proceed somewhat differently.

To illustrate another technique we return to our summation formula in (A1.64), (A1.65). Expanding about $\lambda = 0$ we find $F(0; a, b) = 0$ and

$$\begin{aligned} F'(0;a,b) =& -2\pi b - 2\mathcal{R}\ln\left[1-e^{-2\pi(b+ia)}\right] \\ =& -2\pi b - \ln\left[1-e^{-2\pi(b+ia)}\right] - \ln\left[1-e^{-2\pi(b-ia)}\right] \end{aligned} \tag{5.88}$$

where the $'$ on F denotes the derivative with respect to λ. If we now set

$$a = i\,\frac{e\mu\beta}{2\pi}, \tag{5.89}$$

$$b = \frac{\beta E_k}{2\pi}, \tag{5.90}$$

(5.88) becomes

$$F'(0;a,b) = -\beta E_k - \ln\left[1-e^{-\beta(E_k-e\mu)}\right] - \ln\left[1-e^{-\beta(E_k+e\mu)}\right]. \tag{5.91}$$

At this stage we can recognize this as looking very much like the structure of the thermodynamic potential. In fact, from (5.82) we can see that

$$\Omega = -\frac{1}{\beta}\sum_k F'\left(0; i\,\frac{e\mu\beta}{2\pi}, \frac{\beta E_k}{2\pi}\right). \tag{5.92}$$

This suggests that we define a new sum,

$$G(\lambda) = \sum_k \sum_{n=-\infty}^{\infty}\left[\left(n + i\,\frac{e\mu\beta}{2\pi}\right)^2 + \left(\frac{\beta E_k}{2\pi}\right)^2\right]^{-\lambda} \tag{5.93}$$

with

$$\Omega = -\frac{1}{\beta}G'(0). \tag{5.94}$$

The advantage of doing this is that the temperature dependence in $G(\lambda)$ is simple, and our strategy in obtaining the high temperature expansion will be to perform the sum over k first, then expand the result in powers of $\beta = 1/T$, and finally to perform the analytic continuation to $\lambda = 0$. This provides an alternative, and somewhat easier, approach than that

used in Haber and Weldon (1982), and was first used by Actor (1987). We will follow the generalization of Toms (1993).

We will look only at the $D = 3$ case in flat spacetime. Performing the by now familiar method of enclosing the system in a box with the large volume limit taken results in

$$G(\lambda) = V \int \frac{d^3k}{(2\pi)^3} \sum_{n=-\infty}^{\infty} \left[\left(n + ie\bar{\beta}\right)^2 + \bar{\beta}^2(k^2 + m^2) \right]^{-\lambda} \tag{5.95}$$

with

$$\bar{\beta} = \frac{\beta}{2\pi} \tag{5.96}$$

defined for convenience. The integration over k can be performed using the same procedure as in Section 4.2 to give

$$G(\lambda) = \frac{V\,\Gamma\left[\lambda - (3/2)\right]}{(4\pi)^{3/2}\bar{\beta}^3\,\Gamma(\lambda)} \sum_{n=-\infty}^{\infty} \left[\left(n + ie\bar{\beta}\right)^2 + \bar{\beta}^2 m^2 \right]^{(3/2)-\lambda}. \tag{5.97}$$

The next step is to use the binomial expansion to obtain an expansion in powers of $\bar{\beta}$. To this end, we first separate off the $n = 0$ term, and write

$$\begin{aligned} G(\lambda) =& \frac{V\,\Gamma\left[\lambda - (3/2)\right]}{(4\pi)^{3/2}\bar{\beta}^{2\lambda}\,\Gamma(\lambda)} (m^2 - e^2\mu^2)^{(3/2)-\lambda} \\ &+ \frac{V}{(4\pi)^{3/2}\bar{\beta}^3\,\Gamma(\lambda)} \left[S\left(\lambda - \frac{3}{2}, \mu\right) + S\left(\lambda - \frac{3}{2}, -\mu\right) \right] \end{aligned} \tag{5.98}$$

where

$$S(\lambda, \mu) = \Gamma(\lambda) \sum_{n=1}^{\infty} \left[\left(n + ie\bar{\beta}\right)^2 + \bar{\beta}^2 m^2 \right]^{-\lambda}. \tag{5.99}$$

has been defined. The calculation now reduces to an evaluation of $S(\lambda, \mu)$.

If we define(5.99)[9]

$$z_n = \frac{2ie\mu\bar{\beta}}{n} + \bar{\beta}^2 \frac{(m^2 - e^2\mu^2)}{n^2}, \tag{5.100}$$

we can write

$$S(\lambda, \mu) = \Gamma(\lambda) \sum_{n=1}^{\infty} n^{-2\lambda}(1 + z_n)^{-\lambda}. \tag{5.101}$$

[9] This is why we first removed the $n = 0$ term in (5.98).

The binomial expansion gives us

$$(1+z_n)^{-\lambda} = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} \frac{\Gamma(\lambda+k)}{\Gamma(\lambda)} z_n^k. \tag{5.102}$$

We can substitute for z_n on the right-hand side of (5.102) using the definition (5.100), and then use the binomial expansion again to find

$$(1+z_n)^{-\lambda} = \sum_{k=0}^{\infty} \sum_{l=0}^{k} \frac{(-1)^k}{l!(k-l)!} \frac{\Gamma(\lambda+k)}{\Gamma(\lambda)} (2ie\mu)^{k-l} \bar{\beta}^{k+l} (m^2 - e^2\mu^2)^l. \tag{5.103}$$

This second use of the binomial expansion is necessary because $\bar{\beta}$ occurs with different powers in (5.100). After substitution of (5.103), we notice that the summation over n may be performed in terms of the Riemann ζ-function. This gives

$$S(\lambda,\mu) = \sum_{k=0}^{\infty} \sum_{l=0}^{k} \sigma(k,l) \bar{\beta}^{k+l} \tag{5.104}$$

where the coefficients

$$\sigma(k,l) = \frac{(-1)^k}{l!(k-l)!} \Gamma(\lambda+k)(2ie\mu)^{k-l}(m^2 - e^2\mu^2)^l \zeta(2\lambda+k+l) \tag{5.105}$$

have no explicit dependence on temperature.

To identify a particular power of $\bar{\beta}$ in $S(\lambda,\mu)$ is complicated because of the double summation. We can alleviate this complication by the simple expedient of relabelling the summation indices:

$$S(\lambda,\mu) = \sum_{n=0}^{\infty} \sum_{l=0}^{n} \sigma(n-l,l) \bar{\beta}^n. \tag{5.106}$$

Now one of the summation indices (the one over n) gives us the order of $\bar{\beta}$. Finally, it proves advantageous to split the sum up into terms which are even and odd powers of μ. This is because we are really only interested in the combination $S(\lambda,\mu) + S(\lambda,-\mu)$ which is an even function of μ. From (5.105), $\sigma(n-l,l)$ has a μ-dependence of $(i\mu)^{n-2l}$. Therefore all terms in (5.106) with n odd will cancel when we form $S(\lambda,\mu) + S(\lambda,-\mu)$. We can write

$$S(\lambda,\mu) = \sum_{n=0}^{\infty} x_n(\lambda) \bar{\beta}^{2n} + \sum_{n=0}^{\infty} y_n(\lambda) \bar{\beta}^{2n+1}, \tag{5.107}$$

where

$$x_n(\lambda) = \sum_{l=0}^{n} \sigma(2n-l,l), \tag{5.108}$$

$$y_n(\lambda) = \sum_{l=0}^{n} \sigma(2n+1-l,l). \tag{5.109}$$

As explained, $y_n(\lambda)$ will be odd in μ (and hence purely imaginary) and will not be needed. Returning to (5.98), we have found

$$G(\lambda) = \frac{V\,\Gamma\left[\lambda-(3/2)\right]}{(4\pi)^{3/2}\,\Gamma(\lambda)}\,\bar{\beta}^{-2\lambda}(m^2-e^2\mu^2)^{(3/2)-\lambda} + \frac{2V}{(4\pi)^{3/2}\,\Gamma(\lambda)}\sum_{n=0}^{\infty} x_n\left(\lambda-\frac{3}{2}\right)\bar{\beta}^{2n-3}. \tag{5.110}$$

The coefficients $x_n\left[\lambda-(3/2)\right]$ may be found using (5.105) and (5.108). A short calculation leads to the first few terms given by

$$x_0\left(\lambda-\frac{3}{2}\right) = \Gamma\left(\lambda-\frac{3}{2}\right)\zeta(2\lambda-3), \tag{5.111}$$

$$x_1\left(\lambda-\frac{3}{2}\right) = -\left[m^2+2(\lambda-1)e^2\mu^2\right]\Gamma\left(\lambda-\frac{1}{2}\right)\zeta(2\lambda-1), \tag{5.112}$$

$$x_2\left(\lambda-\frac{3}{2}\right) = \frac{1}{6}\left[3m^4+12\lambda m^2e^2\mu^2+4\lambda(\lambda-1)e^4\mu^4\right] \times\Gamma\left(\lambda+\frac{1}{2}\right)\zeta(2\lambda+1). \tag{5.113}$$

We can concentrate on the finite temperature part of the thermodynamic potential here.[10] When $\mu=0$ the thermodynamic potential follows from Section 5.3: it is just the expression in (5.68) multiplied by two (since there are two real scalar fields here, the real and the imaginary parts of the complex field). We have

$$\frac{\Omega_{T\neq0}(\mu=0)}{V} = -\frac{\pi^2}{45}T^4+\frac{1}{12}m^2T^2-\frac{1}{6\pi}m^3T - \frac{m^4}{32\pi^2}\left[2\gamma-\frac{3}{2}+2\ln\left(\frac{\beta m}{4\pi}\right)\right]+\mathcal{O}(T^{-2}). \tag{5.114}$$

[10] As in Section 5.3 we will define this as that part of Ω which does not involve the zero-point energy contribution.

It should be clear that we can write

$$\Omega_{T\neq 0}(\mu) = \Omega_{T\neq 0}(\mu = 0) - \frac{1}{\beta}\left[G'(0) - G'(0)|_{\mu=0}\right] \tag{5.115}$$

from (5.94). Proceeding like this means that we do not have to work out the $\mu = 0$ terms all over again, which shortens the calculation. If we now use the results we have found for $G(\lambda)$ and the results for x_0, x_1, x_2 found in (5.111)–(5.113), it is easy to see that

$$\begin{aligned} G'(0) - G'(0)|_{\mu=0} = {} & \frac{V}{6\pi}\left[\left(m^2 - e^2\mu^2\right)^{3/2} - m^3\right] \\ & + \frac{V}{12\pi}\bar{\beta}\left[e^2\mu^2\bar{\beta}^{-2} + e^2\mu^2(3m^2 - e^2\mu^2) + \mathcal{O}(\bar{\beta}^2)\right]. \end{aligned} \tag{5.116}$$

Combining the results for (5.114) and (5.116) yields our final expression:

$$\begin{aligned} \frac{\Omega_{T\neq 0}}{V} = {} & -\frac{\pi^2}{45}T^4 + \frac{1}{12}(m^2 - 2e^2\mu^2)T^2 - \frac{1}{6\pi}\left(m^2 - e^2\mu^2\right)^{3/2}T \\ & - \frac{m^4}{32\pi^2}\left[2\gamma - \frac{3}{2} + 2\ln\left(\frac{m}{4\pi T}\right)\right] - \frac{1}{24\pi^2}e^2\mu^2(3m^2 - e^2\mu^2) \\ & + \mathcal{O}(T^{-2}) \end{aligned} \tag{5.117}$$

at high temperatures. In the next chapter we will use this expression to study Bose–Einstein condensation of the relativistic charged gas in the high temperature limit. Although we have restricted our attention to the case $D = 3$, the reader should have no trouble repeating the analysis for other spatial dimensions.

5.5 Non-relativistic field

5.5.1 Non-relativistic limit

In previous chapters we considered a system of non-relativistic bosons by postulating that the theory was described by a Schrödinger field Ψ. Here we wish to discuss this in a bit more detail beginning with a complex scalar field as in the previous section and by considering the non-relativistic limit.

First of all we are usually interested in low temperatures for non-relativistic systems. Specifically we have $kT << mc^2$ in conventional units, or $\beta m >> 1$ in natural units.[11] Physically what $kT << mc^2$ means is that

[11] Under normal laboratory experimental conditions the temperature is usually much smaller than the rest mass energy of an atom.

there is not enough thermal energy present to create particle–antiparticle pairs.[12] Since we deal primarily with particles rather than antiparticles, the implication of $kT << mc^2$ is that the number of particles is conserved to a good approximation in this temperature range. The number of particles N_+ and the number of antiparticles N_- with energy E_n are given by the Bose–Einstein distribution functions

$$N_\pm = [e^{\beta(E_n \mp e\mu)} - 1]^{-1}. \tag{5.118}$$

If $N \simeq N_+$, then $N_- << N_+$ giving from (5.118)

$$e^{2\beta e\mu} >> 1, \tag{5.119}$$

and hence

$$\beta e\mu >> 1. \tag{5.120}$$

We can treat $e\mu$ as positive here. Since $e\mu$ has dimensions of mass, we have kT much smaller than both mass scales m and $e\mu$ in the theory.

As T is reduced, if $N \simeq N_+$ is to remain fixed, $e\mu$ must increase. Since we have $e\mu \leq E_0 = \sqrt{\sigma_0 + m^2}$, $e\mu$ must approach its maximum value at low temperatures. The non-relativistic energy was defined by $\varepsilon_n = \sigma_n/2m$. We use ε_n to distinguish the non-relativistic from the relativistic value of E_n. We have

$$E_n = \sqrt{2m\varepsilon_n + m^2}, \tag{5.121}$$

that for $\varepsilon_n << m$ gives

$$E_n \simeq m + \varepsilon_n + \cdots, \tag{5.122}$$

showing the usual relation between the relativistic and the non-relativistic energies. We can conclude that $E_0 \simeq m + \varepsilon_0 \simeq m$ in the non-relativistic limit, and therefore $e\mu \to m$. A natural definition for the chemical potential in the non-relativistic limit is

$$e\mu_{nr} = e\mu - m, \tag{5.123}$$

which should be small at low temperatures.

The thermodynamic potential (5.82) involves $E_n \pm e\mu$. Using (5.122) and (5.123) it is seen that

$$E_n - e\mu \simeq \varepsilon_n - e\mu_{nr}, \tag{5.124}$$

[12] Of course, this cannot happen for the free field theory we are considering here anyway, but we should view the free theory as the model for a realistic theory with interactions present.

and

$$E_n + e\mu \simeq 2m + \varepsilon_n + e\mu_{nr}. \tag{5.125}$$

This last result shows that the antiparticle contribution to the thermodynamic potential contained in $T\sum_n \ln[1 - e^{-\beta(E_n+e\mu)}]$ is very small since $\varepsilon_n + e\mu_{nr} << 2m$ and $\beta m >> 1$. We can drop the antiparticle contribution to the thermodynamic potential leaving us with

$$\Omega_{nr} \simeq \sum_n \varepsilon_n + T\sum_n \ln[1 - e^{-\beta(\varepsilon_n - e\mu_{nr})}]. \tag{5.126}$$

In the zero-point energy contribution we have used (5.122) and dropped the rest mass energy. The rest mass energy only adds a constant term to Ω which cannot affect any physically relevant expressions computed from the various derivatives of Ω.

The Hamiltonian for the relativistic field (5.69) contains both particle and antiparticle contributions. As we have already discussed, the non-relativistic limit can be regarded as a theory which is free of antiparticles. Thus the states in the non-relativistic theory $|\psi\rangle$ satisfy $B_n^\dagger B_n|\psi\rangle = 0$. Since $B_n B_n^\dagger - B_n^\dagger B_n = 1$, we can think of $B_n B_n^\dagger$ as acting like the identity operator in the non-relativistic limit. Using (5.69) we have

$$H_{nr} \simeq \sum_n \varepsilon_n (A_n^\dagger A_n + 1) \tag{5.127}$$

if we make use of (5.122) and drop the rest mass energy. For the case of the Schrödinger theory in Section 3.8 we had (see (3.272))

$$H = \sum_n \varepsilon_n A_n^\dagger A_n. \tag{5.128}$$

The only difference between (5.127) and (5.128) is the presence of the zero-point energy term. We can think of H given by the Schrödinger field theory in Section 3.8 as the normal-ordered expression for H_{nr}.

To sum up, the Schrödinger theory follows as the non-relativistic limit of the complex relativistic scalar field theory if we drop the antiparticle contribution to the thermodynamic potential, neglect the rest mass energy, and drop the zero-point energy. In addition we must restrict ourselves to temperatures which satisfy $kT << mc^2$. Whether or not we wish to neglect the zero-point energy depends on exactly what calculation we are performing. If the only role of the zero-point energy is to add on a constant term to Ω, then it may be safely ignored; however, as we will see later this is not always the case.

5.5.2 Thermodynamic potential for bosons

For bosons we assume that the creation and annihilation operators satisfy commutation relations as described in Section 3.8. Because the Hamiltonian in (5.127) is the sum of simple harmonic oscillator Hamiltonians we can follow the same procedure as we did in Section 5.2 to show that the thermodynamic potential is given by (5.126).[13]

When we take the space Σ to represent flat space it is easy to evaluate Ω much as we did for the relativistic fields. By imposing box normalization we have (using E_n rather than ε_n from here on)

$$E_n = \frac{1}{2m}\sum_{j=1}^{D}\left(\frac{2\pi n_j}{L_j}\right)^2 \tag{5.129}$$

where $n_j = 0, \pm 1, \pm 2, \ldots$. With the large box limit taken we have the finite temperature part of Ω given as

$$\Omega_{T\neq 0} = T\int d^D n \ln\left[1 - e^{-\beta(E_n-\mu)}\right]. \tag{5.130}$$

The zero-point energy contribution is an irrelevant constant in this case even if we do not normal order the Hamiltonian operator. We have defined $\mu = e\mu_{nr}$ here so that our results apply to neutral particles.

To evaluate (5.130) we can expand the logarithm in its Taylor series as we did in Sections 5.3 and 5.4 obtaining

$$\Omega_{T\neq 0} = -\frac{V}{\beta}\int \frac{d^D p}{(2\pi)^D}\sum_{k=1}^{\infty}\frac{1}{k}e^{-k\beta\left[p^2/(2m)-\mu\right]} \tag{5.131}$$

after changing variables $n_j \to p_j L_j/2\pi$. The momentum integral is just a Gaussian evaluated to give

$$\Omega_{T\neq 0} = -\frac{V}{\beta}\left(\frac{m}{2\pi\beta}\right)^{D/2}\sum_{k=1}^{\infty}\frac{e^{k\beta\mu}}{k^{1+D/2}}. \tag{5.132}$$

Note that we need $\mu \leq E_0 = 0$ to avoid negative occupation numbers so that the sum in (5.132) is convergent. It is convenient to define the polylogarithm function

$$\mathrm{Li}_p(z) = \sum_{n=1}^{\infty}\frac{z^n}{n^p}, \tag{5.133}$$

[13] Use of (5.128) instead of (5.127) will lead to (5.126) with the zero-point energy term removed.

for all p if $|z| < 1$, and for $p > 1$ if $z = 1$. Some of the properties of this function are examined in Section A1.4. With this definition we have

$$\Omega_{T\neq 0} = -\frac{V}{\beta}\left(\frac{m}{2\pi\beta}\right)^{D/2} \mathrm{Li}_{1+D/2}(e^{\beta\mu}). \tag{5.134}$$

We will return to discuss some of the physical consequences of this later.

5.5.3 Thermodynamic potential for fermions

Non-relativistic fermions are described by operators A_n and $A_n^\dagger$ which obey the anti-commutation relations (3.249) and (3.250). The Hamiltonian is still given by (5.128) (after normal ordering), and the number operator is $\mathcal{N} = \sum_n A^\dagger A_n$ just as for bosons. To compute the thermodynamic potential we proceed as in Section 5.2. We have

$$\bar{H} = H - \mu\mathcal{N} = \sum_n (E_n - \mu) A_n^\dagger A_n. \tag{5.135}$$

We can use the anti-commutation relations (3.249) and (3.250) to compute

$$\begin{aligned}
[\bar{H}, A_n] &= \sum_{n'} (E_{n'} - \mu)[A_{n'}^\dagger A_{n'}, A_n] \\
&= \sum_{n'} (E_{n'} - \mu)\left\{A_{n'}^\dagger [A_{n'}, A_n]_+ - [A_{n'}^\dagger, A_n]_+ A_{n'}\right\} \\
&= -(E_n - \mu) A_n.
\end{aligned} \tag{5.136}$$

In the middle line we have used the identity (3.245). We can now use (3.163) and (3.165) to obtain

$$e^{-\beta\bar{H}} A_n e^{\beta\bar{H}} = e^{\beta(E_n - \mu)} A_n. \tag{5.137}$$

Taking the Hermitian conjugate of this last result gives

$$e^{-\beta\bar{H}} A_n^\dagger e^{\beta\bar{H}} = e^{-\beta(E_n - \mu)} A_n^\dagger. \tag{5.138}$$

We can now deduce that

$$\langle A_n \rangle = 0 = \langle A_n^\dagger \rangle. \tag{5.139}$$

This conclusion follows from (5.137) and (5.138) using the same argument as in Section 5.2.

We can also calculate

$$\begin{aligned}\langle A_n^\dagger A_{n'}\rangle &= \mathfrak{Z}^{-1}\mathrm{tr}\left(e^{-\beta\bar{H}}A_n^\dagger A_{n'}\right)\\ &= \mathfrak{Z}^{-1}e^{-\beta(E_n-\mu)}\mathrm{tr}\left(A_n^\dagger e^{-\beta\bar{H}}A_{n'}\right)\\ &= e^{-\beta(E_n-\mu)}\langle A_{n'}A_n^\dagger\rangle. \end{aligned} \tag{5.140}$$

We have used (5.138) to obtain the middle line, and the cyclic property of the trace has been used in the last line. This result is identical to that found for bosons (see (5.53)) since the commutation or anti-commutation relations for the creation and annihilation operators are not used. The difference between bosons and fermions comes when we use (5.140) to compute $\langle A_{n'}A_n^\dagger\rangle$. For fermions we use (3.250), $A_{n'}A_n^\dagger + A_n^\dagger A_{n'} = \delta_{n'n}$, to find

$$\langle A_{n'}A_n^\dagger\rangle = \delta_{nn'}\left[1+e^{-\beta(E_n-\mu)}\right]^{-1}, \tag{5.141}$$

$$\langle A_n^\dagger A_{n'}\rangle = \delta_{nn'}\left[e^{\beta(E_n-\mu)}+1\right]^{-1}. \tag{5.142}$$

Since $A_n^\dagger A_n$ is the number operator for the nth mode, (5.142) shows the familiar Fermi–Dirac distribution function. The results of (5.141) and (5.142) can be contrasted with (5.55) and (5.56) for bosons. The origin of the difference between the two distribution functions is clearly traced to the use of commutation relations for the creation and annihilation operators for bosons versus anti-commutation relations for fermions.

From (5.135) we find

$$\frac{\partial\bar{H}}{\partial E_n} = A_n^\dagger A_n. \tag{5.143}$$

Following the same procedure as led to (5.57) we can show

$$\langle A_n^\dagger A_n\rangle = -\frac{1}{\beta}\frac{\partial q}{\partial E_n} = -\frac{\partial\Omega}{\partial E_n}. \tag{5.144}$$

Integration of this expression using (5.142) gives

$$\Omega_{T\neq 0} = T\sum_n \ln[1+e^{-\beta(E_n-\mu)}] \tag{5.145}$$

as the finite temperature part of the thermodynamic potential. If we do not include the zero-point energy term in the Hamiltonian, then this is the complete expression for Ω. We will see in the next section how (5.145) is related to the non-relativistic limit of the Dirac theory.

5.6 Dirac field

We begin with the Hamiltonian given in (3.310). We have interpreted $a^\dagger_{n\lambda}a_{n\lambda}$ as the number operator for particles of energy E_n in the spin state λ with $b^\dagger_{n\lambda}b_{n\lambda}$ as the number operator for antiparticles. The charge operator is therefore

$$Q = e\sum_{n,\lambda}(a^\dagger_{n\lambda}a_{n\lambda} - b^\dagger_{n\lambda}b_{n\lambda}). \tag{5.146}$$

(The result has been normal ordered so that $\langle 0|Q|0\rangle = 0$.) We form

$$\bar{H} = H - \mu Q = \sum_{n,\lambda}\Big[(E_n - e\mu)a^\dagger_{n\lambda}a_{n\lambda} + (E_n + e\mu)b^\dagger_{n\lambda}b_{n\lambda} - 1\Big]. \tag{5.147}$$

Because of the anti-commutation relations (3.305) and (3.306) obeyed by the creation and annihilation operators we find

$$[\bar{H}, a_{n\lambda}] = -(E_n - e\mu)a_{n\lambda}, \tag{5.148}$$
$$[\bar{H}, b_{n\lambda}] = -(E_n + e\mu)b_{n\lambda}. \tag{5.149}$$

The identity (3.165) with (3.163) now gives

$$e^{-\beta\bar{H}}a_{n\lambda}e^{\beta\bar{H}} = e^{\beta(E_n - e\mu)}a_{n\lambda}, \tag{5.150}$$
$$e^{-\beta\bar{H}}b_{n\lambda}e^{\beta\bar{H}} = e^{\beta(E_n + e\mu)}b_{n\lambda}. \tag{5.151}$$

As in previous cases we find

$$\langle a_{n\lambda}\rangle = \langle a^\dagger_{n\lambda}\rangle = \langle b_{n\lambda}\rangle = \langle b^\dagger_{n\lambda}\rangle = 0. \tag{5.152}$$

The calculation which led to (5.140) and (5.142) can again be followed to show that

$$\langle a^\dagger_{n\lambda}a_{n'\lambda'}\rangle = e^{-\beta(E_n - e\mu)}\langle a_{n'\lambda'}a^\dagger_{n\lambda}\rangle, \tag{5.153}$$
$$\langle b^\dagger_{n\lambda}b_{n'\lambda'}\rangle = e^{-\beta(E_n + e\mu)}\langle b_{n'\lambda'}b^\dagger_{n\lambda}\rangle. \tag{5.154}$$

Using the anti-commutation relations (3.306) we find

$$\langle a^\dagger_{n\lambda}a_{n'\lambda'}\rangle = \delta_{nn'}\delta_{\lambda\lambda'}[e^{\beta(E_n - e\mu)} + 1]^{-1}, \tag{5.155}$$
$$\langle b^\dagger_{n\lambda}b_{n'\lambda'}\rangle = \delta_{nn'}\delta_{\lambda\lambda'}[e^{\beta(E_n + e\mu)} + 1]^{-1}. \tag{5.156}$$

The thermodynamic potential is

$$\Omega = -\sum_{n,\lambda}E_n + T\sum_{n,\lambda}\Big\{\ln[1 + e^{-\beta(E_n - e\mu)}] + \ln[1 + e^{-\beta(E_n + e\mu)}]\Big\}. \tag{5.157}$$

Given that the energy levels E_n do not depend on the spin label λ for the free Dirac theory, the sum over λ in (5.157) just results in a numerical factor of $2^{[(D+1)/2]}$ as in Section 3.9.

We can take the non-relativistic limit of the theory just as we did for the complex scalar field in Section 5.5.1. The conditions $\beta m >> 1$ and $\beta e\mu >> 1$ follow for exactly the same reasons as before. The antiparticle contribution to the thermodynamic potential is suppressed at such low temperatures and we recover the result of (5.145) with the addition of the zero-point energy, and the extra sum over λ because the Dirac theory has spin built into it.

5.7 Electromagnetic field

Photons are neither charged nor is their particle number conserved. The quantization of the electromagnetic field was discussed in Section 3.10. We have the Hamiltonian operator

$$H = \frac{1}{2}\sum_{n,\lambda} E_n(a_{n\lambda}a^\dagger_{n,\lambda} + a^\dagger_{n\lambda}a_{n\lambda}), \tag{5.158}$$

where λ runs over $(D-1)$ possible values. Apart from the extra label λ, related to the spin states of the electromagnetic field, the Hamiltonian is like that for a massless real scalar field. The thermodynamic potential therefore follows from (5.58) as

$$\Omega = \frac{1}{2}\sum_{n,\lambda} E_n + T\sum_{n,\lambda}\ln(1-e^{-\beta E_n}). \tag{5.159}$$

If we concentrate on flat space with the zero-point energy removed, we have

$$\Omega = \frac{V}{\beta}(D-1)\int \frac{d^Dp}{(2\pi)^D}\,\ln(1-e^{-\beta p}) \tag{5.160}$$

from (5.60). (The factor of $(D-1)$ comes from the sum over λ.) Unlike previous examples, we can perform the integral to obtain an analytical result for the thermodynamic potential in this case. Expanding the logarithm in its Taylor series gives

$$\Omega = -\frac{V}{\beta}(D-1)\sum_{k=1}^{\infty}\frac{1}{k}\int\frac{d^Dp}{(2\pi)^D}e^{-k\beta p}. \tag{5.161}$$

If we switch to polar coordinates in momentum space we have

$$\int\frac{d^Dp}{(2\pi)^D} = S_D\int_0^\infty dp\,p^{D-1}, \tag{5.162}$$

where S_D is the area of the unit $(D-1)$-sphere divided by $(2\pi)^D$. We can evaluate S_D by considering

$$I = \int \frac{d^D p}{(2\pi)^D} e^{-p^2} = (4\pi)^{-D/2} \tag{5.163}$$

where the integral has been evaluated by expressing it as the product of D one-dimensional Gaussians. On the other hand, if we use (5.162) we have

$$\begin{aligned} I &= S_D \int_0^\infty dp\, p^{D-1} e^{-p^2} \\ &= S_D \frac{1}{2} \Gamma\left(\frac{D}{2}\right), \end{aligned} \tag{5.164}$$

from the definition of the Γ-function (see Section A1.1). Comparing (5.163) and (5.164) allows us to deduce

$$S_D = \frac{2}{(4\pi)^{D/2}\Gamma(D/2)}. \tag{5.165}$$

Returning to (5.161) we can write

$$\begin{aligned} \Omega &= -\frac{2V(D-1)}{\beta(4\pi)^{D/2}\Gamma(D/2)} \sum_{k=1}^{\infty} \frac{1}{k} \int_0^\infty dp\, p^{D-1} e^{-k\beta p} \\ &= -\frac{2V(D-1)}{\beta(4\pi)^{D/2}\Gamma(D/2)} \beta^{-D} \Gamma(D) \zeta_R(D+1), \end{aligned} \tag{5.166}$$

using results from Sections A1.1 and A1.2. The internal energy follows from (5.22) and (5.26) as

$$E = \frac{\partial}{\partial \beta}(\beta\Omega) = \frac{2VD(D-1)\Gamma(D)}{(4\pi)^{D/2}\Gamma(D/2)} \beta^{-D-1} \zeta_R(D+1). \tag{5.167}$$

In the special case $D = 3$ we find

$$E = \frac{\pi^2}{15} V T^4, \tag{5.168}$$

which is the standard blackbody radiation result.

Notes

Obviously we can only discuss the basics of quantum statistical mechanics in a short chapter like this. A selection of references is given in Section 5.1. I first learned of the utility of the Mellin–Barnes integral representation from Klaus Kirsten (Kirsten and Toms, 1996b).

6
Effective action at finite temperature

6.1 Condensate contribution

In Section 4.1 we discussed how the effective action could be used to formulate an equation of motion which incorporated quantum corrections to the classical theory. The effective action was stationary under arbitrary variations of the mean field to first order. At finite temperature we can also define the effective action and use it exactly as we did at zero temperature. In fact it is possible, with a slight modification of Section 5.1, to relate the effective action to the thermodynamic potential Ω, or the q-potential.

We will deal first with the non-relativistic Schrödinger field Ψ. If we allow Ψ to represent charged particles in a background magnetic field described by the vector potential $\mathbf{A}$, and a potential represented by $U(\mathbf{x})$, then we can write

$$H = \int_\Sigma d\sigma_x \left[\frac{1}{2m} |\mathbf{D}\Psi|^2 + U(\mathbf{x}) |\Psi|^2 \right], \tag{6.1}$$

as the Hamiltonian. (Here $\mathbf{D} = \nabla - ie\mathbf{A}$ is the gauge covariant derivative.) The charge Q is

$$Q = e \int_\Sigma d\sigma_x |\Psi|^2, \tag{6.2}$$

so that

$$\bar{H} = H - \mu Q = \int_\Sigma d\sigma_x \left[\frac{1}{2m} |\mathbf{D}\Psi|^2 - e\mu|\Psi|^2 + U(\mathbf{x}) |\Psi|^2 \right] \tag{6.3}$$

is the combination which enters the statistical mechanics. Because of this it proves convenient to let $\bar{H}$ rather than H determine the dynamics. We

can either write down the Heisenberg equations of motion for Ψ and $\Psi^\dagger$ or else use the action functional

$$\bar{S}=\int_{t_1}^{t_2}\int_\Sigma d\sigma_x\left[\frac{i}{2}\left(\Psi^\dagger\dot{\Psi}-\dot{\Psi}^\dagger\Psi\right)-\frac{1}{2m}|\mathbf{D}\Psi|^2+e\mu|\Psi|^2-U(\mathbf{x})|\Psi|^2\right]. \tag{6.4}$$

Either of these two approaches results in the equation of motion

$$0=i\dot{\Psi}+\frac{1}{2m}\mathbf{D}^2\Psi+e\mu\Psi-U(\mathbf{x})\Psi, \tag{6.5}$$

and its Hermitian conjugate. The only difference between this result and the Schrödinger equation is the presence of the term in μ.

If we proceed as we did in the previous chapter by expanding Ψ and $\Psi^\dagger$ in terms of creation and annihilation operators, we will find $\langle\Psi\rangle=0=\langle\Psi^\dagger\rangle$ since we have shown that $\langle A_n\rangle=0=\langle A_n^\dagger\rangle$. This will not allow for the possibility of a condensate. To broaden our formalism to incorporate a condensate we can write

$$\bar{\Psi}=\langle\Psi\rangle,\qquad \bar{\Psi}^\dagger=\langle\Psi^\dagger\rangle. \tag{6.6}$$

A non-zero condensate will be characterized by $\bar{\Psi}\neq 0$. The full field operator Ψ can be expressed as

$$\Psi=\bar{\Psi}+\psi \tag{6.7}$$

where by construction $\langle\psi\rangle=0$. $\bar{\Psi}$ plays the role of the background field at finite temperature and is a function rather than an operator. ψ is a field operator which contains fluctuations about the background. We will assume $\bar{\Psi}$ has no time dependence here as appropriate to thermal equilibrium.

In our considerations of the thermodynamic potential in the previous chapter, we assumed $\langle\bar{\Psi}\rangle=0$, and therefore only calculated the contributions from ψ. If $\bar{\Psi}\neq 0$, then there should be a term in Ω containing $\bar{\Psi}$. From (6.3) the contribution of $\bar{\Psi}$ to $\bar{H}$ is

$$\bar{H}_0=\int_\Sigma d\sigma_x\left[\frac{1}{2m}\left|\mathbf{D}\bar{\Psi}\right|^2-e\mu|\bar{\Psi}|^2+U(\mathbf{x})\left|\bar{\Psi}\right|^2\right]. \tag{6.8}$$

Because this is a number, rather than an operator, from (5.10) we find that it corresponds to the q-potential

$$q_0=-\beta\bar{H}_0,$$

and hence contributes

$$\Omega_0 = \bar{H}_0 \tag{6.9}$$

to the thermodynamic potential. The full thermodynamic potential is therefore

$$\Omega = \int_\Sigma d\sigma_x \left[\frac{1}{2m} \left| \mathbf{D}\bar{\Psi} \right|^2 - e\mu |\bar{\Psi}|^2 + U(\mathbf{x}) \left| \bar{\Psi} \right|^2 \right] + \Omega_{T=0} + \Omega_{T\neq 0}, \tag{6.10}$$

where $\Omega_{T=0}$ and $\Omega_{T\neq 0}$ were given in the previous chapter. These last two parts of Ω do not contain any dependence on $\bar{\Psi}$. By demanding that $\bar{\Psi}$ provides a stationary value of Ω with μ, V, β fixed we find

$$0 = \frac{1}{2m}\mathbf{D}^2\bar{\Psi} + e\mu\bar{\Psi} - U(\mathbf{x})\bar{\Psi} \tag{6.11}$$

(and its complex conjugate). This equation is completely equivalent to taking (6.5), performing the statistical average using $\langle\psi\rangle = 0$, and utilizing the time independence of $\bar{\Psi}$.

After having gone to all this trouble to deal with $\bar{\Psi}$ we can see that $\bar{\Psi} = 0$ is a solution to (6.11). If this is the only solution, then we are clearly back to the situation of the previous chapter. However, there may be solutions to (6.11) with $\bar{\Psi} \neq 0$. To see this suppose that we expand

$$\bar{\Psi}(\mathbf{x}) = \sum_n C_n f_n(\mathbf{x}) \tag{6.12}$$

where $\{f_n(\mathbf{x})\}$ is a complete orthonormal set of solutions to

$$\left[-\frac{1}{2m}\mathbf{D}^2 + U(\mathbf{x}) \right] f_n(\mathbf{x}) = E_n f_n(\mathbf{x}). \tag{6.13}$$

The C_n represent some expansion coefficients to be determined. Substitution of (6.12) into (6.11) using (6.13) gives

$$\sum_n (E_n - e\mu) C_n f_n(\mathbf{x}) = 0. \tag{6.14}$$

Because the $\{f_n(\mathbf{x})\}$ is a complete orthonormal set of functions we must have

$$(E_n - e\mu)C_n = 0, \tag{6.15}$$

holding for all n. We have already restricted $e\mu \leq E_0$ to avoid negative occupation numbers. Define a critical value for μ by

$$e\mu_c = E_0. \tag{6.16}$$

We then note that if $\mu < \mu_c$ the only solution to (6.15) is for $C_n = 0$ for all n. From (6.12) we see that $\bar{\Psi} = 0$ and there is no condensate present.

On the other hand, suppose that it is possible for μ to reach the critical value of μ defined in (6.16). In this case C_0 in (6.15) is not determined; however, $C_n = 0$ for all $n \neq 0$ since $E_n > E_0$ in this case. (E_0 is the smallest energy eigenvalue.) The background field is given by

$$\bar{\Psi}(\mathbf{x}) = C_0 f_0(\mathbf{x}) \tag{6.17}$$

and is therefore determined by the eigenfunction of lowest eigenvalue; that is, by the ground state. This corresponds to symmetry breaking since the background field is non-zero: the background field has picked out a direction in the space of all fields. We have therefore found a necessary condition for $\bar{\Psi}$ to be non-zero and determined its value up to an overall multiplicative constant.

The as yet undetermined constant C_0 can be fixed in terms of the charge (or particle number). The total charge is given by (5.30),

$$Q = -\left(\frac{\partial \Omega}{\partial \mu}\right)\Big|_{T,V}.$$

With Ω given by (6.10) we have

$$Q = Q_0 + Q_1 \tag{6.18}$$

where

$$Q_0 = e\int_\Sigma d\sigma_x |\bar{\Psi}|^2 = e|C_0|^2 \tag{6.19}$$

if we use (6.17), and

$$Q_1 = -\left(\frac{\partial \Omega_{T\neq 0}}{\partial \mu}\right)\Big|_{T,V}. \tag{6.20}$$

The results in (6.18) and (6.19) show the contribution of the condensate to the total charge. Once we know $Q_0 = Q - Q_1$ we can fix C_0 using (6.19).

6.2 Free homogeneous non-relativistic Bose gas

We will consider the space $\Sigma = \mathbb{R}^D$ and take the gas to be uncharged so that we can speak of the total particle number rather than the charge. In place of (6.18)–(6.20) we have

$$N = N_0 + N_1 \tag{6.21}$$

where

$$N_0 = e\int_\Sigma d\sigma_x |\bar{\Psi}|^2 = |C_0|^2 \tag{6.22}$$

and

$$N_1 = -\left(\frac{\partial \Omega_{T\neq 0}}{\partial \mu}\right)\Bigg|_{T,V}. \tag{6.23}$$

The finite temperature part of the thermodynamic potential was calculated in Section 5.5.2, the result found in (5.134) in terms of the polylogarithm. The energy levels were given in (5.129) and lead to $E_0 = 0$ as the lowest energy eigenvalue of $-(1/2m)\nabla^2$ with corresponding eigenfunction

$$f_0(\mathbf{x}) = V^{-1/2}. \tag{6.24}$$

We then know that $\mu \leq 0$, with $\mu = 0$ the critical value. The boundary conditions (periodic on the walls of the large box) lead to a background field $\bar{\Psi}$ which is constant. Later we will examine a system for which $\bar{\Psi}$ is not constant. Using (5.134), we then find from (6.23) that

$$N_1 = V\left(\frac{m}{2\pi\beta}\right)^{D/2} Li_{D/2}(e^{\beta\mu}). \tag{6.25}$$

Suppose that we have $\bar{\Psi} = 0$. This means that $C_0 = 0$ and hence $N_0 = 0$ from (6.22). The total number of particles is then given by $N = N_1$, so that

$$N = V\left(\frac{m}{2\pi\beta}\right)^{D/2} Li_{D/2}(e^{\beta\mu}) \tag{6.26}$$

$$= V\left(\frac{m}{2\pi\beta}\right)^{D/2} \sum_{k=1}^{\infty} \frac{e^{\beta\mu}}{k^{D/2}}. \tag{6.27}$$

This last result determines μ in terms of N, T, V although we cannot solve explicitly for μ. For $\mu < 0$ the sum in (6.27) converges for all values of D; however, as $\mu \to 0$ the sum will only converge if $D > 2$. We will assume that $D \geq 3$ here and come back to the cases of $D = 1, 2$ later. With $D \geq 3$ it is clear that because $\mu \leq 0$ the sum in (6.27) is bounded above by the maximum value obtained when $\mu = 0$:

$$Li_{D/2}(e^{\beta\mu}) = \sum_{k=1}^{\infty} \frac{e^{\beta\mu}}{k^{D/2}} \leq \sum_{k=1}^{\infty} \frac{1}{k^{D/2}} = \zeta(D/2). \tag{6.28}$$

Because the sum in (6.27) converges when $D \geq 3$ for all $\mu \leq 0$, it is clear that no matter how large the particle number density N/V is we

can always make T large enough so that we can solve (6.27) for μ with $\mu < 0$. Thus for T large enough, since $\mu < 0$, we do have $\bar{\Psi} = 0$. There is no condensate in this case.

Now consider what happens if T is reduced from very high values with N/V fixed. As T reduces the factor of $(m/2\pi\beta)^{D/2}$ reduces. But because N on the left-hand side of (6.26) must remain fixed, $Li_{D/2}(e^{\beta\mu})$ must therefore increase. This means that μ must increase towards the critical value of $\mu = 0$. However, (6.28) shows us that $Li_{D/2}(e^{\beta\mu}) \leq \zeta(D/2)$ implying that there is a limit on how much $Li_{D/2}(e^{\beta\mu})$ can increase. We will define the critical temperature T_c as the value of T at which $\mu = 0$. From (6.26) and (6.28) we have

$$N = V\left(\frac{mT_c}{2\pi}\right)^{D/2}\zeta(D/2). \tag{6.29}$$

Solving for T_c we find

$$T_c = \frac{2\pi}{m}\left[\frac{N}{V\zeta(D/2)}\right]^{2/D}. \tag{6.30}$$

As T is reduced below T_c, μ cannot increase above its critical value of $\mu_c = 0$. This means that we can no longer solve $N = N_1$. We have

$$\begin{aligned} N_1 &= V\left(\frac{m}{2\pi\beta}\right)^{D/2}\zeta(D/2) \\ &= N\left(\frac{T}{T_c}\right)^{D/2} \end{aligned} \tag{6.31}$$

for $T < T_c$. From (6.21) we find

$$N_0 = N - N_1 = N\left[1 - \left(\frac{T}{T_c}\right)^{D/2}\right] \tag{6.32}$$

and using (6.22) obtain

$$|C_0| = \sqrt{N_0} = \sqrt{N}\left[1 - \left(\frac{T}{T_c}\right)^{D/2}\right]^{1/2}. \tag{6.33}$$

Therefore when $T < T_c$ we have

$$\bar{\Psi} = \sqrt{\frac{N}{V}}\left[1 - \left(\frac{T}{T_c}\right)^{D/2}\right]^{1/2} \tag{6.34}$$

using (6.17) with (6.24) and (6.33).

These results can be given a physical interpretation. When T is high enough there is sufficient thermal energy so that it is easy for transitions to occur between the ground state and the excited states. As T is reduced it starts to become harder for these transitions to occur. We can estimate this by using a simple argument based on the uncertainty principle. For N bosons confined in a box of volume V each boson has a volume $V/N = L^D$ available to it. Because of the confinement each boson has a zero-point energy $E_0 = p^2/(2m)$. The uncertainty principle gives $pL \sim 1$ ($\hbar = 1$ here), so we find $E_0 \sim 1/(2mL^2) \sim \frac{1}{2m}(N/V)^{2/D}$. The spacing between the ground state and the first excited level will be of the order of E_0. If $T > E_0$ there is sufficient thermal energy for there to be many transitions between the ground and the excited states. However, once T drops below $T_c \sim E_0$ this is no longer the case and particles would be expected to drop into the ground state. Our estimate shows $T_c \sim \frac{1}{2m}(N/V)^{2/D}$ which agrees with (6.30) apart from the numerical factor. The non-zero value for $\bar{\Psi}$ can be interpreted as condensation of the bosons into the ground state. N_0 in (6.32) then represents the average number of particles in the ground state, and N_1 in (6.31) represents the average number of particles in excited states. This is the phenomenon of Bose–Einstein condensation first predicted by Einstein.

Before studying the properties of the $D \geq 3$ Bose gas in more detail in the next section, we will return to the cases $D = 1, 2$. In these two cases the sum in (6.27) is not bounded as $\mu \to 0$ and this means that we can always solve (6.26) or (6.27) for μ with $\mu < 0$ no matter what T and N are. This means that $\bar{\Psi} = 0$ and that Bose–Einstein condensation in the sense we have discussed does not occur. When $D = 2$ the sum (6.27) can be evaluated explicitly and we have

$$N = -V\left(\frac{m}{2\pi\beta}\right)\ln\left(1 - e^{\beta\mu}\right). \tag{6.35}$$

Solving for μ we find

$$\mu = T\ln\left[1 - e^{-(2\pi N/mVT)}\right]. \tag{6.36}$$

For any finite particle density and non-zero temperature we always have $\mu < 0$. It is never possible for μ to reach the critical value of $\mu = 0$ necessary for a non-zero condensate $\bar{\Psi}$. For very small T, by expanding the logarithm in (6.36) we find

$$\mu \simeq -Te^{-(2\pi N/mVT)}, \tag{6.37}$$

showing that μ can become arbitrarily close to the critical value of $\mu = 0$ but can never reach it.

For $D = 1$, (6.26) gives us

$$N = V\sqrt{\frac{m}{2\pi\beta}}Li_{1/2}(e^{\beta\mu}). \tag{6.38}$$

Although $Li_{1/2}$ cannot be evaluated in elementary terms, it can be seen from the asymptotic expansion given in (A1.73) that the leading order term as $\mu \to 0$ is

$$Li_{1/2}(e^{\beta\mu}) \simeq \sqrt{-\frac{\pi}{\beta\mu}} + \cdots .$$

Just as we found for $D = 2$, it is never possible for μ to reach the critical value of $\mu = 0$ required for a non-zero condensate for any finite particle density.

6.3 Internal energy and specific heat

We will continue our study of the thermodynamics of the ideal Bose gas by evaluating the specific heat and studying its behaviour in different spatial dimensions. The internal energy follows from (5.22) and (5.26) as

$$E = \left[\frac{\partial(\beta\Omega)}{\partial\beta}\right]\Bigg|_{\beta\mu,V,\bar{\Psi}}. \tag{6.39}$$

Using (6.10) we find

$$E = E_0 + E_1, \tag{6.40}$$

where

$$E_0 = \int_\Sigma d\sigma_x \left[\frac{1}{2m}|\mathbf{D}\bar{\Psi}|^2 + U(\mathbf{x})|\bar{\Psi}|^2\right], \tag{6.41}$$

$$E_1 = \left[\frac{\partial(\beta\Omega_{T\neq 0})}{\partial\beta}\right]\Bigg|_{\beta\mu,V,\bar{\Psi}} = \sum_n E_n \left[e^{\beta(E_n-\mu)} - 1\right]^{-1}. \tag{6.42}$$

In the absence of a condensate ($\bar{\Psi} = 0$) we are left with $E = E_1$ which is the familiar expression for the internal energy from elementary statistical mechanics. The condensate contribution (6.41) takes the form of the energy of a classical field described by $\bar{\Psi}$. (See (6.1).)

For the free Bose gas $\mathbf{D} = \nabla$, $U(\mathbf{x}) = 0$ and we have $\bar{\Psi}$ constant so that $E_0 = 0$. Even if $\bar{\Psi} \neq 0$ there will be no direct contribution of the condensate to the internal energy as can be seen from (6.41) and (6.42). (However, a non-zero value for $\bar{\Psi}$ will still affect the internal energy

indirectly through the chemical potential μ.) For the free Bose gas we therefore have

$$E = \left[\frac{\partial(\beta\Omega_{T\neq 0})}{\partial\beta}\right]\Bigg|_{\beta\mu,V,\bar{\Psi}}. \tag{6.43}$$

Using (5.134) (recall that $\beta = 1/T$), we find

$$E = \frac{DV}{2\beta}\left(\frac{m}{2\pi\beta}\right)^{D/2} Li_{1+D/2}(e^{\beta\mu}). \tag{6.44}$$

(Because $\beta\mu$ is held fixed when using Ω to compute E, the polylogarithm in (5.134) involving $\beta\mu$ is fixed. The only temperature dependence is through the factor of $\beta^{-D/2}$ in front of the polylogarithm.)

We will assume $D \geq 3$ here so that there is a critical temperature T_c below which a condensate is present. We can use (6.29) to write E in (6.44) as

$$E = \frac{DN}{2\beta}\left(\frac{\beta_c}{\beta}\right)^{D/2} \frac{Li_{1+D/2}(e^{\beta\mu})}{\zeta(D/2)}. \tag{6.45}$$

With N and V fixed, we can regard β_c as fixed since it is given by (6.30) ($\beta_c = 1/T_c$). For $T < T_c$ we have $\mu = 0$ so that

$$E_< = \frac{DN}{2\beta}\left(\frac{\beta_c}{\beta}\right)^{D/2} \frac{\zeta(1+D/2)}{\zeta(D/2)}. \tag{6.46}$$

We will use the subscript $<$ ($>$) to denote the temperature range $T < T_c$ ($T > T_c$). Although the internal energy E is continuous at $T = T_c$ because of the behaviour of μ, derivatives of E with respect to T may not be continuous. We will examine the specific heat at constant volume defined by

$$C = \left(\frac{\partial E}{\partial T}\right)\Bigg|_{V,N,\bar{\Psi}}. \tag{6.47}$$

For $T < T_c$ it is easy to see from (6.46) that

$$\frac{C_<}{N} = \frac{D}{2}\left(\frac{D}{2}+1\right)\frac{\zeta(1+D/2)}{\zeta(D/2)}\left(\frac{\beta_c}{\beta}\right)^{D/2}. \tag{6.48}$$

For $T > T_c$ the computation of the specific heat is more difficult because (6.45) involves an explicit μ-dependence. We need to compute the derivative of E with respect to T holding N fixed. The expression for N is given in (6.26). If we use (6.29) we find

$$Li_{D/2}(e^{\beta\mu}) = \left(\frac{\beta}{\beta_c}\right)^{D/2}\zeta\left(\frac{D}{2}\right). \tag{6.49}$$

Because β_c is fixed, if we vary both sides of (6.49) with respect to β we find

$$\delta Li_{D/2}(e^{\beta\mu}) = \frac{D}{2\beta}\left(\frac{\beta}{\beta_c}\right)^{D/2}\zeta\left(\frac{D}{2}\right)\delta\beta.$$

The properties of the polylogarithm give $\delta Li_p(z) = z^{-1}Li_{p-1}(z)\delta z$. We therefore find

$$\left[\frac{\partial(\beta\mu)}{\partial\beta}\right]\Bigg|_{N,V,\bar{\Psi}} = \frac{D}{2\beta}\left(\frac{\beta}{\beta_c}\right)^{D/2}\frac{\zeta(D/2)}{Li_{D/2-1}(e^{\beta\mu})}. \tag{6.50}$$

It is now straightforward to show from (6.45) and (6.47) that

$$\frac{C_>}{N} = \frac{D}{2}\left(\frac{D}{2}+1\right)\left(\frac{\beta_c}{\beta}\right)^{D/2}\frac{Li_{D/2+1}(e^{\beta\mu})}{\zeta(D/2)} - \frac{D^2}{4}\frac{Li_{D/2}(e^{\beta\mu})}{Li_{D/2-1}(e^{\beta\mu})}. \tag{6.51}$$

By taking $\beta \to \beta_c$ in (6.51) using $\mu \to 0$, because $Li_{1+D/2}(e^{\beta\mu}) \to \zeta(1+D/2)$, the first term agrees with the $\beta \to \beta_c$ limit of (6.48). Whether or not the specific heat is continuous at $T = T_c$ is determined by the behaviour of the second term in (6.51). We know that $Li_{D/2-1}(e^{\beta\mu}) \to \zeta(D/2-1)$ only for $D/2-1 > 1$, or $D \geq 5$. Therefore for $D \geq 5$ the specific heat will not be continuous at the critical temperature. For $D = 3, 4$ $Li_{D/2-1}(e^{\beta\mu}) \to \infty$ as $\mu \to 0$ so that the specific heat is continuous at $T = T_c$. By computing further derivatives of the specific heat it is easy to show that for $D = 3$ the first derivative of the specific heat is discontinuous at $T = T_c$, and for $D = 4$ although the first derivative of the specific heat is continuous, the second derivative is discontinuous at $T = T_c$. If $D = 1, 2$, where there is no condensate present, it is easy to show that the specific heat is a perfectly smooth function of temperature. Thus there is a direct link between the presence of a non-zero condensate and the non-smooth behaviour of the specific heat. The specific heat is plotted in Fig. 6.1 for the case of $D = 3$.

6.4 Bose gas in a harmonic oscillator confining potential

Advances in the cooling and trapping of atomic gases have led to a number of important experiments performed on systems of bosons at low temperatures.[1] A good model for these systems is a number of bosons in a harmonic oscillator confining potential. We will confine ourselves to $D = 3$ in this section. The trapping potential will be written as

$$U(\mathbf{x}) = \frac{1}{2}m(\omega_1^2x^2 + \omega_2^2y^2 + \omega_3^2z^2), \tag{6.52}$$

[1] See Pethick and Smith (2002) for a review of some of the original work in this area.

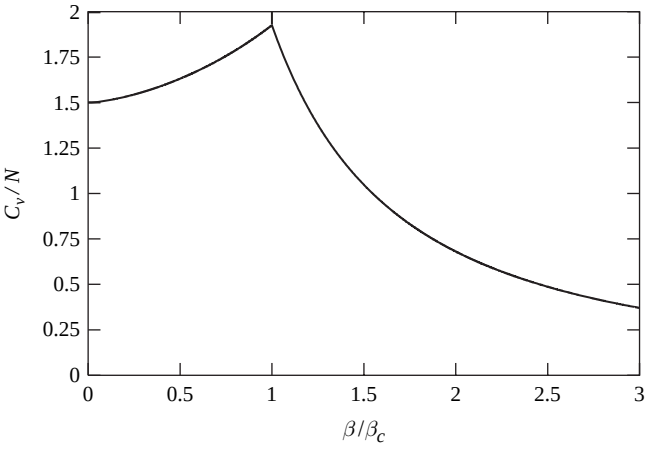

Fig. 6.1 The specific heat for the free three-dimensional Bose gas. The behaviour of the specific heat changes at the critical temperature $T = T_c$ in a continuous, but not smooth, way.

where $\omega_1, \omega_2, \omega_3$ are the angular frequencies characterizing the harmonic oscillator potential. The energy levels of the system are[2]

$$E_n = \left(n_1 + \frac{1}{2}\right)\omega_1 + \left(n_2 + \frac{1}{2}\right)\omega_2 + \left(n_3 + \frac{1}{2}\right)\omega_3, \tag{6.53}$$

where $n_j = 0, 1, 2, \ldots$ for $j = 1, 2, 3$. The critical value of μ at which a non-zero condensate might occur is

$$\mu_c = E_0 = \frac{1}{2}(\omega_1 + \omega_2 + \omega_3). \tag{6.54}$$

We will show that μ can never reach this value and so a condensate characterized by a non-zero value for $\bar{\Psi}$ will not occur. Nevertheless we will see that there is still a sense in which Bose–Einstein condensation can be said to occur.

To simplify the analysis we will look first at the isotropic oscillator by setting $\omega_1 = \omega_2 = \omega_3 = \omega$. The critical value of μ is now

$$\mu_c = \frac{3}{2}\omega. \tag{6.55}$$

[2] The generalization to an arbitrary dimension D should be obvious.

The thermodynamic potential is (ignoring the potential condensate contribution)

$$\Omega = T \sum_{n_1=0}^{\infty} \sum_{n_2=0}^{\infty} \sum_{n_3=0}^{\infty} \ln \left[1 - e^{-\beta(E_n - \mu)} \right]. \tag{6.56}$$

It is advantageous to introduce dimensionless variables x and ϵ by

$$x = \beta\omega, \tag{6.57}$$

$$\mu = \omega \left(\frac{3}{2} - \epsilon \right). \tag{6.58}$$

Because the spacing of adjacent energy levels is of the order of ω, x is a measure of the size of the thermal energy in relation to the energy level spacing. ϵ is a measure of how far μ is from the critical value in (6.55).

Because we are assuming an isotropic potential, we can write the triple sum in (6.56) as a single sum. We can write

$$n_1 + n_2 + n_3 = k,$$

where $k = 0, 1, 2, \ldots$, since each of n_1, n_2 and n_3 is a non-negative integer. We can also let

$$n_2 + n_3 = l,$$

where $l = 0, 1, 2, \ldots$. Because $n_2 \geq 0$ we must have $n_3 \leq l$. Also $n_1 = k - l$ and since $n_1 \geq 0$ the range on l is restricted to $l = 0, 1, \ldots, k$. Thus we have the identity

$$\sum_{n_1=0}^{\infty} \sum_{n_2=0}^{\infty} \sum_{n_3=0}^{\infty} f(n_1 + n_2 + n_3) = \sum_{k=0}^{\infty} \sum_{l=0}^{k} \sum_{n_3=0}^{l} f(k)$$

for any function f. Using $\displaystyle\sum_{n_3=0}^{l} 1 = l + 1$ and $\displaystyle\sum_{l=0}^{k} l = \frac{1}{2}k(k+1)$ we find

$$\sum_{n_1=0}^{\infty} \sum_{n_2=0}^{\infty} \sum_{n_3=0}^{\infty} f(n_1 + n_2 + n_3) = \sum_{k=0}^{\infty} \frac{1}{2}k(k+1) f(k). \tag{6.59}$$

Applying this to Ω in (6.56) gives

$$\Omega = T \sum_{k=0}^{\infty} \frac{1}{2}k(k+1) \ln \left[1 - e^{-(k+\epsilon)x} \right] \tag{6.60}$$

if the result is written in terms of the dimensionless variables x and ϵ. The factor of $(1/2)k(k+1)$ represents the degeneracy of the energy levels $E_k = [k + (3/2)]\omega$ for the isotropic harmonic oscillator. It should be clear why the isotropic case is so much simpler than the anisotropic case: unless the oscillator frequencies are all rational multiples of each other it is impossible to reduce the triple sum (6.56) to a single one. We will return to the general case later.

The result in (6.60) can be evaluated in much the same way as we have done before. Begin by expanding the logarithm in its Taylor series to give

$$\Omega = -T \sum_{k=0}^{\infty} \frac{1}{2} k(k+1) \sum_{n=1}^{\infty} \frac{e^{-n(k+\epsilon)}}{n}. \tag{6.61}$$

The sum over k now just involves a geometric series. If we let

$$S(y) = \sum_{k=0}^{\infty} e^{-ky} = (1 - e^{-y})^{-1}, \tag{6.62}$$

then simple differentiations with respect to y give

$$\sum_{k=0}^{\infty} k e^{-ky} = -S'(y) = (1 - e^{-y})^{-2} e^{-y}, \tag{6.63}$$

$$\sum_{k=0}^{\infty} k^2 e^{-ky} = S''(y) = (1 - e^{-y})^{-2} e^{-y} + 2(1 - e^{-y})^{-3} e^{-2y}. \tag{6.64}$$

Using (6.62)–(6.64) we find

$$\sum_{k=0}^{\infty} \frac{1}{2} k(k+1) e^{-ky} = (1 - e^{-y})^{-3}. \tag{6.65}$$

This last result leads to

$$\Omega = -T \sum_{n=1}^{\infty} \frac{e^{-n\epsilon x}}{n} (1 - e^{-nx})^{-3}. \tag{6.66}$$

The average number of particles N is given in (5.30). With T and ω fixed we have from (6.58) that $\delta\mu = -\omega\delta\epsilon$. Thus we find

$$\begin{aligned} N &= \frac{1}{\omega} \left(\frac{\partial \Omega}{\partial \epsilon} \right) \Bigg|_x \\ &= \sum_{n=1}^{\infty} e^{-n\epsilon x} (1 - e^{-nx})^{-3}. \end{aligned} \tag{6.67}$$

For $x > 0$ and $n \geq 1$ we have the inequality

$$1 < (1 - e^{-nx})^{-3} \leq (1 - e^{-x})^{-3}, \tag{6.68}$$

which shows that

$$N > \sum_{n=1}^{\infty} e^{-n\epsilon x} = (e^{\epsilon x} - 1)^{-1}. \tag{6.69}$$

Although we have derived this result in a purely mathematical way, the inequality (6.69) is obvious on physical grounds. The average number of particles is

$$\begin{aligned} N &= \sum_{n_1=0}^{\infty} \sum_{n_2=0}^{\infty} \sum_{n_3=0}^{\infty} \left[e^{\beta(E_n - \mu)} - 1 \right]^{-1} \\ &= \sum_{n_1=0}^{\infty} \sum_{n_2=0}^{\infty} \sum_{n_3=0}^{\infty} \left[e^{x(n_1+n_2+n_3+\epsilon)} - 1 \right]^{-1}. \end{aligned} \tag{6.70}$$

This shows that the average number of particles in the ground state is

$$N_{gr} = (e^{\epsilon x} - 1)^{-1}. \tag{6.71}$$

The inequality (6.69) states the obvious: $N > N_{gr}$.

We have now obtained enough results to show that $\bar{\Psi}$ remains fixed at $\bar{\Psi} = 0$. To do this all that we need to show is that $\mu < \mu_c$ for all temperatures, or equivalently that ϵ can never vanish. From (6.71) we can solve for

$$\epsilon = \frac{1}{x} \ln \left(1 + \frac{1}{N_{gr}} \right). \tag{6.72}$$

Because we have already established that $N_{gr} < N$, we have

$$\epsilon > \frac{1}{x} \ln \left(1 + \frac{1}{N} \right). \tag{6.73}$$

So long as T is never 0 (so that x defined in (6.57) is always finite), and the number of particles is finite, ϵ will always be positive. This proves that $\bar{\Psi} = 0$. The presence of the confining potential has drastically altered the behaviour of the system from what we found in Section 6.2 for the unconfined gas. In the case of a trapping potential there is no temperature at which a critical temperature associated with a phase transition can be identified.

If this was the whole story, then we could stop here and go on to other more interesting examples. However, there is still some extremely interesting physics to be found in the trapped gas. Even if we have shown

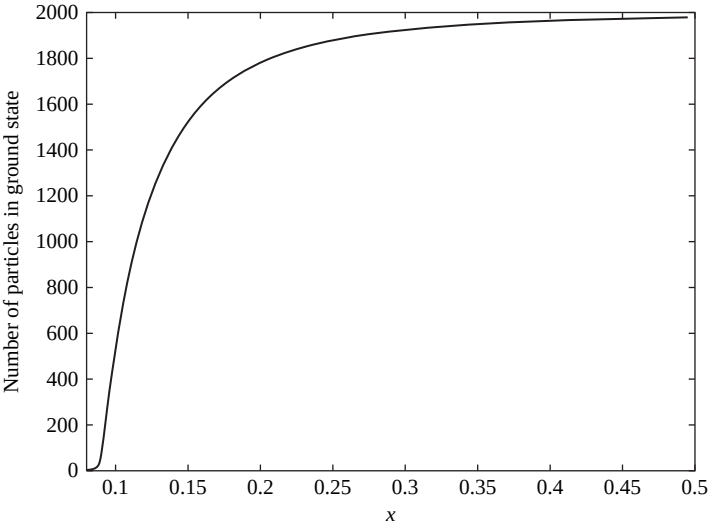

Fig. 6.2 This shows the number of particles in the ground state as a function of $x = \hbar\omega/(kT)$. The total number of particles is 2000.

that ϵ can never reach the value of $\epsilon = 0$ necessary for a phase transition, if ϵ can become very small then (6.71) shows us that there will be a large build-up of particles in the ground state. This is very much like what happened below the critical temperature for the free Bose gas in Section 6.2, and it is in this sense, namely a large build-up of particles in the ground state, that the trapped Bose gas can be said to exhibit Bose–Einstein condensation. As we will see, this build-up can occur very suddenly over a small temperature range so that the system looks very much like it has undergone a phase transition like that occurring in the free Bose gas. Numerical calculation shows that over a very small range of x, ϵ undergoes a drastic decrease from large values to very small ones.[3] The number of particles in the ground state is shown in Fig. 6.2. Because the curve is smooth there is no unique way to assign a critical temperature to Bose–Einstein condensation; however, the sudden growth in the number of particles in the ground state is remarkable.

A natural thing to try, rather than perform laborious numerical computations, is to attempt to obtain analytical approximations for the relevant expressions. The interesting behaviour can be seen from Fig. 6.2 to occur at small values of x. This makes the numerical evaluation of sums like

[3] The calculations involve solving (6.67) with fixed N for ϵ as a function of x.

(6.67) difficult because they converge extremely slow. Instead, following Kirsten and Toms (1996b), we will obtain an accurate asymptotic expansion using the Mellin–Barnes integral representation (5.62).

We will start with (6.61). Although it is possible to apply the Mellin–Barnes integral representation immediately to the exponential that occurs in (6.61), it is better to separate off the $k = 0$ term for special treatment. On physical grounds this is natural because the $k = 0$ term corresponds to the ground state contribution, and it is this we are attempting to study. We will write

$$\Omega = \Omega_{\rm gr} + \Omega_{\rm ex} \tag{6.74}$$

where

$$\Omega_{\rm gr} = -T \sum_{n=1}^{\infty} \frac{e^{-n\epsilon x}}{n} = T \ln(1 - e^{-\epsilon x}) \tag{6.75}$$

is the ground state contribution, and

$$\Omega_{\rm ex} = -T \sum_{k=1}^{\infty} \frac{1}{2}(k+1)(k+2) \sum_{n=1}^{\infty} \frac{e^{-n(k+1)\epsilon x}}{n} \tag{6.76}$$

is the contribution from excited states. Using the integral representation (5.62) for the exponential on the right-hand side of (6.76) enables the sums over k and n to be performed in terms of Riemann and Hurwitz ζ-functions respectively. (See Appendix A1.2.) The result is

$$\begin{aligned}\Omega_{\rm ex} = -T \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} d\alpha\, \Gamma(\alpha) x^{-\alpha} \zeta(1+\alpha) \Big[& \zeta(\alpha - 2, 1+\epsilon) \\ & + (3-2\epsilon)\zeta(\alpha-1, 1+\epsilon) + (1-\epsilon)(2-\epsilon)\zeta(\alpha, 1+\epsilon) \Big]\end{aligned} \tag{6.77}$$

if we take $c > 3$ to avoid the poles of the integrand. The contour is then closed in the left-hand side of the complex α-plane and the result evaluated by residues. There are simple poles at $\alpha = 3, 2, 1$ coming from the Hurwitz ζ-functions, at $\alpha = -1, -2, \ldots$ coming from the Γ-function, and a double pole at $\alpha = 0$ coming from the combination $\Gamma(\alpha)\zeta(1+\alpha)$. The first few terms of the expansion of Ω_{ex} are

$$-\beta\Omega_{\rm ex} \simeq \frac{\zeta(4)}{x^3} + \left(\frac{3}{2} - \epsilon\right)\zeta(3)x^{-2} + \frac{1}{2}(1-\epsilon)(2-\epsilon)\zeta(2)x^{-1} + \cdots . \tag{6.78}$$

(The next term is of order $\ln x$ and is very complicated. See Kirsten and Toms (1996b).)

A similar procedure can be applied to find the particle number. Defining

$$N = N_{\rm gr} + N_{\rm ex} \tag{6.79}$$

where $N_{\rm gr}$ is the number of particles in the ground state given in (6.71), and $N_{\rm ex}$ is the contribution from excited states, we find

$$N_{\rm ex} \simeq \zeta(3)x^{-3} + \left(\frac{3}{2} - \epsilon\right)\zeta(2)x^{-2} + \cdots \tag{6.80}$$

for the two leading terms at small x. Obviously it is possible to extend expansions in (6.80) or (6.78) to any desired order in x.

In order to get an estimate of the temperature associated with Bose–Einstein condensation we can say that the condensation temperature is characterized by the temperature at which $N_{\rm gr}$ changes from very small values to values close to the total number of particles N. Suppose we define x_B by saying $N_{\rm gr} \simeq 0$, or equivalently $N_{\rm ex} \simeq N$. Since x is small and $\epsilon \simeq 0$ we can see from (6.80) that

$$x_B \simeq \left[\frac{\zeta(3)}{N}\right]^{1/3}. \tag{6.81}$$

In terms of the temperature, this results in

$$T_B \simeq \hbar\omega \left[\frac{N}{\zeta(3)}\right]^{1/3}. \tag{6.82}$$

For the original experiment (Anderson *et al.*, 1995) with rubidium gas, $N \simeq 2000$ and $\hbar\omega/(2\pi) \simeq 60\,\text{Hz}$, and we find $T_B \simeq 34\,\text{nK}$ which is very close to the value quoted in the experiment.

Of course the approximations that led up to (6.82) were quite rough, since we set $N_{\rm gr} = 0$ and $N_{\rm ex} = N$ and dropped the term of order x^{-2} in (6.80). We can obtain a better result as follows. Let f be the fraction of the total number of particles in the ground state:

$$N_{\rm gr} = fN. \tag{6.83}$$

From (6.71) we find

$$\epsilon x = \ln\left(1 + \frac{1}{fN}\right) \tag{6.84}$$

which determines ϵ for a given x, f, N. Using this in (6.79) and (6.80) we find

$$(1-f)Nx^3 - \frac{3}{2}\zeta(2)x + \left[\zeta(2)\ln\left(1 + \frac{1}{fN}\right) - \zeta(3)\right] = 0. \tag{6.85}$$

If we now write

$$x = x_B(1 + \eta) \tag{6.86}$$

with η small (since we know x_B is close to the experimental temperature) we find

$$\frac{T - T_B}{T} \simeq -\eta \tag{6.87}$$

where

$$\eta \simeq \frac{1}{3}f + \frac{\zeta(2)}{2[\zeta(3)]^{2/3}}N^{-1/3}. \tag{6.88}$$

Ignoring f and taking $N = 2000$ we find that this more accurate result reduces the temperature by around 10%. It can be seen that the greater the number of particles, the closer T becomes to T_B.

We will now calculate the specific heat for the trapped Bose gas and compare the result with that for the free Bose gas considered in Section 6.3. The internal energy, defined by

$$E = \sum_k E_k \left[e^{\beta(E_k - \mu)} - 1\right]^{-1},$$

becomes

$$E = \omega \sum_{k=0}^{\infty} \frac{1}{2}(k+1)(k+2)\left(k + \frac{3}{2}\right)\left[e^{(k+\epsilon)x} - 1\right]^{-1} \tag{6.89}$$

when written in terms of x and ϵ defined in (6.57) and (6.58). The term in (6.89) that involves 3/2 can be recognized as proportional to the number of particles from (6.70) if we use (6.59). This gives

$$E = \frac{3}{2}\omega N + 3\omega E_1 \tag{6.90}$$

where

$$E_1 = \frac{1}{6}\sum_{k=1}^{\infty} k(k+1)(k+2)\left[e^{(k+\epsilon)x} - 1\right]^{-1}. \tag{6.91}$$

The term E_1 may be dealt with by first using the binomial expansion and then performing the sum over k using

$$\sum_{k=1}^{\infty} k(k+1)(k+2)e^{-ky} = 6(1 - e^{-y})^{-4}e^{-y} \tag{6.92}$$

which follows from differentiating (6.65). We find

$$E_1 = \sum_{n=1}^{\infty} e^{-n(\epsilon+1)x}(1-e^{-nx})^{-4}. \tag{6.93}$$

The specific heat is defined by

$$C = \left(\frac{\partial E}{\partial T}\right)\Big|_{N,\omega}. \tag{6.94}$$

Here ω plays the role of the volume for the free Bose gas (compare with (6.47)). Because N is held fixed when we differentiate E, only the term in E_1 will contribute to the specific heat. Because the temperature enters $x = \beta\omega = \omega/T$, we have

$$C = -3x^2 \left(\frac{\partial E_1}{\partial x}\right)\Big|_{N,\omega}. \tag{6.95}$$

We must be careful when computing C because N is fixed rather than ϵ. We have

$$N = \sum_{n=1}^{\infty} e^{-n\epsilon x}(1-e^{-nx})^{-3} \tag{6.96}$$

which defines ϵ implicitly as a function of N and x. Differentiating both sides of (6.96) with respect to x holding N fixed gives us

$$\left[\frac{\partial(\epsilon x)}{\partial x}\right]\Big|_N = -3\frac{S_2}{S_1} \tag{6.97}$$

where

$$S_1 = \sum_{n=1}^{\infty} n e^{-n\epsilon x}(1-e^{-nx})^{-3}, \tag{6.98}$$

$$S_2 = \sum_{n=1}^{\infty} n e^{-n(\epsilon+1)x}(1-e^{-nx})^{-4}. \tag{6.99}$$

Performing the differentiation in (6.95) using (6.97) results in

$$C = 3x^2\left\{4S_3 + S_2 - 3\frac{S_2^2}{S_1}\right\}, \tag{6.100}$$

where

$$S_3 = \sum_{n=1}^{\infty} n e^{-n(\epsilon+2)x}(1 - e^{-nx})^{-5}. \tag{6.101}$$

We may use (6.100) to compute the specific heat numerically. The procedure is to first solve (6.96) for ϵ as a function of x for fixed N. Knowing ϵ and x the three sums S_1, S_2 and S_3 may be performed and the results used in (6.100). We show the result of this calculation in Fig. 6.3. It can be seen that specific heat is a perfectly smooth function of temperature in contrast to the result found in Section 6.3 for the free Bose gas which had a discontinuous first derivative. A feature which the specific heat has in common with the free Bose gas is that there is a well-defined maximum. The maximum can be seen to occur very close to the temperature at which the number of particles in the ground state starts rise. We can therefore identify the maximum in the specific with the onset of Bose–Einstein condensation.

It is possible to obtain analytical approximations for the specific heat by using the Mellin–Barnes transform method discussed earlier to obtain

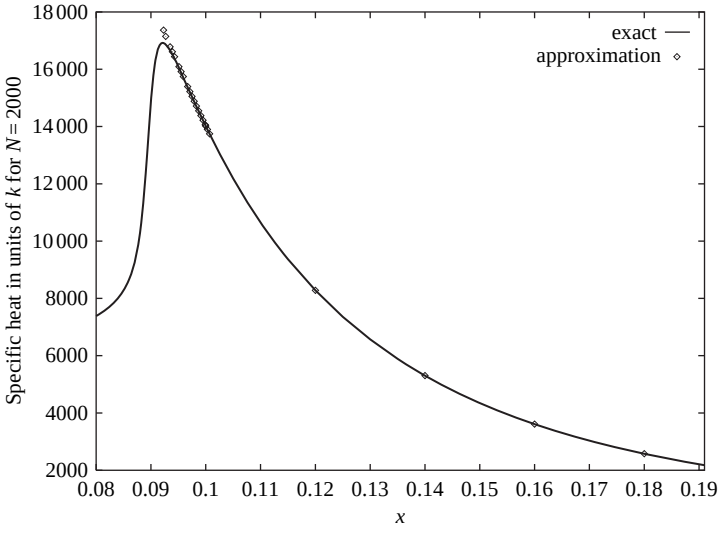

Fig. 6.3 The specific heat computed numerically for the isotropic harmonic oscillator is shown as the solid curve. The diamonds show the result using our approximation. The units for the specific heat are in factors of the Boltzmann constant k. The particle number is $N = 2000$. The maximum occurs for $x \simeq 0.0921$. Our approximation breaks down for x below the point where the specific heat maximum occurs.

asymptotic expansions for sums S_1, S_2, S_3. If we assume $x << 1$ and $\epsilon << 1$ it is possible to show

$$C \simeq 12\zeta(4)x^{-3} - 9\zeta(3)x^{-2} + 2\zeta(2)x^{-1} - 12\epsilon\zeta(3)x^{-2}$$
$$-18\epsilon^2\zeta(2)\zeta(3)x^{-3} - 9\epsilon^2\zeta^2(3)x^{-4} + 9\epsilon^4\zeta^2(3)x^{-6} + \cdots . \quad (6.102)$$

The result of using this to calculate the specific heat is shown as diamonds in Fig. 6.3. It can be seen that at temperatures below the point where the specific heat has its maximum, the approximation is quite good. For values of $x < x_m \simeq 0.0921$ the assumption that ϵ is small is no longer true and the approximation breaks down. In this case it is possible to proceed slightly differently, and the interested reader is referred to Kirsten and Toms (1996b) and Haugset *et al.* (1998). It is also possible to deal with the anisotropic oscillator using the same methods as we have discussed here (Kirsten and Toms, 1996b); however, we will present another method for this in the next section.

6.5 Density of states method

6.5.1 Isotropic harmonic oscillator potential

A commonly used procedure when faced with sums in physics is to approximate them with integrals.[4] In order to illustrate this we will look at the isotropic harmonic oscillator example discussed in the last section. The number of particles in excited states was

$$N_{\rm ex} = \frac{1}{2}\sum_{k=1}^{\infty}(k+1)(k+2)\left[e^{(k+\epsilon)x} - 1\right]^{-1}. \quad (6.103)$$

For small values of x we can replace the sum over k with an integral and replace $(k+1)(k+2)$ with k^2 to give

$$\begin{aligned} N_{\rm ex} &\approx \frac{1}{2}\int_0^{\infty} dk k^2 \left[e^{(k+\epsilon)x} - 1\right]^{-1} \\ &= \frac{1}{2}\sum_{n=1}^{\infty}\int_0^{\infty} dk k^2 e^{-n(k+\epsilon)x} \\ &= \frac{1}{2}\sum_{n=1}^{\infty} e^{-n\epsilon x}\Gamma(3)(nx)^{-3} \\ &= x^{-3}{\rm Li}_3(e^{-\epsilon x}). \end{aligned} \quad (6.104)$$

[4] This is not to be confused with what we did earlier in the book where sums were expressed as contour integrals which is an exact procedure.

We have freely used results from Sections (A1.1)–(A1.4) in obtaining this. If we say that we are interested only in temperatures for which ϵ is very small, we may set $\epsilon = 0$ in (6.104) and obtain

$$N_{\rm ex}^{bulk} = x^{-3}\zeta(3). \tag{6.105}$$

Following Toms (1997) we will call this the bulk approximation. Sometimes it is referred to as the thermodynamic limit. Because we have set $\epsilon = 0$, the approximation really only holds if $N \to \infty$. (See the discussion around (6.80).)

As we discussed in Section 6.4, the bulk approximation gives a result which is close to the value characterizing the Bose–Einstein condensation temperature (see (6.81) and (6.82)). The ground state particle number is (for $x \gg x_B$)

$$\begin{aligned} N_{\rm gr}^{bulk} &= N - N_{\rm ex}^{bulk} \\ &= N\left[1 - \left(\frac{x_B}{x}\right)^3\right] \\ &= N\left[1 - \left(\frac{T}{T_B}\right)^3\right] \end{aligned} \tag{6.106}$$

with the bulk approximation. Although this becomes closer to the true result as T is decreased to smaller values below T_B, it deviates substantially from the true value as $T \to T_B$.[5] This should not be too surprising given the rough approximations we have made.

We can also see what happens if the bulk approximation is used to calculate the specific heat. If we use (6.90) and (6.91), replace the sum on k with an integral, and approximate $k(k+1)(k+2) \approx k^3$ we obtain

$$\begin{aligned} E^{bulk} &= \frac{3}{2}\omega N + \frac{\omega}{2}\int_0^\infty dk\, k^3 \left[e^{(k+\epsilon)x} - 1\right]^{-1} \\ &= \frac{3}{2}\omega N + 3\omega x^{-4}{\rm Li}_4(e^{-\epsilon x}) \end{aligned} \tag{6.107}$$

for the internal energy. For $T < T_B$ we approximate $\epsilon = 0$, so

$$E_<^{bulk} = \frac{3}{2}\omega N + 3\omega x^{-4}\zeta(4) \tag{6.108}$$

is the internal energy in this temperature range. The specific heat for $T < T_B$ is

[5] See Kirsten and Toms (1996b).

$$C_<^{bulk} = \left(\frac{\partial E_<^{bulk}}{\partial T}\right)\Big|_{N,\omega}$$
$$= 12\zeta(4)x^{-3}. \tag{6.109}$$

This can be observed to correspond to only the first term on the right-hand side of (6.102).

The bulk approximation for the specific heat when $T > T_B$ is more involved. T_B is defined by setting $\epsilon = 0$ in (6.104) giving $N_{\rm gr}^{bulk} = 0$. From (6.105) we then have

$$N = x_B^{-3}\zeta(3). \tag{6.110}$$

Eliminating N between (6.110) and (6.105) results in

$$\mathrm{Li}_3(e^{-\epsilon x}) = \zeta(3)\left(\frac{T_B}{T}\right)^3. \tag{6.111}$$

We can use (6.107) to give

$$C_>^{bulk} = 3\omega^{-3}\left(\frac{k}{\hbar\omega}\right)^3 \frac{\partial}{\partial T}\left[T^4\mathrm{Li}_4(e^{-\epsilon x})\right]\Big|_{N,\omega}.$$

By differentiating the polylogarithm it is easy to see that

$$\frac{\partial}{\partial T}\mathrm{Li}_4(e^{-\epsilon x})\Big|_{N,\omega} = -\left[\frac{\partial(\epsilon x)}{\partial T}\right]_{N,\omega}\mathrm{Li}_3(e^{-\epsilon x}).$$

Differentiating (6.111) with respect to T holding N and ω fixed results in

$$\left[\frac{\partial(\epsilon x)}{\partial T}\right]\Big|_{N,\omega} = \frac{3\zeta(3)T_B^3}{\mathrm{Li}_2(e^{-\epsilon x})T^4}.$$

Putting these last three results together shows that

$$\frac{C_>^{bulk}}{N} = 12\frac{\mathrm{Li}_4(e^{-\epsilon x})}{\mathrm{Li}_3(e^{-\epsilon x})} - 9\frac{\mathrm{Li}_3(e^{-\epsilon x})}{\mathrm{Li}_2(e^{-\epsilon x})}. \tag{6.112}$$

For comparison, if we use N given in (6.110) in (6.109) we obtain

$$\frac{C_<^{bulk}}{N} = 12\frac{\zeta(4)}{\zeta(3)}\left(\frac{T}{T_B}\right)^3. \tag{6.113}$$

Taking the limit $T \to T_B$ in (6.112) and (6.113) shows that

$$\frac{C_<^{bulk}}{N} \to 12\frac{\zeta(4)}{\zeta(3)}$$
$$\frac{C_>^{bulk}}{N} \to 12\frac{\zeta(4)}{\zeta(3)} - 9\frac{\zeta(3)}{\zeta(2)}.$$

Thus the bulk approximation leads to a discontinuous result for the specific heat, as obtained in Bagnato *et al.* (1987). This contrasts with the true result shown in Fig. 6.3 which is perfectly continuous and smooth. Although the bulk approximation leads to a result for T_B which is close to the temperature characterizing Bose–Einstein condensation, the approximation shows features not present in the system. Leaving aside the question of the discontinuity, it was shown in Kirsten and Toms (1996b) that the result (6.113) was not particularly good when compared with the exact result for $T < T_B$.

6.5.2 General method

It is reasonable to ask if there is a more systematic way of approximating sums with integrals. The method used in Section 6.5.1 was very heuristic, and, for example, it is not easy to see what to do in the case of the anisotropic oscillator potential where triple sums arise, or for more general potentials where the explicit energy levels may not be known. Following Kirsten and Toms (1996a, 1999) we will present a general approach to this problem.

Let H be the Hamiltonian operator for some system with E_n the energy levels. Let $\mathcal{N}(E)$ be the number of energy levels for which $E_n \leq E$. We can write

$$\mathcal{N}(E) = \sum_n \theta(E - E_n), \tag{6.114}$$

where $\theta(x)$ is the Heaviside distribution (or step function) defined by

$$\theta(x) = \begin{cases} 1, & x > 0; \\ 0, & x < 0; \\ \frac{1}{2}, & x = 0. \end{cases} \tag{6.115}$$

The aim is to treat the energy levels, or at least some part of the energy spectrum, as a continuous set rather than a discrete set by introducing the density of states

$$\begin{aligned} \rho(E)dE &= \mathcal{N}(E + dE) - \mathcal{N}(E) \\ &= \frac{d\mathcal{N}(E)}{dE}\, dE. \end{aligned} \tag{6.116}$$

It is easy to show that $\theta'(x) = \delta(x)$. (Just integrate $\theta'(x)f(x)$ over all space with $f(x)$ an arbitrary test function that is finite as $|x| \to \infty$ and show that the result is $f(0)$.) This means we can use (6.114) in (6.116) to obtain

$$\rho(E) = \sum_n \delta(E - E_n). \tag{6.117}$$

Now define

$$K(t) = \int_0^\infty dE e^{-tE} \rho(E), \tag{6.118}$$

which is just the Laplace transform of the density of states. If we use (6.117), then $K(t)$ becomes

$$K(t) = \sum_n e^{-tE_n}. \tag{6.119}$$

(If we take $t = \beta$, then $K(t)$ is recognized as the partition function for the canonical ensemble.) The inversion formula for Laplace transforms gives

$$\rho(E) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} dt\, e^{tE} K(t), \tag{6.120}$$

for $c \in \mathbb{R}$ with $c > 0$. We can present a heuristic derivation of (6.120) as follows. First of all we can use the representation of the Dirac delta distribution $\delta(E - E_n) = \int (dk/2\pi) e^{ik(E-E_n)}$ to obtain

$$\rho(E) = \sum_n \int_{-\infty}^{\infty} \frac{dk}{2\pi}\, e^{ik(E-E_n)} = \sum_n \frac{1}{2\pi i} \int_{-i\infty}^{i\infty} dt\, e^{t(E-E_n)}. \tag{6.121}$$

(The second equality has followed by changing variables from k to $-it$.) We may now translate the integration contour in (6.121) to the right by an amount c where $c \in \mathbb{R}$ with $c > 0$. Assuming that it is permissable to interchange the order of summation and integration leads to (6.120) with $K(t)$ given by (6.119).

The importance of (6.118) or (6.120) is that if we can evaluate $K(t)$ given in (6.119) then the density of states may be found. The problem of evaluating (6.119) for a given E_n is sometimes not too difficult, as in the case of the harmonic oscillator. We will do this in Section 6.5.3 below.

Even if it is not possible to perform the sum in (6.119) exactly, it is still possible to obtain a knowledge of the density of states. This is because the density of states is determined by the asymptotic behaviour of $K(t)$ as $t \to 0$ which is known for a wide class of operators (see Kirsten (2001) for example). We will assume that as $t \to 0$

$$K(t) \simeq \sum_{i=1}^{k} c_i t^{-r_i} + \mathcal{O}(t^{-r_k+1}), \tag{6.122}$$

for some coefficients c_i and powers r_i with $r_1 > r_2 > \cdots r_k > 0$. Noting that

$$t^{-r_i} = \frac{1}{\Gamma(r_i)} \int_0^\infty dE\, E^{r_i-1} e^{-tE}, \tag{6.123}$$

for $r_i > 0$ it is easy to see from (6.118) that

$$\rho(E) \simeq \sum_{i=1}^{k} \frac{c_i}{\Gamma(r_i)} E^{r_i - 1}. \tag{6.124}$$

Thus a knowledge of the coefficients c_i in (6.122) gives us the density of states.[6]

6.5.3 Application to the anisotropic harmonic oscillator potential

We will show how the density of states method may be used to obtain results for the anisotropic harmonic oscillator potential. The thermodynamic potential is

$$\Omega = \Omega_{\rm gr} + \Omega_{\rm ex}, \tag{6.125}$$

where

$$\Omega_{\rm gr} = T \ln \left(1 - z e^{-\beta E_0}\right) \tag{6.126}$$

is the lowest mode or ground state contribution, and

$$\Omega_{\rm ex} = T \sum_{n>0} \ln \left(1 - z e^{-\beta E_n}\right) \tag{6.127}$$

represents the contribution from the excited states. Here $z = e^{\beta\mu}$ is called the 'fugacity'. We can write

$$\Omega_{\rm ex} = -T \sum_{k=1}^{\infty} \frac{e^{k\beta(\mu - \mu_c)}}{k} \sum_{n>0} e^{-k\beta(E_n - E_0)}, \tag{6.128}$$

since $\mu_c = E_0$. We now convert the sum over n in (6.128) into an integral with the use of the density of states:

$$\Omega_{\rm ex} \simeq -T \sum_{k=1}^{\infty} \frac{e^{k\beta(\mu - \mu_c)}}{k} \int_{E_1 - E_0}^{\infty} dE\, \rho(E) e^{-k\beta E}. \tag{6.129}$$

The lower limit on the integral corresponds to the first term in the sum over n in (6.128).

[6] The result may be extended to $r_i < 0$ but it requires a more powerful method than Laplace transforms. See Baltes and Hilf (1976) for a discussion of this.

We now need $\rho(E)$. To obtain this we first calculate $K(t)$ defined by

$$K(t) = \sum_{n>0} e^{-t(E_n - E_0)}. \tag{6.130}$$

This differs slightly from (6.119) because we have chosen to separate off the ground state. Because we only want the behaviour of $K(t)$ for negative powers of t we can add back the $n = 0$ term to obtain

$$\begin{aligned} K(t) &= \sum_{n_1=0}^{\infty} \sum_{n_2=0}^{\infty} \sum_{n_3=0}^{\infty} e^{-t(n_1\omega_1 + n_2\omega_2 + n_3\omega_3)} - 1 \\ &= \prod_{j=1}^{3} \left(1 - e^{-t\omega_j}\right)^{-1} - 1. \end{aligned} \tag{6.131}$$

The energy levels given in (6.53) have been used here. It is now straightforward to expand $K(t)$ in powers of t using[7]

$$(1 - e^{-x})^{-1} = \frac{1}{x} + \frac{1}{2} + \frac{x}{12} + \mathcal{O}(x^3). \tag{6.132}$$

We find

$$K(t) \simeq c_1 t^{-3} + c_2 t^{-2} + c_3 t^{-1} + \mathcal{O}(1), \tag{6.133}$$

where

$$c_1 = (\omega_1\omega_2\omega_3)^{-1}, \tag{6.134}$$

$$c_2 = \frac{1}{2}\left(\frac{1}{\omega_1\omega_2} + \frac{1}{\omega_2\omega_3} + \frac{1}{\omega_3\omega_1}\right), \tag{6.135}$$

$$c_3 = \frac{1}{12}\left(\frac{\omega_3}{\omega_1\omega_2} + \frac{\omega_2}{\omega_1\omega_3} + \frac{\omega_1}{\omega_2\omega_3} + \frac{3}{\omega_1} + \frac{3}{\omega_2} + \frac{3}{\omega_3}\right). \tag{6.136}$$

We can now use (6.124) to find

$$\rho(E) \simeq \frac{1}{2} c_1 E^2 + c_2 E + c_3. \tag{6.137}$$

Finally we note that for the isotropic oscillator we have $c_1 = \omega^{-3}, c_2 = (3/2)\omega^{-2}$ and $c_3 = \omega^{-1}$ which agrees with a direct conversion of the

[7] This expansion is given in (A1.48) and just involves the Bernoulli numbers.

degeneracy factor $(1/2)(k+1)(k+2)$. This goes beyond the approximation used in Section 6.5.1 by including a more accurate density of states. It was first discussed in Grossmann and Holthaus (1995).

The energy levels were defined in (6.53) with μ_c given by (6.54). In place of the single dimensionless variable x defined by (6.57) we will define

$$x_i = \beta\omega_i \quad (i = 1, 2, 3). \tag{6.138}$$

We will also define

$$\omega = \frac{1}{3}(\omega_1 + \omega_2 + \omega_3) \tag{6.139}$$

to be the average of the three oscillator frequencies. x will still be defined by (6.57), so that in this case

$$x = \frac{1}{3}(x_1 + x_2 + x_3). \tag{6.140}$$

We also retain the definition of ϵ in (6.58).

Returning to the evaluation of $\Omega_{\rm ex}$ in (6.129) using (6.137) we will make the simplifying assumption that $\beta(E_1 - E_0) << 1$. This allows us to replace the lower limit on the integral with zero. We then have

$$\begin{aligned}\Omega_{\rm ex} &= \sum_{k=1}^{\infty} \frac{e^{k\beta(\mu-\mu_c)}}{k} \int_0^{\infty} dE \Big(\frac{1}{2}c_1 E^2 + c_2 E + c_3\Big) e^{-k\beta E} \\ &= \sum_{k=1}^{\infty} \frac{e^{-kx\epsilon}}{k} \left[\frac{c_1}{(k\beta)^3} + \frac{c_2}{(k\beta)^2} + \frac{c_3}{(k\beta)}\right].\end{aligned} \tag{6.141}$$

The sums in (6.141) are just polylogarithms, and we obtain

$$\begin{aligned}\Omega_{\rm ex} = {} & c_1\beta^{-3}{\rm Li}_4(e^{-x\epsilon}) + c_2\beta^{-2}{\rm Li}_3(e^{-x\epsilon}) \\ & + c_3\beta^{-1}{\rm Li}_2(e^{-x\epsilon}).\end{aligned} \tag{6.142}$$

This expression can be used to give an accurate evaluation of the thermodynamic potential. A simpler analytical approximation may be found by expanding the polylogarithm functions in powers of $\beta\omega\epsilon$ (assuming that this quantity is small). A simple expansion of $\Omega_{\rm ex}$ using the properties of the polylogarithm given in Section A1.4 results in

$$\begin{aligned}\Omega_{\rm ex} \simeq {} & -\frac{T}{x_1x_2x_3}\left[\zeta(4) - \zeta(3)x\epsilon + \frac{1}{2}\zeta(2)x^2\epsilon^2\right] \\ & -\frac{T}{2}\left(\frac{1}{x_1x_2} + \frac{1}{x_2x_3} + \frac{1}{x_1x_3}\right)[\zeta(3) - \zeta(2)x\epsilon] \\ & -\frac{T}{12}\left(\frac{x_3}{x_1x_2} + \frac{x_2}{x_1x_3} + \frac{x_1}{x_2x_3} + \frac{3}{x_1} + \frac{3}{x_2} + \frac{3}{x_3}\right)\zeta(2) + \cdots .\end{aligned} \tag{6.143}$$

Here we have treated all of the x_i as the same order of magnitude as x, and have kept terms only up to order x^{-1}.

The average number of particles in excited states is

$$N_{\rm ex} = -\left(\frac{\partial \Omega_{\rm ex}}{\partial \mu}\right)\Big|_{T,\omega_i} = \frac{\beta}{x}\left(\frac{\partial \Omega_{\rm ex}}{\partial \epsilon}\right)\Big|_{x_i}$$
$$\simeq \frac{\zeta(3)}{x_1 x_2 x_3} + \frac{\zeta(2)}{x_1 x_2 x_3}\left(\frac{3}{2} - \epsilon\right) x. \tag{6.144}$$

It is possible to approximate the specific heat and other thermodynamic quantities in a similar way to what we did for the isotropic oscillator. Details may be found in Kirsten and Toms (1996b).

As a rough estimate of the Bose–Einstein condensation temperature (in place of looking at the maximum of the specific heat) we may say $\epsilon << 3/2$ and $N_{\rm ex} \approx N$. This gives

$$N \approx aT^3 + bT^2, \tag{6.145}$$

where

$$a = \frac{\zeta(3)}{\omega_1 \omega_2 \omega_3}, \tag{6.146}$$

$$b = \frac{3\omega\zeta(2)}{2\omega_1 \omega_2 \omega_3}. \tag{6.147}$$

Since N is large and T is small, we may assume

$$T = \left(\frac{N}{a}\right)^{1/3}(1+\eta), \tag{6.148}$$

with η small. It is straightforward to obtain

$$T \approx \omega\left[\frac{N}{\zeta(3)}\right]^{1/3}\left[1 - \frac{x\zeta(2)}{2\omega\zeta^{2/3}(3)}\,N^{-1/3}\right]. \tag{6.149}$$

As before, the second term in (6.149) represents the correction to the bulk result. Because we have assumed $N_{\rm ex} = N$, there will be a small correction to this if we compare the result with the specific heat maximum due to the fact that at the specific heat maximum there is a non-zero occupation for the ground state particle number. Taking $N = 2000$ and the frequencies $\omega_1 = \omega_2 = 240\pi/\sqrt{8}\,{\rm s}^{-1}$ and $\omega_3 = 240\pi\,{\rm s}^{-1}$ as quoted in Anderson *et al.* (1995) gives $T \simeq 31.9\,{\rm nK}$ resulting in a 6% reduction from the bulk value.[8] More details on the anisotropic oscillator may be found in Kirsten and Toms (1996b).

[8] For comparison, the specific heat maximum occurs at $T \simeq 30.9\,{\rm nK}$ in this case.

6.6 Charged non-relativistic Bose gas in a constant magnetic field

We will study the behaviour of the magnetized non-relativistic Bose gas in three spatial dimensions here. The first correct analysis of this problem was presented by Schafroth (1955) who was motivated by the desire to understand superconductivity.[9] We will first evaluate the thermodynamic potential, then use it to examine Bose–Einstein condensation and the Meissner–Ochsenfeld effect.

Our starting point is

$$\Omega_{T\neq 0} = T\sum_n \ln\left[1 - e^{-\beta(E_n - e\mu)}\right] \tag{6.150}$$

with E_n the energy levels for a charged spin-0 boson in a constant magnetic field. We solved for the energy levels and their degeneracy in Section 4.5, and found (see (4.88) and (4.108))

$$E_{n,j} = \frac{1}{2m}\left[(2n+1)eB + \left(\frac{2\pi j}{L_3}\right)^2\right] \tag{6.151}$$

where $n = 0, 1, 2, \ldots$ and $j = 0, \pm 1, \ldots$ with degeneracy $eBL_1L_2/(2\pi)$.

Here $V = L_1L_2L_3$ is the volume of the normalizing box, and we will take the infinite volume limit. This means that the sum over j may be approximated with an integral, and after a change variables we have

$$\Omega_{T\neq 0} = \frac{eBVT}{2\pi}\sum_{n=0}^{\infty}\int_{-\infty}^{\infty}\frac{dp}{2\pi}\ln\left(1 - e^{-\beta\left\{[n+(1/2)]\frac{eB}{m} + \frac{p^2}{2m} - e\mu\right\}}\right). \tag{6.152}$$

As for the harmonic oscillator confining potential in Section 6.4, it is convenient to define dimensionless parameters. We will define

$$x = \beta\frac{eB}{m} \tag{6.153}$$

which has the interpretation as the ratio of the energy gap between successive energy levels (eB/m) to the thermal energy kT. The critical value of the chemical potential, as discussed in Section 6.2 (see (6.16)), is determined by the lowest energy level. With (6.151) for the energy levels we find

$$e\mu_c = E_{0,0} = \frac{eB}{2m}. \tag{6.154}$$

[9] This is prior to its eventual solution which has nothing to do with the charged Bose gas.

We will define the dimensionless chemical potential ϵ by

$$e\mu = \frac{eB}{m}\left(\frac{1}{2} - \epsilon\right). \tag{6.155}$$

To see if a phase transition occurs we must study the behaviour of the system as $\epsilon \to 0$. The procedure is very similar to that in Section 6.4 for the trapped Bose gas. With dimensionless variables used we have

$$\Omega_{T\neq 0} = \frac{eBVT}{2\pi}\sum_{n=0}^{\infty}\int_{-\infty}^{\infty}\frac{dp}{2\pi}\ln\left\{1 - e^{-[\beta p^2/(2m)-(n+\epsilon)x]}\right\}. \tag{6.156}$$

Expanding the logarithm in its Taylor series, and performing the integration over p results in

$$\Omega_{T\neq 0} = \frac{eBV}{m}\left(\frac{mT}{2\pi}\right)^{3/2}\sum_{n=0}^{\infty}\sum_{l=1}^{\infty} l^{-3/2}e^{-l(n+\epsilon)x}. \tag{6.157}$$

The sum over n is recognized as a geometric series, and we can easily see that

$$\Omega_{T\neq 0} = \frac{eBV}{m}\left(\frac{T}{2\pi}\right)^{3/2}\sum_{l=1}^{\infty}\frac{e^{-l\epsilon x}}{l^{3/2}(1-e^{-lx})}. \tag{6.158}$$

This is observed to be very similar in form to the expression we analysed in Section 6.4, so we would expect that the same techniques used there should be applicable here.

We want to first of all see whether or not Bose–Einstein condensation, in the sense of symmetry breaking with non-zero condensate, can occur. The complete thermodynamic potential is obtained by adding together the condensate contribution and $\Omega_{T\neq 0}$. We defined

$$Q_1 = -\left(\frac{\partial}{\partial\mu}\Omega_{T\neq 0}\right)\Big|_{T,V} \tag{6.159}$$

before, with Q_0 the possible condensate contribution to the charge (see (6.20)). To see if Bose–Einstein condensation occurs we wish to see if it is possible to solve $Q_1 = Q$ for μ for all T. Using (6.158) we calculate

$$Q_1 = \frac{e^2BV}{2\pi}\left(\frac{mT}{2\pi}\right)^{1/2}\sum_{l=1}^{\infty}\frac{e^{-l\epsilon x}}{l^{1/2}(1-e^{-lx})}. \tag{6.160}$$

Since $\epsilon \geq 0$, we can use the inequality $1 < (1 - e^{-lx})^{-1}$ to conclude that

$$Q_1 > \frac{e^2 BV}{2\pi} \left(\frac{mT}{2\pi} \right)^{1/2} \sum_{l=1}^{\infty} l^{-1/2} e^{-l\epsilon x}. \tag{6.161}$$

As $\epsilon \to 0$, corresponding to $\mu \to \mu_c$, the sum on the right-hand side diverges. What this means is that no matter what value we pick for Q, it will always be possible to solve $Q = Q_1$ for μ and satisfy $\mu < \mu_c$.[10] Therefore, unlike the case of the free Bose gas, there is no Bose–Einstein condensation in the sense of a non-zero condensate and symmetry breaking here.

As an aside, we can consider what happens if we make the spatial dimension larger, say D. The energy levels are just augmented with additional components of momentum (as we found in Section 4.5), giving $D - 2$ momentum integrals in (6.156). It is easy to show that this results in $l^{-D/2}$ in (6.157) and $l^{1-D/2}$ in (6.161). The additional factors of l arising change the convergence or divergence of the sum in (6.161). If $D \geq 5$ the expression for Q_1 will converge as $\epsilon \to 0$. This is like the situation for the free Bose gas, and means that μ can reach its critical value of μ_c, corresponding to a critical temperature and the development of a condensate. Therefore the behaviour of the system is crucially dependent on the spatial dimension. For more details, Standen and Toms (1998, 1999) can be consulted.

Although the analysis we have just presented is undoubtedly correct, as is the conclusion that the presence of a non-zero magnetic field, no matter how small, destroys the Bose–Einstein condensation found for the free Bose gas, there is something unsettling. On physical grounds, it would be expected that as the magnetic field is reduced the system should start to look more and more like the free Bose gas. For infinitesimally small magnetic fields we would expect that the magnetized gas should look almost indistinguishable from a free gas. Yet we know that the magnetized gas will never have a condensate so long as $B \neq 0$. In order to study what happens as $B \to 0$ we will look at the specific heat.

We start with the internal energy which, since there is no condensate, is given by

$$E = \frac{\partial}{\partial \beta} (\beta \Omega). \tag{6.162}$$

[10] Contrast this to the discussion in Section 6.2 for the free Bose gas.

To shorten expressions we will define a class of sums by

$$\Sigma_\kappa\left[\alpha,\delta\right]=\sum_{l=1}^{\infty}\frac{l^{\alpha/2}e^{-lx(\epsilon+\delta)}}{(1-e^{-lx})^\kappa}. \tag{6.163}$$

With this notation, we have (from (6.158) and (6.160)),

$$\Omega_{T\neq 0}=\frac{eBV}{m}\left(\frac{mT}{2\pi}\right)^{3/2}\Sigma_1[-3,0], \tag{6.164}$$

$$Q=\frac{e^2BV}{2\pi}\left(\frac{mT}{2\pi}\right)^{1/2}\Sigma_1[-1,0]. \tag{6.165}$$

(Note, as already discussed, that $Q=Q_1$ here since there is no condensate.) It is easy to show that

$$E=\frac{BQ}{2m}+\frac{eBV}{m}\left(\frac{mT}{2\pi}\right)^{3/2}\left(x\Sigma_2[-1,1]+\frac{1}{2}\Sigma_1[-3,0]\right). \tag{6.166}$$

The specific heat is given in terms of the internal energy by (6.47). Using (6.166), and $N=Q/e$ with Q given by (6.165) results in the rather lengthy expression

$$\begin{aligned}C_V/N=\frac{1}{\Sigma_1[-1,0]}\Big\{&x\Sigma_2[-1,1]+\frac{3}{4}\Sigma_1[-3,0]+x^2\Sigma_2[1,1]\\&+2x^2\Sigma_3[1,2]-x^2\frac{\Sigma_2^2[1,1]}{\Sigma_1[1,0]}\Big\}\\&-\frac{1}{4}\frac{\Sigma_1[-1,0]}{\Sigma_1[1,0]}-x\frac{\Sigma_2[1,1]}{\Sigma_1[1,0]}.\end{aligned} \tag{6.167}$$

In computing this we have been careful to keep Q (or N) fixed. The calculation is very similar to that done in Section 6.4 for the harmonic oscillator confining potential.

Before approximating (6.167) we will study it by numerical computation for different values of the magnetic field. The calculation is done by solving (6.165) for ϵ as a function of x after fixing B. The result can then be used in (6.167) with all sums computed numerically. The result of this calculation of the specific heat is plotted in Fig. 6.4. For comparison we have also plotted the specific heat for the free Bose gas. The first observation is that for $B\neq 0$ the specific heat is a perfectly smooth function, with smooth derivatives. There is no 'point' like that present for the free Bose gas illustrated in Fig. 6.1 signalling a critical temperature. Given the discussion above, this is what we would expect. The second observation

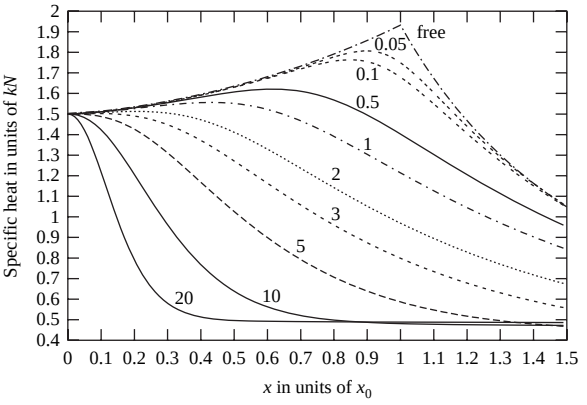

Fig. 6.4 This shows the specific heat for the magnetized Bose gas in units of kN. The curve labelled free is the result for the uncharged Bose gas. The x coordinate in the figure is $x = \hbar\omega/T$ in units of $x_0 = \hbar\omega/T_0$ with T_0 the critical temperature for the free Bose gas. The numbers labelling the curves are the values for x_0. The smaller numbers indicate lower values for the magnetic field.

is that as we decrease the value of B the specific heat starts to develop a more pronounced maximum, and the curve starts to come closer to that for the free Bose gas. The temperature at which the specific heat has a maximum becomes closer to the critical temperature of the free Bose gas. A similar conclusion holds for the number of particles in the ground state. This is consistent with the expectation that as B is reduced, the system should start to look more and more like a system of uncharged bosons. It can also be observed that as $x \to 0$, corresponding to $T \to \infty$, $C_V \to (3/2)N$ as would be expected for a three-dimensional gas. If we increase the magnetic field, the peak in the specific heat moves to smaller values of x, corresponding to values of T larger than T_0. The maximum of C_V decreases in magnitude. For very large values of B the graphs show that before the specific heat rises and approaches $(3/2)N$, there is a dip at $(1/2)N$. This is the Maxwell–Boltzmann result for a one-dimensional gas. Thus for large values of B, at low temperatures, the specific heat resembles that of a free one-dimensional Bose gas. A heuristic classical argument can be used to understand why this might happen. Classically the motion of a charged particle is a spiral around the magnetic field direction. The radius of the orbit is inversely proportional to the magnetic field; thus as B is increased the motion starts to look more and more like linear motion.

It is also possible to study the behaviour of the specific heat analytically for small values of B, and for T close to T_0. This provides concrete back-up for the observations based on the numerical calculations that we

have just described. The critical temperature for the free Bose gas was defined by (6.30) where we set $D = 3$ and call the critical temperature T_0 in place of T_c. For $B \neq 0$, we have $N = Q/e$ where Q is given in (6.165). Equating this with the result for N in (6.29) gives

$$x\Sigma_1[-1,0] = \left(\frac{x}{x_0}\right)^{3/2} \zeta(\frac{3}{2}). \tag{6.168}$$

We wish to solve this for ϵ when the magnetic field is weak and T is close to T_0 (meaning that x is close to $x_0 = eB/(mT_0)$). We have

$$\begin{aligned}\Sigma_1[-1,0] &= \sum_{l=1}^{\infty} l^{-1/2} e^{-l\epsilon x}(1-e^{-lx})^{-1} \\ &= \sum_{l=1}^{\infty}\sum_{n=0}^{\infty} l^{-1/2} e^{-lx(n+\epsilon)}.\end{aligned}$$

This can be approximated using the Mellin–Barnes integral representation (5.62):

$$\Sigma_1[-1,0] = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} d\alpha\, \Gamma(\alpha) x^{-\alpha} \zeta\left(\alpha+\frac{1}{2}\right)\zeta(\alpha,\epsilon) \tag{6.169}$$

$$\begin{aligned}&\simeq \zeta\left(\frac{3}{2}\right)x^{-1} + \sqrt{\pi}x^{-1/2}\zeta\left(\frac{1}{2},\epsilon\right) \\ &\quad +\zeta\left(\frac{1}{2}\right)\left(\frac{1}{2}-\epsilon\right) + \mathcal{O}(x),\end{aligned} \tag{6.170}$$

where in the second line we have just kept the first three terms in the expansion. Using this expansion in (6.168) leads to

$$\left(\frac{x}{x_0}\right)^{3/2}\zeta\left(\frac{3}{2}\right) \simeq \zeta\left(\frac{3}{2}\right) + (\pi x)^{1/2}\zeta\left(\frac{1}{2},\epsilon\right) + \zeta\left(\frac{1}{2}\right)\left(\frac{1}{2}-\epsilon\right)x + \cdots \tag{6.171}$$

as our approximation.

Suppose that we concentrate first on $T = T_0$. Call the value of ϵ at $T = T_0$, ϵ_0. Then (6.171) gives us

$$0 = \zeta\left(\frac{1}{2},\epsilon_0\right) + \pi^{-1/2}\zeta\left(\frac{1}{2}\right)\left(\frac{1}{2}-\epsilon_0\right)x_0^{1/2} + \cdots. \tag{6.172}$$

(The next term is of order $x_0^{3/2}$ and could easily be calculated if needed.) If we let $B \to 0$, corresponding to $x_0 \to 0$, then we must have $\epsilon \to a$ where a is the solution to

$$\zeta(1/2, a) = 0. \tag{6.173}$$

The value of a can be calculated numerically from this definition, with the result $a \simeq 0.302721829$. For small, but non-zero, values of B we can try to solve (6.172) for ϵ as a function of x_0. It should be clear that we must have

$$\epsilon_0 = a + a_1 x_0^{1/2} + a_2 x_0 + \cdots \tag{6.174}$$

for some coefficients a_1, a_2. This is because x_0 is arbitrary and (6.172) must hold for arbitrary values of x_0. By expanding the Hurwitz ζ-function about $\epsilon_0 = a$, using (6.174) we find

$$\zeta\left(\frac{1}{2}, \epsilon_0\right) \simeq -\frac{1}{2} a_1 x_0^{1/2} \zeta\left(\frac{3}{2}, a\right) + \mathcal{O}(x_0). \tag{6.175}$$

Using (6.174) and (6.175) in (6.172) fixes

$$a_1 = \frac{2\zeta(1/2)}{\sqrt{\pi}\zeta(3/2, a)} \left(\frac{1}{2} - a\right). \tag{6.176}$$

(Numerically the result is $a_1 \simeq -0.039874213$.) It should be clear how we can extend this result to higher orders and find a_2 in (6.174).

If we generalize slightly and look at temperatures close to T_0, it is easy to show that

$$\epsilon \simeq a + a_1 x_0^{1/2} + \frac{6\zeta(3/2)}{\sqrt{\pi}\zeta(3/2, a)} x_0^{-1/2} \left[1 - \left(\frac{x}{x_0}\right)^{1/2}\right] + \cdots. \tag{6.177}$$

In order that this expression be consistent, we must require

$$1 - \left(\frac{x}{x_0}\right)^{1/2} << x_0^{1/2}. \tag{6.178}$$

In particular, we see that the expansion is good at $T = T_0$.

We can now proceed to the specific heat given in (6.167). All of the sums can be evaluated in the same way as we approximated $\Sigma_1[-1, 0]$. The details are left to the interested reader.[11] At $T = T_0$ we find

$$C_V/N \simeq \frac{15\zeta(5/2)}{4\zeta(3/2)} - x_0^{1/2} \frac{9\zeta(3/2)}{2\sqrt{\pi}\zeta(3/2, a)}$$

[11] See Standen and Toms (1999) for some general results.

$$+x_0\Big[\frac{3}{4}\left(\frac{1}{2}-a\right)+\frac{9\zeta(1/2)\zeta(3/2)}{\pi\zeta^2(3/2,a)} - \frac{27\zeta(1/2)\zeta(3/2)\zeta(5/2,a)}{2\pi\zeta^3(3/2,a)}\left(\frac{1}{2}-a\right)\Big]+\mathcal{O}(x_0^{3/2}). \tag{6.179}$$

The coefficients appearing in this expression can be evaluated numerically to give

$$C_V/N \simeq 1.925671 - 0.813529x_0^{1/2} + 0.106553x_0.$$

If we let $B \to 0$, we are left with just the first term on the right-hand side which agrees with what we found in Section 6.3 for the free Bose gas. This proves analytically what appeared from the numerical results: as $B \to 0$ the specific heat becomes equal to that for the free Bose gas. It also shows that the specific heat for a non-zero magnetic field is smaller than for $B = 0$. An expression for T close to, but not equal to, T_0 can also be found (Standen and Toms (1999)).

A well-known feature of a superconductor is that when a magnetic field is applied to a sample it is possible to find that there is no magnetic field in the sample provided that the applied magnetic field is larger than a critical value. This is called the 'Meissner–Ochsenfeld effect'. What we will do here is examine this phenomenon using the formalism we have developed.

The simplest way to study the magnetization is to study the field equations for electromagnetism. They will follow from the stationary values of the thermodynamic potential. However, we must add in a term coming from the classical Maxwell action which has played no part up until now because it is independent of any condensate and also independent of the chemical potential.

From Section 2.3.4 we can conclude that the classical thermodynamic potential coming from the magnetic field is

$$\Omega_{em} = \int_\Sigma d\sigma_x \left(\frac{1}{4}F_{ij}F^{ij} - J^i_{ext}A_i\right). \tag{6.180}$$

Here $F_{ij} = \partial_i A_j - \partial_j A_i$ represents the magnetic field and J^i_{ext} is the current density responsible for setting up the externally applied magnetic field. For $\mathbf{B}$ directed in the z-direction we have $F_{12} = -F_{21} = B$, so that $F_{ij}F^{ij} = 2B^2$. The result (6.180) is in agreement with basic electromagnetism where $(1/2)B^2$ is the energy density for a magnetic field. We do not yet assume that B is constant.

The thermodynamic potential is

$$\Omega = \Omega_{em} + \Omega_{T\neq 0}. \tag{6.181}$$

If we vary Ω with respect to A_i, we find

$$\partial_j F^{ij} = J^i_{ext} + J^i_{ind} \tag{6.182}$$

where we define

$$\delta\Omega_{T\neq 0} = -\int_\Sigma d\sigma_x J^i_{ind}\delta A_i. \tag{6.183}$$

The physical interpretation of J^i_{ind} is that it represents the current density induced by quantum corrections to the classical theory. We have computed $\Omega_{T\neq 0}$ as a function of B, or F_{ij}, so it would be easier to find J^i_{ind} if the variation in (6.183) was with respect to F_{ij}, rather than A_i. Using the definition of functional differentiation (see Section 2.4),

$$\delta\Omega_{T\neq 0} = \int_\Sigma d\sigma_x \frac{\delta\Omega_{T\neq 0}}{\delta B(\mathbf{x})}\delta B(\mathbf{x}) \tag{6.184}$$

where we assume the magnetic field is in the z-direction with strength $B(\mathbf{x})$: $F_{12} = B,\ F_{21} = -B$. If we write (6.184) in terms of F_{ij} then we should take

$$\begin{aligned}
\delta\Omega_{T\neq 0} &= \frac{1}{2}\int_\Sigma d\sigma_x \left(\frac{\delta\Omega_{T\neq 0}}{\delta F_{12}}\delta F_{12} + \frac{\delta\Omega_{T\neq 0}}{\delta F_{21}}\delta F_{21}\right) \\
&= \frac{1}{2}\int_\Sigma d\sigma_x \frac{\delta\Omega_{T\neq 0}}{\delta F_{ij}}\delta F_{ij} \\
&= \frac{1}{2}\int_\Sigma d\sigma_x \frac{\delta\Omega_{T\neq 0}}{\delta F_{ij}}\left(\partial_i\delta A_j - \partial_j\delta A_i\right) \\
&= -\int_\Sigma d\sigma_x \frac{\delta\Omega_{T\neq 0}}{\delta F_{ij}}\partial_j\delta A_i \\
&= \int_\Sigma d\sigma_x \partial_j\left(\frac{\delta\Omega_{T\neq 0}}{\delta F_{ij}}\right)\delta A_i.
\end{aligned} \tag{6.185}$$

In the first line we have used the fact that only F_{12} and F_{21} are non-zero; this is rewritten using the summation convention in the second line. The third line uses the definition of F_{ij} in terms of A_i. The fourth line uses the antisymmetry, $F_{ij} = -F_{ji}$. The last line is obtained from an integration by parts. Comparison of (6.185) with (6.183) shows that

$$J^i_{ind} = -\partial_j\left(\frac{\delta\Omega_{T\neq 0}}{\delta F_{ij}}\right). \tag{6.186}$$

If we use this expression in (6.182), we can rearrange the result to read

$$\partial_j H^{ij} = J^i_{ext} \tag{6.187}$$

where

$$H^{ij} = F^{ij} + \frac{\delta\Omega_{T\neq 0}}{\delta F_{ij}}. \tag{6.188}$$

This is a generalization of the standard electromagnetic result

$$\mathbf{H} = \mathbf{B} - \mathbf{M} \tag{6.189}$$

where $\mathbf{M}$ is the magnetization.[12] Since only one component of the magnetic field is non-zero, we will define

$$M = -\frac{\delta\Omega_{T\neq 0}}{\delta B}. \tag{6.190}$$

Further simplification occurs here if we now take $B(\mathbf{x}) = B$ to be constant. We have $\delta\Omega_{T\neq 0} = (\partial\Omega_{T\neq 0}/\partial B)\delta B$ in this case, where normal partial derivatives occur. Comparison with (6.184) leads to

$$M = -\frac{1}{V}\frac{\partial\Omega_{T\neq 0}}{\partial B} \tag{6.191}$$

when B is constant.

This approach makes it clear what the physical interpretation of the various fields is, and avoids any possible confusion over what was referred to by Schafroth (1955) as the acting and microscopic magnetic fields. From (6.187) it can be seen that H_{ij}, or $H = B - M$ in the case we have here, is the field set up by the external current. It is therefore the externally applied field. B is the magnetic field felt by the particles, and is therefore the magnetic field present in the sample. These two fields are of course different because the externally applied field causes the charged particles to move, which gives rise to an induced current J^i_{ind} in the sample. This induced current changes the overall magnetic field. For the Meissner–Ochsenfeld effect to occur, we need to know if it is possible for $B \to 0$ (so the charged particles feel no field) when H (the external field) is changed.

We can now use (6.164) to compute the magnetization. It is easy to show that

$$M = -\frac{\rho}{2m} + \frac{e}{m}\left(\frac{mT}{2\pi}\right)^{3/2}\left(\Sigma_1\left[-3,0\right] - x\Sigma_2\left[-1,1\right]\right), \tag{6.192}$$

where $\rho = Q/V$ is the charge density. Using the Mellin–Barnes technique as before, the sums appearing in (6.192) result in

[12] See, for example, Jackson (1962) where different units are used.

$$\Sigma_1[-3,0] - x\Sigma_2[-1,1] \simeq \frac{1}{2}\zeta\left(\frac{3}{2}\right) - \sqrt{\pi}x^{1/2}\left[3\zeta\left(-\frac{1}{2},\epsilon\right) - \epsilon\zeta\left(\frac{1}{2},\epsilon\right)\right] - \frac{1}{2}\zeta\left(\frac{1}{2}\right)x\left(\epsilon - \frac{1}{3}\right) + \mathcal{O}(x^2). \tag{6.193}$$

From the definition of T_0 in (6.30) (recall that we are using T_0 in place of T_c) and $Q = \rho V$, we have

$$e\left(\frac{mT}{2\pi}\right)^{3/2}\zeta\left(\frac{3}{2}\right) = \rho\left(\frac{T}{T_0}\right)^{3/2}. \tag{6.194}$$

Using (6.193) in (6.192), along with (6.194) results in

$$M \simeq -\frac{\rho}{2m}\left[1 - \left(\frac{T}{T_0}\right)^{3/2}\right] + \frac{\rho}{m\zeta(3/2)}\left(\frac{T}{T_0}\right)^{3/2} \times\Big\{ - \sqrt{\pi}x^{1/2}\left[3\zeta\left(-\frac{1}{2},\epsilon\right) - \epsilon\zeta\left(\frac{1}{2},\epsilon\right)\right] - \frac{1}{2}\zeta\left(\frac{1}{2}\right)x\left(\epsilon - \frac{1}{3}\right) + \cdots\Big\} \tag{6.195}$$

as our approximate expression for the magnetization. At this stage we can see that the Meissner–Ochsenfeld effect does occur. If we let $B \to 0$, then because $x \sim B$ all of the terms on the right-hand side of (6.195) will vanish, apart from the first. The result may be used in (6.189) to see that

$$H \simeq B + \frac{\rho}{2m}\left[1 - \left(\frac{T}{T_0}\right)^{3/2}\right]. \tag{6.196}$$

Thus for $T < T_0$, we can have $B = 0$ for $H \geq H_c$, where

$$H_c = \frac{\rho}{2m}\left[1 - \left(\frac{T}{T_0}\right)^{3/2}\right]. \tag{6.197}$$

This is the classic result for the Meissner–Ochsenfeld effect.[13]

If we examine the magnetization at $T = T_0$ we find that it does not vanish identically, so that the approximation we made in getting to

[13] See the discussion in Pippard (1957), for example.

(6.196) and (6.197) breaks down. Setting $T = T_0$ in (6.195), recalling our definition of ϵ_0 gives

$$M|_{T=T_0} \simeq -\frac{3\sqrt{\pi}\zeta(-1/2,a)}{\zeta(3/2)}\frac{\rho}{m}x_0^{1/2} + \cdots \tag{6.198}$$

showing a dependence on $B^{1/2}$ for the magnetization. This behaviour was first demonstrated in Daicic and Frankel (1996), but in a temperature range which did not include $T = T_0$. Note that this result contrasts with the strictly classical Meissner–Ochsenfeld effect for the magnetization (first term of (6.195)) which would vanish at $T = T_0$. A number of generalizations are possible, some of which are explored in Standen and Toms (1998, 1999).[14]

6.7 The interacting Bose gas

6.7.1 General results

Although the neglect of interactions among particles may be justified as an approximation, it cannot be justified at the fundamental level. After all, if we do not allow the particles in a real physical system to interact with each other, then it is hard to imagine how statistical equilibrium could be achieved. In addition, without allowing for the possibility of interactions it would be impossible for us to ever make a measurement on the system.

The role of interactions on the behaviour of the non-relativistic Bose gas was studied in great detail in the late 1950s.[15] Some of the methods used in these original studies are described in the textbooks Huang (1987) and Pathria (1972). The purpose of the present section is to show how the methods used in this book can be applied to the interacting Bose gas.

We will take the action functional to be

$$S[\Psi,\Psi^\dagger] = \int dt \int_\Sigma d\sigma_x \Big[\frac{i}{2}(\Psi^\dagger\dot{\Psi} - \dot{\Psi}^\dagger\Psi) + \frac{1}{2m}|\nabla\Psi|^2 + \mu|\Psi|^2 - U(|\Psi|^2)\Big], \tag{6.199}$$

in place of (6.4). Here $U(|\Psi|^2)$ represents an arbitrary real function which contains details of the interaction. The equation of motion for Ψ follows

[14] A fairly extensive list of references to work on thermodynamics in magnetic fields can be found in the last of these two citations.

[15] Classic references include Lee and Yang (1957), Brueckner and Sawada (1957), Lee *et al.* (1957), and Lee and Yang (1958).

as usual from applying the principle of stationary action to (6.199) and is

$$0 = i\dot{\Psi} + \frac{1}{2m}\nabla^2\Psi + \mu\Psi - U'(|\Psi|^2)\Psi, \tag{6.200}$$

(There is also an equation for $\Psi^\dagger$ which is just the Hermitian conjugate of (6.200).) Just as in Section 6.1, we can expand the field Ψ about the mean field $\bar{\Psi}$ as in (6.7). We will take $\bar{\Psi}$ to be constant. Working to first order in the fluctuation ψ, we have

$$\begin{aligned} 0 = & i\dot{\psi} + \frac{1}{2m}\nabla^2\psi + \mu\psi - U'(|\bar{\Psi}|^2)\psi \\ & -U''(|\bar{\Psi}|^2)\left(|\bar{\Psi}|^2\psi + \bar{\Psi}^2\psi^\dagger\right), \end{aligned} \tag{6.201}$$

$$\begin{aligned} 0 = & -i\dot{\psi}^\dagger + \frac{1}{2m}\nabla^2\psi^\dagger + \mu\psi^\dagger - U'(|\bar{\Psi}|^2)\psi^\dagger \\ & -U''(|\bar{\Psi}|^2)\left(|\bar{\Psi}|^2\psi^\dagger + (\bar{\Psi}^\dagger)^2\psi\right), \end{aligned} \tag{6.202}$$

from (6.200) and its conjugate.

We will now define $\{f_k(\mathbf{x})\}$ to be a complete orthonormal set of solutions to

$$-\nabla^2 f_k(\mathbf{x}) = \sigma_k f_k(\mathbf{x}) \tag{6.203}$$

as usual. We can expand the fluctuation $\psi(t, \mathbf{x})$

$$\psi(t, \mathbf{x}) = \sum_k A_k e^{-iE_k t} f_k(\mathbf{x}), \tag{6.204}$$

$$\psi^\dagger(t, \mathbf{x}) = \sum_k B_k e^{-iE_k t} f_k(\mathbf{x}), \tag{6.205}$$

for independent expansion coefficients A_k and B_k. E_k can be interpreted as the excitation energy, and it is this energy that we are after. Because of the assumption of completeness for the $f_k(\mathbf{x})$, substitution of (6.204) and (6.205) into (6.201) and (6.202) results in the coupled set of equations

$$\begin{aligned} 0 = & \left[E_k - \frac{\sigma_k}{2m} + \mu - U'(|\bar{\Psi}|^2) - |\bar{\Psi}|^2 U''(|\bar{\Psi}|^2)\right] A_k \\ & -\bar{\Psi}^2 U''(|\bar{\Psi}|^2) B_k, \end{aligned} \tag{6.206}$$

$$\begin{aligned} 0 = & \left[-E_k - \frac{\sigma_k}{2m} + \mu - U'(|\bar{\Psi}|^2) - |\bar{\Psi}|^2 U''(|\bar{\Psi}|^2)\right] B_k \\ & -(\bar{\Psi}^\dagger)^2 U''(|\bar{\Psi}|^2) A_k. \end{aligned} \tag{6.207}$$

For a non-trivial solution the expansion coefficients A_k and B_k should not vanish. We either use the result from linear algebra that the matrix

of coefficients must have a vanishing determinant, or more simply solve for A_k in terms of B_k in the first equation and substitute the result into the second equation. In either case, this results in

$$E_k = \left[\frac{\sigma_k}{2m} - \mu + U'(|\bar{\Psi}|^2)\right]^{1/2} \times \left[\frac{\sigma_k}{2m} - \mu + U'(|\bar{\Psi}|^2) + 2|\bar{\Psi}|^2 U''(|\bar{\Psi}|^2)\right]^{1/2}. \tag{6.208}$$

As a check on the result (6.208), if we take the limit $U \to 0$, then $E_k \to \sigma_k/(2m) - \mu$ which is exactly the expression that enters the thermodynamic potential for the free theory considered earlier.

The full thermodynamic potential can be written as in (6.10) if we only work to order $\hbar$. We have

$$\Omega = \Omega_{\text{class}} + \Omega^{(1)}_{T=0} + \Omega^{(1)}_{T\neq 0}, \tag{6.209}$$

where

$$\begin{aligned}\Omega_{\text{class}} &= \int_\Sigma d\sigma_x \left[\frac{1}{2m}|\nabla\bar{\Psi}|^2 - \mu|\bar{\Psi}|^2 + U(|\bar{\Psi}|^2)\right] \\ &= V\left[U(|\bar{\Psi}|^2) - \mu|\bar{\Psi}|^2\right]\end{aligned} \tag{6.210}$$

if $\bar{\Psi}$ is constant, with V the volume of the system. $\Omega^{(1)}_{T=0} + \Omega^{(1)}_{T\neq 0}$ represents the first-order quantum correction (order $\hbar$) to the classical result. The zero temperature contribution $\Omega^{(1)}_{T=0}$ is formally given as the sum of the zero-point energy

$$\Omega^{(1)}_{T=0} = \frac{\hbar}{2}\sum_k E_k \tag{6.211}$$

and

$$\Omega^{(1)}_{T\neq 0} = \hbar T \sum_k \ln(1 - e^{-\beta E_k}) \tag{6.212}$$

is the finite temperature correction to this. In our earlier discussion of the free Bose gas we neglected the zero-temperature contribution as being of no significance (since there was no dependence on the condensate or the temperature). For the interacting gas, because the energies E_k in (6.208) have a non-trivial dependence on $\bar{\Psi}$ we should not neglect $\Omega^{(1)}_{T=0}$. We will see later that our neglect of $\Omega^{(1)}_{T=0}$ for the free theory was fully justified. As we have done many times previously, we can define $\Omega^{(1)}_{T=0}$ by using an energy ζ-function and taking

$$\Omega^{(1)}_{T=0} = \frac{\hbar}{2}E(0). \tag{6.213}$$

This will be evaluated later.

The number of particles is given by

$$N = -\left(\frac{\partial\Omega}{\partial\mu}\right)\Big|_{\beta,V,\bar{\Psi}}, \tag{6.214}$$

and the internal energy density ρ is contained in

$$\rho V = \frac{\partial}{\partial\beta}(\beta\Omega)\Big|_{\beta\mu,V,\bar{\Psi}} \tag{6.215}$$

(See (5.30) and (6.39) respectively. Because ρ is constant, the internal energy is just ρV.) A more useful expression for ρ can be achieved by noting that if F is any function of β and μ then

$$\delta F = \frac{\partial F}{\partial\beta}\Big|_{\mu}\delta\beta + \frac{\partial F}{\partial\mu}\Big|_{\beta}\delta\mu \tag{6.216}$$

represents the change in F under any arbitrary change of β and μ. If F is changed holding $\beta\mu$ fixed, then

$$\delta(\beta\mu) = 0 = \delta\beta\ \mu + \beta\ \delta\mu. \tag{6.217}$$

Eliminating $\delta\mu$ in (6.216) using (6.217) results in

$$\delta F = \left(\frac{\partial F}{\partial\beta}\Big|_{\mu} - \frac{\mu}{\beta}\ \frac{\partial F}{\partial\mu}\Big|_{\beta}\right)\delta\beta$$

or equivalently

$$\frac{\partial F}{\partial\beta}\Big|_{\beta\mu} = \frac{\partial F}{\partial\beta}\Big|_{\mu} - \frac{\mu}{\beta}\ \frac{\partial F}{\partial\mu}\Big|_{\beta}. \tag{6.218}$$

Using the identity (6.218) to evaluate the right-hand side of (6.215) leads to

$$\rho V = \frac{\partial}{\partial\beta}(\beta\Omega)\Big|_{\mu,V,\bar{\Psi}} + \mu N \tag{6.219}$$

if (6.214) is used.

The mean field, or condensate, $\bar{\Psi}$ satisfies the equation obtained from

$$0 = \frac{\partial\Omega}{\partial\bar{\Psi}}\Big|_{\beta,V,\mu}. \tag{6.220}$$

This is extremely complicated due to the involved nature of the $\bar{\Psi}$ dependence in the energy levels E_k in (6.208). However we are only working to

order $\hbar$; from (6.209) and (6.210) we can conclude that for $\bar{\Psi} \neq 0$ (6.220) results in

$$\mu = U'(|\bar{\Psi}|^2) + \mathcal{O}(\hbar). \tag{6.221}$$

This means that if we have an expression which is already of order $\hbar$ we can simplify it using only the first term of (6.221). For an expression which is of lower order in $\hbar$ we must know something about the $\mathcal{O}(\hbar)$ part of μ in (6.222) if we are to work consistently to $\mathcal{O}(\hbar)$. We will deal with this later.

The number density is just the number of particles per unit volume: $n = N/V$. Using (6.214) with (6.209) and (6.210) we can write

$$n = |\bar{\Psi}|^2 + n^{(1)}_{T=0} + n^{(1)}_{T\neq 0}, \tag{6.222}$$

with

$$n^{(1)}_{T=0} = -\frac{1}{V}\left[\frac{\partial \Omega^{(1)}_{T=0}}{\partial \mu}\right]\Bigg|_{\beta,V,\bar{\Psi}} \tag{6.223}$$

and a similar expression holding for $n^{(1)}_{T\neq 0}$. Since $n^{(1)}_{T=0}$ and $n^{(1)}_{T\neq 0}$ are both of order $\hbar$, it is obvious from (6.222) that we have

$$|\bar{\Psi}|^2 = n + \mathcal{O}(\hbar). \tag{6.224}$$

It follows from (6.224) that we can set $|\bar{\Psi}|^2 = n$ in any expression that is already of order $\hbar$.[16]

6.7.2 Ground state energy

From the energy density in (6.218), we find using (6.209), (6.210), and (6.222) that

$$\begin{aligned}\rho = U(|\bar{\Psi}|^2) + \frac{1}{V}\Omega^{(1)}_{T=0} + \frac{1}{V}\frac{\partial}{\partial \beta}\left[\beta \Omega^{(1)}_{T\neq 0}\right]\Bigg|_{\mu,V,\bar{\Psi}} \\ +\mu\left[n^{(1)}_{T=0} + n^{(1)}_{T\neq 0}\right].\end{aligned} \tag{6.225}$$

If we use (6.222) for $|\bar{\Psi}|^2$ in $U(|\bar{\Psi}|^2)$ and expand to order $\hbar$ we find

$$U(|\bar{\Psi}|^2) = U(n) - U'(n)\left[n^{(1)}_{T=0} + n^{(1)}_{T\neq 0}\right] + \cdots. \tag{6.226}$$

[16] Remember that we are working consistently to order $\hbar$.

The last term of (6.225) may be simplified using (6.221) to give

$$\mu\left[n_{T=0}^{(1)}+n_{T\neq 0}^{(1)}\right]=U'(n)\left[n_{T=0}^{(1)}+n_{T\neq 0}^{(1)}\right]+\cdots, \tag{6.227}$$

again working only to order $\hbar$. Using (6.226) and (6.227) to simplify (6.246) results in

$$\rho=U(n)+\frac{1}{V}\Omega_{T=0}^{(1)}+\frac{1}{V}\frac{\partial}{\partial\beta}\left[\beta\Omega_{T\neq 0}^{(1)}\right]\Big|_{\mu,V,\bar{\Psi}}. \tag{6.228}$$

All that is necessary now is the evaluation of the last two terms of this result and we will have the ground-state energy density expressed in terms of the number density.

We turn first to $\Omega_{T=0}^{(1)}$ which will give us the quantum correction to the energy density at zero temperature. We will evaluate the energy ζ-function defined by

$$E(s)=\sum_k E_k(\ell E_k)^{-s}. \tag{6.229}$$

A direct evaluation using the energy levels in (6.208) is difficult. However because we are only working to order $\hbar$, and $\Omega_{T=0}^{(1)}$ is already of order $\hbar$, we can simplify the excitation energies using $\mu=U'(n)$ and $|\bar{\Psi}|^2=n$ as given in (6.221) and (6.224). Doing this in (6.208) results in

$$E_k=\left(\frac{\sigma_k}{2m}\right)^{1/2}\left[\frac{\sigma_k}{2m}+2nU''(n)\right]^{1/2}. \tag{6.230}$$

This simplification makes the evaluation of the energy ζ-function fairly straightforward. If we take the large volume limit and replace $\sigma_k\to k^2$ and $\sum_k\to V\int d^3k/(2\pi)^3$, the energy ζ-function reads[17]

$$E(s)=\frac{V}{\ell^s}\int\frac{d^3k}{(2\pi)^3}\left(\frac{k^2}{2m}\right)^{(1-s)/2}\left[\frac{k^2}{2m}+2nU''(n)\right]^{(1-s)/2}. \tag{6.231}$$

The integral in (6.231) can be evaluated using the representation of the Γ-function (see Section A1.1). We write

$$\left[\frac{k^2}{2m}+2nU''(n)\right]^{(1-s)/2}=\frac{1}{\Gamma\left[(s-1)/2\right]}\int_0^\infty dt\,t^{(s-3)/2}e^{-t\left[k^2/(2m)+2nU''(n)\right]}.$$

[17] Note that the energy spectrum in (6.230) with $\sigma_k\to k^2$ was first given by Bogoliubov (1947).

This result may be substituted into (6.231) and the order of integrations changed. The integration over k may be performed using

$$\begin{aligned}\int \frac{d^3k}{(2\pi)^3}\left(\frac{k^2}{2m}\right)^{(1-s)/2} e^{-tk^2/(2m)} &= \frac{(2m)^{3/2}}{2\pi^2}\int_0^\infty dk\, k^2 (k^2)^{(1-s)/2} e^{-tk^2} \\ &= \frac{(2m)^{3/2}}{4\pi^2}\int_0^\infty d\kappa\, \kappa^{1-s/2} e^{-t\kappa} \\ &= \frac{(2m)^{3/2}}{4\pi^2}\Gamma(2-s/2)t^{5/2-s}.\end{aligned}$$

In the first equality we have rescaled $k \to (2m)^{1/2}k$, switched to spherical polar coordinates, and performed the angular integrations (so $d^3k \to 4\pi k^2 dk$). In the second equality we have changed variables from k^2 to $k = \kappa^{1/2}$. The final equality has made use of the integral representation for the Γ-function again. The energy ζ-function now reads

$$E(s) = \frac{V(2m)^{3/2}}{4\pi^2\ell^s}\frac{\Gamma[2-s/2]}{\Gamma[s-5/2]}\int_0^\infty dt\, t^{s-7/2} e^{-t[2nU''(n)]}.$$

We use the integral representation for the Γ-function a final time to give the closed form result

$$E(s) = \frac{V(2m)^{3/2}}{4\pi^2\ell^s}\frac{\Gamma[2-s/2]\Gamma[s-5/2]}{\Gamma[(s-1)/2]}[2nU''(n)]^{5/2-s}. \tag{6.232}$$

This expression is analytic at $s = 0$ with the value

$$E(0) = \frac{16}{15\pi^2}m^{3/2}V[nU''(n)]^{5/2}. \tag{6.233}$$

We therefore find

$$\frac{1}{V}\Omega^{(1)}_{T=0} = \frac{8\hbar}{15\pi^2}m^{3/2}[nU''(n)]^{5/2} \tag{6.234}$$

from (6.213).

To evaluate the last term of (6.228) we can use (6.212) to obtain

$$\begin{aligned}\rho^{(1)}_{T\neq 0} &= \frac{1}{V}\frac{\partial}{\partial\beta}[\beta\Omega^{(1)}_{T\neq 0}]\Big|_{\mu,V,\bar{\Psi}} \\ &= \frac{\hbar}{V}\sum_k E_k(e^{\beta E_k}-1)^{-1}.\end{aligned} \tag{6.235}$$

This may be recognized as the usual expression for the internal energy density from statistical mechanics. As in our evaluation of $\Omega^{(1)}_{T=0}$, we are

allowed to use the simplified result for the energy levels given in (6.230). In the large volume limit, after switching to spherical polar coordinates, performing the angular integration, and rescaling $k \to (2mT)^{1/2}k$ we obtain

$$\rho^{(1)}_{T\neq 0} = \frac{\hbar}{2\pi^2\beta}\left(\frac{2m}{\beta}\right)^{3/2}\int_0^\infty dk\, k^3 \frac{\sqrt{k^2+2\beta n U''(n)}}{\left[e^{k\sqrt{k^2+2\beta n U''(n)}}-1\right]}. \tag{6.236}$$

Although it is not possible to evaluate the integral here exactly, it is relatively straightforward to obtain an expansion valid at low temperatures. To do this we will take $2\beta n U''(n) >> 1$, or equivalently $T << 2nU''(n)$. Define

$$\epsilon = [2\beta n U''(n)]^{-2} \tag{6.237}$$

and rescale $k \to \epsilon^{-1/4}k$ in (6.236):

$$\rho^{(1)}_{T\neq 0} = \frac{\hbar T}{2\pi^2}(2mT)^{3/2} I \tag{6.238}$$

where

$$I = \epsilon^{3/4}\int_0^\infty dk\, k^2\sqrt{1+\epsilon k^2}\left(e^{k\sqrt{1+\epsilon k^2}}-1\right)^{-1}. \tag{6.239}$$

We can now notice that the dominant contribution to the integral I comes from values of k close to $k = 0$ because that is where the factor involving the exponential is largest. We can expand $\sqrt{1+\epsilon k^2}$ about $k = 0$, or equivalently in powers of the small parameter ϵ. The resulting integrals are then all of the form $\int_0^\infty dk\, k^n (e^k - 1)^{-1}$ for various values of n. From Section A1.2 such integrals can be done in terms of the Riemann ζ-function, and the results expressed in terms of Bernoulli numbers. After a bit of calculation it can be shown that

$$I \simeq \frac{\pi^4}{15}\epsilon^{3/4} - \frac{20\pi^6}{63}\epsilon^{7/4} + \frac{21\pi^8}{5}\epsilon^{11/4} + \cdots. \tag{6.240}$$

As ϵ becomes smaller, the difference between this approximation and the result found by a numerical evaluation of (6.239) becomes virtually negligible. The low temperature expansion of $\rho^{(1)}_{T\neq 0}$ reads

$$\rho^{(1)}_{T\neq 0} \simeq \frac{\hbar\pi^2}{30}\left[\frac{m}{nU''(n)}\right]^{3/2} T^4\left\{1 - \frac{25\pi^2}{21}[\beta n U''(n)]^{-2} + \cdots\right\}. \tag{6.241}$$

This result vanishes as $T \to 0$ as expected.

If we wish to make contact with the standard results (Brueckner and Sawada, 1957; Lee and Yang, 1957; Lee *et al.*, 1957; Lee and Yang, 1958) we must specialize the potential to be

$$U(|\bar{\Psi}|^2) = \frac{2\pi a}{m}|\bar{\Psi}|^4. \tag{6.242}$$

a is called the 's-wave scattering length'. In this case it follows from (6.228) and (6.234) that

$$\rho(T=0) = \frac{2\pi a n^2}{m}\left(1 + \frac{128\hbar}{15\sqrt{\pi}}\sqrt{na^3}\right) \tag{6.243}$$

is the ground-state energy density at $T = 0$. The finite temperature correction, at low temperatures (low means $T << 2nU''(n)$ here), is

$$\rho^{(1)}_{T\neq 0} \simeq \frac{\hbar m^3 T^4}{240\sqrt{\pi}}(na^3)^{-3/2}\left[1 - \frac{25}{336}\left(\frac{mT}{na}\right)^2 + \cdots\right]. \tag{6.244}$$

The result in (6.243) agrees with the classic calculations of Lee and Yang (1957), Brueckner and Sawada (1957), and Lee *et al.* (1957) for the zero temperature gas. The first term of (6.244) reproduces the leading correction at low temperature found in Lee and Yang (1958). (Note that Lee and Yang (1958) chose units with $m = 1/2$.)

6.7.3 Equation of state

The pressure was defined in terms of the thermodynamic potential by (5.29). It is clear in the large volume limit that $\Omega \propto V$ so that we have

$$P = -\frac{\Omega}{V}. \tag{6.245}$$

Using (6.209) and (6.210) this becomes

$$P = \mu|\bar{\Psi}|^2 - U(|\bar{\Psi}|^2) - \frac{\Omega^{(1)}_{T=0} + \Omega^{(1)}_{T\neq 0}}{V}. \tag{6.246}$$

Using (6.222) and (6.224) to eliminate $|\bar{\Psi}|^2$ we find (to order $\hbar$)

$$P = \mu n - U(n) - \frac{\Omega^{(1)}_{T=0} + \Omega^{(1)}_{T\neq 0}}{V} \tag{6.247}$$

where we can set $|\bar{\Psi}|^2 = n$ in $\Omega^{(1)}_{T=0}$ and $\Omega^{(1)}_{T\neq 0}$ since these two terms are already of order $\hbar$. What makes the calculation of P more difficult than

that of ρ is that we cannot simply use (6.221) for μ in the first term; we must know the $\mathcal{O}(\hbar)$ contribution to μ coming from the quantum corrections to the classical field equation for $\bar{\Psi}$.

Because we are interested only in the condensed phase, we can replace (6.220) with

$$0 = \left(\frac{\partial\Omega}{\partial|\bar{\Psi}|^2}\right)\Bigg|_{\beta,V,\mu}. \tag{6.248}$$

This leads to

$$\mu = U'(|\bar{\Psi}|^2) + \frac{1}{V}\frac{\partial[\Omega^{(1)}_{T=0} + \Omega^{(1)}_{T\neq 0}]}{\partial|\bar{\Psi}|^2}\Bigg|_{\mu,T,V}. \tag{6.249}$$

We use (6.224) in the first term to obtain

$$\mu = U'(n) + \frac{1}{V}\left\{\frac{\partial[\Omega^{(1)}_{T=0} + \Omega^{(1)}_{T\neq 0}]}{\partial|\bar{\Psi}|^2} + U''(n)\frac{\partial[\Omega^{(1)}_{T=0} + \Omega^{(1)}_{T\neq 0}]}{\partial\mu}\right\}. \tag{6.250}$$

This result may be used in (6.247) to give

$$\begin{aligned} P = nU'(n) - U(n) + \frac{1}{V}\left[n\frac{\partial\Omega^{(1)}_{T=0}}{\partial|\bar{\Psi}|^2} + nU''(n)\frac{\partial\Omega^{(1)}_{T=0}}{\partial\mu} - \Omega^{(1)}_{T=0}\right] \\ + \frac{1}{V}\left[n\frac{\partial\Omega^{(1)}_{T\neq 0}}{\partial|\bar{\Psi}|^2} + nU''(n)\frac{\partial\Omega^{(1)}_{T\neq 0}}{\partial\mu} - \Omega^{(1)}_{T\neq 0}\right] \end{aligned} \tag{6.251}$$

for the pressure to order $\hbar$. The last term of (6.251) displays the finite temperature correction to the zero temperature result. In the last two terms of (6.251) we can set $|\bar{\Psi}|^2 = n$ and $\mu = U'(n)$ since they are of order $\hbar$.[18]

We define $\Omega^{(1)}_{T=0}$ by the energy ζ-function method as before. From the excitation energy (6.208) it is easy to see that

$$\frac{\partial E_k}{\partial\mu} = -\frac{1}{E_k}\left[\frac{\sigma_k}{2m} + nU''(n)\right] \tag{6.252}$$

$$\frac{\partial E_k}{\partial|\bar{\Psi}|^2} = \frac{1}{E_k}\left\{\left[2U''(n) + nU'''(n)\right]\frac{\sigma_k}{2m} + n(U''(n))^2\right\}. \tag{6.253}$$

[18] Of course it is necessary to perform the indicated differentiations before doing any such simplifications.

It then follows from (6.213) and the definition of the energy ζ-function that

$$\frac{n}{V}\left[\frac{\partial\Omega^{(1)}_{T=0}}{\partial|\bar{\Psi}|^2}+U''(n)\frac{\partial\Omega^{(1)}_{T=0}}{\partial\mu}\right]=\frac{\hbar n(1-s)}{2V\ell^s}[U''(n)+nU'''(n)] \times\sum_k\frac{\sigma_k}{2mE_k^{1+s}} \tag{6.254}$$

with the right-hand side defined by analytic continuation to $s=0$. Taking the large volume limit and evaluating the resulting integral using the same procedure as that which led to (6.232) gives

$$\begin{aligned}\frac{n}{V}\left[\frac{\partial\Omega^{(1)}_{T=0}}{\partial|\bar{\Psi}|^2}+U''(n)\frac{\partial\Omega^{(1)}_{T=0}}{\partial\mu}\right]&=\frac{\hbar n}{8\pi^2}(2m)^{3/2}\left[U''(n)+nU'''(n)\right]\ell^{-s}\\ &\times(1-s)\frac{\Gamma(2-s/2)\Gamma(s-3/2)}{\Gamma\left[(1+s)/2\right]}\left[2mU''(n)\right]^{3/2-s}\\ &=\frac{4\hbar n}{3\pi^2}\left[U''(n)+nU'''(n)\right]\left[mnU''(n)\right]^{3/2}\end{aligned} \tag{6.255}$$

after analytic continuation to $s=0$.

The pressure of the zero temperature gas follows as

$$\begin{aligned}P_{T=0}=&nU'(n)-U(n)+\frac{4\hbar}{5\pi^2}m^{3/2}[nU''(n)]^{5/2}\\ &+\frac{4\hbar}{3\pi^2}n^2U'''(n)[mnU''(n)]^{3/2}.\end{aligned} \tag{6.256}$$

Specializing the potential as in (6.242) results in

$$P_{T=0}=\frac{2\pi an^2}{m}\left(1+\frac{64\hbar}{5\sqrt{\pi}}\sqrt{na^3}\right) \tag{6.257}$$

in agreement with the standard results (Lee and Yang, 1957; Lee *et al.*, 1957).

To evaluate the finite temperature part of the pressure, we use (6.212) along with (6.252) and (6.253) to find

$$\frac{n}{V}\left[\frac{\partial\Omega^{(1)}_{T\neq0}}{\partial|\bar{\Psi}|^2}+U''(n)\frac{\partial\Omega^{(1)}_{T\neq0}}{\partial\mu}\right]=\frac{\hbar n}{V}\left[U''(n)+nU'''(n)\right] \times\sum_k(e^{\beta E_k}-1)^{-1}\left[\frac{\sigma_k}{\sigma_k+4mnU''(n)}\right]^{1/2}.$$

The simplified energy levels in (6.230) can be used to evaluate the right-hand side at low temperatures using the same procedure as that for $\rho^{(1)}_{T\neq 0}$ in (6.241). A short calculation leads to

$$\frac{n}{V}\left[\frac{\partial\Omega^{(1)}_{T\neq 0}}{\partial|\bar{\Psi}|^2}+U''(n)\frac{\partial\Omega^{(1)}_{T\neq 0}}{\partial\mu}\right]=\frac{\hbar\pi^2T^4}{60}\left[\frac{m}{nU''(n)}\right]^{3/2}\left[1+\frac{nU'''(n)}{U''(n)}\right]\times\left\{1-\frac{5\pi^2}{3}[\beta nU''(n)]^{-2}+\cdots\right\} \tag{6.258}$$

assuming $\beta nU''(n) >> 1$. In a similar way the low temperature expansion of (6.212) gives

$$-\frac{\Omega^{(1)}_{T\neq 0}}{V}=\frac{\pi^2\hbar}{90}T^4\left[\frac{m}{nU''(n)}\right]^{3/2}\left\{1-\frac{5\pi^2}{7}[\beta nU''(n)]^{-2}+\cdots\right\}. \tag{6.259}$$

Combining (6.258) and (6.259) we have

$$P_{T\neq 0}\simeq\frac{\pi^2\hbar}{36}T^4\left[\frac{m}{nU''(n)}\right]^{3/2}\left\{1+\frac{3nU'''(n)}{5U''(n)}-\pi^2\left[\frac{9}{7}+\frac{nU'''(n)}{U''(n)}\right][\beta nU''(n)]^{-2}+\cdots\right\} \tag{6.260}$$

as the low temperature correction to the zero-temperature expression for the pressure given in (6.256). When we look at the special case $U(n) = 2\pi an^2/m$ given in (6.242) we find

$$P_{T\neq 0}\simeq\hbar\frac{\sqrt{\pi}}{288}m^3T^4(na)^{-3/2}\left[1-\frac{9}{118}\left(\frac{m}{\beta na}\right)^2+\cdots\right]. \tag{6.261}$$

The leading term agrees with the earlier calculation in Lee and Yang (1958).

6.8 The relativistic non-interacting charged scalar field

For the relativistic scalar field we can proceed along the same lines as we did in Section 6.1 for the non-relativistic case. The Hamiltonian for the charged scalar field follows from (2.52) in Section 2.3.2 as

$$H=\int_\Sigma d\sigma_x\left(|\Pi|^2+|\nabla\Phi|^2+m^2|\Phi|^2\right), \tag{6.262}$$

and there is a conserved charge (see (3.222) in Section 3.7) given by

$$Q = ie \int_\Sigma d\sigma_x \left(\Phi^\dagger \dot{\Phi} - \dot{\Phi}^\dagger \Phi \right). \tag{6.263}$$

The canonical momentum is $\Pi = \dot{\Phi}$, and so it is easy to write the charge in terms of fields and momentum. We then form

$$\bar{H} = H - \mu Q = \int_\Sigma d\sigma_x \left[|\Pi|^2 + |\nabla \Phi|^2 + m^2 |\Phi|^2 + ie\mu \left(\Pi\Phi - \Phi^\dagger \Pi^\dagger \right) \right] \tag{6.264}$$

as in (6.3).

In order to obtain the equations of motion we will use the Heisenberg equations for the field operators Π and Φ. The only difference with what we have seen already in Chapter 3 is that $\bar{H}$ will be used here in (3.37) instead of simply H:

$$i\dot{\Phi} = [\Phi, \bar{H}], \tag{6.265}$$

$$i\dot{\Pi} = [\Pi, \bar{H}]. \tag{6.266}$$

We need the field commutation relation

$$[\Phi(t, \mathbf{x}), \Pi(t, \mathbf{x}')] = i\delta(\mathbf{x}, \mathbf{x}'),$$

and find in a straightforward way

$$\dot{\Phi} = \Pi^\dagger + ie\mu\Phi, \tag{6.267}$$

$$\dot{\Pi} = \nabla^2 \Phi^\dagger - m^2 \Phi^\dagger - ie\mu\Pi, \tag{6.268}$$

from (6.265) and (6.266) respectively. There are also two more equations which are simply the Hermitian conjugates of (6.267) and (6.268). If we use (6.267) in the Hermitian conjugate of (6.268) we can obtain an uncoupled equation for Φ alone:

$$\ddot{\Phi} - 2ie\mu\dot{\Phi} - \nabla^2 \Phi + (m^2 - e^2\mu^2)\Phi = 0. \tag{6.269}$$

As we described in Section 6.1, we can allow for a possible non-zero condensate $\bar{\Phi}$ which is defined by

$$\bar{\Phi} = \langle \Phi \rangle. \tag{6.270}$$

Bose–Einstein condensation can be characterized by whether or not $\bar{\Phi}$ vanishes. In equilibrium we will assume that $\bar{\Phi}$ has no time dependence.

If the condensate does not vanish, then there will be a contribution to the thermodynamic potential as in Section 6.1 which is determined by $\bar{H}$ evaluated for the condensate; call it $\bar{H}_0$. Using (6.267) for $\bar{\Phi}$ with $\dot{\bar{\Phi}} = 0$ we find $\bar{\Pi} = ie\mu\bar{\Phi}$. This gives

$$\Omega_0 = \bar{H}_0 = \int_\Sigma d\sigma_x \left[|\nabla\bar{\Phi}|^2 + (m^2 - e^2\mu^2)|\bar{\Phi}|^2 \right]. \tag{6.271}$$

The full thermodynamic potential is

$$\Omega = \int_\Sigma d\sigma_x \left[|\nabla\bar{\Phi}|^2 + (m^2 - e^2\mu^2)|\bar{\Phi}|^2 \right] + \Omega_{T=0} + \Omega_{T\neq 0}, \tag{6.272}$$

where $\Omega_{T=0}$ is the zero temperature contribution given as the sum of the zero-point energy, and $\Omega_{T\neq 0}$ represents the finite temperature contribution. For the non-interacting field considered here the explicit dependence on the condensate is contained entirely in the first term of (6.272). $\bar{\Phi}$, which makes the thermodynamic potential stationary, must therefore satisfy

$$0 = -\nabla^2\bar{\Phi} + (m^2 - e^2\mu^2)\bar{\Phi}. \tag{6.273}$$

Obviously $\bar{\Phi} = 0$ is a solution to (6.273). To see if there are any other allowed solutions, we can use the method described in Section 6.1. Let $\{f_n(\mathbf{x})\}$ be a complete orthonormal set of solutions to

$$-\nabla^2 f_n(\mathbf{x}) = \sigma_n f_n(\mathbf{x}), \tag{6.274}$$

where the solutions obey the required boundary conditions on the space Σ. The condensate, or background field, $\bar{\Phi}$ may be expanded in terms of the $f_n(\mathbf{x})$:

$$\bar{\Phi}(\mathbf{x}) = \sum_n C_n f_n(\mathbf{x}). \tag{6.275}$$

Because the $f_n(\mathbf{x})$ are complete, if we substitute (6.275) into (6.273) we must have

$$(\sigma_n + m^2 - e^2\mu^2)C_n = 0 \tag{6.276}$$

holding for all n. We will define a critical value for μ, called μ_c, by

$$e\mu_c = \sqrt{\sigma_0 + m^2} \tag{6.277}$$

where σ_0 is the smallest eigenvalue of (6.274). It can be noted that $E_n = \sqrt{\sigma_n + m^2}$ gives the energy of the nth mode (see Section 3.7), so (6.277) is exactly the same result as we found in the non-relativistic case in (6.16).

To avoid negative occupation numbers in the Bose–Einstein distribution function we must have $|e\mu| \leq E_0$; that is, $|\mu| < \mu_c$. As we found

before, if $\mu < \mu_c$ then the only solution to (6.276) is for $C_n = 0$ for all values of n. This corresponds to $\bar{\Phi} = 0$ and there is no condensate. If it is possible for μ to attain the critical value of μ_c then C_0 is undetermined by (6.276) and we have

$$\bar{\Phi}(\mathbf{x}) = C_0 f_0(\mathbf{x}). \tag{6.278}$$

We will now specialize to the case $\Sigma = \mathbb{R}^3$. The total charge is given by $Q = -(\partial\Omega/\partial\mu)|_{T,V,\bar{\Phi}}$. Using (6.272) we can conveniently split Q up into two parts:

$$\begin{aligned} Q_0 &= -\left(\frac{\partial\Omega_0}{\partial\mu}\right)\Big|_{T,V,\bar{\Phi}} \\ &= 2e^2\mu \int_\Sigma d\sigma_x |\bar{\Phi}|^2 \\ &= 2e^2\mu |C_0|^2 \end{aligned} \tag{6.279}$$

using (6.278), and

$$Q_1 = -\left(\frac{\partial\Omega_{T\neq 0}}{\partial\mu}\right)\Big|_{T,V,\bar{\Phi}}. \tag{6.280}$$

($\Omega_{T=0}$ does not involve μ, so makes no contribution to the total charge.) In this case, using box normalization, $f_0(\mathbf{x}) = V^{-1/2}$ with V the volume of Σ. (As usual we will assume that the infinite volume limit is taken at the end.) The corresponding eigenvalue is $\sigma_0 = 0$, so that $e\mu_c = m$ here.

We now use the high temperature expansion for $\Omega_{T\neq 0}$ that we found in Section 5.4. Using (5.117) we find

$$Q_1 \simeq \frac{1}{3} e^2 \mu V T^2 \tag{6.281}$$

as the leading contribution at high temperature. This means that for sufficiently large T, no matter what the total charge Q is, we can always solve $Q = Q_1$ for μ with $\mu < \mu_c$. A consequence of this is that at very high T we have $\bar{\Phi} = 0$, so no condensation occurs. As T decreases, μ must increase if $Q_1 = Q$ is to remain fixed. However μ can never increase beyond $\mu = \mu_c = m$. This means that we can define a critical temperature T_c by

$$Q = \frac{1}{3} m e^2 V T_c^2 \tag{6.282}$$

or explicitly

$$T_c = \left(\frac{3Q}{me^2V}\right)^{1/2}. \tag{6.283}$$

For $T < T_c$, μ must remain fixed at $\mu = \mu_c = m$ and it is impossible to satisfy $Q = Q_1$. If we take $\mu = \mu_c = m$ in (6.281) and use (6.282) we obtain

$$Q_1 = Q\left(\frac{T}{T_c}\right)^2 \tag{6.284}$$

for $T < T_c$. Because $Q = Q_0 + Q_1$ we find

$$Q_0 = Q\left[1 - \left(\frac{T}{T_c}\right)^2\right] \tag{6.285}$$

as the charge in the condensate. From (6.279), because $\mu = \mu_c = m$ for $T < T_c$, we find

$$|C_0| = \left(\frac{Q}{2me^2}\right)^{1/2}\left[1 - \left(\frac{T}{T_c}\right)^2\right]^{1/2} \tag{6.286}$$

$$= \left(\frac{1}{6}V\right)^{1/2}\left(T_c^2 - T^2\right)^{1/2} \tag{6.287}$$

if we use (6.282) in the second line. The temperature dependence of the condensate is

$$\bar{\Phi} = \frac{1}{\sqrt{6}}\left(T_c^2 - T^2\right)^{1/2} \tag{6.288}$$

if we use (6.278) with $f_0(\mathbf{x}) = V^{-1/2}$.

We can conclude that the non-interacting charged gas has a critical temperature T_c which is determined by the total charge density in (6.283). This is valid at high temperatures. For $T > T_c$ there is no condensate. As the temperature drops below T_c a phase transition occurs, corresponding to symmetry breaking, and a condensate develops. This is the direct counterpart to the non-relativistic calculation performed in Section 6.1. It has been suggested by Madsen (1992) that Bose–Einstein condensation could play a role in the early universe.

6.9 The interacting relativistic field

What we will do in this section is to generalize the analysis of Section 6.8 to include interactions. We will add a potential term to (6.262) and take

$$H = \int_\Sigma d\sigma_x \left[|\Pi|^2 + |\nabla\Phi|^2 + m^2|\Phi|^2 + U(|\Phi|^2)\right] \tag{6.289}$$

where we assume that $U(|\Phi|^2)$ is real and depends only on $|\Phi|^2$. This means that the theory has a rigid $U(1)$ gauge invariance. In place of (6.264) we have

$$\bar{H} = \int_\Sigma d\sigma_x \left[|\Pi|^2 + |\nabla\Phi|^2 + m^2|\Phi|^2 + U(|\Phi|^2) + ie\mu \left(\Pi\Phi - \Phi^\dagger\Pi^\dagger \right) \right] \tag{6.290}$$

noting that the charge operator is still given by (6.263). The Heisenberg equations of motion are given by (6.265) and (6.266). Equation (6.265) leads to (6.267) again, but from (6.266), in place of (6.268), we find

$$\dot{\Pi} = \nabla^2\Phi^\dagger - m^2\Phi^\dagger - ie\mu\Pi - U'(|\Phi|^2)\Phi^\dagger. \tag{6.291}$$

Here $U'(|\Phi|^2) = (\partial/\partial|\Phi|^2)U(|\Phi|^2)$.[19] As before, we can eliminate Π and find an equation of motion that involves only $\Phi(t, \mathbf{x})$:

$$0 = \ddot{\Phi} - \nabla^2\Phi - 2ie\mu\dot{\Phi} + (m^2 - e^2\mu^2)\Phi + U'(|\Phi|^2)\Phi. \tag{6.292}$$

As in Section 6.7, we will calculate the excitation energies by substituting $\Phi = \bar{\Phi} + \psi$ into (6.292) with $\bar{\Phi}$ the possible condensate. We linearize in the excitation ψ:

$$\begin{aligned} 0 = {} & \ddot{\psi} - 2ie\mu\dot{\psi} - \nabla^2\psi + (m^2 - e^2\mu^2)\psi \\ & + U'(|\bar{\Phi}|^2)\psi + U''(|\bar{\Phi}|^2)\left(|\bar{\Phi}|^2\psi + \bar{\Phi}^2\psi^\dagger \right). \end{aligned} \tag{6.293}$$

There is also the equation satisfied by $\psi^\dagger$ which is just the Hermitian conjugate of (6.293):

$$\begin{aligned} 0 = {} & \ddot{\psi}^\dagger + 2ie\mu\dot{\psi}^\dagger - \nabla^2\psi^\dagger + (m^2 - e^2\mu^2)\psi^\dagger \\ & + U'(|\bar{\Phi}|^2)\psi^\dagger + U''(|\bar{\Phi}|^2)\left[|\bar{\Phi}|^2\psi^\dagger + \left(\bar{\Phi}^\dagger\right)^2\psi \right]. \end{aligned} \tag{6.294}$$

The procedure is basically the same as in Section 6.7. With $f_n(\mathbf{x})$ defined as in (6.274) we will write

$$\Psi(t, \mathbf{x}) = \sum_n A_n e^{-iE_n t} f_n(\mathbf{x}), \tag{6.295}$$

$$\Psi^\dagger(t, \mathbf{x}) = \sum_n B_n e^{-iE_n t} f_n(\mathbf{x}), \tag{6.296}$$

with A_n and B_n as arbitrary independent expansion coefficients. Substitution of (6.295) and (6.296) into (6.293) and (6.294), assuming that $\bar{\Phi}$ is constant, results in two coupled equations for the expansion coefficients:

[19] The last term in the above equation is easy to obtain using $\Pi(t, \mathbf{x}) = -i[\delta/\delta\Phi(t, \mathbf{x})]$ which follows from the field canonical commutation relations.

$$0 = \left[(E_n + e\mu)^2 - \sigma_n - m^2 - U' - |\bar{\Phi}|^2 U''\right] A_n - \bar{\Phi}^2 U'' B_n, \tag{6.297}$$

$$0 = \left[(E_n - e\mu)^2 - \sigma_n - m^2 - U' - |\bar{\Phi}|^2 U''\right] B_n - (\bar{\Phi}^\dagger)^2 U'' A_n. \tag{6.298}$$

In order that these equations have a non-trivial solution for A_n and B_n the 2×2 matrix of coefficients of A_n and B_n found from (6.297) and (6.298) must have a vanishing determinant. This leads to the result $E_n^\pm$ for the excitation energies, where

$$E_n^\pm = \left\{ M_n^2 + e^2\mu^2 \pm \left[4e^2\mu^2 M_n^2 + |\bar{\Phi}|^4 (U'')^2\right]^{1/2} \right\}^{1/2} \tag{6.299}$$

with

$$M_n^2 = \sigma_n + m^2 + U' + |\Phi|^2 U''. \tag{6.300}$$

This agrees with the results of Bernstein and Dodelson (1991) and Benson *et al.* (1991) if we specialize to flat space with the potential quartic in the fields, and write the results in terms of real (rather than complex) fields. A useful check on the result is to let $U \to 0$, corresponding to a non-interacting theory, where it is easy to see that $E_n^\pm \to \sqrt{\sigma_n + m^2} \pm e\mu$, which is correct.

The finite temperature part of the thermodynamic potential is

$$\Omega_{T\neq 0} = T \sum_n \left[\ln\left(1 - e^{-\beta E_n^+}\right) + \ln\left(1 - e^{-\beta E_n^-}\right) \right]. \tag{6.301}$$

There is also a zero temperature part given as the sum over the zero-point energies we will ignore, since we are interested in what happens at high temperature. A complete evaluation of (6.301) is not likely to be possible, since even for the free theory we had to resort to a high temperature expansion (see Section 5.4). However the leading behaviour of $\Omega_{T\neq 0}$ at high temperature is relatively easy to obtain given our knowledge of the free field result.

Begin by defining

$$\omega_n = \sqrt{\sigma_n + m^2}, \tag{6.302}$$

$$M_n^2 = \omega_n^2 + \delta M^2 \tag{6.303}$$

with

$$\delta M^2 = U'(|\bar{\Phi}|^2) + |\bar{\Phi}|^2 U''(|\bar{\Phi}|^2). \tag{6.304}$$

Now take the excitation energies (6.299) and expand to first order in the potential that occurs in δM^2:

$$E_n^{\pm} = \omega_n \pm e\mu + \frac{\delta M^2}{2\omega_n} + \cdots . \tag{6.305}$$

We can use this approximation in (6.301), and expand to first order in δM^2. The zeroth-order term will just be the finite temperature part of the thermodynamic potential for the free theory:

$$\Omega_{T\neq 0}^{\text{free}} = T\sum_n \left\{ \ln\left[1 - e^{-\beta(\omega_n - e\mu)}\right] + \ln\left[1 - e^{-\beta(\omega_n + e\mu)}\right] \right\}. \tag{6.306}$$

The first-order term results in

$$\Omega_{T\neq 0} = \Omega_{T\neq 0}^{\text{free}} + \sum_n \frac{\delta M^2}{2\omega_n} \left\{ \left[e^{\beta(\omega_n - e\mu)} - 1\right]^{-1} + \left[e^{\beta(\omega_n + e\mu)} - 1\right]^{-1} \right\}. \tag{6.307}$$

It is now possible to relate the second term in (6.307) to $\Omega_{T\neq 0}^{\text{free}}$ if we first note that

$$T\frac{\partial}{\partial m^2} \ln\left[1 - e^{-\beta(\omega_n - e\mu)}\right] = \frac{1}{2\omega_n} \left[e^{-\beta(\omega_n - e\mu)} - 1\right]^{-1}. \tag{6.308}$$

Using this identity in (6.307) shows that

$$\Omega_{T\neq 0} = \Omega_{T\neq 0}^{\text{free}} + \delta M^2 \frac{\partial}{\partial m^2} \Omega_{T\neq 0}^{\text{free}} + \cdots . \tag{6.309}$$

With just the two leading terms in (5.117) kept, we obtain

$$\begin{aligned} \frac{\Omega_{T\neq 0}}{V} \simeq & -\frac{\pi^2}{45} T^4 \\ & + \frac{1}{12} T^2 \left[m^2 - 2e^2\mu^2 + U'(|\bar{\Phi}|^2) + |\bar{\Phi}|^2 U''(|\bar{\Phi}|^2) \right] + \cdots \end{aligned} \tag{6.310}$$

as the dominant terms at high temperature.

To the expression in (6.310) we must add the condensate contribution as in (6.209). In the interacting case, from (6.290), we find

$$\frac{\Omega_0}{V} = (m^2 - e^2\mu^2)|\bar{\Phi}|^2 + U(|\bar{\Phi}|^2). \tag{6.311}$$

We will now choose

$$U(|\bar{\Phi}|^2) = \frac{\lambda}{6}|\bar{\Phi}|^4. \tag{6.312}$$

Our approximate thermodynamic potential is then

$$\frac{\Omega}{V} \simeq (m^2 - e^2\mu^2)|\bar{\Phi}|^2 + \frac{\lambda}{6}|\bar{\Phi}|^4 - \frac{\pi^2}{45}T^4 + \frac{1}{12}T^2\left(m^2 - 2e^2\mu^2 + \frac{2\lambda}{3}|\bar{\Phi}|^4\right) + \cdots . \tag{6.313}$$

The condensate $\bar{\Phi}$ should obey $(\partial/\partial\bar{\Phi})\Omega = 0$, which gives rise to the equation

$$0 \simeq (m^2 - e^2\mu^2)\bar{\Phi} + \frac{\lambda}{3}|\bar{\Phi}|^2\bar{\Phi} + \frac{\lambda}{18}T^2\bar{\Phi}. \tag{6.314}$$

There are two possible solutions to this. We either have $\bar{\Phi} = 0$, corresponding to the symmetric phase, or else

$$|\bar{\Phi}|^2 \simeq \frac{3}{\lambda}\left(e^2\mu^2 - m^2 - \frac{\lambda}{18}T^2\right) \tag{6.315}$$

corresponding to the broken symmetry.[20] The total charge density is given by

$$\rho = -\frac{1}{V}\left(\frac{\partial\Omega}{\partial\mu}\right)\Big|_{T,V,\bar{\Phi}} \simeq 2e^2\mu|\bar{\Phi}|^2 + \frac{1}{3}e^2\mu T^2. \tag{6.316}$$

If we define

$$\rho_0 = 2e^2\mu|\bar{\Phi}|^2, \tag{6.317}$$

$$\rho_1 = \frac{1}{3}e^2\mu T^2, \tag{6.318}$$

we can interpret ρ_0 as the charge density of the condensate. These results can be seen to be identical to those found for the free theory in (6.279) and (6.281). In the symmetric phase we have $\bar{\Phi} = 0$ so that $\rho_0 = 0$ and all of the charge is given by

$$\rho \simeq \frac{1}{3}e^2\mu T^2. \tag{6.319}$$

As T decreases from large values, for a fixed charge density μ will increase until we reach the critical value set by

$$e^2\mu_c^2 = m^2 + \frac{\lambda}{18}T_c^2 \tag{6.320}$$

[20] The symmetry which is broken by this solution is the rigid $U(1)$ symmetry of the classical theory.

at the critical temperature T_c. This is the temperature at which the symmetry is broken (see (6.315)). For $T < T_c$ we have μ fixed at the value μ_c, and from (6.315),

$$|\bar{\Phi}|^2 \simeq \frac{1}{6}\left(T_c^2 - T^2\right). \tag{6.321}$$

This is also the same as we found earlier in (6.288) for the free theory.

At the critical temperature we have

$$\rho \simeq \frac{1}{3} e^2 \mu_c T_c^2 \tag{6.322}$$

using (6.319). Thus when $T < T_c$ we find

$$\rho_1 \simeq \rho \left(\frac{T}{T_c}\right)^2,$$

and hence

$$\rho_0 \simeq \rho \left[1 - \left(\frac{T}{T_c}\right)^2\right].$$

These last two results are exactly the same as we found for the free Bose gas, although the critical temperature is different in the two cases. The interacting gas also undergoes Bose–Einstein condensation. Some caution must be used in applying these results when T is too close to the critical temperature. As described originally by Weinberg (1974) in the quantum field theory setting, naive perturbation expansions, such as we have done, become unreliable as the critical temperature of a phase transition is approached. This is because higher-order terms in the expansion can become the same size as lower-order terms.

6.10 Fermi gases at finite temperature in a magnetic field

At first sight it might be thought that it would be very easy to generalize the analysis of the thermodynamic potential of Section 6.6 to fermions. After all, the energy levels are unchanged, and all that happens is that the distribution function becomes Fermi–Dirac, rather than Bose–Einstein. The thermodynamic potential is therefore

$$\Omega = -\frac{eBVT}{2\pi} \sum_{n=0}^{\infty} \int_{-\infty}^{\infty} \frac{dp}{2\pi} \ln\left[1 + e^{-\beta p^2/(2m) - (n+\epsilon)x}\right] \tag{6.323}$$

where we adopt (6.153) and (6.155) again. One fundamental difference with fermions is that there are no bounds at all on the chemical potential,

since the Fermi–Dirac distribution function

$$F(E) = \left[e^{\beta(E-e\mu)} + 1\right]^{-1} \tag{6.324}$$

is positive for all values of μ. This means that ϵ in (6.323) can be negative corresponding to large positive values of μ, a possibility which did not occur for bosons. A consequence of this is that we can no longer expand the logarithm in (6.323) since the exponential can be large, a step that made it easy to evaluate Ω in Section 6.6. Instead a different approach is needed. An elegant method was presented by Sondheimer and Wilson (1951). In this section we will present their method for the D-dimensional Fermi gas.

The thermodynamic potential for fermions can be written as (see (5.145))

$$\Omega = -T \sum_n f(E_n), \tag{6.325}$$

where

$$f(E) = \ln\left[1 + e^{-\beta(E-e\mu)}\right]. \tag{6.326}$$

Define

$$Z(\beta) = \sum_n e^{-\beta E_n}, \tag{6.327}$$

which can be recognized as the partition function for the $\mu = 0$ system. Define $\phi(\beta)$ to be the Laplace transform of $f(E)$:

$$\phi(\beta) = \int_0^\infty dE\, e^{-\beta E} f(E), \tag{6.328}$$

and $\mathsf{z}(E)$ by the requirement that $\beta^{-2}Z(\beta)$ is its Laplace transform:

$$Z(\beta) = \beta^2 \int_0^\infty dE\, e^{-\beta E} \mathsf{z}(E). \tag{6.329}$$

We can use the inverse Laplace transform to obtain

$$\mathsf{z}(E) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} d\beta\, e^{\beta E} \beta^{-2} Z(\beta), \tag{6.330}$$

$$f(E) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} d\beta\, e^{\beta E} \phi(\beta). \tag{6.331}$$

Here c is a constant chosen so that all singularities of the integrand lie to the left of the integration path.

We now use (6.331) in (6.325) to obtain

$$\begin{aligned}\Omega &= -\sum_n \frac{T}{2\pi i}\int_{c-i\infty}^{c+i\infty} d\beta\, e^{\beta E_n}\phi(\beta)\\ &= -\frac{T}{2\pi i}\int_{c-i\infty}^{c+i\infty} d\beta\, Z(-\beta)\phi(\beta)\end{aligned}$$

with the second line following from the definition (6.327). Note that it is necessary to view $Z(\beta)$ as a function of β with β regarded as a complex variable. $Z(-\beta)$ then represents the analytic continuation of the sum (6.327) to $\mathcal{R}(\beta) < 0$. Now use (6.329) to obtain

$$\Omega = -\frac{T}{2\pi i}\int_{c-i\infty}^{c+i\infty} d\beta\, \phi(\beta)\beta^2 \int_0^\infty dE\, e^{\beta E}\mathsf{z}(E).$$

The use of (6.331) results in

$$\begin{aligned}\Omega &= -T\int_0^\infty dE\, \mathsf{z}(E)\frac{\partial^2 f(E)}{\partial E^2}\\ &= \int_0^\infty dE\, \mathsf{z}(E)\frac{\partial F(E)}{\partial E}\end{aligned} \tag{6.332}$$

with the second line following from (6.324) and (6.326) along with $\beta T = 1$.

The basic idea behind the method is to find $\mathsf{z}(E)$ and then use (6.332) to obtain an integral representation for the thermodynamic potential. We can calculate $\mathsf{z}(E)$ using (6.330) if we first know the partition function $Z(\beta)$ for $\mu = 0$. In our case

$$\begin{aligned}Z(\beta) &= \frac{eBV}{2\pi}\sum_{n=0}^\infty \int \frac{d^{D-2}}{(2\pi)^{D-2}}\, e^{-\beta\{p^2/(2m)+[n+1/2]eB/m\}}\\ &= \frac{eBV}{2\pi}\left(\frac{m}{2\pi\beta}\right)^{D/2-1}\frac{e^{-\beta\omega}}{(1-e^{-2\beta\omega})}\end{aligned} \tag{6.333}$$

with

$$\omega = \frac{eB}{2m} \tag{6.334}$$

half of the classical cyclotron frequency.[21] We then obtain

$$\mathsf{z}(E) = \frac{eBV}{2\pi}\left(\frac{m}{2\pi}\right)^{D/2-1}\frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} d\beta\, \beta^{-1-D/2}\frac{e^{\beta(E-\omega)}}{(1-e^{-2\beta\omega})}. \tag{6.335}$$

[21] The steps leading up to (6.333) consist of doing the momentum integral, which is Gaussian, and the sum over n, which is a geometric series.

We now need to perform the contour integral to obtain $\mathsf{z}(E)$. The structure of the singularities of the integrand depends upon whether D is even or odd. When D is even the power of β is a negative integer. For small β the integrand behaves like $\beta^{-D/2-2}$; thus for D even there is a pole of order $D/2+2$ at $\beta = 0$. For odd D, $\beta = 0$ is a branch point and we must introduce a branch cut, which we take along the negative real axis. There are also simple poles of the integrand which can occur when $e^{2\beta\omega} = 1$, or

$$\beta = \beta_k = i\pi\frac{k}{\omega} \tag{6.336}$$

for $k = \pm 1, \pm 2, \ldots$. For $\beta > 0$ the integrand is analytic in β, so with $c > 0$ we satisfy the condition for the Laplace transform that all singularities lie to the left of the integration path. We will take the contour $\mathcal{C}$ pictured in Fig. 6.5. For odd D there is a branch cut along the negative real axis. We will choose $|\arg\beta| \leq \pi$, with $\arg\beta = \pi$ on the top of the branch cut, and $\arg\beta = -\pi$ on the bottom. For even D the portions of the contour above and below the negative real axis will cancel, and only the pole at $\beta = 0$ will make a contribution. For odd D the integrand

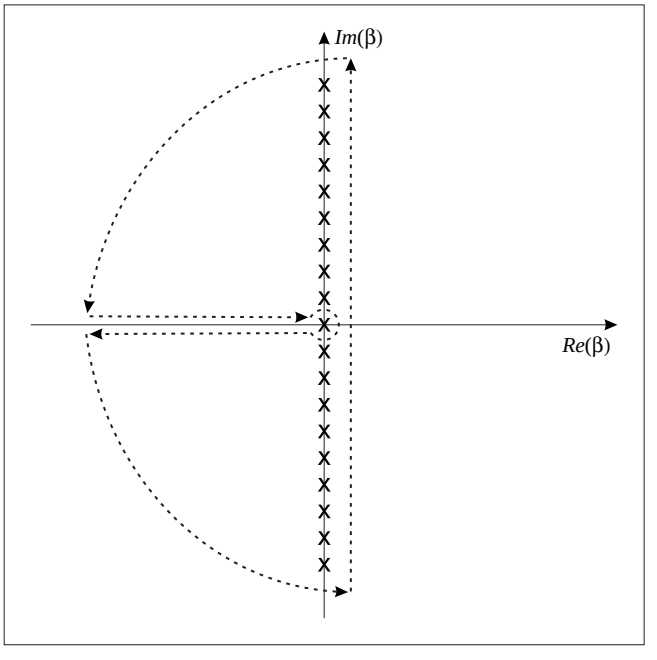

Fig. 6.5 This shows the contour $\mathcal{C}$ used in the evaluation of $\mathsf{z}(E)$. The poles are indicated by the crosses that extend along the imaginary axis. For odd D, there is a branch cut along the negative real axis.

will take different values above and below the negative real axis, and the contributions to the contour integral will not cancel.

Consider

$$\mathfrak{J} = \frac{1}{2\pi i}\int_{\mathcal{C}} d\beta\, \beta^{-1-D/2}\frac{e^{\beta(E-\omega)}}{1-e^{-2\beta\omega}}, \tag{6.337}$$

with $\mathcal{C}$ the contour pictured in Fig. 6.5. Let σ be that portion of the contour which circles the negative real axis.[22] By assuming that the circular portions of the contour vanish as we expand the radius to infinity, we find

$$\frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} d\beta\, \beta^{-1-D/2}\frac{e^{\beta(E-\omega)}}{(1-e^{-2\beta\omega})} = \mathfrak{J} - \frac{1}{2\pi i}\int_{\sigma} d\beta\, \beta^{-1-D/2}\frac{e^{\beta(E-\omega)}}{(e^{2\beta\omega}-1)}.$$

Changing variables in the last term, and making use of the representation of the Hurwitz ζ-function in (A1.52), we obtain

$$\begin{aligned}&\frac{1}{2\pi i}\textstyle\int_{c-i\infty}^{c+i\infty} d\beta\, \beta^{-1-D/2}\dfrac{e^{\beta(E-\omega)}}{(1-e^{-2\beta\omega})}\\ &= \mathfrak{J} - (2\omega)^{D/2}\frac{\zeta\left[-D/2, 1/2+E/(2\omega)\right]}{\Gamma\left[1+D/2\right]}.\end{aligned} \tag{6.338}$$

Using this in (6.335) allows us to write

$$\mathsf{z}(E) = \mathsf{z}_0(E) + \mathsf{z}_1(E) \tag{6.339}$$

where

$$\mathsf{z}_0(E) = -\frac{2\pi V}{m}\left(\frac{eB}{2\pi}\right)^{D/2+1}\frac{\zeta\left[-D/2, 1/2+E/(2\omega)\right]}{\Gamma\left[1+D/2\right]} \tag{6.340}$$

and

$$\mathsf{z}_1(E) = \frac{eBV}{2\pi}\left(\frac{m}{2\pi}\right)^{D/2-1}\mathfrak{J}. \tag{6.341}$$

We can evaluate $\mathsf{z}_1(E)$ using the residue theorem. The residue at $\beta = \beta_k$ of the integrand in (6.335) is given by

$$\begin{aligned}r_k &= \lim_{\beta\to\beta_k}(\beta-\beta_k)\beta^{-D/2-1}\frac{e^{\beta(E-\omega)}}{1-e^{-2\beta\omega}}\\ &= \frac{1}{2\omega}\beta_k^{-D/2-1}e^{\beta_k(E-\omega)}.\end{aligned} \tag{6.342}$$

[22] This is opposite in orientation to the choice made in Sondheimer and Wilson (1951).

For $k > 0$ we have $\arg\beta = \pi/2$, while for $k < 0$ we have $\arg\beta = -\pi/2$ (since we chose $|\arg\beta| \leq \pi$). This means that we can write β_k in (6.336) as

$$\beta_k = \frac{\pi}{\omega}|k|e^{i\,\arg\beta_k}. \tag{6.343}$$

Summing over all residues results in

$$\mathsf{z}_1(E) = \frac{eBV}{\pi m}\left(\frac{m\omega}{2\pi^2}\right)^{D/2}\sum_{k=1}^{\infty}\frac{(-1)^k}{k^{D/2+1}}\sin\left(\pi k\frac{E}{\omega} - \frac{\pi}{4}D\right) \tag{6.344}$$

after some simplification. Note that the sum in (6.344) is absolutely convergent for all $D \geq 1$. In the case of $D = 3$ this expression agrees with the result of Sondheimer and Wilson (1951) after some trigonometry.

We can now use our results for $\mathsf{z}_0(E)$ and $\mathsf{z}_1(E)$ to calculate Ω. If we substitute (6.339) into (6.332) we can write

$$\Omega = \Omega_0 + \Omega_1 \tag{6.345}$$

where

$$\Omega_1 = \int_0^{\infty} dE\,\mathsf{z}_1(E)\frac{\partial F(E)}{\partial E} \tag{6.346}$$

with Ω_0 given by a similar expression with $\mathsf{z}_0(E)$ in place of $\mathsf{z}_1(E)$.

Differentiating (6.324) leads to

$$\Omega_1 = -\frac{eBV}{\pi m}\beta\left(\frac{m\omega}{2\pi^2}\right)^{D/2}\sum_{k=1}^{\infty}\frac{(-1)^k}{k^{D/2+1}}I_k \tag{6.347}$$

where

$$I_k = \int_0^{\infty} dE\,e^{\beta(E-e\mu)}\frac{\sin\left[\pi kE/\omega - (\pi/4)D\right]}{\left[e^{\beta(E-e\mu)}+1\right]^2}. \tag{6.348}$$

The integral I_k can be written as

$$I_k = \frac{1}{2}T\int_{-(1/2)\beta e\mu}^{\infty} d\eta\,\frac{\sin\left[(2\pi kT/\omega)\eta + (\pi k/\omega)e\mu - (\pi/4)D\right]}{\cosh^2\eta} \tag{6.349}$$

where we have defined

$$\eta = \frac{1}{2}\beta(E - e\mu). \tag{6.350}$$

We will now make the approximation $T \ll e\mu$ or $e\mu \gg 1$, which should be valid at low temperatures. This enables us to replace the lower limit of (6.349) with $-\infty$, and we approximate

$$I_k \sim \frac{1}{2}T\int_{-\infty}^{\infty} d\eta\,\frac{\sin(a\eta + b)}{\cosh^2\eta} \tag{6.351}$$

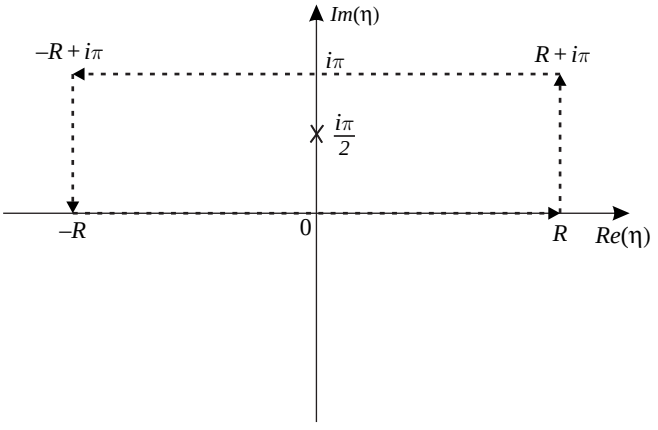

Fig. 6.6 This shows the contour used in the evaluation of $\mathcal{I}$. The cross indicates the location of a simple pole.

where

$$a = \frac{2\pi kT}{\omega}, \tag{6.352}$$

$$b = \frac{\pi k}{\omega} e\mu - \frac{\pi}{4} D. \tag{6.353}$$

I_k can be evaluated by considering the contour integral

$$\mathcal{I} = \oint \frac{e^{ia\eta}}{\cosh^2 \eta}\, d\eta \tag{6.354}$$

with the contour shown in Fig. 6.6. The integrand of (6.354) has a simple pole enclosed by the contour at $\eta = i\pi/2$ with residue r.[23] Then

$$\mathcal{I} = 2\pi i r.$$

By writing the contour integral out explicitly along the four sides of the contour we have

$$\int_{-R}^{R} \frac{e^{ia\eta}}{\cosh^2 \eta}\, d\eta + \int_0^{\pi} \frac{e^{ia(R+i\theta)}\, id\theta}{\cosh^2(R+i\theta)} + \int_R^{-R} \frac{e^{ia(x+i\pi)}}{\cosh^2(x+i\pi)}\, dx + \int_{\pi}^{0} \frac{e^{ia(-R+i\theta)}\, id\theta}{\cosh^2(-R+i\theta)} = 2\pi i r. \tag{6.355}$$

[23] We will evaluate r momentarily.

For large R, $\cosh(\pm R + i\theta) \sim (1/2)e^R$. This means that as $R \to \infty$ the contributions from the vertical portions of the contour will vanish. We also have $\cosh(x + i\pi) = -\cosh x$, so by taking $R \to \infty$ in (6.355) we find

$$(1 - e^{-\pi a}) \int_{-\infty}^{\infty} d\eta \, \frac{e^{ia\eta}}{\cosh^2 \eta} = 2\pi i r. \tag{6.356}$$

We now need r, the residue of $e^{ia\eta}/\cosh^2 \eta$ at $\eta = i\pi/2$. This can be found by setting $\eta = i\pi/2 + \epsilon$ and expanding about $\epsilon = 0$. It is easy to show that

$$\frac{e^{ia\eta}}{\cosh^2 \eta} = -\frac{e^{-\pi a/2}}{\epsilon^2} \left[1 + ia\epsilon + \mathcal{O}(\epsilon^2)\right],$$

and we conclude

$$r = -iae^{-(\pi/2)a}. \tag{6.357}$$

Using (6.351) and (6.354) we have

$$\begin{aligned} I_k &\simeq \frac{1}{2} T \, \Im \int_{-\infty}^{\infty} d\eta \, \frac{e^{i(a\eta + b)}}{\cosh^2 \eta} \\ &= \frac{1}{2} T \, \Im \left[e^{ib} \frac{\pi a}{\sinh(\pi a/2)} \right] \\ &= \frac{1}{2} T \, \frac{\pi a \sin b}{\sinh(\pi a/2)}. \end{aligned} \tag{6.358}$$

Using the results for a, b in (6.352) and (6.353) leads to

$$\Omega_1 \simeq -2\pi TV \frac{(eB)^{D/2}}{(2\pi)^D} \sum_{k=1}^{\infty} \frac{(-1)^k}{k^{D/2}} \frac{\sin\left[\pi k(e\mu/\omega) - (\pi/4)D\right]}{\sinh\left[\pi^2 kT/\omega\right]}. \tag{6.359}$$

This result holds for all $D \geq 1$.

Before discussing the implications of the result we will return to the evaluation of Ω_0:

$$\Omega_0 = \int_0^{\infty} dE \, \mathsf{z}_0(E) \frac{\partial F(E)}{\partial E}. \tag{6.360}$$

The result for $\mathsf{z}_0(E)$ given in (6.340) is exact; however, when we substitute this into (6.360) it is not possible to express the resulting integral in simple form. By making use of the definition (6.324) of $F(E)$, along with a change of variable $E = e\mu + 2\eta/\beta$, we find

$$\Omega_0 = -\frac{1}{2} \int_{-\beta e\mu/2}^{\infty} d\eta \, \frac{\mathsf{z}_0\left(e\mu + 2T\eta\right)}{\cosh^2 \eta}. \tag{6.361}$$

We have already assumed $\beta e\mu \gg 1$ in obtaining Ω_1. If we make the same approximation here, then we can replace the lower limit of the integral with $-\infty$ up to exponentially small terms. It is still not possible to evaluate Ω_0 in closed form; however, due to the presence of the factor of $\cosh^2\eta$ in the denominator we can argue that the dominant contribution to the result should come from small values of η. We can approximate $\mathsf{z}_0\,(e\mu + 2T\eta)$ with its Maclaurin–Taylor expansion about $\eta = 0$ to find

$$\Omega_0 \simeq -\frac{1}{2}\int_{-\infty}^{\infty}\frac{d\eta}{\cosh^2\eta}\left[\mathsf{z}_0(e\mu) + 2T^2\eta^2\mathsf{z}_0''(e\mu) + \frac{2}{3}T^4\eta^4\mathsf{z}_0^{(iv)}(e\mu) + \cdots\right]. \tag{6.362}$$

Note that all of the terms that have odd-order derivatives of $\mathsf{z}_0(e\mu)$ will vanish because they involve the integration of an odd function of η. The remaining integrals can be evaluated by residues as in the evaluation of I_k above, or else more simply by making use of

$$\int_{-\infty}^{\infty} d\eta\,\frac{\sin(a\eta+b)}{\cosh^2\eta} = \frac{\pi a\sin b}{\sinh(\pi a/2)}, \tag{6.363}$$

as follows from (6.351) and (6.358). If we differentiate both sides of (6.363) with respect to b we find

$$\int_{-\infty}^{\infty} d\eta\,\frac{\cos(a\eta+b)}{\cosh^2\eta} = \frac{\pi a\cos b}{\sinh(\pi a/2)}. \tag{6.364}$$

The integrals that we require to obtain Ω_0 in (6.362) may all be found by setting $b = 0$ in (6.364) and then expanding both sides about $a = 0$ with terms of equal order in a equated on both sides. The result of this leads to

$$\Omega_0 \simeq -\mathsf{z}_0(e\mu) - \frac{\pi^2T^2}{24}\mathsf{z}_0''(e\mu) - \frac{7\pi^4T^4}{360}\mathsf{z}_0^{(iv)}(e\mu) + \cdots. \tag{6.365}$$

This is usually referred to as the 'Sommerfeld expansion' (see Pathria (1972); Ashcroft and Mermin (1976); Huang (1987) for different derivations). As a check on this result, we can calculate the first term in the expansion very simply. For $e\mu \gg T$, the Fermi–Dirac distribution function is approximately a step function, $F(E) \simeq \theta(e\mu - E)$, and so $F'(E) \simeq -\delta(E - e\mu)$. If we use $F'(E) \simeq -\delta(E - e\mu)$ in (6.360) we obtain the first term on the right-hand side of (6.365). For our purposes here the first term on the right-hand side of (6.365) is sufficiently accurate. We have

$$\Omega_0 \simeq \frac{2\pi V}{m}\left(\frac{eB}{2\pi}\right)^{D/2+1}\frac{\zeta\left[-D/2, 1/2 + e\mu/(2\omega)\right]}{\Gamma\left[1 + D/2\right]}. \tag{6.366}$$

For $e\mu \gg \omega$ we can further expand this result using the method described in Section A1.2 which led up to the approximation (A1.49). Start with the integral expression for the ζ-function in (A1.29) and take $a = (1/2) + \vartheta$; $\vartheta = e\mu/(2\omega)$ will be taken to be large. Use the expansion

$$e^{-(t/2)}(1 - e^{-t})^{-1} \simeq t^{-1} - \frac{t}{24} + \frac{7t^3}{5760} - \frac{31t^5}{967\,680} + \cdots$$

and integrate the result term by term using the definition of the Γ-function in (A1.1). This gives

$$\zeta\left(z, \frac{1}{2} + \vartheta\right) \simeq \frac{\vartheta^{1-z}}{z-1} - \frac{z}{24}\,\vartheta^{-1-z} + \frac{7z(z+1)(z+2)}{5760}\,\vartheta^{-3-z} + \cdots . \tag{6.367}$$

Setting $z = -3/2$ results in

$$\zeta\left(-\frac{3}{2}, \frac{1}{2} + \vartheta\right) \simeq -\frac{2}{5}\,\vartheta^{5/2} + \frac{1}{16}\,\vartheta^{1/2} + \frac{7}{15\,360}\,\vartheta^{-3/2} + \cdots . \tag{6.368}$$

This is the expression relevant to $D = 3$. There is no difficulty extending the analysis to other dimensions, but we will concentrate on $D = 3$ from now on.[24] With $D = 3$ in (6.366) we find

$$\begin{aligned}\Omega_0 \simeq \frac{2^{3/2}V}{15\pi^2 m}\Big[&- (me\mu)^{5/2} + \frac{5}{32}(eB)^2(me\mu)^{1/2} \\ &+ \frac{7}{6144}(eB)^4(me\mu)^{-3/2} + \cdots\Big]\end{aligned} \tag{6.369}$$

as the leading terms in the expansion. The second term contains the leading order correction to the expression for a non-zero magnetic field.

The oscillatory behaviour of the thermodynamic potential (6.359) is evident from the dependence on the sin factor. The period between oscillations is seen to be proportional to $1/\omega \propto 1/B$. The factor of sinh that occurs in (6.359) may be interpreted as modulating the amplitude of this oscillatory factor. The physical effects of the oscillations can be observed in the behaviour of the magnetization of the Fermi gas at low temperatures, as we will now show. If we use (6.191) to compute the magnetization, it is clear that there will be an oscillatory term present whose origin is that part of the thermodynamic potential given by (6.359). This can be important in practical studies of the Fermi surface of metals.[25]

[24] When D is even the expansion will terminate, consistent with our earlier observation that the result could be written in terms of Bernoulli polynomials.

[25] See Ashcroft and Mermin (1976) for a discussion of some of the applications.

In (6.191) we take $\Omega_{T\neq 0} = \Omega_0 + \Omega_1$. This allows us to split up the magnetization as $M = M_0 + M_1$ using an obvious notation. With (6.369) used for Ω in (6.191), we find

$$M_0 \simeq -\frac{e^2 B (me\mu)^{1/2}}{3\pi^2 m 2^{5/2}} \left[1 + \frac{35}{96} e^2 B^2 (me\mu)^{-2} + \cdots\right]. \tag{6.370}$$

Since we have assumed that μ is very large, the dominant term in M_0 should be the first one. Taking $\Omega = \Omega_1$ and using (6.359) for Ω_1, we find

$$\begin{aligned} M_1 \simeq & -\frac{T e^{3/2} m\mu}{2\pi B^{1/2}} \sum_{k=1}^{\infty} \frac{(-1)^k \cos\left[(2\pi k m\mu/B) - (3\pi/4)\right]}{k^{1/2} \sinh\left[2\pi^2 k m T/(eB)\right]} \\ & + \frac{3T}{8\pi^2} e^{3/2} B^{1/2} \sum_{k=1}^{\infty} \frac{(-1)^k \sin\left[(2\pi k m\mu/B) - (3\pi/4)\right]}{k^{3/2} \sinh\left[2\pi^2 k m T/(eB)\right]} + \frac{T^2 m e^{1/2}}{2B^{1/2}} \\ & \times \sum_{k=1}^{\infty} \frac{(-1)^k \sin\left[(2\pi k m\mu/B) - (3\pi/4)\right] \cosh\left[2\pi^2 k m T/(eB)\right]}{k^{1/2} \sinh^2\left[2\pi^2 k m T/(eB)\right]}. \end{aligned} \tag{6.371}$$

In order to obtain a complete expression for the magnetization we must eliminate the chemical potential from expressions (6.370) and (6.371). To do this we will use

$$N = -\left[\frac{\partial \Omega}{\partial(e\mu)}\right]\Bigg|_T$$

to solve for the chemical potential in terms of the particle number N (see (5.30)). Because we have written $\Omega = \Omega_0 + \Omega_1$, we can split up N into two contributions, one from Ω_0 that we will call N_0, and one from Ω_1 that we will call N_1. The particle density $\rho = N/V$ has a similar decomposition, and we find

$$\rho_0 \simeq \frac{\sqrt{2}}{3\pi^2} (me\mu)^{3/2} \left[1 - \frac{1}{32} (eB)^2 (me\mu)^{-2} + \cdots\right]. \tag{6.372}$$

Again, for large μ only the first term will contribute. For ρ_1 we find

$$\rho_1 \simeq \frac{mT}{2\pi} (eB)^{1/2} \sum_{k=1}^{\infty} \frac{(-1)^k \cos\left[(2\pi k m\mu/B) - (3\pi/4)\right]}{k^{1/2} \sinh\left[2\pi^2 k m T/(eB)\right]}. \tag{6.373}$$

For large μ, specifically $m\mu \gg B$, the particle density is dominated by the first term in ρ_0; the oscillating part of the density is negligible in comparison. We can therefore approximate

$$me\mu \simeq \left(\frac{3\pi^2 \rho}{\sqrt{2}}\right)^{2/3}, \tag{6.374}$$

and use this result to eliminate μ from the expression for the magnetization. In contrast with the particle density just discussed, in the expression for the magnetization the oscillatory term is not negligible for large μ and makes a significant and observable contribution to the magnetization.[26] The magnetization exhibits oscillations in $1/B$, as well as in the particle density. As mentioned above, because of the presence of the hyperbolic factors in M_1, the oscillations will only manifest themselves at low temperatures. This phenomenon is referred to as the de Haas–van Alphen effect.

6.11 Trapped Fermi gases

We have already presented a discussion of trapped Bose gases in Section 6.4. Due to the advances made in the cooling and trapping of atomic gases it is possible to prepare atoms in states that obey Fermi–Dirac statistics.[27] The purpose of this section is to consider trapped Fermi gases following Toms (2004, 2005).

6.11.1 Thermodynamic potential

If we model the trapping potential by a harmonic oscillator potential (6.52) the energy levels are as in (6.53). The only difference is that due to our assumption of Fermi–Dirac statistics the thermodynamic potential is given by

$$\Omega = -T \sum_{\mathbf{n}} \ln \left\{ 1 + \exp \left[-\beta (E_{\mathbf{n}} - \mu) \right] \right\}. \tag{6.375}$$

The fact that the energy levels are similar to those in Section 6.10 that were responsible for the de Haas–van Alphen effect means that we would expect there to be an oscillatory part of Ω that could lead to observable results. This analogy was first discussed in Toms (2004).

We will concentrate on the case $D = 3$ and use the method of Sondheimer and Wilson (1951), following our discussion in Section 6.10. The thermodynamic potential can be expressed as (6.332) with $\mathsf{z}(E)$ the inverse Laplace transform of the partition function. For the energy levels in (6.53) we have

$$Z(\beta) = \prod_{j=1}^{3} \frac{e^{-\beta\omega_j/2}}{(1 - e^{-\beta\omega_j})}. \tag{6.376}$$

[26] Again, we refer the reader to Ashcroft and Mermin (1976) for a discussion of this, and for the application to more realistic models.

[27] See Pethick and Smith (2002) for an overview.

We need to know the pole structure of $\beta^{-2}e^{\beta E}Z(\beta)$ in order to calculate $\mathsf{z}(E)$. It is obvious that the integrand of (6.330) has a pole of order 5 at $\beta = 0$. As in Section 6.10 we will call the contribution from the pole at $\beta = 0$, $\mathsf{z}_0(E)$. There is also a series of poles along the imaginary β-axis away from the origin at values of β that satisfy $e^{\beta\omega_j} = 1$ for $j = 1, 2, 3$. We use $\mathsf{z}_1(E)$ to denote the contribution from these poles to $\mathsf{z}(E)$. The evaluation of $\mathsf{z}_1(E)$ will be deferred until we have considered $\mathsf{z}_0(E)$.

By expanding $Z(\beta)$ in (6.376) about $\beta = 0$ it can be shown that

$$\mathsf{z}_0(E) = \frac{1}{5760\omega_1\omega_2\omega_3}\Big[240E^4 - 120E^2(\omega_1^2+\omega_2^2+\omega_3^2) \\ +7(\omega_1^4+\omega_2^4+\omega_3^4) + 10(\omega_1^2\omega_2^2+\omega_2^2\omega_3^2+\omega_3^2\omega_1^2)\Big]. \tag{6.377}$$

We have (6.361) holding (if we set $e = 1$ there). The low temperature approximation $\beta\mu \gg 1$ (or $T \ll \mu$) leads to

$$\Omega_0 \simeq -\frac{1}{2}\int_{-\infty}^{\infty} d\eta\, \frac{\mathsf{z}_0(\mu + 2T\eta)}{\cosh^2\eta}. \tag{6.378}$$

Because $\mathsf{z}_0(E)$ here is a polynomial in E, the integrals that result when (6.377) is used in (6.378) may all be evaluated without any further approximation using the result (6.364) as described in Section 6.10. The result is

$$\Omega_0 \simeq -\frac{\mu^4}{24\omega_1\omega_2\omega_3} + \frac{\mu^2}{48\omega_1\omega_2\omega_3}(\omega_1^2+\omega_2^2+\omega_3^2-4\pi^2T^2) \\ -\frac{1}{5760\omega_1\omega_2\omega_3}\Big[7(\omega_1^4+\omega_2^4+\omega_3^4) + 10(\omega_1^2\omega_2^2+\omega_2^2\omega_3^2+\omega_3^2\omega_1^2) \\ -40\pi^2T^2(\omega_1^2+\omega_2^2+\omega_3^2) + 112\pi^4T^4\Big]. \tag{6.379}$$

We now turn to the evaluation of Ω_1. The poles of $Z(\beta)$ for $\beta \neq 0$ occur at values of $\beta = 2\pi ik/\omega_j$ for $j = 1, 2, 3$ and $k = \pm1, \pm2, \ldots$. The nature of these poles depends upon the relative magnitude of the trap frequencies ω_j. If any of the trap frequencies are rational multiples of each other the poles will not be simple. The general situation is considered in Toms (2005). To keep things simple here, we will only examine the isotropic potential described by $\omega_1 = \omega_2 = \omega_3 = \omega$. It is then obvious that $Z(\beta)$ in (6.376) has triple poles at $\beta = 2\pi ik/\omega$ for $k = \pm1, \pm2, \ldots$. The residues at these poles may be evaluated in a straightforward way, and after a bit of calculation it will be found that

$$\mathsf{z}_1(E) = \sum_{k=1}^{\infty} \frac{(-1)^k \omega}{16\pi^4 k^4} \left(6 + \pi^2 k^2 - \frac{4\pi^2 k^2 E^2}{\omega^2} \right) \cos\left(\frac{2\pi k E}{\omega} \right) + \sum_{k=1}^{\infty} \frac{(-1)^k E}{2\pi^3 k^3} \sin\left(\frac{2\pi k E}{\omega} \right). \tag{6.380}$$

This can be compared with the simpler expression (6.344) found in the de Haas–van Alphen case. Making use of the integrals (6.363) and (6.364) and derivatives of these results with respect to the parameter a results in (for $T \ll \mu$)

$$\begin{aligned} \Omega_1 \simeq -\frac{1}{8\pi^2 \beta^3 \omega^2} \sum_{k=1}^{\infty} \frac{(-1)^k}{k^3 \sinh\left[2\pi^2 k/(\beta\omega)\right]} \Big\{ \Big[& 8\pi^4 k^2 \operatorname{csch}^2\Big(\frac{2\pi^2 k}{\beta\omega}\Big) \\ & + 4\pi^2 k \beta\omega \coth\Big(\frac{2\pi^2 k}{\beta\omega}\Big) + 2\beta^2\omega^2 \\ & + \pi^2 k^2 (4\pi^2 + \beta^2\omega^2 - 4\beta^2\mu^2) \Big] \cos\left(\frac{2\pi k\mu}{\omega}\right) \\ & + 4\pi k\beta\mu \Big[\beta\omega + 2\pi^2 k \coth\Big(\frac{2\pi^2 k}{\beta\omega}\Big) \Big] \sin\left(\frac{2\pi k\mu}{\omega}\right) \Big\}. \end{aligned} \tag{6.381}$$

This can be contrasted with the de Haas–van Alphen result (6.359). The more complicated result found here is a consequence of the higher-order poles along the imaginary β-axis that were found.

6.11.2 Chemical potential

The particle number is defined in terms of Ω by (5.30). We can split up $N = N_0 + N_1$ if we take $\Omega = \Omega_0 + \Omega_1$. With (6.379) used for Ω_0 we find

$$N_0 \simeq \frac{\mu^3}{6\omega_1\omega_2\omega_3} - \frac{\mu}{24\omega_1\omega_2\omega_3}(\omega_1^2 + \omega_2^2 + \omega_3^2 - 4\pi^2 T^2). \tag{6.382}$$

We will temporarily ignore the possible contribution from N_1 (an omission that will be remedied later in this section). If we set $N \simeq N_0$ we can solve for μ. Rather than write down a complicated expression involving the root of the cubic equation that results, we will assume that μ is large. To leading order in μ we will have

$$\mu^3 \simeq 6\omega_1\omega_2\omega_3 N, \tag{6.383}$$

showing that $\mu \propto N^{1/3}$. This result was first given in Butts and Rokhsar (1997) where it was found by approximating the sum over discrete energy

levels with integrals. It is possible to find the finite temperature correction to (6.383) as follows. Write

$$\mu = (6\omega_1\omega_2\omega_3 N)^{1/3}(1+\epsilon), \tag{6.384}$$

with $|\epsilon| \ll 1$. Substitution of (6.384) into (6.382) (with $N_0 = N$ assumed) and working to first order in ϵ results in

$$\frac{\mu^3}{\omega_1\omega_2\omega_3} \simeq 6N\left[1 + \frac{(\omega_1^2+\omega_2^2+\omega_3^2-4\pi^2T^2)}{4(6N\omega_1\omega_2\omega_3)^{2/3}}\right]. \tag{6.385}$$

This shows that for large values of N, that lead to large values of μ consistent with what we have assumed, the correction to (6.383) becomes increasingly unimportant. It is customary to define the Fermi energy E_F by

$$E_F = \mu(T=0). \tag{6.386}$$

If we do this then it is easy to show that (6.385) can be rewritten to give

$$\mu \simeq E_F\left(1 - \frac{\pi^2T^2}{3E_F^2}\right). \tag{6.387}$$

The contribution of Ω_1 to the particle number N is found using (6.381) to be (assuming an isotropic potential with $\omega_1 = \omega_2 = \omega_3 = \omega$)

$$\begin{aligned} N_1 \simeq \frac{\pi}{4\beta^3\omega^3}\sum_{k=1}^{\infty}\frac{(-1)^k}{\sinh\left[2\pi^2k/\left(\beta\omega\right)\right]}\Big\{\Big[&4\beta^2\mu^2 - 4\pi^2 - \beta^2\omega^2 \\ &-8\pi^2\mathrm{csch}^2\left(\frac{2\pi^2k}{\beta\omega}\right)\Big]\sin\left(\frac{2\pi k\mu}{\omega}\right) \\ &+8\pi\beta\mu\coth\left(\frac{2\pi^2k}{\beta\omega}\right)\cos\left(\frac{2\pi k\mu}{\omega}\right)\Big\}. \end{aligned} \tag{6.388}$$

One major difference here from the de Haas–van Alphen expression found from (6.373) (apart from the obvious complication) is that N_1 for the trapped gas involves an explicit dependence on μ outside of the trigonometric functions. In fact, the leading-order term here involves μ^2 as compared with μ^3 found in N_0; it is therefore important to consider the possible influence that N_1 might have on the chemical potential.

If we take $T \ll \mu$, and in addition assume that $\mu \gg \omega$, then we can approximate N_1 by the first term on the right-hand side of (6.388). For $\beta\omega \leq 1$ (or $T \geq \omega$) the sum that occurs in N_1 is well approximated by taking just the $k = 1$ term, and it is clear that the oscillations, although present, will have only a very small amplitude due to the behaviour of

the sinh factor. This means that for $T \geq \omega$ we would expect that $N \simeq N_0$ would be a good approximation, and therefore that (6.383) or (6.387) would provide a reliable approximation for the chemical potential. However as the temperature is reduced below $T = \omega$ the amplitude of the oscillations starts to increase and their effects can be quite marked. We therefore need to consider the behaviour of N_1 as $T \to 0$.

One way to evaluate N_1 at low temperature is to make use of the Poisson summation formula.[28] If $\varphi(x)$ is assumed to be a continuous function defined for all real values of x and we form

$$\Phi(x) = \sum_{k=-\infty}^{\infty} \varphi(x + 2\pi k), \tag{6.389}$$

with the assumption that the sum is convergent, then $\Phi(x + 2\pi) = \Phi(x)$ is a periodic function. As a consequence, we can express $\Phi(x)$ as a Fourier series

$$\Phi(x) = \sum_{n=-\infty}^{\infty} \Phi_n e^{inx}, \tag{6.390}$$

where the Fourier coefficients Φ_n are given by

$$\Phi_n = \frac{1}{2\pi} \int_0^{2\pi} dx\, e^{-inx} \Phi(x). \tag{6.391}$$

If we substitute (6.389) into (6.391) and interchange the order of summation and integration, we find

$$\begin{aligned} \Phi_n &= \frac{1}{2\pi} \sum_{k=-\infty}^{\infty} \int_0^{2\pi} dx\, e^{-inx} \varphi(x + 2\pi k) \\ &= \frac{1}{2\pi} \sum_{k=-\infty}^{\infty} \int_{2\pi k}^{2\pi(k+1)} dy\, e^{-in(y-2\pi k)} \varphi(y) \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} dy\, e^{-iny} \varphi(y). \end{aligned} \tag{6.392}$$

In the middle equality we made the change of variable $x = y - 2\pi k$ in the integral, and in the last equality we noted that $e^{2\pi ink} = 1$ since n and k

[28] See Whittaker and Watson (1928) for a rigorous derivation applied to the θ-function. We will present a non-rigorous derivation here.

are both integers. Equating the two expressions (6.389) and (6.390) for $\Phi(x)$ shows that

$$\sum_{k=-\infty}^{\infty} \varphi(x+2\pi k) = \sum_{n=-\infty}^{\infty} \Phi_n e^{inx} \tag{6.393}$$

with Φ_n defined in terms of $\varphi(y)$ by (6.392). This is referred to as the 'Poisson summation formula'.

For large μ we can approximate N_1 in (6.388) by its first term. This can be written as

$$N_1 \simeq \frac{\pi\mu^2}{\beta\omega^3} S\left(\frac{\mu}{\omega}, \frac{T}{\omega}\right), \tag{6.394}$$

where

$$S(q,b) = \sum_{k=1}^{\infty} \frac{\sin(2\pi qk - \pi k)}{\sinh(2\pi^2 kb)}. \tag{6.395}$$

Because $S(q,b)$ is periodic in q with period 1, we will initially restrict $0 \le q < 1$. We can apply the Poisson summation formula to $S(q,b)$ with $x = 0$ taken in (6.393) to find

$$S(q,b) = \sum_{n=-\infty}^{\infty} \Phi_n, \tag{6.396}$$

with

$$\Phi_n = \frac{1}{2\pi} \int_{-\infty}^{\infty} dy\; e^{-iny}\, \frac{\sin(qy - y/2)}{\sinh(\pi by)}. \tag{6.397}$$

It is now easy to evaluate the integral in (6.397) using the contour integral method that led to (6.363). To do this first note that when we expand $e^{-iny} = \cos(ny) - i\sin(ny)$, the imaginary part will vanish because it involves an integrand that is an odd function of y. By writing

$$\cos ny\;\sin(qy - y/2) = \frac{1}{2}\Big\{ \sin\left[(q+n-1/2)y\right] + \sin\left[(q-n-1/2)y\right] \Big\},$$

and making use of

$$\int_{-\infty}^{\infty} \frac{\sin(\alpha x)}{\sinh(\beta x)}\, dx = \frac{\pi}{\beta} \tanh\left(\frac{\pi\alpha}{2\beta}\right), \tag{6.398}$$

we find

$$\Phi_n = \frac{1}{4\pi b}\left[\tanh\left(\frac{q+n-1/2}{2b}\right) + \tanh\left(\frac{q-n-1/2}{2b}\right)\right] \tag{6.399}$$

$$= \frac{1}{2\pi b}\, \frac{\sinh[(q-1/2)/b]}{\cosh(n/b) + cosh[(q-1/2)/b]} \tag{6.400}$$

after some algebra. We can now split the sum that occurs in (6.396) as

$$\begin{aligned} S(q,b) &= \Phi_0 + 2\sum_{n=1}^{\infty}\Phi_n \\ &= \frac{1}{4\pi b}\tanh\left(\frac{2q-1}{4b}\right) - \frac{2q-1}{4\pi b} \\ &\quad + \frac{\sinh\left[(2q-1)/2b\right]}{2\pi b}\sum_{n=1}^{\infty}\left[\cosh\left(\frac{n}{b}\right)+\cosh\left(\frac{2q-1}{2b}\right)\right]^{-1} \end{aligned} \tag{6.401}$$

if it is noted from (6.400) that $\Phi_{-n} = \Phi_n$. At first sight this has done nothing but convert one infinite sum that we cannot evaluate in closed form into another one; however, the dependence on T/ω in each of the two expressions is the relevant feature. In the original sum (6.395) each term increases in magnitude as $T \to 0$; whereas in the transformed expression (6.401) the terms get smaller exponentially fast, behaving roughly like $e^{-c\,\omega/T}$ as $T \to 0$ for some constant c. Thus (6.401) is better suited to study the low temperature limit than (6.395). To a very good approximation, if we are only interested in very low values of T, we can neglect the infinite sum that appears in (6.401) and keep only the first two analytical terms. A bit of care must be exercised at this stage because we have assumed that $0 \le q < 1$. If we wish the result to apply for arbitrary values of q then we must ensure that the result has the same periodicity in q as the original expression (6.395). This will be the case if we take q in (6.401) to be $q - [q]$ where $[q]$ denotes the greatest integer whose value does not exceed q. In this case we have the approximation

$$S(q,b) \simeq \frac{1}{4\pi b}\tanh\left\{\frac{1}{2b}\left(q-[q]-\frac{1}{2}\right)\right\} - \frac{1}{2\pi b}\left(q-[q]-\frac{1}{2}\right), \tag{6.402}$$

that we expect to be good for small values of b.[29]

The result in (6.402) can be simplified further if we look at $T \to 0$. From writing the tanh factor in terms of exponentials, it can be seen that

$$\tanh\left\{\frac{1}{2b}\left(q-[q]-\frac{1}{2}\right)\right\} \to \begin{cases} 1 & \text{if } q-[q] > \frac{1}{2}, \\ -1 & \text{if } q-[q] < \frac{1}{2}. \end{cases} \tag{6.403}$$

If we write

$$\bar{q} = q - [q], \tag{6.404}$$

[29] This can be checked by numerical evaluation of (6.395) and comparison with (6.402), a task we leave to the reader.

then it can be seen that

$$S(q,b) \simeq -\frac{1}{2\pi b}\left(\bar{q} - \left[\bar{q} + \frac{1}{2}\right]\right), \tag{6.405}$$

as $b \to 0$. We can use either (6.402) or (6.405) back in (6.394) to obtain an approximate analytical result for N_1:

$$\begin{aligned} N_1 \simeq & \frac{\mu^2}{4\omega^2}\left\{\tanh\left(\frac{\beta\omega}{2}\left(\frac{\mu}{\omega} - \left[\frac{\mu}{\omega}\right] - \frac{1}{2}\right)\right)\right. \\ & \left. +1 - 2\left(\frac{\mu}{\omega} - \left[\frac{\mu}{\omega}\right]\right)\right\} \qquad (6.406) \\ \simeq & \frac{\mu^2}{2\omega^2}\left(\left[\frac{\mu}{\omega} + \frac{1}{2}\right] - \frac{\mu}{\omega}\right). \qquad (6.407) \end{aligned}$$

If we now include the limiting form (6.407) for N_1 and solve $N = N_0 + N_1$ with the first term of (6.382) used for N_0, it is possible to see that an approximate solution for large μ is given by

$$\frac{\mu}{\omega} \simeq \left[(6N)^{1/3}\right] + 1/2. \tag{6.408}$$

The presence of the greatest integer function in (6.408) shows that the chemical potential will go through steps when $(6N)^{1/3}$ changes by an integer. This behaviour was first found in numerical studies done in Schneider and Wallis (1998) and confirmed by the analytical method we have just described in Toms (2005). In Fig. 6.7 we plot μ/ω as a function of N for various temperatures and compare the result with the simple approximation (6.383) that ignores the oscillatory de Haas–van Alphen type contributions, as well as the zero temperature limit we found in (6.408). It can be seen that the approximation (6.383) captures the general behaviour of μ, but misses the step-like behaviour altogether. As the temperature is reduced, (6.408) starts to become a very good approximation. The step-like behaviour has its origins in the same type of expressions as that which led to the de Haas–van Alphen effect discussed in Section 6.10.

6.11.3 Specific heat

It is natural to ask if the oscillatory, or step-like, behaviour found for the chemical potential carries over into any of the observable thermodynamic quantities. To see that it does we will examine the specific heat.

The internal energy is defined in terms of the thermodynamic potential by combining (5.22) and (5.26). Because we have written $\Omega = \Omega_0 + \Omega_1$ we will have a similar split of the internal energy $E = E_0 + E_1$. It follows using (6.379) for Ω_0 that

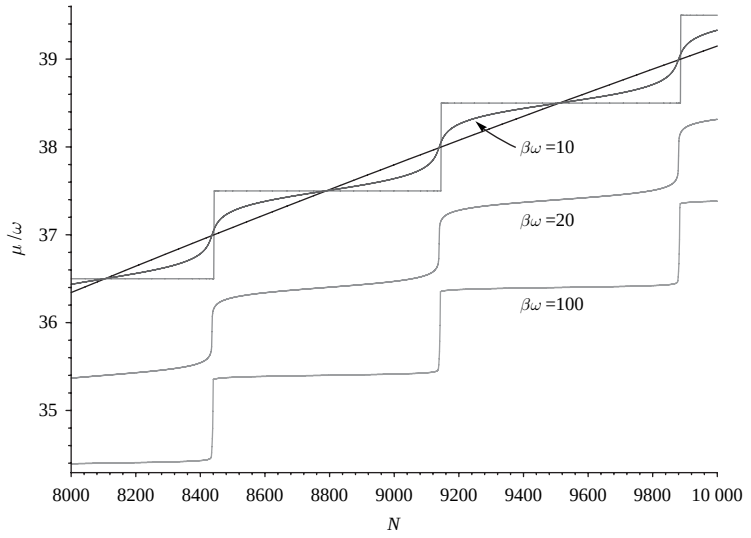

Fig. 6.7 This plot shows μ/ω plotted over a range of N for three sample temperatures. The solid, almost straight, line shows the result found using the continuum approximation (6.383) for the particle number, $\mu/\omega = (6N)^{1/3}$. The step-function superimposed shows the result found from the very low temperature approximation of (6.408). The smooth sinuous curves give the results for $T = 0.1\omega, T = 0.05\omega$, and $T = 0.01\omega$. The last two curves have been displaced from the first one for clarity.

$$E_0 = \frac{\partial}{\partial\beta}(\beta\Omega_0)\bigg|_{\beta\mu,\omega} \tag{6.409}$$

$$= \frac{\mu^4}{8\omega^3} - \frac{\mu^2}{16\omega^3}(\omega^2 - 4\pi^2T^2) + \frac{1}{1920\omega^3}(17\omega^4 + 40\pi^2\omega^2T^2 - 112\pi^4T^4). \tag{6.410}$$

If we use (6.381) for Ω_1 to compute E_1 (just replace Ω_0 in (6.409) with Ω_1) the result is rather lengthy so we will just give the two leading terms in μ since they are the ones we will need to calculate the specific heat. After some calculation, it can be shown that

$$E_1 \simeq \frac{\pi\mu^3}{\beta\omega^3}\sum_{k=1}^{\infty}\frac{(-1)^k}{\sinh\left[2\pi^2k/(\beta\omega)\right]}\sin\left(\frac{2\pi k\mu}{\omega}\right) + \frac{3\pi^2\mu^2}{\beta^2\omega^3}\sum_{k=1}^{\infty}\frac{(-1)^k\cosh\left[2\pi^2k/(\beta\omega)\right]}{\sinh^2\left[2\pi^2k/(\beta\omega)\right]}\cos\left(\frac{2\pi k\mu}{\omega}\right). \tag{6.411}$$

The specific heat is defined by

$$C = \left(\frac{\partial E}{\partial T}\right)\Big|_{N,\omega}. \tag{6.412}$$

We have E expressed as a function of T and μ, so it would be more useful to have an expression for C that involved holding μ rather than N fixed in the differentiation. One easy way to get this is to consider how E varies under small changes in T and μ with N held fixed. We have

$$\delta E = \left(\frac{\partial E}{\partial T}\right)\Big|_{\mu} \delta T + \left(\frac{\partial E}{\partial \mu}\right)\Big|_{T} \delta\mu, \tag{6.413}$$

$$0 = \delta N = \left(\frac{\partial N}{\partial T}\right)\Big|_{\mu} \delta T + \left(\frac{\partial N}{\partial \mu}\right)\Big|_{T} \delta\mu. \tag{6.414}$$

Eliminating $\delta\mu$ in (6.413) using (6.414) results in

$$C = \left(\frac{\partial E}{\partial T}\right)\Big|_{\mu,\omega} - \frac{(\partial E/\partial\mu)|_{T,\omega}\,(\partial N/\partial T)|_{\mu,\omega}}{(\partial N/\partial\mu)|_{T,\omega}}, \tag{6.415}$$

and the result is now directly useful for calculating C.[30]

Because we are assuming large μ, we will obtain an expansion for C in powers of μ. Using (6.410) we find

$$\left(\frac{\partial E}{\partial T}\right)\Big|_{\mu,\omega} \simeq \frac{\pi^2\mu^2 T}{3\omega^3} + \left(\frac{\partial E_1}{\partial T}\right)\Big|_{\mu,\omega}, \tag{6.416}$$

$$\left(\frac{\partial E}{\partial \mu}\right)\Big|_{T,\omega} \simeq \frac{\mu^3}{2\omega^3} + \left(\frac{\partial E_1}{\partial \mu}\right)\Big|_{T,\omega}. \tag{6.417}$$

Using (6.382) with $\omega_1 = \omega_2 = \omega_3 = \omega$ we find

$$\left(\frac{\partial N}{\partial T}\right)\Big|_{\mu,\omega} \simeq \frac{\pi^2\mu T}{3\omega^3} + \left(\frac{\partial N_1}{\partial T}\right)\Big|_{\mu,\omega}, \tag{6.418}$$

$$\left(\frac{\partial N}{\partial \mu}\right)\Big|_{T,\omega} \simeq \frac{\mu^2}{2\omega^3} + \left(\frac{\partial N_1}{\partial \mu}\right)\Big|_{T,\omega}. \tag{6.419}$$

[30] This procedure is equivalent to what we did in Section 6.4 for the Bose gas.

If we ignore the oscillatory contributions to the specific heat (the terms on the right-hand side of (6.416)–(6.419) that involve E_1 and N_1) then it is easy to show that $C = C_0$ with

$$C_0 \simeq \frac{\pi^2 T \mu^2}{6\omega^3}. \tag{6.420}$$

For low T, this shows that the specific heat would be expected to behave linearly with T. However if we include the oscillatory terms the result becomes less obvious.

If we use (6.411) for E_1 it can be seen that

$$\left(\frac{\partial E_1}{\partial T}\right)\bigg|_{\mu,\omega} \simeq \alpha_3 \mu^3 + \alpha_2 \mu^2 + \cdots, \tag{6.421}$$

$$\left(\frac{\partial E_1}{\partial \mu}\right)\bigg|_{T,\omega} \simeq \beta_3 \mu^3 + \beta_2 \mu^2 + \cdots, \tag{6.422}$$

where $\alpha_3, \alpha_2, \beta_3, \beta_2$ involve sums that can easily be found by the indicated differentiation. Thus the oscillatory contributions to C, when expanded in powers of μ, would be expected to be of order μ^3 rather than the μ^2 behaviour that was found in (6.420). Similar expansions for the derivatives of N_1 that appear in (6.418) and (6.419) result in

$$\left(\frac{\partial N_1}{\partial T}\right)\bigg|_{\mu,\omega} \simeq \gamma_2 \mu^2 + \gamma_1 \mu + \cdots, \tag{6.423}$$

$$\left(\frac{\partial N_1}{\partial \mu}\right)\bigg|_{T,\omega} \simeq \delta_2 \mu^2 + \delta_1 \mu + \cdots, \tag{6.424}$$

with $\gamma_2, \gamma_1, \delta_2, \delta_1$ expressed as various sums. By substituting the expansions (6.421)–(6.424) into (6.416)–(6.419), and then using the results in (6.415) with an expansion in powers of μ, it can be seen, after a bit of work, that

$$C \simeq \frac{\pi^2 T \mu^2}{6\omega^3}\left(1 + \Sigma_1 - 12\frac{\Sigma_2^2}{\Sigma_3}\right), \tag{6.425}$$

with

$$\Sigma_1 = 12\sum_{k=1}^{\infty}(-1)^k \left[\frac{\cosh\theta_k}{\sinh^2\theta_k} - \frac{\pi^2 kT}{\omega}\left(\frac{1}{\sinh\theta_k} + \frac{2}{\sinh^3\theta_k}\right)\right] \times \cos\left(2\pi k\frac{\mu}{\omega}\right), \tag{6.426}$$

$$\Sigma_2 = \sum_{k=1}^{\infty} (-1)^k \left(\frac{1}{\sinh \theta_k} - \frac{2\pi^2 kT}{\omega} \frac{\cosh \theta_k}{\sinh^2 \theta_k} \right) \sin\left(2\pi k \frac{\mu}{\omega} \right), \quad (6.427)$$

$$\Sigma_3 = 1 + \sum_{k=1}^{\infty} \frac{(-1)^k 4\pi^2 k}{\beta\omega \sinh \theta_k} \cos\left(2\pi k \frac{\mu}{\omega} \right), \quad (6.428)$$

where

$$\theta_k = \frac{2\pi^2 k}{\beta\omega}. \quad (6.429)$$

As a check on this result, if we drop all of the terms that arose from the oscillatory part of Ω (namely $\Sigma_{1,2,3}$) we recover (6.420).

It remains to study how the appearance of the oscillatory terms in (6.425) alters the behaviour of the specific heat from the linear temperature dependence. It is possible to evaluate the asymptotic expansion of the three sums defined in (6.426)–(6.428) for large values of $\beta\omega$ in a similar way to what we did in Section 6.11.2. Leaving out the technical details of this for brevity, we find the approximate forms

$$\Sigma_1 \simeq \frac{3\beta^3\omega^3(2\bar{\mu}-1)^2}{16\pi^2 \cosh^2(\beta\omega/4)(2\bar{\mu}-1)} - 1, \quad (6.430)$$

$$\Sigma_2 \simeq -\frac{\beta^2\omega^2(2\bar{\mu}-1)}{16\pi \cosh^2(\beta\omega/4)(2\bar{\mu}-1)}, \quad (6.431)$$

$$\Sigma_3 \simeq \frac{\beta\omega}{4\cosh^2(\beta\omega/4)(2\bar{\mu}-1)}, \quad (6.432)$$

with $\bar{\mu}$ defined by

$$\bar{\mu} = \frac{\mu}{\omega} - \left[\frac{\mu}{\omega} \right]. \quad (6.433)$$

The results in (6.430)–(6.432) can be checked against a direct numerical evaluation of the sums defined by (6.426)–(6.428) and found to be accurate for $\beta\omega \simeq 10$ and $\bar{\mu}$ not too close to 0 or 1. Once $\beta\omega \simeq 100$ the results become very accurate even for $\bar{\mu}$ close to 0 and 1. Thus for $T \leq \omega/100$, the simple expressions in (6.430)–(6.432) become reliable approximations for $\Sigma_{1,2,3}$.

If we use (6.430)–(6.432) in the expression for the specific heat in (6.425) the result can be shown to vanish. The de Haas–van Alphen contribution to the specific heat cancels the continuum approximation as found in (6.420) to the leading order we are working to. The specific heat therefore vanishes as $T \to 0$ faster than T. This is completely consistent with the numerical results found in Schneider and Wallis (1998). Because the de Haas–van Alphen approximation as well as the asymptotic evaluation of the sums leading to (6.430)–(6.432) neglect terms that are exponentially suppressed, we expect that the specific heat vanishes like $e^{-\alpha\omega/T}$ for some constant α as $T \to 0$. This was shown rigorously for the one-dimensional gas in Toms (2005).

For $T \geq \omega/100$, but still small, the results in (6.430)–(6.432) start to become less reliable. As a check on our results against the numerical ones of Schneider and Wallis (1998) we plot the specific heat as found from (6.425) to demonstrate the de Haas–van Alphen oscillations. This is shown in Fig. 6.8. As the temperature increases we do find, as expected, that the contribution from $\Sigma_{1,2,3}$ becomes smaller exponentially, and the linear behaviour with temperature is regained. The analogue of the de Haas–van Alphen effect for trapped gases can therefore lead to potentially observable consequences at very low temperature.

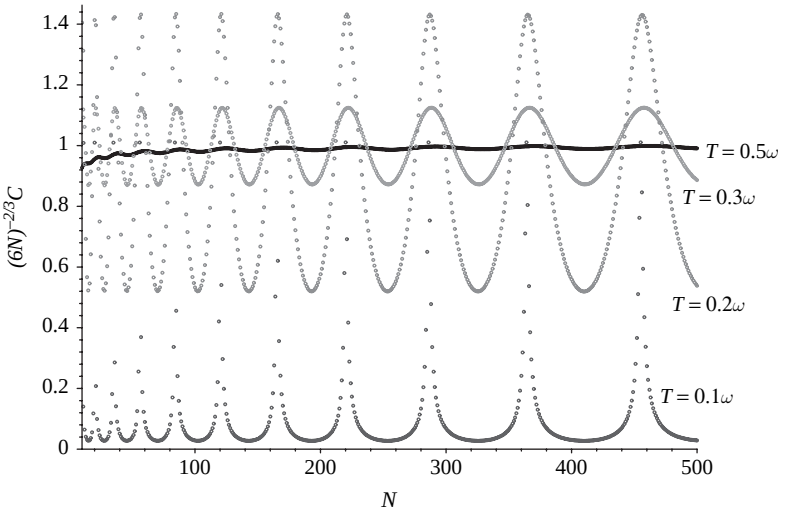

Fig. 6.8 This plot shows $C/(6N)^{2/3}$ plotted over a range of N for four sample temperatures $T = 0.1\omega, T = 0.2\omega, T = 0.3\omega$, and $T = 0.5\omega$. As the temperature increases the oscillation amplitude decreases and the curves approach the continuum limit of 1 in the scaled specific heat. As the temperature decreases there are significant deviations from the result found from using the continuum limit, and for very small temperatures the specific heat starts to become vanishingly small.

Notes

The basic idea that Bose–Einstein condensation can be viewed as symmetry breaking, like the Higgs mechanism in particle physics, was discussed by Kapusta (1981, 1989). The general version presented here was given in Toms (1992). The method described in Section 6.9 was first presented in Kirsten and Toms (1995). A very complete discussion of Bose–Einstein condensation for the relativistic interacting scalar field is Benson *et al.* (1991). This paper shows very clearly how the non-relativistic result follows by taking a careful limit from the relativistic result.

7

Further applications of the Schwinger action principle

In this chapter we return to the Schwinger action principle that we introduced in Chapter 3 and consider some further applications. This not only illustrates the utility of the method, but also helps to set the stage for the final chapter where we return to quantum field theory and provide a general definition for the effective action.

7.1 Integration of the action principle

Consider $\langle a'|F(A,B)|b''\rangle$ where A and B each represent a complete set of mutually compatible observables, and $F(A,B)$ is some function. We do not assume that observables from the two different sets commute with each other. In general if $F(A,B)$ contains terms like BA there is no way to evaluate the above matrix element in terms of the eigenvalues of the operators, since there is no possible way to reorder A and B to place them next to their respective eigenstates unless A and B satisfy some particular commutation relations. If $[B,A]$ is known, it is always possible to reorder the operators in $F(A,B)$ so that all of the A's stand to the left of all of the B's, allowing us to evaluate $\langle a'|F(A,B)|b''\rangle$ in terms of the eigenvalues of the operators. Let

$$\mathcal{F}(A,B) = F(A,B) \tag{7.1}$$

denote the operator where the commutation relation for $[A,B]$ has been used to move all occurrences of A in $F(A,B)$ to the left of all occurrences of B. $\mathcal{F}(A,B)$ is said to be well-ordered.[1] In this case we have

$$\langle a'|F(A,B)|b''\rangle = \mathcal{F}(a',b'')\langle a'|b''\rangle. \tag{7.2}$$

[1] See Dirac, 1958, Section 32.

The matrix element of $F(A, B)$ is then seen to be directly related to the transformation function $\langle a'|b''\rangle$.

We can apply the idea of well-ordered operators to the action principle (3.52). Define

$$\delta\mathcal{W}_{21} = \delta W_{21} \tag{7.3}$$

to be the well-ordered form of δW_{21}. Then in (3.52) we have

$$\delta\langle a_2', t_2|a_1', t_1\rangle = \frac{i}{\hbar}\delta\mathcal{W}_{21}'\langle a_2', t_2|a_1', t_1\rangle \tag{7.4}$$

where $\delta\mathcal{W}_{21}'$ denotes the replacement of all operators with their eigenvalues as in (7.2). Integration of (7.4) gives

$$\langle a_2', t_2|a_1', t_1\rangle = \exp\left(\frac{i}{\hbar}\mathcal{W}_{21}'\right). \tag{7.5}$$

Any constant of integration can be absorbed into $\mathcal{W}_{21}'$ and fixed by taking the limit $t_2 \to t_1$, and using $\langle a_2', t_1|a_1', t_1\rangle = \delta(a_2', a_1')$. $\mathcal{W}_{21}'$ depends only on the observables at the initial and final times, and on the initial and final times themselves.

It is now possible to use the action principle to make contact with the Hamilton–Jacobi equation discussed in Section 1.4.2. Using (3.61) and (3.73) in the action principle (3.52) we have

$$\begin{aligned}\delta\langle a_2', t_2|a_1', t_1\rangle =& \frac{i}{\hbar}\delta x^i(t_2)\langle a_2', t_2|p_i(t_2)|a_1', t_1\rangle - \frac{i}{\hbar}\delta t_2\langle a_2', t_2|H(t_2)|a_1', t_1\rangle \\ &- \frac{i}{\hbar}\delta x^i(t_1)\langle a_2', t_2|p_i(t_1)|a_1', t_1\rangle + \frac{i}{\hbar}\delta t_1\langle a_2', t_2|H(t_1)|a_1', t_1\rangle.\end{aligned} \tag{7.6}$$

In comparing this with (7.4) it can be noted that we may write

$$\delta\langle a_2', t_2|a_1', t_1\rangle = \frac{i}{\hbar}\langle a_2', t_2|\delta\mathcal{W}_{21}|a_1', t_1\rangle \tag{7.7}$$

since $\delta\mathcal{W}_{21}$ is well-ordered. Comparison with (7.6) leads to

$$\frac{\partial\mathcal{W}_{21}}{\partial x^i(t_2)} = p_i(t_2), \tag{7.8}$$

$$\frac{\partial\mathcal{W}_{21}}{\partial t_2} = -H(t_2), \tag{7.9}$$

$$\frac{\partial\mathcal{W}_{21}}{\partial x^i(t_1)} = -p_i(t_1), \tag{7.10}$$

$$\frac{\partial\mathcal{W}_{21}}{\partial t_1} = H(t_1). \tag{7.11}$$

These results may be recognized as operator versions of the Hamilton–Jacobi equations. If $H = H[x(t), p(t), t]$, then from (7.8)–(7.11) we have

$$\frac{\partial \mathcal{W}_{21}}{\partial t_2} + H\Big[x(t_2), \frac{\partial \mathcal{W}_{21}}{\partial x^i(t_2)}, t_2\Big] = 0, \tag{7.12}$$

$$-\frac{\partial \mathcal{W}_{21}}{\partial t_1} + H\Big[x(t_1), -\frac{\partial \mathcal{W}_{21}}{\partial x^i(t_1)}, t_1\Big] = 0. \tag{7.13}$$

Suppose that we concentrate on $\langle \mathbf{x}'', t_2 | \mathbf{x}', t_1 \rangle$ which we will call the propagator and study in more depth in Section 7.5. We then have

$$\langle \mathbf{x}'', t_2 | \mathbf{x}', t_1 \rangle = \exp\Big(\frac{i}{\hbar}\mathcal{W}'_{21}\Big) \tag{7.14}$$

from (7.5). The arbitrary constant of integration that we said had been absorbed into $\mathcal{W}'_{21}$ can be determined from the requirement

$$\langle \mathbf{x}'', t_1 | \mathbf{x}', t_1 \rangle = \delta(\mathbf{x}'', \mathbf{x}'). \tag{7.15}$$

The more general transformation function $\langle a'_2, t_2 | a'_1, t_1 \rangle$ can always be recovered from

$$\langle a'_2, t_2 | a'_1, t_1 \rangle = \int d^D x'' \int d^D x' \langle a'_2, t_2 | \mathbf{x}'', t_2 \rangle \langle \mathbf{x}'', t_2 | \mathbf{x}', t_1 \rangle \langle \mathbf{x}', t_1 | a'_1, t_1 \rangle \tag{7.16}$$

which follows by the completeness relation for the position eigenstates.

7.2 Application of the action principle to the free particle

We will now illustrate the action principle by applying it to the evaluation of the propagator for a free particle. The Hamiltonian operator is simply

$$H = \frac{1}{2m}p^2, \tag{7.17}$$

where p is the momentum operator. Because H has no explicit dependence on time, the Heisenberg equations of motion (3.90) or (3.48) give us

$$\frac{\partial}{\partial t}H = \frac{d}{dt}H = 0, \tag{7.18}$$

and hence we find $H(t_1) = H(t_2)$ by integration from $t = t_1$ to $t = t_2$. This corresponds to the classical conservation of energy. It therefore follows that

$$p(t_1) = p(t_2) = p, \tag{7.19}$$

where p is a constant operator. This can also be deduced directly from the Heisenberg equation of motion (3.92) since $[H, p] = 0$.

If we abbreviate $x_1 = x(t_1)$ and $x_2 = x(t_2)$, then (7.8)–(7.11) become

$$\frac{\partial}{\partial x_2}\mathcal{W}_{21} = p = -\frac{\partial}{\partial x_1}\mathcal{W}_{21}, \tag{7.20}$$

$$\frac{\partial}{\partial t_2}\mathcal{W}_{21} = -\frac{p^2}{2m} = -\frac{\partial}{\partial t_1}\mathcal{W}_{21}. \tag{7.21}$$

Integration of these partial differential equations in a straightforward way leads to

$$\mathcal{W}_{21} = p(x_2 - x_1) - \frac{p^2}{2m}(t_2 - t_1) + C \tag{7.22}$$

where C is a constant operator.

The constant value of momentum can be related to the positions x_1 and x_2 by solving the Heisenberg equations of motion (3.91). We have

$$\begin{aligned} \dot{x} &= \frac{i}{\hbar}[H, x] = \frac{i}{2m\hbar}[p^2, x] \\ &= \frac{i}{2m\hbar}\Big[p(p, x) + (p, x)p\Big] \\ &= \frac{1}{m}p \end{aligned} \tag{7.23}$$

using the canonical commutation relation (3.95). Since p is a constant operator, (7.23) can be integrated to give

$$x(t) = \frac{1}{m}pt + C_0 \tag{7.24}$$

where C_0 is a constant operator. Applying the conditions $x_1 = x(t_1)$ and $x_2 = x(t_2)$ leads to

$$x_2 - x_1 = \frac{1}{m}p(t_2 - t_1), \tag{7.25}$$

so that p can be eliminated in (7.22) to give

$$\mathcal{W}_{21} = \frac{m(x_2 - x_1)^2}{2(t_2 - t_1)} + C. \tag{7.26}$$

The result in (7.26) is not in well-ordered form since

$$(x_2 - x_1)^2 = x_2^2 - x_2x_1 - x_1x_2 + x_1^2. \tag{7.27}$$

It is necessary to order the term in x_1x_2 as x_2x_1 to obtain a well-ordered form for $\mathcal{W}_{21}$. To do this, note that

$$-x_1x_2 = [x_2, x_1] - x_2x_1. \tag{7.28}$$

Also from (7.25) we know that

$$\begin{aligned}[x_2, x_1] &= \left[x_1 + \frac{1}{m}p(t_2 - t_1), x_1\right] \\ &= \frac{1}{m}(t_2 - t_1)[p, x_1] \\ &= -\frac{i\hbar}{m}(t_2 - t_1)\end{aligned} \tag{7.29}$$

using (3.95) and (3.103). Combining (7.27)–(7.29), and using the result in (7.26), gives

$$\mathcal{W}_{21} = \frac{m}{2(t_2 - t_1)}(x_2^2 - 2x_2x_1 + x_1^2) - \frac{i}{2}\hbar + C \tag{7.30}$$

which is now well-ordered.

Because $\mathcal{W}_{21}$ in (7.30) is now well-ordered, we can replace the operators in (7.30) with their eigenvalues. We have from (7.14)

$$\langle x_2', t_2 | x_1', t_1\rangle = \exp\left(\frac{i}{\hbar}\mathcal{W}_{21}'\right) \tag{7.31}$$

where

$$\mathcal{W}_{21}' = \frac{m(x_2' - x_1')^2}{2(t_2 - t_1)} - \frac{i\hbar}{2} + C. \tag{7.32}$$

The last task remaining is to find the constant C. This can be done by using (7.15). To do this define

$$\delta_\alpha(z) = (i\pi\alpha)^{-1/2}\exp\left(\frac{i}{\alpha}z^2\right) \tag{7.33}$$

and consider

$$I(\alpha) = \int_{-\infty}^{\infty} dz\, \delta_\alpha(z) f(z). \tag{7.34}$$

Here $\alpha > 0$ is a real number and $f(z)$ is any function for which the integral $I(\alpha)$ exists. We have, upon a simple change of variable $z \to \alpha^{1/2}z$,

$$I(\alpha) = (i\pi)^{-1/2}\int_{-\infty}^{\infty} dz\, e^{iz^2} f(\alpha^{1/2}z).$$

By taking the limit $\alpha \to 0$ in $I(\alpha)$, and interchanging the order of the limit and the integration, we find

$$I(0) = f(0)$$

since $\int_{-\infty}^{\infty} dz\, e^{iz^2} = (i\pi)^{1/2}$. This shows that $\lim_{\alpha\to 0} \delta_\alpha(z)$ has the property of the Dirac delta distribution. We may therefore define

$$\lim_{\alpha\to 0} (i\pi\alpha)^{-1/2} \exp\left(\frac{i}{\alpha} z^2\right) = \delta(z). \tag{7.35}$$

Using (7.35) it is now easy to see that (7.15) holds only if

$$C = \frac{i\hbar}{2}\Big\{1 - \ln\Big[\frac{m}{2\pi i\hbar(t_2 - t_1)}\Big]\Big\}, \tag{7.36}$$

giving

$$\mathcal{W}'_{21} = \frac{m}{2(t_2 - t_1)}(x'_2 - x'_1)^2 - \frac{i\hbar}{2}\ln\Big[\frac{m}{2\pi i\hbar(t_2 - t_1)}\Big], \tag{7.37}$$

and

$$\mathcal{W}_{21} = \frac{m}{2(t_2 - t_1)}(x_2^2 - 2x_2x_1 + x_1^2) - \frac{i\hbar}{2}\ln\Big[\frac{m}{2\pi i\hbar(t_2 - t_1)}\Big]. \tag{7.38}$$

The propagator for a free particle is therefore

$$\langle x'_2, t_2 | x'_1, t_1\rangle = \Big[\frac{m}{2\pi i\hbar(t_2 - t_1)}\Big]^{1/2} \exp\Big[\frac{im(x'_2 - x'_1)^2}{2\hbar(t_2 - t_1)}\Big]. \tag{7.39}$$

We can also work out the action operator W_{21} defined by

$$W_{21} = \int_{t_1}^{t_2} dt\Big\{\frac{1}{2}\Big[p(t)\dot{x}(t) + \dot{x}(t)p(t)\Big] - H\Big\}. \tag{7.40}$$

Because $p(t) = p$ is constant, the integration in (7.40) is trivial and gives

$$W_{21} = \frac{1}{2}p(x_2 - x_1) + \frac{1}{2}(x_2 - x_1)p - \frac{p^2}{2m}(t_2 - t_1). \tag{7.41}$$

Utilizing (7.25) results in

$$W_{21} = \frac{m}{2(t_2 - t_1)}(x_2 - x_1)^2. \tag{7.42}$$

This operator is Hermitian, as it must be; however, it is not well-ordered. Using (7.27)–(7.29) again shows that

$$W_{21} = \frac{m}{2(t_2 - t_1)}(x_2^2 - 2x_2x_1 + x_1^2) - \frac{i\hbar}{2}. \tag{7.43}$$

Comparing (7.43) with (7.38) shows very clearly that $\mathcal{W}_{21}$ is not obtained from W_{21} by the process of well-ordering the operators. The formalism tells us that $\delta\mathcal{W}_{21}$ must be obtained from δW_{21} by well-ordering the operators, and it is easy to verify that this is the case for this example.

Finally we note that by taking the classical limit (i.e. $\hbar \to 0$) we have

$$\lim_{\hbar\to 0} \mathcal{W}_{21} = \lim_{\hbar\to 0} W_{21} = S_{21} \tag{7.44}$$

where S_{21} is Hamilton's principle function.[2] The fact that $\mathcal{W}_{21}$ and W_{21} coincide in the limit $\hbar \to 0$ is a consequence of the fact that x_1 and x_2 commute in this limit.

7.3 Application to the simple harmonic oscillator

The Hamiltonian was given earlier in (3.129) as

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2. \tag{7.45}$$

The Heisenberg equations of motion for the position and momentum read (see (3.48) and (3.90))

$$\dot{x} = -\frac{i}{\hbar}[x, H] = -\frac{i}{2\hbar m}[x, p^2] = \frac{1}{m}p, \tag{7.46}$$

and

$$\dot{p} = -\frac{i}{\hbar}[p, H] = -\frac{i}{2\hbar}m\omega^2[p, x^2] = -m\omega^2 x. \tag{7.47}$$

These two equations are easily integrated with the results

$$x(t) = C_1 \cos\omega t + C_2 \sin\omega t, \tag{7.48}$$

$$p(t) = m\dot{x}(t) = m\omega(-C_1 \sin\omega t + C_2 \cos\omega t). \tag{7.49}$$

Here C_1 and C_2 are constant operators to be fixed by the two conditions $x(t_1) = x_1$ and $x(t_2) = x_2$. We have from (7.48)

$$\begin{pmatrix} x_2 \\ x_1 \end{pmatrix} = \begin{pmatrix} \cos\omega t_2 & \sin\omega t_2 \\ \cos\omega t_1 & \sin\omega t_1 \end{pmatrix} \begin{pmatrix} C_1 \\ C_2 \end{pmatrix},$$

[2] S_{21} is the classical action functional evaluated along the classical path.

which upon inversion of the 2×2 matrix gives

$$C_1 = \frac{1}{\sin\omega(t_2 - t_1)}[x_1 \sin\omega t_2 - x_2 \sin\omega t_1], \tag{7.50}$$

$$C_2 = \frac{1}{\sin\omega(t_2 - t_1)}[x_2 \cos\omega t_1 - x_1 \cos\omega t_2]. \tag{7.51}$$

By taking $t = t_1$ and $t = t_2$ in (7.49), and using the expressions for C_1 and C_2 we have just found, the following results are obtained:

$$p_1 = \frac{m\omega}{\sin\omega(t_2 - t_1)}[x_2 - x_1 \cos\omega(t_2 - t_1)], \tag{7.52}$$

$$p_2 = \frac{m\omega}{\sin\omega(t_2 - t_1)}[-x_1 + x_2 \cos\omega(t_2 - t_1)]. \tag{7.53}$$

Since the canonical commutation relations give $[x_2, p_2] = i\hbar$, we have from (7.53) that

$$[x_1, x_2] = \frac{i\hbar}{m\omega} \sin\omega(t_2 - t_1). \tag{7.54}$$

This result may be used to express any monomial in x_1 and x_2 in well-ordered form.

A straightforward calculation using

$$H_2 = \frac{p_2^2}{2m} + \frac{1}{2}m\omega^2 x_2^2$$

with p_2 substituted from (7.53) shows that

$$H_2 = \frac{m\omega^2}{2\sin^2\omega(t_2 - t_1)}[x_1^2 + x_2^2 - (x_1x_2 + x_2x_1)\cos\omega(t_2 - t_1)].$$

As for the free particle considered in the previous section, because the Hamiltonian does not have an explicit dependence on the time, we have $H_1 = H_2$, and it does not matter which time we use to evaluate the Hamiltonian. H_2 can be written in well-ordered form using (7.54) as

$$H_2 = \frac{m\omega^2}{2\sin^2\omega(t_2 - t_1)}[x_1^2 + x_2^2 - 2x_2x_1\cos\omega(t_2 - t_1)] - \frac{i\hbar\omega\cos\omega(t_2 - t_1)}{2\sin\omega(t_2 - t_1)}. \tag{7.55}$$

We can now solve the equations (7.9) and (7.11) with p_1 and p_2 given by (7.52) and (7.53) to find

$$\mathcal{W}_{21} = \frac{m\omega}{2\sin\omega(t_2-t_1)}[(x_1^2+x_2^2)\cos\omega(t_2-t_1)-2x_2x_1]+F(t_2,t_1), \quad (7.56)$$

where $F(t_2,t_1)$ is an arbitrary function with no dependence on x_1 or x_2. It should be noted that because of (7.54) it does not matter which order we write the term in x_2x_1 since $x_2x_1 - x_1x_2$ is a function of t_2, t_1 only. It is most convenient to take the order of x_1 and x_2 so that $\mathcal{W}_{21}$ is well-ordered.

The result in (7.56) must also solve (7.8). From (7.56) we find

$$\frac{\partial\mathcal{W}_{21}}{\partial t_2} = -\frac{m\omega^2}{2\sin^2\omega(t_2-t_1)}[x_1^2+x_2^2-2x_2x_1\cos\omega(t_2-t_1)] + \frac{\partial F(t_2,t_1)}{\partial t_2}.$$

Since the right-hand side must equal $-H_2$ with H_2 given in (7.55), this tells us that

$$\frac{\partial}{\partial t_2}F(t_2,t_1) = \frac{i\hbar\omega\cos\omega(t_2-t_1)}{2\sin\omega(t_2-t_1)}.$$

This last result may be integrated to yield

$$F(t_2,t_1) = \frac{i\hbar}{2}\ln\sin\omega(t_2-t_1) + f(t_1),$$

where $f(t_1)$ is an arbitrary function of integration. Finally we require (7.10) to be satisfied. Since $H_1 = H_2$ it is easy to show that $f(t_1)$ must be a constant. This constant can be found from noting that as $\omega \to 0$ the result for $\mathcal{W}_{21}$ should reproduce the result for the free particle found in (7.38). This results in

$$\begin{aligned}\mathcal{W}_{21} = &\frac{m\omega}{2\sin\omega(t_2-t_1)}[(x_1^2+x_2^2)\cos\omega(t_2-t_1)-2x_2x_1] \\ &+\frac{i\hbar}{2}\ln\Big[\frac{2\pi i\hbar\sin\omega(t_2-t_1)}{m\omega}\Big]. \end{aligned} \quad (7.57)$$

The propagator for the simple harmonic oscillator now follows from (7.14) as

$$\langle x_2', t_2 | x_1', t_1 \rangle = \Big[\frac{m\omega}{2\pi i\hbar \sin\omega(t_2 - t_1)}\Big]^{1/2} \exp\Big\{\frac{im\omega}{2\hbar \sin\omega(t_2 - t_1)} \times [(x_1'^2 + x_2'^2)\cos\omega(t_2 - t_1) - 2x_2'x_1']\Big\}. \tag{7.58}$$

7.4 Application to the forced harmonic oscillator

In this section we wish to show how the Schwinger action principle can be used to obtain the propagator for the forced harmonic oscillator. In the next chapter we will show how this result is useful in a quantum field theory setting.

The Hamiltonian reads

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 - J(t)x \tag{7.59}$$

where $J(t)$ denotes the driving, or forcing, term. We will assume that $J(t) = 0$ for $t \leq t_-$ and for $t \geq t_+$ where $t_+ > t_-$. The Heisenberg equations of motion give

$$\dot{x} = \frac{i}{\hbar}[H, x] = \frac{p}{m}, \tag{7.60}$$

as in (7.46); however,

$$\dot{p} = \frac{i}{\hbar}[H, p] = -m\omega^2 x + J(t), \tag{7.61}$$

in contrast with (7.47). Differentiating (7.60) with respect to t, and using (7.61) results in

$$\ddot{x}(t) + \omega^2 x(t) = \frac{1}{m}J(t), \tag{7.62}$$

and the interpretation of $J(t)$ as the driving force should be obvious. The equation of motion we have just obtained is valid for $x(t)$ an operator, but is identical to the classical equation of motion for a driven oscillator. Probably the easiest way of solving (7.62) is to reduce it to a system of first-order equations by factoring the differential operator

$$\frac{d^2}{dt^2} + \omega^2 = \Big(\frac{d}{dt} - i\omega\Big)\Big(\frac{d}{dt} + i\omega\Big)$$

that occurs on the left-hand side first. This leads us to define

$$y(t) = \frac{dx(t)}{dt} + i\omega x(t), \tag{7.63}$$

with $y(t)$ satisfying

$$\frac{dy(t)}{dt} - i\omega y(t) = \frac{1}{m}J(t). \tag{7.64}$$

Multiplying both sides of (7.64) by the integrating factor $e^{-i\omega t}$ and integrating from t_1 to t results in

$$y(t) = e^{i\omega(t-t_1)}y(t_1) + \frac{1}{m}\int_{t_1}^{t} d\tau\, J(\tau)e^{i\omega(t-\tau)}. \tag{7.65}$$

If we take $t_1 < t_-$, then the lower limit on the integral in (7.65) can be taken as t_- since $J(\tau) = 0$ for $\tau < t_-$. Using (7.63) and taking the imaginary part of both sides of (7.65) leads to

$$x(t) = x_1 \cos\omega(t-t_1) + \frac{1}{\omega}\dot{x}(t_1)\sin\omega(t-t_1) + \frac{1}{m\omega}\int_{t_-}^{t} d\tau\, J(\tau)\sin\omega(t-\tau). \tag{7.66}$$

We can now use $x(t_2) = x_2$ and (7.60) to find

$$\begin{aligned} p_1 = m\dot{x}(t_1) = {} & \frac{m\omega}{\sin\omega(t_2-t_1)}[x_2 - x_1\cos\omega(t_2-t_1)] \\ & - \frac{1}{\sin\omega(t_2-t_1)}\int_{t_-}^{t_+} d\tau\, J(\tau)\sin\omega(t_2-\tau). \end{aligned} \tag{7.67}$$

We have chosen $t_2 > t_+$ so that the upper limit in the integral may be taken as t_+ instead of t_2.

We can find p_2 from $p_2 = m\dot{x}(t_2)$ with $\dot{x}(t_2)$ found by first differentiating (7.66) with respect to t and then setting $t = t_2$. This results in

$$\begin{aligned} p_2 = {} & \frac{m\omega}{\sin\omega(t_2-t_1)}[x_2\cos\omega(t_2-t_1) - x_1] \\ & + \frac{1}{\sin\omega(t_2-t_1)}\int_{t_-}^{t_+} d\tau\, J(\tau)\sin\omega(\tau-t_1). \end{aligned} \tag{7.68}$$

With $J(\tau) = 0$, the results for p_1 and p_2 reduce to those in (7.52) and (7.53). We also note that because the source only alters the solution for $x(t)$ by an additive term which is a multiple of the identity operator, the result for $[x(t), x(t')]$ will be unchanged from that of the simple harmonic oscillator. In particular, (7.54) still applies.

We now wish to evaluate $\mathcal{W}_{21}$. First of all, note that from (7.8) and (7.10) with p_1 and p_2 determined by (7.67) and (7.68) we have

$$\mathcal{W}_{21} = \frac{m\omega}{2\sin\omega(t_2-t_1)}[(x_1^2+x_2^2)\cos\omega(t_2-t_1) - 2x_2x_1] + \frac{i\hbar}{2}\ln\Big[\frac{2\pi i\hbar\sin\omega(t_2-t_1)}{m\omega}\Big] + \frac{1}{\sin\omega(t_2-t_1)}[x_2I_1 + x_1I_2] + F(t_2,t_1) \tag{7.69}$$

where

$$I_1 = \int_{t_-}^{t_+} d\tau\, J(\tau)\sin\omega(\tau - t_1), \tag{7.70}$$

$$I_2 = \int_{t_-}^{t_+} d\tau\, J(\tau)\sin\omega(t_2 - \tau), \tag{7.71}$$

with $F(t_2,t_1)$ some as yet unknown function of t_1 and t_2. The first two terms in (7.69) are just those found for the simple harmonic oscillator in (7.57).

We now need to solve (7.9) and (7.11). Unlike the free particle or the simple harmonic oscillator where $H(t_2) = H(t_1)$, this time the energy of the oscillator is not conserved because of the external forcing term. From $(d/dt)H(t) = (\partial/\partial t)H(t)$ we find

$$\frac{d}{dt}H(t) = -\dot{J}(t)x(t), \tag{7.72}$$

if (7.59) is used. Integration of both sides of (7.72) from $t = t_1$ to $t = t_2$ gives

$$\begin{aligned} H(t_2) &= H(t_1) - \int_{t_1}^{t_2} d\tau \frac{dJ(\tau)}{d\tau}x(\tau) \\ &= H(t_1) + \int_{t_-}^{t_+} d\tau\, J(\tau)\dot{x}(\tau). \end{aligned} \tag{7.73}$$

The last line has followed from the previous one by integrating by parts and using the fact that $J(\tau)$ vanishes for $\tau < t_-$ and $\tau > t_+$.

We can evaluate $H(t_2)$ directly from (7.59) and (7.68) to be

$$H(t_2) = \frac{m\omega^2}{2\sin^2\omega(t_2-t_1)}[x_1^2 + x_2^2 - (x_1x_2 + x_2x_1)\cos\omega(t_2-t_1)] + \frac{\omega}{\sin^2\omega(t_2-t_1)}[x_2\cos\omega(t_2-t_1) - x_1]I_1 + \frac{I_1^2}{2m\sin^2\omega(t_2-t_1)}. \tag{7.74}$$

Partial differentiation of (7.69) with respect to t_2 and comparison with $-H(t_2)$ results in

$$\frac{\partial}{\partial t_2}F(t_2,t_1) = -\frac{I_1^2}{2m\sin^2\omega(t_2-t_1)}. \tag{7.75}$$

(Note that (7.54) was used to write $H(t_2)$ in (7.74) in well-ordered form.)

We can also find $H(t_1)$ in a similar manner to be

$$\begin{aligned} H(t_1) = &\frac{m\omega^2}{2\sin^2\omega(t_2-t_1)}[x_1^2+x_2^2-(x_1x_2+x_2x_1)\cos\omega(t_2-t_1)] \\ &-\frac{\omega}{\sin^2\omega(t_2-t_1)}[x_2\cos\omega(t_2-t_1)-x_1]I_2 \\ &+\frac{I_2^2}{2m\sin^2\omega(t_2-t_1)}. \end{aligned} \tag{7.76}$$

Partial differentiation of (7.69) with respect to t_1 and comparison with $H(t_1)$ results in

$$\frac{\partial}{\partial t_1}F(t_2,t_1) = \frac{I_2^2}{2m\sin^2\omega(t_2-t_1)}. \tag{7.77}$$

To integrate (7.75) and (7.77) we will first consider I_2^2. Using (7.71) we have

$$I_2^2 = \int_{t_-}^{t_+} d\tau \int_{t_-}^{t_+} d\tau' J(\tau)J(\tau')\sin\omega(t_2-\tau)\sin\omega(t_2-\tau').$$

The following trigonometric identity

$$\sin\omega(t_2-\tau) = \sin\omega(t_1-\tau)\cos\omega(t_2-t_1) + \cos\omega(t_1-\tau)\sin\omega(t_2-t_1)$$

may be used to give

$$I_2^2 = -\cos\omega(t_2-t_1)I_1I_2 - \frac{1}{\omega}\sin\omega(t_2-t_1)I_2\frac{\partial}{\partial t_1}I_1, \tag{7.78}$$

noting (7.70). Because I_2 does not involve t_1, we can write (7.77) as

$$\frac{\partial}{\partial t_1}F(t_2,t_1) = -\frac{1}{2m\omega}\frac{\partial}{\partial t_1}\Big[\frac{I_1I_2}{\sin\omega(t_2-t_1)}\Big] \tag{7.79}$$

where the right-hand side is now a complete partial derivative.

In a similar way, from (7.70) we have

$$I_1^2 = \int_{t_-}^{t_+} d\tau \int_{t_-}^{t_+} d\tau' J(\tau)J(\tau') \sin\omega(\tau - t_1) \sin\omega(\tau' - t_1)$$
$$= -\cos\omega(t_2 - t_1) I_1 I_2 + \frac{1}{\omega} \sin\omega(t_2 - t_1) I_1 \frac{\partial}{\partial t_2} I_2. \tag{7.80}$$

Because I_1 does not depend on t_2 we can write (7.75) as

$$\frac{\partial}{\partial t_2} F(t_2, t_1) = -\frac{1}{2m\omega} \frac{\partial}{\partial t_2} \Big[\frac{I_1 I_2}{\sin\omega(t_2 - t_1)} \Big]. \tag{7.81}$$

It now follows from (7.79) and (7.81) that

$$F(t_2, t_1) = -\frac{I_1 I_2}{2m\omega \sin\omega(t_2 - t_1)}. \tag{7.82}$$

Requiring $\mathcal{W}_{21}$ to reduce to the result for the simple harmonic oscillator when $J(t) = 0$ fixes the constant of integration in (7.82) to vanish. We therefore have

$$\mathcal{W}_{21} = \frac{m\omega}{2\sin\omega(t_2 - t_1)} [(x_1^2 + x_2^2)\cos\omega(t_2 - t_1) - 2x_2 x_1]$$
$$+ \frac{i\hbar}{2} \ln \Big[\frac{2\pi i\hbar \sin\omega(t_2 - t_1)}{m\omega} \Big]$$
$$+ \frac{1}{\sin\omega(t_2 - t_1)} \int_{t_-}^{t_+} d\tau\, J(\tau) [x_2 \sin\omega(\tau - t_1) + x_1 \sin\omega(t_2 - \tau)]$$
$$- \frac{1}{2m\omega \sin\omega(t_2 - t_1)} \int_{t_-}^{t_+} d\tau \int_{t_-}^{t_+} d\tau' J(\tau)J(\tau')$$
$$\times \sin\omega(\tau - t_1) \sin\omega(t_2 - \tau'). \tag{7.83}$$

We can also work out how much energy is transferred to the oscillator by the forcing term. From (7.63) and (7.73) we have

$$\Delta E = H(t_2) - H(t_1) = \mathcal{R} \int_{t_-}^{t_+} dt\, J(t) y(t). \tag{7.84}$$

Using (7.65) it can be seen that

$$\Delta E = \int_{t_-}^{t_+} dt \int_{t_-}^{t} dt' J(t)J(t') \frac{1}{m} \cos\omega(t - t')$$
$$+ \mathcal{R} \int_{t_-}^{t_+} dt\, J(t) e^{i\omega(t - t_1)} y(t_1). \tag{7.85}$$

If the oscillator is initially at rest, then we find

$$\Delta E = \int_{t_-}^{t_+} dt \int_{t_-}^{t} dt' J(t) J(t') \frac{1}{m} \cos \omega (t - t') \tag{7.86}$$

which is identical to the result found for the classical forced harmonic oscillator.

7.5 Propagators and energy levels

So far we have only calculated the propagator. Often in quantum theory we are interested in the energy spectrum of a given system rather than the transition amplitude between two states. The Schwinger action principle, although ideally suited for the calculation of transition amplitudes, does not yield the energy spectrum in any immediately obvious way. Since all of the information that we might be interested in should be contained in the propagator, there must be some way of extracting the energy spectrum from it. This is the main goal of this section. We will present a general discussion of advanced and retarded propagators, followed by applications to the free particle and simple harmonic oscillator to show how everything works.

7.5.1 Advanced and retarded propagators

The propagator is an example of a Green's function. Green function techniques are useful not only in classical physics, such as electromagnetic theory (Jackson, 1962), but are also central to the development of quantum field theory.[3] So apart from studying the role of Green's functions in the extraction of the energy levels, it is also useful to know a bit more about them for later developments.

The propagator $\langle \mathbf{x}'', t_2 | \mathbf{x}', t_1 \rangle$ has been defined to be the transition amplitude between two position eigenstates in the Heisenberg picture. It proves convenient to change notation slightly and adopt

$$K(t'', \mathbf{x}''; t', \mathbf{x}') = \langle \mathbf{x}'', t'' | \mathbf{x}', t' \rangle. \tag{7.87}$$

By taking $t'' \to t'$ in (7.87) we see that

$$K(t', \mathbf{x}''; t', \mathbf{x}') = \delta(\mathbf{x}'', \mathbf{x}'). \tag{7.88}$$

[3] See Bjorken and Drell (1964, 1965) for example.

The propagator can be expressed in terms of Schrödinger picture eigenstates by making use of the time evolution operator $U(t'', t')$ as found in (3.40). This gives

$$K(t'', \mathbf{x}''; t', \mathbf{x}') = \langle \mathbf{x}'' | U(t'', t') | \mathbf{x}' \rangle. \tag{7.89}$$

If we now specialize to time-independent Hamiltonians, then we know from (3.22) that $U(t'', t') = \exp\left[-(i/\hbar)(t'' - t')H\right]$. Energy eigenstates $|n'\rangle$ of the Hamiltonian can be defined by

$$H|n'\rangle = E_{n'}|n'\rangle, \tag{7.90}$$

where $E_{n'}$ are the energy levels of the system. The identification of $E_{n'}$ from the propagator $K(t'', \mathbf{x}''; t', \mathbf{x}')$ is one of our main goals. By inserting a complete set of energy eigenstates into (7.89) and noting that

$$U(t'', t')|n'\rangle = \exp\left[-\frac{i}{\hbar}(t'' - t')E_{n'}\right]|n'\rangle,$$

we find

$$K(t'', \mathbf{x}''; t', \mathbf{x}') = \sum_{n'} e^{-(i/\hbar)(t''-t')E_{n'}} \langle \mathbf{x}''|n'\rangle\langle n'|\mathbf{x}'\rangle. \tag{7.91}$$

This provides one way of identifying $E_{n'}$ from a knowledge of the propagator $K(t'', \mathbf{x}''; t', \mathbf{x}')$; simply take $K(t'', \mathbf{x}''; t', \mathbf{x}')$ as calculated from the Schwinger action principle, write it in the form (7.91), and read off $E_{n'}$. However, if you look back at the propagators for a free particle in (7.39) or the simple harmonic oscillator in (7.58) it is not immediately transparent how to rewrite the results in the form of (7.91). It would therefore be easier if we could find a more direct and general method starting with the propagator $K(t'', \mathbf{x}''; t', \mathbf{x}')$ in any form and identifying the energy levels.

We are typically interested in Hamiltonians that are local in the sense that

$$\langle \mathbf{x}'|H|n'\rangle = H_{\mathbf{x}'}\langle \mathbf{x}'|n'\rangle, \tag{7.92}$$

for some differential operator $H_{\mathbf{x}'}$. For example, the standard Hamiltonian of non-relativistic quantum mechanics $H = \mathbf{p}^2/(2m) + V(\mathbf{x})$ obeys (7.92) with $H_{\mathbf{x}'} = -(\hbar^2/2m)\nabla'^2 + V(\mathbf{x}')$. Operating on both sides of (7.90) with $\langle \mathbf{x}'|$ and using (7.92) gives

$$H_{\mathbf{x}'}\langle \mathbf{x}'|n'\rangle = E_{n'}\langle \mathbf{x}'|n'\rangle, \tag{7.93}$$

which can be recognized as the time-independent Schrödinger equation with $\langle \mathbf{x}'|n'\rangle$ the wave function written in Dirac notation. It follows from (7.91) and (7.93) that

$$i\hbar\frac{\partial}{\partial t''}K(t'', \mathbf{x}''; t', \mathbf{x}') = H_{\mathbf{x}''}K(t'', \mathbf{x}''; t', \mathbf{x}'), \tag{7.94}$$

showing that the propagator satisfies the time-dependent Schrödinger equation.[4]

The usual situation is that we are interested in $t'' > t'$ in order to study how a state evolves with time. However, in all that we have written down it makes no difference whether we take $t'' > t'$ or $t'' < t'$. We will define the retarded propagator $K_r(t'', \mathbf{x}''; t', \mathbf{x}')$ by

$$K_r(t'', \mathbf{x}''; t', \mathbf{x}') = \begin{cases} 0, & \text{if } t'' < t'; \\ K(t'', \mathbf{x}''; t', \mathbf{x}'), & \text{if } t'' \geq t'; \end{cases} \tag{7.95}$$

and the advanced propagator $K_a(t'', \mathbf{x}''; t', \mathbf{x}')$ by

$$K_a(t'', \mathbf{x}''; t', \mathbf{x}') = \begin{cases} K(t'', \mathbf{x}''; t', \mathbf{x}'), & \text{if } t'' \leq t'; \\ 0, & \text{if } t'' > t'. \end{cases} \tag{7.96}$$

By defining the step function, or Heaviside distribution, $\theta(\tau)$ by

$$\theta(\tau) = \begin{cases} 1, & \text{if } \tau > 0; \\ 0, & \text{if } \tau < 0; \end{cases} \tag{7.97}$$

and

$$\theta(0) = \lim_{\tau \to 0} \theta(\tau), \tag{7.98}$$

with the limit taken from above if $\tau > 0$ and from below if $\tau < 0$, we can write (7.95) and (7.96) succinctly as

$$K_r(t'', \mathbf{x}''; t', \mathbf{x}') = \theta(t'' - t') K(t'', \mathbf{x}''; t', \mathbf{x}'), \tag{7.99}$$

$$K_a(t'', \mathbf{x}''; t', \mathbf{x}') = \theta(t' - t'') K(t'', \mathbf{x}''; t', \mathbf{x}'). \tag{7.100}$$

A useful integral representation for $\theta(\tau)$ when $\tau \neq 0$ is

$$\theta(\tau) = -\frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{e^{-i\omega\tau}}{\omega + i\epsilon} \, d\omega, \tag{7.101}$$

where $\epsilon \to 0$ is understood. The equivalence of (7.101) with (7.97) can be shown by considering a contour in the complex ω-plane extending along the real ω-axis and closed with a semi-circle in either the upper or lower half-plane. Writing the complex variable $\omega = \omega_R + i\omega_I$ with $\omega_R(\omega_I)$ the real (imaginary) parts we have $e^{-i\omega\tau} = e^{\omega_I \tau} e^{-i\omega_R \tau}$. It then follows that if $\tau > 0$ we must close the contour in the lower half-plane to ensure that the contribution coming from the semi-circle vanishes as the radius is extended to infinity. This encloses a simple pole at $\omega = -i\epsilon$ and the

[4] This result can also be deduced from (7.89) and (3.20).

residue theorem gives the result of $+1$ for the contour integral.[5] When $\tau < 0$ we must close the contour in the upper half-plane in order that the contribution coming from the semi-circular arc vanishes as the radius extends to infinity. This time no poles are enclosed, and the residue theorem (or Cauchy's theorem) tells us that the contour integral vanishes. This proves the equivalence between (7.101) and (7.97).

If we differentiate (7.97) it is obvious that $\theta'(\tau)$ vanishes everywhere except at $\tau = 0$ where it is discontinuous. This indicates a possible connection with the Dirac δ-distribution. One way to see this connection is to differentiate (7.101) with respect to τ, let $\epsilon \to 0$, and note that we are left with the integral representation of the Dirac δ-distribution. To establish this connection in another way, let $f(\tau)$ be any differentiable function which is well behaved as $\tau \to \pm\infty$ and at $\tau = 0$. Consider $\int_{-\infty}^{\infty} \theta'(\tau) f(\tau) d\tau$ and perform an integration by parts, followed by use of the definition (7.97)

$$\begin{aligned}\int_{-\infty}^{\infty} d\tau \theta'(\tau) f(\tau) &= \int_{-\infty}^{\infty} d\tau \left\{ \frac{d}{d\tau} \left[\theta(\tau) f(\tau)\right] - \theta(\tau) f'(\tau) \right\} \\ &= \theta(\tau) f(\tau)|_{-\infty}^{\infty} - \int_{0}^{\infty} d\tau f'(\tau) \\ &= f(0). \end{aligned} \tag{7.102}$$

The second term on the right-hand side in the second line has used the property (7.97) of $\theta(\tau)$ to replace the lower limit of the integral with 0. The last line has used the assumed finiteness of $f(\tau)$ at $\tau = 0, \infty$. From (7.102) it can be seen that $\theta'(\tau)$ has exactly the same property as the Dirac δ-distribution, so we have established the distributional identity

$$\theta'(\tau) = \delta(\tau). \tag{7.103}$$

If we now differentiate both sides of (7.99) with respect to t'' and use (7.103) we find that the retarded propagator satisfies

$$\left(i\hbar \frac{\partial}{\partial t''} - H_{\mathbf{x}''} \right) K_r(t'', \mathbf{x}''; t', \mathbf{x}') = i\hbar \delta(t'' - t') \delta(\mathbf{x}'', \mathbf{x}'). \tag{7.104}$$

We have also used the results (7.88) and (7.94) for $K(t'', \mathbf{x}''; t', \mathbf{x}')$ here. In a similar way, from (7.100) we find

$$\left(i\hbar \frac{\partial}{\partial t''} - H_{\mathbf{x}''} \right) K_a(t'', \mathbf{x}''; t', \mathbf{x}') = -i\hbar \delta(t'' - t') \delta(\mathbf{x}'', \mathbf{x}'). \tag{7.105}$$

[5] Note that there is a factor of -1 because the contour is traversed in the clockwise sense.

Note the sign difference on the right-hand side of (7.105) when compared with (7.104) comes about because

$$\frac{\partial}{\partial t''}\theta(t'-t'') = -\delta(t'-t'')$$

from (7.103). It can be seen from (7.95) and (7.96), or else from (7.99) and (7.100) with $\theta(\tau)+\theta(-\tau)=1$, that

$$K_r(t'',\mathbf{x}'';t',\mathbf{x}') + K_a(t'',\mathbf{x}'';t',\mathbf{x}') = K(t'',\mathbf{x}'';t',\mathbf{x}'). \tag{7.106}$$

Now suppose that we set $t''=t'+\tau$ in $K_r(t'',\mathbf{x}'';t',\mathbf{x}')$, so that we have $\tau\geq 0$, and take the Fourier transform:

$$K_r(\mathbf{x}'',\mathbf{x}';E) = \int_{-\infty}^{\infty} d\tau\, \exp\left(\frac{i}{\hbar}E\tau\right) K_r(t'+\tau,\mathbf{x}'';t',\mathbf{x}'). \tag{7.107}$$

(Note that there is no harm in extending the integration range to $-\infty$ because $K_r(t'',\mathbf{x}'';t',\mathbf{x}')$ vanishes if $\tau<0$.) The inverse of (7.107) reads

$$K_r(t'+\tau,\mathbf{x}'';t',\mathbf{x}') = \int_{-\infty}^{\infty} \frac{dE}{2\pi\hbar}\, \exp\left(-\frac{i}{\hbar}E\tau\right) K_r(\mathbf{x}'',\mathbf{x}';E). \tag{7.108}$$

By making use of the fact that $K_r(t'+\tau,\mathbf{x}'';t',\mathbf{x}')$ satisfies (7.104) it is easy to show that

$$(H_{\mathbf{x}''}-E)\,K_r(\mathbf{x}'',\mathbf{x}';E) = -i\hbar\delta(\mathbf{x}'',\mathbf{x}'). \tag{7.109}$$

We may now write

$$K_r(\mathbf{x}'',\mathbf{x}';E) = \sum_{n'}\langle\mathbf{x}''|n'\rangle\langle n'|\mathbf{x}'\rangle K_r(E;n'), \tag{7.110}$$

and using (7.109) along with (7.93) find

$$(E_{n'}-E)\,K_r(E;n') = -i\hbar. \tag{7.111}$$

This shows that $K_r(E;n')$ has simple poles at $E\neq E_{n'}$. It is therefore necessary to give a prescription for dealing with the poles at $E=E_{n'}$. This can be found by demanding that all of the results that we have found for $K_r(t'',\mathbf{x}'';t',\mathbf{x}')$ be consistent. If we combine (7.111), (7.110) and (7.108) we find (restoring $t''=t'+\tau$)

$$K_r(t'',\mathbf{x}'';t',\mathbf{x}') = i\sum_{n'}\langle\mathbf{x}''|n'\rangle\langle n'|\mathbf{x}'\rangle \int_{-\infty}^{\infty}\frac{dE}{2\pi}\,\frac{\exp\left[-(i/\hbar)E(t''-t')\right]}{E-E_{n'}}.$$

The integral that appears on the right-hand side must result in

$$\theta(t''-t')\exp\left[-\frac{i}{\hbar}(t''-t')E_{n'}\right]$$

as can be seen from (7.91) and (7.99). In order that this be so, from the integral representation of the step function in (7.101) it follows that we should replace E with $E+i\epsilon$ in the denominator. This motivates the definition

$$K_r(E;n') = \frac{i\hbar}{E-E_{n'}+i\epsilon} \tag{7.112}$$

with $\epsilon \to 0$ understood. This choice of an $i\epsilon$ prescription ensures that we will obtain the retarded propagator.

We can obtain a similar result for the advanced propagator. Leaving out the details, since they are very similar to what we have just discussed, we have

$$K_a(E;n') = \frac{-i\hbar}{E-E_{n'}-i\epsilon} \tag{7.113}$$

with the label r interchanged with a in (7.110). The overall sign change here relative to (7.112) is attributable to that in front of $\delta(t''-t')$ in (7.105). The different $i\epsilon$ prescription ensures that the advanced propagator is obtained.

The results in (7.112) and (7.113) show us another way to identify the energy levels of a system; namely, study the analytical properties of the Fourier transform of the advanced or retarded propagators. In the $\epsilon \to 0$ limit, the Fourier transforms of these propagators develop poles corresponding to the energy levels of the system. We will illustrate this with two examples.

7.5.2 Free particle

The propagator was derived from the Schwinger action principle in (7.39). We then have

$$K(t'+\tau,x'';t',x') = \left[\frac{m}{2\pi i\hbar\tau}\right]^{1/2}\exp\left[\frac{im(x''-x')^2}{2\hbar\tau}\right] \tag{7.114}$$

if we take $t''=t'+\tau$. By restricting $\tau>0$ we can identify (7.114) with the retarded propagator $K_r(t'+\tau,x'';t',x')$. Using (7.114) in the result (7.107) gives us

$$K_r(x'',x';E) = \int_0^\infty d\tau\left[\frac{m}{2\pi i\hbar\tau}\right]^{1/2}\exp\left[\frac{i}{\hbar}E\tau+\frac{im(x''-x')^2}{2\hbar\tau}\right] \tag{7.115}$$

where E is understood to be $E + i\epsilon$ here due to the $i\epsilon$ prescription discussed in the previous subsection.[6]

The analogue of (7.110) in this case is just the Fourier transform

$$K_r(x'', x'; E) = \int_{-\infty}^{\infty} \frac{dk}{2\pi}\, e^{ik(x''-x')} K_r(E, k). \tag{7.116}$$

Inverting (7.116) and using (7.115) results in

$$\begin{aligned} K_r(E; k) &= \int_0^{\infty} d\tau \Big[\frac{m}{2\pi i\hbar\tau}\Big]^{1/2} e^{(i/\hbar)E\tau} \\ &\quad \times \int_{-\infty}^{\infty} dx'' e^{\left\{\left[im(x''-x')^2/2\hbar\tau\right]-ik(x''-x')\right\}} \\ &= \int_0^{\infty} d\tau\; e^{(i/\hbar)\left[E-(\hbar^2/2m)k^2\right]\tau} \qquad (7.117) \\ &= \frac{i\hbar}{E-(\hbar^2/2m)k^2}. \qquad (7.118) \end{aligned}$$

The last line has followed from the fact that E contains a small positive imaginary part as mentioned above. This ensures that the integration in (7.117) converges.

The result in (7.118) shows us that the energy associated with a system consisting of a single free particle is given by $(\hbar^2 k^2/(2m)$. Identifying the eigenvalue of momentum operator p by $p' = \hbar k$, we see that the energy is the standard result $p'^2/(2m)$ as in classical mechanics.

7.5.3 Simple harmonic oscillator

The propagator was found from the Schwinger action principle in (7.58) and reads

$$\begin{aligned} K(t'+\tau, x''; t', x') &= \Big[\frac{m\omega}{2\pi i\hbar \sin\omega\tau}\Big]^{1/2} \\ &\quad \times \exp\Big\{\frac{im\omega}{2\hbar\sin\omega\tau}[(x'^2+x''^2)\cos\omega\tau - 2x'x'']\Big\}. \end{aligned} \tag{7.119}$$

with the replacement $t'' = t' + \tau$. Assuming $\tau > 0$, this can be viewed as the retarded propagator $K_r(t'+\tau, x''; t', x')$, and can be used in (7.107) to express $K_r(x'', x'; E)$ as an integral. We are after $K_r(E; n')$ since the

[6] Note that because $K_r(t'+\tau, x''; t', x')$ vanishes for $\tau < 0$, the lower limit on the integration in (7.107) can be replaced with 0.

poles of this as a function of E determines the energy spectrum. This can be found most easily by setting $x'' = x'$ in (7.110) and integrating both sides with respect to x':

$$\int_{-\infty}^{\infty} dx' K_r(x', x'; E) = \sum_{n'} K_r(E; n') \tag{7.120}$$

$$= \sum_{n'} \frac{i\hbar}{E - E_{n'}} \tag{7.121}$$

We have used the completeness of the position eigenstates and (7.112). If we use (7.119) in (7.107) and perform the integration over x', but not over τ, we find

$$\int_{-\infty}^{\infty} dx' K_r(x', x'; E) = \int_0^{\infty} d\tau \; e^{(i/\hbar)E\tau} \left[2(\cos\omega\tau - 1)\right]^{-1/2}. \tag{7.122}$$

Noting that

$$\left[2(\cos\omega\tau - 1)\right]^{-1/2} = \sum_{n=0}^{\infty} e^{-i(n+1/2)\omega\tau},$$

we obtain

$$\int_{-\infty}^{\infty} dx' K_r(x', x'; E) = \sum_{n=0}^{\infty} \frac{i\hbar}{E - (n + 1/2)\hbar\omega}, \tag{7.123}$$

again using the $i\epsilon$ prescription that gives E a small positive imaginary part. From (7.123) we can read off the quantized energy levels $(n+1/2)\hbar\omega$ that agree with the more standard derivation in Section 3.5.

7.6 General variation of the Lagrangian

In the applications of the Schwinger action principle that have been considered in Chapter 3 and in the present chapter we have only considered variations of the transformation function in the end times or positions. However the action principle is claimed to be valid for any type of variation. One type of variation that we have not considered is one in which the structure of the Lagrangian itself is altered. For the free particle or simple harmonic oscillator the only variables in the Lagrangian that we can alter are the mass or frequency which are both constant. This does not lead to anything new. However for the forced harmonic oscillator considered in Section 7.4 we can alter the driving force $J(t)$. This variation is not simply related to the endpoint variations that were utilized earlier.

We will show how a variation in the structure of the Lagrangian can be used as the basis for a perturbative treatment of the theory.

We had

$$\delta\langle a_2', t_2|a_1', t_1\rangle = \frac{i}{\hbar}\langle a_2', t_2|\delta W_{21}|a_1', t_1\rangle \tag{7.124}$$

as our expression of the Schwinger action principle. (This was the result in (3.52) of Section 3.2). Suppose that the variation in (7.124) refers to a variation in the structure of the Lagrangian of the system with the endpoints held fixed. In this case we can write

$$\delta W_{21} = \int_{t_1}^{t_2} dt\, \delta L(t), \tag{7.125}$$

with $\delta L(t)$ representing the variation of the Lagrangian operator, whatever that might be. The general action principle, expressed in (7.124), can then be written as

$$\delta\langle a_2', t_2|a_1', t_1\rangle = \frac{i}{\hbar}\int_{t_1}^{t_2} dt\langle a_2', t_2|\delta L(t)|a_1', t_1\rangle. \tag{7.126}$$

By inserting complete sets of states taken at the time t in the manner indicated below, this last result can be rewritten as

$$\delta\langle a_2', t_2|a_1', t_1\rangle = \frac{i}{\hbar}\int_{t_1}^{t_2} dt \sum_{b_1'}\sum_{b_2'}\langle a_2', t_2|b_2', t\rangle\langle b_2', t|\delta L(t)|b_1', t\rangle\langle b_1', t|a_1', t_1\rangle. \tag{7.127}$$

Now suppose that we perform another infinitesimal variation of the Lagrangian, independent of the one that we have just done. If we denote the first variation that resulted in (7.127) by δ_1, and use δ_2 to denote the second variation, we find

$$\begin{aligned}\delta_2\delta_1\langle a_2', t_2|a_1', t_1\rangle = \frac{i}{\hbar}\int_{t_1}^{t_2} dt \sum_{b_1'}\sum_{b_2'}\Big[&(\delta_2\langle a_2', t_2|b_2', t\rangle)\,\langle b_2', t|\delta_1 L(t)|b_1', t\rangle \\ &\times\langle b_1', t|a_1', t_1\rangle + \langle a_2', t_2|b_2', t\rangle\langle b_2', t|\delta_1 L(t)|b_1', t\rangle \\ &\times(\delta_2\langle b_1', t|a_1', t_1\rangle)\Big].\end{aligned} \tag{7.128}$$

(Note that since the second variation in the structure of the Lagrangian is independent of the first, there is no term like $\delta_2\langle b_2', t|\delta_1 L(t)|b_1', t\rangle$ in (7.128).) The terms that involve the variation δ_2 that occur on the right-hand side of (7.128) can be expressed as

$$\delta_2\langle a_2', t_2|b_2', t\rangle = \frac{i}{\hbar}\int_{t_1}^{t_2} dt'\langle a_2', t_2|\delta_2 L(t')|b_2', t\rangle,$$
$$\delta_2\langle b_1', t|a_1', t_1\rangle = \frac{i}{\hbar}\int_{t_1}^{t_2} dt'\langle b_1', t|\delta_2 L(t')|a_1', t_1\rangle,$$

if we use (7.126). The completeness relation for the kets $|b_1', t\rangle$ and $|b_2', t\rangle$ allows us to write (7.128) as

$$\begin{aligned}\delta_2\delta_1\langle a_2', t_2|a_1', t_1\rangle = &\left(\frac{i}{\hbar}\right)^2\int_{t_1}^{t_2} dt\int_{t}^{t_2} dt'\langle a_2', t_2|\delta_2 L(t')\delta_1 L(t)|a_1', t_1\rangle \\ &+\left(\frac{i}{\hbar}\right)^2\int_{t_1}^{t_2} dt\int_{t_1}^{t} dt'\langle a_2', t_2|\delta_1 L(t)\delta_2 L(t')|a_1', t_1\rangle.\end{aligned} \tag{7.129}$$

If we utilize the time-ordering symbol introduced in Section 3.1.2, the result in (7.129) can be expressed in a more compact form. We have, by definition of time ordering,

$$T\left[\delta_1 L(t)\delta_2 L(t')\right] = \theta(t-t')\delta_1 L(t)\delta_2 L(t') + \theta(t'-t)\delta_2 L(t')\delta_1 L(t). \tag{7.130}$$

(Compare this with (3.27).) Using the time-ordering symbol, it is easy to see that (7.129) can be rewritten as

$$\delta_2\delta_1\langle a_2', t_2|a_1', t_1\rangle = \left(\frac{i}{\hbar}\right)^2\int_{t_1}^{t_2} dt\int_{t}^{t_2} dt'\langle a_2', t_2|T\left[\delta_1 L(t)\delta_2 L(t')\right]|a_1', t_1\rangle. \tag{7.131}$$

From this result it is clear that the order in performing the two variations is irrelevant. The extension of (7.131) to an arbitrary number of variations is straightforward and results in

$$\begin{aligned}\delta_1\cdots\delta_n\langle a_2', t_2|a_1', t_1\rangle = &\left(\frac{i}{\hbar}\right)^n\int_{t_1}^{t_2} dt_1'\cdots\int_{t}^{t_2} dt_n' \\ &\times\langle a_2', t_2|T\left[\delta_1 L(t_1')\cdots\delta_n L(t_n')\right]|a_1', t_1\rangle.\end{aligned} \tag{7.132}$$

Here $\delta_1, \ldots, \delta_n$ represent n independent variations.

In order to show the utility of this result, we can use it to make contact with the time-development operator in the interaction picture. Suppose that the Lagrangian operator can be written as

$$L(t) = L_0(t) + L_1(t) \tag{7.133}$$

for some operators $L_0(t)$ and $L_1(t)$. Furthermore, suppose that when we set $L_1(t) = 0$ the transition amplitude for the Lagrangian $L_0(t)$ is known.

We can evaluate the amplitude for the theory whose Lagrangian is given by (7.133) by treating $L_1(t)$ perturbatively. In order to do this, introduce a continuous parameter λ and write

$$L_\lambda(t) = L_0(t) + \lambda L_1(t). \tag{7.134}$$

If we take $\lambda = 0$, then $L_\lambda(t)$ reduces to $L_0(t)$ with a known transition amplitude. When we take $\lambda = 1$, $L_\lambda(t)$ becomes the Lagrangian in (7.133) whose amplitude we wish to know.

When the Lagrangian is taken as in (7.134), we can regard the amplitude $\langle a_2', t_2 | a_1', t_1\rangle$ as a function of λ. The aim is to compute this amplitude as a Taylor series in λ. From (7.126) we have

$$\frac{\partial}{\partial\lambda}\langle a_2', t_2 | a_1', t_1\rangle = \frac{i}{\hbar}\int_{t_1}^{t_2} dt \langle a_2', t_2 | L_1(t) | a_1', t_1\rangle. \tag{7.135}$$

Using (7.132) we find

$$\frac{\partial^n}{\partial\lambda^n}\langle a_2', t_2 | a_1', t_1\rangle = \left(\frac{i}{\hbar}\right)^n \int_{t_1}^{t_2} dt_1' \cdots \int_{t_1}^{t_2} dt_n' \langle a_2', t_2 | T\left[L_1(t_1') \cdots L_1(t_n')\right] | a_1', t_1\rangle. \tag{7.136}$$

We now expand $\langle a_2', t_2 | a_1', t_1\rangle$ in a Taylor series in λ about $\lambda = 0$ to obtain

$$\begin{aligned}\langle a_2', t_2 | a_1', t_1\rangle &= \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} \frac{\partial^n}{\partial\lambda^n}\langle a_2', t_2 | a_1', t_1\rangle\Big|_{\lambda=0} \\ &= \sum_{n=0}^{\infty} \frac{\lambda^n}{n!}\left(\frac{i}{\hbar}\right)^n \int_{t_1}^{t_2} dt_1' \cdots \int_{t_1}^{t_2} dt_n' \\ &\quad \times \langle a_2', t_2 | T\left[L_1(t_1') \cdots L_1(t_n')\right] | a_1', t_1\rangle|_{\lambda=0}. \end{aligned} \tag{7.137}$$

If we set $\lambda = 1$, so that the Lagrangian operator becomes equal to that in (7.133), we find

$$\langle a_2', t_2 | a_1', t_1\rangle = \langle a_2', t_2 | T\left[\exp\frac{i}{\hbar}\int_{t_1}^{t_2} dt' L_1(t')\right] | a_1', t_1\rangle\Big|_{\lambda=0} \tag{7.138}$$

by summing the series and using the definition of the time-ordered exponential function defined earlier in Section 3.1.2. The states that appear on the right-hand side of (7.138) have their time development determined by using the Hamiltonian H_0 that is obtained from the Lagrangian L_0, since the right-hand side is evaluated at $\lambda = 0$. This is equivalent to using the interaction picture described in Appendix 3.

7.7 The vacuum-to-vacuum transition amplitude

In this section we will show how the Schwinger action principle may be used to evaluate the vacuum persistence amplitude for the forced harmonic oscillator. The result will then be compared with that found using the interaction picture described in Appendix 3.

The equation of motion for the position operator for the forced harmonic oscillator is (see (7.62))

$$\ddot{x}(t) + \omega^2 x(t) = \frac{1}{m} J(t). \tag{7.139}$$

Consider $t_1 < t_-$ and $t_2 > t_+$ where $J(t)$, that we will call the source, can be non-zero only for $t_- \leq t \leq t_+$ as before. Let $|\text{in}\rangle$ denote the ground state for $t < t_-$ and $|\text{out}\rangle$ denote the ground state for $t > t_+$. We are interested in $\langle \text{out}|\text{in}\rangle$, and in particular its dependence on the driving force, or source, $J(t)$. This transition amplitude is referred to as the 'vacuum persistence amplitude'.

Suppose that we define

$$\langle F(t)\rangle = \frac{\langle \text{out}|F(t)|\text{in}\rangle}{\langle \text{out}|\text{in}\rangle}, \tag{7.140}$$

where $t_- \leq t \leq t_+$ for any operator $F(t)$. By taking the inner product of (7.139) between the states $|\text{in}\rangle$ and $|\text{out}\rangle$, we have

$$\left(\frac{d^2}{dt^2} + \omega^2\right) \langle x(t)\rangle = \frac{1}{m} J(t). \tag{7.141}$$

The general solution to this can be written as

$$\langle x(t)\rangle = h(t) + \frac{1}{m} \int_{t_-}^{t_+} dt'\, G(t,t') J(t'), \tag{7.142}$$

where $h(t)$ is any solution to the homogeneous equation obtained by setting $J(t) = 0$ in (7.141) and $G(t,t')$ is a solution to

$$\left(\frac{d^2}{dt^2} + \omega^2\right) G(t,t') = \delta(t-t'). \tag{7.143}$$

That is, $G(t,t')$ is a Green function that we must specify.

At this stage we can consider the boundary conditions. If we take $J(t) = 0$, then the ground states $|\text{in}\rangle$ and $|\text{out}\rangle$ are identical, and we will

have $\langle x(t)\rangle = 0$.[7] This means that we must choose $h(t) = 0$ in (7.142).[8] We therefore have

$$\langle x(t)\rangle = \frac{1}{m}\int_{t_-}^{t_+} dt'\, G(t,t')J(t'). \tag{7.144}$$

By taking the functional derivative of this last result with respect to the source $J(t')$ we find

$$\frac{\delta}{\delta J(t')}\langle x(t)\rangle = \frac{1}{m}G(t,t'). \tag{7.145}$$

Note that $G(t,t')$ as defined in (7.143) is independent of $J(t)$, so that further functional derivatives of (7.145) must vanish.

Next, let us write

$$\langle \text{out}|\text{in}\rangle = \exp\left[\frac{i}{\hbar}W[J]\right], \tag{7.146}$$

for some $W[J]$. If we vary both sides of this with respect to $J(t)$ we find

$$\delta\langle \text{out}|\text{in}\rangle = \frac{i}{\hbar}\delta W[J]\exp\left[\frac{i}{\hbar}W[J]\right]. \tag{7.147}$$

The Schwinger action principle (7.126) gives us

$$\begin{aligned}\delta\langle \text{out}|\text{in}\rangle &= \frac{i}{\hbar}\langle \text{out}|\int_{t_1}^{t_2}\delta L(t)dt\ |\text{in}\rangle \\ &= \frac{i}{\hbar}\int_{t_-}^{t_+} dt\,\delta J(t)\langle \text{out}|x(t)|\text{in}\rangle,\end{aligned} \tag{7.148}$$

since $\delta L(t) = \delta J(t)x(t)$ here. Combining (7.147) and (7.148), and making use of the definition (7.140), we find

$$\frac{\delta W[J]}{\delta J(t)} = \langle x(t)\rangle. \tag{7.149}$$

If we now differentiate both sides of (7.149) and use (7.145) we obtain

$$\frac{\delta^2 W[J]}{\delta J(t')\delta J(t)} = \frac{1}{m}G(t,t'). \tag{7.150}$$

[7] This is true because the operator $x(t)$ involves a sum of terms with the creation and annihilation operators a and $a^\dagger$ whose vacuum expectation values both vanish.

[8] Note that as $h(t)$ satisfies the homogeneous equation, it must be independent of the source $J(t)$.

Because $G(t,t')$ is independent of $J(t)$, the solution to this equation may be seen to be

$$W[J] = \frac{1}{2m}\int_{-\infty}^{\infty} dt \int_{-\infty}^{\infty} dt'\, G(t,t')J(t)J(t'). \tag{7.151}$$

Note that $W[J=0]=1$ by (7.146) since the states $|\text{in}\rangle$ and $|\text{out}\rangle$ coincide in this case, and $\left.\dfrac{\delta W[J]}{\delta J(t)}\right|_{J=0} = 0$ from (7.149). We have chosen to extend the limits of integration to $-\infty$ and $+\infty$ since $J(t)$ vanishes as $t \to \pm\infty$ by assumption. The only remaining thing is to discuss which Green function enters here.

We can find the general solution to (7.143) by solving first for $t > t'$ then for $t < t'$ and matching up the two solutions at $t = t'$. Let

$$G(t,t') = \begin{cases} G_<(t,t') & \text{for } t < t', \\ G_>(t,t') & \text{for } t > t'. \end{cases} \tag{7.152}$$

We will require $G(t,t')$ to be continuous at $t = t'$:

$$G_<(t',t') = G_>(t',t'). \tag{7.153}$$

By integrating both sides of (7.143) from $t = t' - \epsilon$ to $t = t' + \epsilon$, followed by taking the $\epsilon \to 0$ limit, we find a second condition

$$\left.\frac{\partial G_>(t,t')}{\partial t}\right|_{t=t'} - \left.\frac{\partial G_<(t,t')}{\partial t}\right|_{t=t'} = 1 \tag{7.154}$$

that the Green function must satisfy.[9]

It is obvious that we can write the solutions to (7.143) when $t \neq t'$ as

$$G_>(t,t') = A_>(t')e^{-i\omega t} + B_>(t')e^{i\omega t}, \tag{7.155}$$

$$G_<(t,t') = A_<(t')e^{-i\omega t} + B_<(t')e^{i\omega t}, \tag{7.156}$$

for some functions $A_>(t'), A_<(t'), B_>(t'), B_<(t')$. The continuity conditions (7.153) and (7.154) at $t = t'$ give us two equations for the four unknown functions. We therefore need two further conditions to specify the solution completely. The conditions that we will choose are that for $t > t_+$, $\langle x(t)\rangle$ contains only positive frequencies (i.e. has a time dependence $e^{-i\omega t}$) and that for $t < t_-$, $\langle x(t)\rangle$ contains only negative frequencies (i.e. has a time dependence $e^{i\omega t}$). As noted by Schwinger (1951c,

[9] The continuity condition implies that the ω^2 term in (7.143) makes no contribution when we let $\epsilon \to 0$.

1953b) the Green function satisfies '... the temporal analogue of the outgoing wave or radiation condition familiar in the spatial description of a harmonic source'. We therefore impose

$$B_>(t') = 0 = A_<(t'). \tag{7.157}$$

The two continuity conditions (7.153) and (7.154) at $t = t'$ give us

$$A_>(t')e^{-i\omega t'} = B_<(t')e^{i\omega t'}, \tag{7.158}$$

and

$$-i\omega A_>(t')e^{-i\omega t'} - i\omega B_<(t')e^{i\omega t'} = 1, \tag{7.159}$$

respectively. The solution to (7.158) and (7.159) is

$$A_>(t') = \frac{i}{2\omega}e^{i\omega t'}, \tag{7.160}$$

$$B_<(t') = \frac{i}{2\omega}e^{-i\omega t'}, \tag{7.161}$$

and therefore

$$G(t,t') = \begin{cases} \frac{i}{2\omega}e^{-i\omega(t-t')} & \text{if } t \geq t', \\ \frac{i}{2\omega}e^{i\omega(t-t')} & \text{if } t \leq t'. \end{cases} \tag{7.162}$$

Alternatively, we can combine the two time intervals of this result and write the single equation

$$G(t,t') = \frac{i}{2\omega}e^{-i\omega|t-t'|}. \tag{7.163}$$

This allows us to see that the result found here for $W[J]$, as a consequence of the boundary conditions employed as described above, agrees with the vacuum persistence amplitude found at the end of Appendix 3.

The particular Green function that we found is known as the 'Feynman Green function' because of its importance in quantum field theory as demonstrated by Feynman (1949a). Because the Feynman Green function plays such a central role in quantum field theory, we will study it a bit further here as a preparation for the next chapter.

Another way to solve (7.143) is by expressing $G(t,t')$ as a Fourier transform. Write

$$G(t,t') = \int_{-\infty}^{\infty} \frac{dk}{2\pi}\, e^{ik(t-t')}G(k). \tag{7.164}$$

We then find

$$(-k^2 + \omega^2)G(k) = 1, \tag{7.165}$$

noting that

$$\delta(t-t') = \int_{-\infty}^{\infty} \frac{dk}{2\pi}\, e^{ik(t-t')}.$$

Provided that $k^2 \neq \omega^2$, the solution for $G(k)$ is obvious; however, the integration goes from $k = -\infty$ to $k = +\infty$ and runs through the points $k = \pm\omega$ where $G(k)$ has simple poles. This means that we must regard (7.164) as a contour integral with an integration path that avoids the poles at $k = \pm\omega$. How we choose this path coincides precisely with the choice that we needed to make in the boundary conditions when we solved for $G(t,t')$ earlier.[10] We therefore must choose a contour that leads us to the result in (7.163).

The contour that we specify in (7.164) can be closed by the addition of a semi-circle of infinite radius. In order that this semi-circle makes no contribution to the result, if $t > t'$ we must close the semi-circle in the upper half of the complex k-plane (so that if $k = iR$, then $e^{ik(t-t')} = e^{-R(t-t')} \to 0$ as $R \to \infty$). Because of our requirement that $G(t,t') \propto e^{-i\omega t}$, this demands that the $k = -\omega$ pole be enclosed. By similar reasoning, for $t < t'$ we choose the semi-circle in the lower half of the complex k-plane and require that $k = \omega$ be enclosed. A simple application of the residue theorem shows that the procedure we have described recovers the Green function in (7.163).

Rather than choose a contour that is indented off the real axis around the poles at $k = \pm\omega$, it is simpler to displace the poles off the real axis and leave the integration as it stands. We need to shift the $k = -\omega$ pole above the real axis (so that it is enclosed by the semi-circle in the upper half of the complex k-plane) and the $k = \omega$ pole below the real axis (so that it is enclosed by the semi-circle in the lower half of the complex k-plane). It is easy to see that this can be accomplished by replacing ω^2 in (7.164) with $\omega^2 - i\epsilon$ with $\epsilon \to 0$ understood. We therefore have the Fourier transform of the Feynman Green function being

$$G(t,t') = -\int_{-\infty}^{+\infty} \frac{dk}{2\pi}\, \frac{e^{ik(t-t')}}{k^2 - \omega^2 + i\epsilon}. \tag{7.166}$$

This '$i\epsilon$' prescription ensures that we obtain the Feynman Green function.

7.8 More general systems

In Chapter 3 we introduced the Schwinger action principle and used it to derive the canonical commutation relations for the position and

[10] Recall that we chose $G(t,t') \propto e^{-i\omega t}$ for $t > t'$ and $G(t,t') \propto e^{i\omega t}$ for $t < t'$.

the momentum, as well as the Heisenberg equations of motion. In these derivations if we assume that the variations of the position and momentum are multiples of the identity operator, so that they commute with all operators, only commutation relations are obtained. If we are to treat fermions, which satisfy anti-commutation relations, our assumption concerning the nature of the infinitesimal variations of position and momentum must be relaxed.[11] In this section we will re-examine the Schwinger action principle in quantum mechanics from a more general standpoint.[12]

If we consider a system of bosons initially, then the Lagrangian operator in (3.68) may be written in the form

$$L = \frac{1}{2}(p\dot{x} + \dot{x}p - \dot{p}x - x\dot{p}) - H(p, x, t) \tag{7.167}$$

if we add an appropriate total time derivative term.[13] If we introduce

$$Q = \begin{pmatrix} x \\ p \end{pmatrix}, \tag{7.168}$$

$$Q^T = (x, p), \tag{7.169}$$

then (7.167) can be rewritten as

$$L = \frac{1}{2}(Q^T A\dot{Q} - \dot{Q}^T AQ) - H(Q, t), \tag{7.170}$$

where

$$A = \frac{1}{2}\begin{pmatrix} 0 & -\mathrm{I} \\ \mathrm{I} & 0 \end{pmatrix}. \tag{7.171}$$

The constant matrix A has the following properties:

$$A^* = A, \qquad A^T = -A, \qquad A^\dagger = -A. \tag{7.172}$$

Suppose that we now consider a more general theory where L is given by (7.170) but where the constant matrix A is not necessarily given by (7.171). We will require A to be independent of Q and $\dot{Q}$, and in order that the Lagrangian operator be Hermitian require

$$A^\dagger = -A. \tag{7.173}$$

[11] This was discussed in Section 3.8 for the Schrödinger field.

[12] This section is not needed for the final chapter and can be omitted by the reader not interested in issues related to the generality of the Schwinger action principle.

[13] We will not bother to explicitly indicate the coordinate indices on the position and momentum here.

The dynamical variables entering L are assumed to be real

$$Q^* = Q. \tag{7.174}$$

We make no further assumptions about the nature of Q, or of the arbitrary variation δQ, at this stage. The action operator is given by

$$W_{21} = \int_{t_1}^{t_2} dt\, L(t), \tag{7.175}$$

with $L(t)$ given in (7.170) and is Hermitian.

Before looking at what the action principle has to say about the quantum theory, we will examine the classical theory based on (7.170) with $A^\dagger = -A$. Any matrix can be decomposed as the sum of a symmetric matrix and an antisymmetric matrix. We can write

$$A = A^s + A^a, \tag{7.176}$$

where

$$A^s = \frac{1}{2}(A + A^T) \tag{7.177}$$

is symmetric, and

$$A^a = \frac{1}{2}(A - A^T) \tag{7.178}$$

is antisymmetric. The Lagrangian L in (7.170) may be written as

$$L = \frac{1}{2}A^s_{ij}(Q_i\dot{Q}_j - \dot{Q}_jQ_i) + \frac{1}{2}A^a_{ij}(Q_i\dot{Q}_j + \dot{Q}_jQ_i) - H(Q,t), \tag{7.179}$$

where the indices i and j are summed over the appropriate range. Even though we are considering a classical theory, we are not making any assumptions about the commutativity properties of the Q_i. Normally we are used to variables where $Q_i\dot{Q}_j = \dot{Q}_jQ_i$. In this case the term in A^s makes no contribution to the Lagrangian and we lose no generality by taking A to be antisymmetric. This was the case for the boson theory we considered in Section 3.3.

There is however another natural possibility for the variables. Consider variables which obey $Q_i\dot{Q}_j = -\dot{Q}_jQ_i$ and $Q_iQ_j = -Q_jQ_i$. With this choice the classical theory is described by anti-commuting coordinates, which although are perhaps strange, are no less consistent than coordinates which commute. We will refer to variables which commute as c-type, and variables which anti-commute as a-type. Schwinger was the first to utilize them in quantum theory, and called them variables of

the first kind and second kind respectively. Our terminology is now more standard.[14]

We will now partition Q into two sets of variables

$$Q = \begin{pmatrix} b \\ f \end{pmatrix} \tag{7.180}$$

where b_i denotes the set of classically commuting variables (i.e. b_i is c-type) and f_α denotes the set of classically anti-commuting variables (i.e. f_α is a-type). We will further assume that the constant matrix A, which obeys (7.173), takes the form

$$A = \begin{pmatrix} A_B & 0 \\ 0 & A_F \end{pmatrix}, \tag{7.181}$$

where

$$A_B^T = -A_B, \tag{7.182}$$

$$A_F^T = A_F. \tag{7.183}$$

More generally, cross-terms in the c-type and a-type variables could be allowed in the Lagrangian. In this case, A is not the direct sum of A_B and A_F as given in (7.181), and the off-diagonal blocks of A must be taken to be a-type matrices. We will not consider this further in what follows.

We will first consider a variation of the initial or the final time. As in Section 3.2 we have

$$\begin{aligned} \delta_t W_{21} &= \int_{t_1+\delta t_1}^{t_2+\delta t_2} dt\, L(t) - \int_{t_1}^{t_2} dt\, L(t) \\ &= \delta t_2\, L(t_2) - \delta t_1\, L(t_1). \end{aligned} \tag{7.184}$$

(We have appended a subscript t to δ on the left-hand side of (7.184) to show that the variation is only with respect to the time.) The result in (7.184) is of the general form in (3.61) with the infinitesimal generator given by

$$G_t(t) = \delta t\, L(t). \tag{7.185}$$

Next, consider a general variation of the dynamical variables $Q(t)$ with the time held fixed. It follows from (7.170) that

$$\delta L(t) = \frac{1}{2}(\delta Q^T A\dot{Q} + Q^T A\delta\dot{Q} - \delta\dot{Q}^T AQ - \dot{Q}^T A\delta Q) - \delta H \tag{7.186}$$

[14] See DeWitt (1984) for example.

where

$$\delta H = H(Q + \delta Q, t) - H(Q, t). \tag{7.187}$$

Equation (7.186) is identical to

$$\delta L(t) = \delta Q^T A \dot{Q} - \dot{Q}^T A \delta Q - \delta H + \frac{1}{2}\frac{d}{dt}(Q^T A \delta Q - \delta Q^T A Q). \tag{7.188}$$

The equations of motion must be contained in

$$\delta Q^T A \dot{Q} - \dot{Q}^T A \delta Q = \delta H, \tag{7.189}$$

and the generator of the infinitesimal transformation of the dynamical variables is

$$G_Q(t) = \frac{1}{2}[Q^T(t) A \delta Q(t) - \delta Q^T(t) A Q(t)]. \tag{7.190}$$

At this stage Schwinger (1970) makes a strong assumption. In computing δH from (7.187), he assumes that it is always possible to write δH in a form where δQ appears on the left or on the right. For conformity with (7.189), this requires δQ to possess simple commutation relations with Q. Furthermore, Schwinger demands that δQ commutes with H. These restrictions are then shown to lead only to commutation or anti-commutation relations for the dynamical variables. It was later realized by other authors (Kibble and Polkinghorne (1958), Kibble (1959), and Bloore and Lovely (1972)) that Schwinger's restrictions could be weakened somewhat, allowing more general possibilities, such as the parastatistics of Green (1953).

We can make a weaker assumption than Schwinger, still based on the form of (7.189), by writing δH in the form

$$\delta H = \delta Q^T H_l + H_r \delta Q \tag{7.191}$$

for some operators H_l and H_r. If δH is to be Hermitian we must require $H_l^\dagger = H_r$. In this case, we have

$$\delta H = \delta Q^T H_l + H_l^\dagger \delta Q. \tag{7.192}$$

It is important to emphasize that this requirement on δH still entails restrictions on the class of allowed variations which may rule out certain theories. If H is more than quadratic in Q, then some assumption must be made about the relation between Q and δQ if δH is to be written in the form (7.192). It is possible to go some way without assuming (7.192),

but at some stage the variations must be restricted in some way if any progress is to be made.[15]

The equations of motion which follow from (7.189) and (7.192) are

$$A\dot{Q} = H_l, \tag{7.193}$$

$$-\dot{Q}^T A = H_l^\dagger. \tag{7.194}$$

It is easy to see that (7.194) is just the Hermitian conjugate of (7.193) if we use the property $A^\dagger = -A$ in (7.173). Assuming that A is invertible, implying that all of the variables are dynamical, we have the solution

$$\dot{Q} = A^{-1} H_l \tag{7.195}$$

to the equations of motion (7.193).

Another possible variation is to alter the structure of $L(t)$ in some way. Suppose that we change $L(t)$ to

$$L_\Lambda(t) = L(t) + \Lambda(t) \tag{7.196}$$

where $\Lambda(t)$ is some arbitrary infinitesimal function which may depend on the dynamical variables. We will take $\Lambda^\dagger = \Lambda$ to be Hermitian. This alters the Hamiltonian to

$$H_\Lambda = H - \Lambda \tag{7.197}$$

changing the equation of motion (7.193) to

$$A\dot{Q}_\Lambda = H_l - \Lambda_l \tag{7.198}$$

if we define

$$\delta\Lambda = \delta Q^T \Lambda_l + \Lambda_l^\dagger \delta Q. \tag{7.199}$$

Writing

$$Q_\Lambda = Q - \delta_\Lambda Q, \tag{7.200}$$

we find that

$$\delta_\Lambda \dot{Q} = A^{-1} \Lambda_l \tag{7.201}$$

using (7.195) and (7.198).

[15] For example, the analysis of Bloore and Lovely (1972), which does not assume (7.192), has the tacit assumption that the variations must be independent of time, and a number of other properties are imposed.

The alteration of the Lagrangian operator in (7.196) changes the action operator by an amount

$$\delta_\Lambda W_{21} = \int_{t_1}^{t_2} dt\, \Lambda(t). \tag{7.202}$$

If we define

$$G_\Lambda(t_2) = \int_{t_1}^{t_2} dt\, \Lambda(t), \tag{7.203}$$

$$G_\Lambda(t_1) = 0, \tag{7.204}$$

then (7.202) is of the general form (3.61) required by the action principle. The change in any observable generated by $G_\Lambda(t_2)$ can be computed using the general result (3.86). In particular we must have

$$\delta_\Lambda Q(t_2) = \frac{i}{\hbar}[G_\Lambda(t_2), Q(t_2)]. \tag{7.205}$$

This result can be compared with (7.201). The two expressions obtained for $\delta_\Lambda Q$ must be consistent. This consistency will lead to the canonical commutation relations.

$\Lambda(t)$ is completely general so far. Suppose that we specialize to the variation considered by Peierls (1952),

$$\Lambda(t) = \lambda(t)\delta(t - t'). \tag{7.206}$$

Then (7.203) and (7.204) give

$$G_\Lambda(t_2) = \begin{cases} 0 & \text{if } t' \notin [t_1, t_2], \\ \lambda(t') & \text{if } t' \in [t_1, t_2]. \end{cases} \tag{7.207}$$

If $\Lambda(t)$ is given by (7.206) we have $G(t_2) = 0$ if $t' > t_2$. From (7.205) we find

$$\delta_\Lambda Q(t_2) = 0 \quad \text{if } t_2 < t'. \tag{7.208}$$

If we set

$$t' = t_2 - \tau \tag{7.209}$$

with $\tau > 0$, then

$$\begin{aligned} \delta_\Lambda Q(t_2) &= \frac{i}{\hbar}[\lambda(t_2 - \tau), Q(t_2)] \\ &\simeq \frac{i}{\hbar}[\lambda(t_2), Q(t_2)] \end{aligned} \tag{7.210}$$

since $\lambda(t_2)$ is already infinitesimal, and we work only to lowest order.

Also from (7.201) and (7.206) we have

$$\delta_\Lambda \dot{Q}(t) = A^{-1}\lambda_l(t)\delta(t-t'). \tag{7.211}$$

Integration of both sides of this result from $t'-\tau$ to $t'+\tau$ where $\tau > 0$ gives

$$\delta_\Lambda Q(t'+\tau) - \delta_\Lambda Q(t'-\tau) = A^{-1}\lambda_l(t'). \tag{7.212}$$

Using (7.208) and (7.209), and again working only to first order in infinitesimals, we have

$$\delta_\Lambda Q(t_2) = A^{-1}\lambda_l(t_2). \tag{7.213}$$

In order that (7.210) be consistent with (7.213) we must have

$$A^{-1}\lambda_l = \frac{i}{\hbar}[\lambda, Q]. \tag{7.214}$$

If we now take

$$\lambda(t) = -H(t)\delta t, \tag{7.215}$$

then $\lambda_l = -H_l\delta t$. Equation (7.214) now leads to

$$-A^{-1}H_l = \frac{i}{\hbar}[-H, Q]$$

which may be recognized as

$$\dot{Q} = \frac{i}{\hbar}[H, Q], \tag{7.216}$$

if (7.195) is used. This is the Heisenberg equation of motion for the dynamical variables.

We can consider other possibilities for λ. If λ is independent of the Q_i then $\delta\lambda = 0$ under a variation of the dynamical variables. From (7.214) we obtain

$$[\lambda, Q_i] = 0. \tag{7.217}$$

After a λ which is independent of Q_i, the next most complicated possibility is to take λ to depend linearly on Q_i. Let

$$\lambda = \epsilon^T Q + Q^T \epsilon \tag{7.218}$$

which is Hermitian if $\epsilon^* = \epsilon$ is real. ϵ is taken to have no dependence on Q. With Q given as in (7.180), we may write

$$\epsilon = \begin{pmatrix} \epsilon_B \\ \epsilon_F \end{pmatrix}, \tag{7.219}$$

and (7.218) becomes

$$\lambda = \epsilon_B^T b + b^T \epsilon_B + \epsilon_F^T f + f^T \epsilon_F. \tag{7.220}$$

Because λ must be c-type (since it is part of the modified action), ϵ_B must be c-type and ϵ_F must be a-type. Variation of (7.220) with respect to b, f shows that

$$\lambda_l = \begin{pmatrix} \epsilon_B \\ \epsilon_F \end{pmatrix} \tag{7.221}$$

and (7.214) results in

$$A_B^{-1}\epsilon_B = \frac{i}{\hbar}[\lambda, b], \tag{7.222}$$

$$A_F^{-1}\epsilon_F = \frac{i}{\hbar}[\lambda, f]. \tag{7.223}$$

Because ϵ_B and ϵ_F may be specified independently, (7.222) and (7.223) give

$$A_B^{-1}\epsilon_B = \frac{i}{\hbar}[\epsilon_B^T b + b^T \epsilon_B, b], \tag{7.224}$$

$$0 = \frac{i}{\hbar}[\epsilon_F^T f + f^T \epsilon_F, b], \tag{7.225}$$

$$A_F^{-1}\epsilon_F = \frac{i}{\hbar}[\epsilon_F^T f + f^T \epsilon_F, f], \tag{7.226}$$

$$0 = \frac{i}{\hbar}[\epsilon_B^T b + b^T \epsilon_B, f]. \tag{7.227}$$

In order to analyse the structure of these four equations we will use the following identity

$$[AB, C] = A[B, C]_q - [C, A]_q B \tag{7.228}$$

where

$$[A, B]_q = AB - qBA \tag{7.229}$$

with q an arbitrary number. Applying this first to (7.224) results in

$$\begin{aligned} -i\hbar(A_B^{-1})_{ij}\epsilon_{Bj} = {} & \epsilon_{Bj}[b_j, b_i]_q - [b_i, \epsilon_{Bj}]_q b_j \\ & + b_j[\epsilon_{Bj}, b_i]_q - [b_i, b_j]_q \epsilon_{Bj}. \end{aligned} \tag{7.230}$$

The aim of this exercise is to obtain a relation for $[b_i, b_j]_q$ in terms of something which is independent of b_i. Suppose that we write

$$[b_i, b_j]_q = T_{ij}(q), \tag{7.231}$$

for some $T_{ij}(q)$ which is independent of the operators b_i. We will show that this can only work if $q = \pm 1$. To do this, note that $T_{ij}(q)$ can be viewed as the elements of a matrix. We can always decompose

$$T_{ij}(q) = T_{(ij)}(q) + T_{[ij]}(q) \tag{7.232}$$

where

$$T_{(ij)}(q) = \frac{1}{2}\Big[T_{ij}(q) + T_{ji}(q)\Big], \tag{7.233}$$

$$T_{[ij]}(q) = \frac{1}{2}\Big[T_{ij}(q) - T_{ji}(q)\Big]. \tag{7.234}$$

By direct computation from (7.231) we have

$$T_{(ij)}(q) = \frac{1}{2}(1-q)\{b_i, b_j\}, \tag{7.235}$$

where $\{b_i, b_j\} = b_i b_j + b_j b_i$ is the anti-commutator. It is also easy to see that

$$T_{[ij]}(q) = \frac{1}{2}(1+q)[b_i, b_j]. \tag{7.236}$$

However, both $T_{(ij)}(q)$ and $T_{[ij]}(q)$ are constructed from $T_{ij}(q)$, which by assumption is independent of the operators b_i. The only way for both $T_{(ij)}(q)$ and $T_{[ij]}(q)$ to be independent of b_i occurs if $q = 1$ or if $q = -1$. No other values of q are allowed. We must now study these two allowed values of q to see if they are consistent.

Returning now to (7.230) we see that if $[b_i, b_j]_q$ with $q = \pm 1$ is a fixed numerical value independent of the operators b_i, then because the left-hand side of the equation is independent of b_i, the two terms on the right-hand side involving b_i must vanish. We may pick

$$[b_i, \epsilon_{Bj}]_q = 0 \tag{7.237}$$

for $q = \pm 1$. If we choose $q = -1$, we are left in (7.230) with $(A_B^{-1})_{ij}\epsilon_{Bj} = 0$. Since we wish to allow $\epsilon_B \neq 0$, there is no solution in the case $q = -1$. We must therefore have $q = 1$, in which case we obtain

$$[b_i, b_j] = \frac{i\hbar}{2}(A_B^{-1})_{ij}. \tag{7.238}$$

In the classical limit, $\hbar \to 0$, we obtain $b_i b_j = b_j b_i$ as expected from our earlier discussion. We also see from (7.237) with $q = 1$ that ϵ_B commutes with b_i and therefore may be regarded as a c-type function. This is consistent with what we found earlier by demanding that λ be c-type.

Given that ϵ_B is an ordinary c-type function which commutes with b_i, (7.227) immediately leads to

$$[b_i, f_\alpha] = 0. \tag{7.239}$$

We can now try to analyse (7.226) in exactly the same way as we did (7.224). The case $q = -1$ leads to $\epsilon_F = 0$ as the only solution. The case $q = 1$ leads to

$$[f_\alpha, \epsilon_{F\beta}] = 0$$

and

$$\frac{i\hbar}{2}(A_F^{-1})_{\alpha\beta}\epsilon_{F\beta} = [f_\alpha, f_\beta]\epsilon_{F\beta}.$$

This time there is no solution if $\epsilon_{F\beta} \neq 0$ because $(A_F^{-1})_{\alpha\beta}$ is symmetric in α and β whereas $[f_\alpha, f_\beta]$ is antisymmetric. So regardless of whether $q = 1$ or $q = -1$, we must have $\epsilon_F = 0$. There is no way to deduce $[f_\alpha, f_\beta]_q$ from a λ which is linear in the dynamical variables. We can note that (7.225) is trivially satisfied by $\epsilon_F = 0$.

To summarize, by taking λ to be linear in the dynamical variables Q, we have shown that λ can only depend on the c-type dynamical variables b_i. The two relations (7.238) and (7.239) must be satisfied for conformity with the Schwinger action principle.

We now examine a λ which is quadratic in the dynamical variables. We will write

$$\lambda = Q^T M Q, \tag{7.240}$$

where M is a c-type Hermitian matrix. We will take

$$M = \begin{pmatrix} M_B & 0 \\ 0 & M_F \end{pmatrix}, \tag{7.241}$$

so that

$$\lambda = b^T M_B b + f^T M_F f. \tag{7.242}$$

We know from (7.238) that $b_i b_j = b_j b_i + (i\hbar/2)(A_B^{-1})_{ij}$. It then follows that

$$\begin{aligned} b^T M_B b &= (M_B)_{ij} b_i b_j \\ &= \frac{1}{2}\Big[(M_B)_{ij} + (M_B)_{ji}\Big] b_i b_j + \frac{i\hbar}{4}(M_B)_{ij}(A_B^{-1})_{ij}. \end{aligned}$$

The last term on the right-hand side is a constant term satisfying (7.217). Accordingly, we lose no generality by assuming that M_B is a symmetric matrix. Because the relation between $f_\alpha f_\beta$ and $f_\beta f_\alpha$ is unknown, we do not impose any symmetry properties on M_F.

By varying λ with respect to the dynamical variables, it is easy to see that

$$\lambda_l = \begin{pmatrix} M_B b \\ M_F f \end{pmatrix}, \tag{7.243}$$

and so (7.214) results in

$$A_B^{-1} M_B b = \frac{i}{\hbar}[\lambda, b], \tag{7.244}$$

$$A_F^{-1} M_F f = \frac{i}{\hbar}[\lambda, f]. \tag{7.245}$$

Because M_B and M_F may be freely specified independently of each other, we must have

$$A_B^{-1} M_B b = \frac{i}{\hbar}[b^T M_B b, b], \tag{7.246}$$

$$0 = \frac{i}{\hbar}[f^T M_F f, b], \tag{7.247}$$

$$0 = \frac{i}{\hbar}[b^T M_B b, f], \tag{7.248}$$

$$A_F^{-1} M_F f = \frac{i}{\hbar}[f^T M_F f, f]. \tag{7.249}$$

It is now straightforward to show that (7.246) is satisfied by virtue of (7.238), and that (7.247) and (7.248) are satisfied by virtue of (7.239). The only equation that can have any new content is (7.249), and we will now analyse this equation.

We can always write $M_F = M_F^a + M_F^s$ where M_F^a is antisymmetric and M_F^s is symmetric. These two parts of M_F can be specified independently of each other, so (7.249) results in

$$A_F^{-1} M_F^s f = \frac{i}{\hbar}[f^T M_F^s f, f], \tag{7.250}$$

$$A_F^{-1} M_F^a f = \frac{i}{\hbar}[f^T M_F^a f, f]. \tag{7.251}$$

If we assume that $M_F^a \neq 0$, then (7.251) gives us

$$(A_F^{-1})_{\alpha\beta} f_\gamma - (A_F^{-1})_{\alpha\gamma} f_\beta = \frac{i}{\hbar}[f_\beta f_\gamma - f_\gamma f_\beta, f_\alpha]. \tag{7.252}$$

(This follows from $(M_F^a)_{\beta\gamma} = -(M_F^a)_{\gamma\beta}$.) Defining

$$[f_\alpha, f_\beta]_q = T_{\alpha\beta}(q), \tag{7.253}$$

in a similar way to (7.231), with $T_{\alpha\beta}(q)$ independent of the operators f_α, we find

$$(A_F^{-1})_{\alpha\beta} f_\gamma - (A_F^{-1})_{\alpha\gamma} f_\beta = -\frac{i}{\hbar}\Big[T_{\alpha\beta}(q) + T_{\beta\alpha}(q)\Big] f_\gamma + \frac{i}{\hbar}\Big[T_{\alpha\gamma}(q) + T_{\gamma\alpha}(q)\Big] f_\beta.$$

The solution to this equation requires

$$T_{\alpha\beta}(q) + T_{\beta\alpha}(q) = i\hbar (A_F^{-1})_{\alpha\beta}. \tag{7.254}$$

Directly from (7.253) we find

$$T_{\alpha\beta}(q) + T_{\beta\alpha}(q) = (1-q)\{f_\alpha, f_\beta\}. \tag{7.255}$$

The results in (7.253)–(7.255) are only consistent with each other, and with the requirement that $T_{\alpha\beta}(q)$ be independent of f_α if $q = -1$. ($q = 1$ results in $A_F^{-1} = 0$ which is not allowed.) We therefore find

$$\{f_\alpha, f_\beta\} = \frac{i\hbar}{2}(A_F^{-1})_{\alpha\beta}. \tag{7.256}$$

In the classical limit, $\hbar \to 0$, the operators f_α reduce to a-type numbers as we found earlier for the classical theory.

Given (7.256), it is now easy to show that the only solution to (7.250) is for $M_F^s = 0$. We therefore find that M_F in (7.242) may be chosen to be antisymmetric.

It is now natural to investigate a λ which is higher order than quadratic in the dynamical variables Q. Consider a general monomial in f_α and b_i. It must contain an even number of the f_α operators if the coefficients of the monomial are to be c-type. Write

$$\lambda = \lambda_{\alpha_1 \cdots \alpha_{2n} i_1 \cdots i_m} f_{\alpha_1} \cdots f_{\alpha_{2n}} b_{i_1} \cdots b_{i_m}, \tag{7.257}$$

where the coefficients $\lambda_{\alpha_1 \cdots \alpha_{2n} i_1 \cdots i_m}$ are c-type, and all repeated indices are summed over appropriate values. Note that because b_i commutes with f_α, we can always arrange the order of the f's and b's as shown in (7.257) without any loss of generality. Furthermore, because $b_i b_j = b_j b_i +$ a c-type number and $f_\alpha f_\beta = -f_\beta f_\alpha +$ a c-type number, we do not lose any generality by taking $\lambda_{\alpha_1 \cdots \alpha_{2n} i_1 \cdots i_m}$ to be totally antisymmetric in $\alpha_1 \cdots \alpha_{2n}$ and totally symmetric in $i_1 \cdots i_m$.

We now wish to compute $\delta\lambda$. In order to do this we need to know the properties of δf_α and δb_i. By varying the canonical commutation relations we have already found in (7.238), (7.239), and (7.256) we obtain

$$[\delta b_i, b_j] + [b_i, \delta b_j] = 0, \tag{7.258}$$

$$[\delta b_i, f_\alpha] + [b_i, \delta f_\alpha] = 0, \tag{7.259}$$
$$\{\delta f_\alpha, f_\beta\} + \{f_\alpha, \delta f_\beta\} = 0. \tag{7.260}$$

The simplest assumption we can make which satisfies (7.258)–(7.260) is that

$$[b_i, \delta b_j] = 0, \tag{7.261}$$
$$[b_i, \delta f_\alpha] = [\delta b_i, f_\alpha] = 0, \tag{7.262}$$
$$\{f_\alpha, \delta f_\beta\} = 0. \tag{7.263}$$

These results hold if the variations δb_i and δf_α are treated as classical c-type or a-type functions.

It is now easy to show that

$$\begin{aligned}\delta\lambda = {} & 2n\lambda_{\alpha_1\cdots\alpha_{2n}i_1\cdots i_m}\delta f_{\alpha_{2n}} f_{\alpha_1}\cdots f_{\alpha_{2n-1}} b_{i_1}\cdots b_{i_m} \\ & + m\lambda_{\alpha_1\cdots\alpha_{2n}i_1\cdots i_m}\delta b_{i_m} f_{\alpha_1}\cdots f_{\alpha_{2n}} b_{i_1}\cdots b_{i_{m-1}}.\end{aligned} \tag{7.264}$$

Because we have imposed the relations (7.261)–(7.263) on the variations, we have

$$\delta\lambda = \delta Q^T \lambda_l + \lambda_l^\dagger \delta Q = 2\delta Q^T \lambda_l. \tag{7.265}$$

Write

$$\lambda_l = \begin{pmatrix} \lambda_{li} \\ \lambda_{l\alpha} \end{pmatrix}, \tag{7.266}$$

where

$$\lambda_{lj} = \frac{m}{2}\lambda_{\alpha_1\cdots\alpha_{2n}i_1\cdots i_{m-1}j} f_{\alpha_1}\cdots f_{\alpha_{2n}} b_{i_1}\cdots b_{i_{m-1}}, \tag{7.267}$$
$$\lambda_{l\beta} = n\lambda_{\alpha_1\cdots\alpha_{2n-1}\beta i_1\cdots i_m} f_{\alpha_1}\cdots f_{\alpha_{2n-1}} b_{i_1}\cdots b_{i_m}. \tag{7.268}$$

The relation (7.214) that must be satisfied if the action principle is to hold gives us

$$(A_B^{-1})_{ij}\lambda_{lj} = \frac{i}{\hbar}[\lambda, b_i], \tag{7.269}$$
$$(A_F^{-1})_{\alpha\beta}\lambda_{l\beta} = \frac{i}{\hbar}[\lambda, f_\alpha]. \tag{7.270}$$

If we make use of (7.239), then

$$[\lambda, b_i] = \lambda_{\alpha_1\cdots\alpha_{2n}i_1\cdots i_m} f_{\alpha_1}\cdots f_{\alpha_{2n}}[b_{i_1}\cdots b_{i_m}, b_i]. \tag{7.271}$$

By repeated use of the identity in (7.228) where we take $q = 1$, along with the fact that $\lambda_{\alpha_1 \cdots \alpha_{2n} i_1 \cdots i_m}$ is symmetric in $i_1 \cdots i_m$, it is easy to see that

$$\begin{aligned}[\lambda, b_i] &= m\lambda_{\alpha_1 \cdots \alpha_{2n} i_1 \cdots i_m} f_{\alpha_1} \cdots f_{\alpha_{2n}} b_{i_1} \cdots b_{i_{m-1}} [b_{i_m}, b_i] \\ &= \frac{i\hbar}{2} m\lambda_{\alpha_1 \cdots \alpha_{2n} i_1 \cdots i_m} f_{\alpha_1} \cdots f_{\alpha_{2n}} b_{i_1} \cdots b_{i_{m-1}} (A_B^{-1})_{i_m i}.\end{aligned}$$

With (7.267) used on the left-hand side of (7.269), the relation (7.269) can be seen to be satisfied. (Recall that $(A_B^{-1})_{ij}$ is antisymmetric).

In a similar way, use of (7.239) leads to

$$[\lambda, f_\alpha] = \lambda_{\alpha_1 \cdots \alpha_{2n} i_1 \cdots i_m} b_{i_1} \cdots b_{i_m} [f_{\alpha_1} \cdots f_{\alpha_{2n}}, f_\alpha].$$

By repeated use of the identity (7.228) with $q = -1$ and the antisymmetry of $\lambda_{\alpha_1 \cdots \alpha_{2n} i_1 \cdots i_m}$ in $\alpha_1 \cdots \alpha_{2n}$, it can be seen that

$$\begin{aligned}[\lambda, f_\alpha] &= 2n\lambda_{\alpha_1 \cdots \alpha_{2n} i_1 \cdots i_m} f_{\alpha_1} \cdots f_{\alpha_{2n-1}} [f_{\alpha_{2n}}, f_\alpha] b_{i_1} \cdots b_{i_m} \\ &= i\hbar n\lambda_{\alpha_1 \cdots \alpha_{2n} i_1 \cdots i_m} f_{\alpha_1} \cdots f_{\alpha_{2n}} (A_F^{-1})_{\alpha_{2n} \alpha} b_{i_1} \cdots b_{i_m}.\end{aligned}$$

The equation resulting in (7.270) can now be seen to be satisfied if we use the result just derived on the right-hand side, and use (7.268) on the left-hand side.

It therefore follows that provided the assumptions (7.261)–(7.263) on the variations of the operators b_i and f_α hold, the relations (7.238), (7.239), and (7.256) may be imposed consistently with the Schwinger action principle for any alteration of the operator Lagrangian which can be expressed as a monomial in the operators b_i and f_α.

The analysis of this section shows that it is too strong to claim that it is possible to derive the canonical commutation relations from the Schwinger action principle, since properties must be imposed on variations of the dynamical variables which cannot be derived from the action principle. (For example, we assumed that the Hamiltonian was always such that its variation could be written in the form (7.189).) A more accurate statement is that it is possible to set up the theory so that a set of commutation and anti-commutation relations may be imposed consistently. Within the constraints we have imposed, it has been shown that only Bose and Fermi statistics are allowed. In order to obtain any other kind of statistics it is necessary to change the form assumed for the Lagrangian, restrict the allowed class of variations of the Lagrangian, or restrict the properties of the allowed variations of the dynamical variables more than we have done.

Notes

The transition amplitude for the free particle appears in Schwinger (1951b). The transition amplitude for the forced harmonic oscillator is presented in Feynman (1948) using the path integral method. The relationship between the more widely known path integral method and the Schwinger action principle is discussed by DeWitt (1965). A very comprehensive treatment of the path integral method in quantum mechanics is Kleinert (2004). For more about Schwinger's approach to quantum mechanics, see Schwinger (2001).

8
General definition of the effective action

This chapter presents the application of the Schwinger action principle to interacting field theory. We concentrate on the case of scalar fields for simplicity. It will be shown how the perturbative expansion of the effective action can be obtained in a systematic manner. The renormalization of interacting scalar fields with a quartic self-interaction is discussed using this formalism to two-loop order. We will see how to incorporate finite temperature effects into the formalism and then discuss Bose–Einstein condensation using a generalization of the effective action due to Callan, Jackiw, and Tomboulis (Cornwall *et al.*, 1974).

8.1 Generating functionals for free field theory

The action integral for a typical theory that we are interested in is local in the sense that it only involves the integral of fields at the same spacetime point. (See the examples of Chapter 2.) When we replace the classical fields with operators, this means that the time-ordering operation is not important in the action. This is also true for the equations of motion. In this section we will follow essentially the same procedure as we did in Section 7.7, but this time for field theory.

Suppose that we consider a free field theory with a field operator denoted by $\phi^I(t, \mathbf{x})$. Here I runs over any type of indices that the field might have. We will initially assume that $\phi^I(t, \mathbf{x})$ is a Bose field to avoid the complication of dealing with anti-commuting numbers. In order to deal with the basic formalism, it proves convenient to adopt DeWitt's (1965) condensed notation with an index, like i, standing for the complete set of labels on a field, including the spacetime coordinates. We will use ϕ^i in condensed notation to be short for $\phi^I(t, \mathbf{x})$ in conventional notation. So the condensed index i is short for $(I, t, \mathbf{x})$. We

have been using the Einstein summation convention in which a repeated index involves a sum over all possible values. In condensed notation we will understand that any repeated index is summed over all values of the normal index I and also involves an integration over the continuous labels t and $\mathbf{x}$. For example, if we have $J_i\phi^i$ in condensed notation, this is shorthand for the lengthier expression $\sum_I \int dt \int d^D x J_I(t,\mathbf{x})\phi^I(t,\mathbf{x})$ in normal notation. An object like A_{ij} in condensed notation that has two (or more) indices must correspond to an object in normal notation with more than one spacetime label: $A_{ij} \leftrightarrow A_{IJ}(t,\mathbf{x};t',\mathbf{x}')$. An expression like $A_{ij}\phi^i\phi^j$ in condensed notation becomes

$$\sum_{I,J} \int dt \int d^D x \int dt' \int d^D x' A_{IJ}(t,\mathbf{x};t',\mathbf{x}')\phi^I(t,\mathbf{x})\phi^J(t',\mathbf{x}')$$

in normal notation. The advantage of using condensed notation, as should be readily evident, is that it shortens many expressions considerably and allows us to manipulate terms in exactly the same way as if they were finite dimensional.

We will consider initially a free field whose action functional is

$$S[\phi] = -\frac{1}{2}A_{ij}\phi^i\phi^j + J_i\phi^i. \tag{8.1}$$

A specific example of this is the real scalar field described in (3.170) where we ignore any self-interaction and add on a coupling to an external source. The external source is a convenience that we introduce for reasons that will become apparent; it can be set to zero at any stage. In this case we have the correspondence

$$A_{ij} \leftrightarrow \left(\Box_x + m^2 - i\epsilon\right)\delta(x,x'). \tag{8.2}$$

Here we have added on the $i\epsilon$ to ensure that when we define the Green function it corresponds to the Feynman Green function as described in Section 7.7.

The equation of motion for the field operator ϕ^i that follows from the action functional (8.1) is

$$A_{ij}\phi^j = J_i. \tag{8.3}$$

If we define the Feynman Green function in condensed notation as G^{ij} where

$$A_{ij}G^{jk} = \delta_i^k, \tag{8.4}$$

we can solve (8.3) with

$$\phi^i = G^{ij}J_j. \tag{8.5}$$

The Schwinger action principle reads

$$\delta\langle \text{out}|\text{in}\rangle = \frac{i}{\hbar}\langle \text{out}|\delta S|\text{in}\rangle. \tag{8.6}$$

Again, because of our assumption that the action only involves the products of fields with the same time coordinate, whether or not we include the time-ordering operation in (8.6) is irrelevant. (See the scalar field action in (3.170) for example.) Suppose that we choose the variation in (8.6) to be with respect to the external source J_i keeping everything else fixed. Then we obtain

$$\frac{\delta}{\delta J_i}\langle \text{out}|\text{in}\rangle = \frac{i}{\hbar}\langle \text{out}|\phi^i|\text{in}\rangle. \tag{8.7}$$

Introduce the notation

$$\langle A[\phi]\rangle = \frac{\langle \text{out}|T(A[\phi])|\text{in}\rangle}{\langle \text{out}|\text{in}\rangle}, \tag{8.8}$$

and

$$\langle \text{out}|\text{in}\rangle = \exp\left(\frac{i}{\hbar}W[J]\right). \tag{8.9}$$

These are the analogues of (7.140) and (7.146) found for the forced harmonic oscillator. Differentiation of both sides of (8.9) results in

$$\frac{\delta}{\delta J_i}\langle \text{out}|\text{in}\rangle = \frac{i}{\hbar}\frac{\delta W}{\delta J_i}\exp\left(\frac{i}{\hbar}W[J]\right). \tag{8.10}$$

Comparison with (8.7) and use of the definition (8.8) shows that

$$\frac{\delta W}{\delta J_i} = \langle \phi^i\rangle. \tag{8.11}$$

From (8.5) we have

$$\frac{\delta W}{\delta J_i} = G^{ij}J_j. \tag{8.12}$$

Regarding this as a functional differential equation for $W\,[J]$, the solution to (8.12) is seen to be

$$W[J] = \frac{1}{2}J_iG^{ij}J_j + W[0], \tag{8.13}$$

where $W[0]$ is independent of the source J_i and is something that we need to determine.

To find $W[0]$, apply the Schwinger action principle (8.6) again, except this time take the variation to be with respect to A_{ij}.[1] From (8.1) we have

$$\delta S = -\frac{1}{2}\delta A_{ij}\phi^i\phi^j. \tag{8.14}$$

Using the results from (8.6), (8.9), and (8.14) we find

$$\delta W = -\frac{1}{2}\delta A_{ij}\frac{\langle \text{out}|T(\phi^i\phi^j)|\text{in}\rangle}{\langle \text{out}|\text{in}\rangle}. \tag{8.15}$$

We have used the locality of the action functional to introduce the time-ordering operation here.[2] We now use the notation of (8.8) and set $J_i = 0$ to find

$$\delta W[0] = -\frac{1}{2}\delta A_{ij}\langle T(\phi^i\phi^j)\rangle. \tag{8.16}$$

As in the previous chapter, see (7.132), we have

$$\frac{\delta^2\langle \text{out}|\text{in}\rangle}{\delta J_i \delta J_j} = \left(\frac{i}{\hbar}\right)^2 \langle \text{out}|T(\phi^i\phi^j)|\text{in}\rangle. \tag{8.17}$$

Making the replacement of $\langle \text{out}|\text{in}\rangle$ in terms of $W[J]$ as defined in (8.9), setting $J_i = 0$, and noting (8.12), it can be seen that

$$\left.\frac{\delta^2 W}{\delta J_i \delta J_j}\right|_{J_i=0} = \frac{i}{\hbar}\exp\left(-\frac{i}{\hbar}W[0]\right)\langle \text{out}|T(\phi^i\phi^j)|\text{in}\rangle. \tag{8.18}$$

Finally, (8.13) may be used on the left-hand side to see that

$$\langle T(\phi^i\phi^j)\rangle = -i\hbar G^{ij}. \tag{8.19}$$

The relationship between the time-ordered product of field operators and the Feynman Green function established in (8.19) may be used back in (8.16) resulting in

$$\delta W[0] = \frac{i\hbar}{2}\delta A_{ij}G^{ij}. \tag{8.20}$$

It proves useful to view the Green function defined by (8.4) as the inverse of A_{ij}. We can then view $\delta A_{ij}G^{ij}$ in (8.20) as the trace of $\delta\mathbf{A}\mathbf{A}^{-1}$ if

[1] Remember that we are allowed to vary with respect to anything that occurs in the Lagrangian of the theory.

[2] It can be introduced at the earlier stage of (8.14) if we like.

we proceed by analogy with what would be found if $\mathbf{A}$ was an ordinary symmetric matrix with components A_{ij}. This gives

$$\begin{aligned}\delta A_{ij}G^{ij} &= \mathrm{tr}(\delta\mathbf{A}\mathbf{A}^{-1}) \\ &= \delta\left[\mathrm{tr}\ln(\ell^2 A_{ij})\right] \qquad (8.21)\\ &= \delta\left[\ln\det(\ell^2 A_{ij})\right] \qquad (8.22)\end{aligned}$$

if we use the matrix identity $\mathrm{tr}\ln = \ln\det$ in the last line.[3] In addition we have introduced an arbitrary constant ℓ^2 to keep the argument of the logarithm dimensionless. This motivates the adoption of

$$\begin{aligned}W[0] &= \frac{i\hbar}{2}\mathrm{tr}\ln(\ell^2 A_{ij}) \qquad (8.23)\\ &= \frac{i\hbar}{2}\ln\det(\ell^2 A_{ij}). \qquad (8.24)\end{aligned}$$

From (8.13) the complete expression for $W[J]$ is now

$$\begin{aligned}W[J] &= \frac{1}{2}J_i G^{ij}J_j + \frac{i\hbar}{2}\ln\det(\ell^2 A_{ij}) \qquad (8.25)\\ &= \frac{1}{2}J_i G^{ij}J_j - \frac{i\hbar}{2}\ln\det\left(\frac{G^{ij}}{\ell^2}\right) \qquad (8.26)\end{aligned}$$

with the second equality making use of the fact that the Green function is the inverse of A_{ij} as shown in (8.4).

The only role of the external source here is to provide us with something to differentiate with respect to. In order to remove the dependence on the source J_i, suppose that we define the background field φ^i by

$$\varphi^i = \langle\phi^i\rangle = \frac{\delta W}{\delta J_i}. \qquad (8.27)$$

We may then perform a Legendre transformation, exactly as we did in passing from a Lagrangian to a Hamiltonian description in classical mechanics, with

$$\Gamma[\varphi] = W[J] - J_i\varphi^i. \qquad (8.28)$$

In this definition it is understood that all of the dependence on the source is eliminated in favour of a dependence on φ^i using (8.27). Making use of (8.5) shows that

$$\varphi^i = G^{ij}J_j. \qquad (8.29)$$

[3] For a symmetric matrix this identity follows simply by diagonalization of the matrix.

By operating on both sides of this with A_{ij} and making use of the definition of the Green function in (8.4) we find

$$J_i = A_{ij}\varphi^j. \tag{8.30}$$

If we now use (8.25) for $W[J]$, eliminate J_i using (8.30), and simplify the result using (8.4), it can be seen that

$$\Gamma[\varphi] = -\frac{1}{2}A_{ij}\varphi^i\varphi^j + \frac{i\hbar}{2}\ln\det(\ell^2 A_{ij}) \tag{8.31}$$

$$= S[\varphi] + \frac{i\hbar}{2}\ln\det(\ell^2 A_{ij}). \tag{8.32}$$

The result for $\Gamma[\varphi]$ is seen to consist of the classical action plus a quantum correction. It is conventional to call $\Gamma[\varphi]$ the 'effective action'. Later we will show how this result is connected with what we have been calling the effective action in earlier chapters.

Before continuing on to consider interacting theories, it is useful to show another way of obtaining $W[J]$. Suppose that we redefine our field operator by

$$\phi^i = \psi^i - \chi^i, \tag{8.33}$$

with χ^i chosen to remove the linear term in the field operator from the action functional (8.1). By a straightforward calculation, making use of the symmetry of A_{ij}, we find

$$S = -\frac{1}{2}A_{ij}\psi^i\psi^j + (J_i + A_{ij}\chi^j)\psi^i - \frac{1}{2}A_{ij}\chi^i\chi^j - J_i\chi^i. \tag{8.34}$$

We will therefore make the choice

$$J_i = -A_{ij}\chi^j, \tag{8.35}$$

or equivalently,

$$\chi^i = -G^{ij}J_j \tag{8.36}$$

if we make use of (8.4). This allows us to simplify (8.34) to

$$S = -\frac{1}{2}A_{ij}\chi^i\chi^j + \frac{1}{2}J_iG^{ij}J_j. \tag{8.37}$$

The last term in (8.37) is independent of the field operators. This means that if we use the Schwinger action principle with the last term on the right-hand side of (8.37) varied, we find

$$\delta\langle\text{out}|\text{in}\rangle[J] = \frac{i}{2\hbar}\delta(J_iG^{ij}J_j)\langle\text{out}|\text{in}\rangle[J_i = 0] \tag{8.38}$$

where we explicitly indicate the dependence on the source. The solution to this is

$$\langle \text{out}|\text{in}\rangle[J] = \exp\left(\frac{i}{2\hbar} J_i G^{ij} J_j\right) \langle \text{out}|\text{in}\rangle[J=0]. \tag{8.39}$$

The analysis of the $J = 0$ amplitude follows as described above. This result is the field theory analogue of what we found for the vacuum persistence amplitude for the forced harmonic oscillator in Section 7.7.

8.2 Interacting fields and perturbation theory

In the previous section we considered the effective action for a free field theory. We now want to see how to deal with the more general case of a theory with interactions. We again use condensed notation with ϕ^i representing the field operators. The action functional $S[\phi]$ can be divided up into two parts:

$$S = S_0 + S_1, \tag{8.40}$$

with S_1 treated as the interaction term.[4] It proves convenient to include a coupling between the field ϕ^i and an external source J_i as we have done before. The Schwinger action principle then gives us

$$\langle \text{out}|\text{in}\rangle[J] = \langle \text{out}|T\left[\exp\left(\frac{i}{\hbar} S_1 + \frac{i}{\hbar} J_i \phi^i\right)\right]|\text{in}\rangle_0 \tag{8.41}$$

where the subscript 0 on the right-hand side is to remind us that the states are evaluated treating only S_0 as the action; the only occurrence of S_1 and J_i on the right-hand side is in the exponential factor. This is discussed at the end of Section 7.6.

Define $W[J]$ exactly as in (8.9), except with (8.41) now used for $\langle \text{out}|\text{in}\rangle$. We can remove the dependence on the external source by adopting (8.27) and (8.28). The difference this time is that in the absence of a closed form expression for $W[J]$ we cannot solve for J_i explicitly in terms of φ^i. Instead we must regard (8.27) as an implicit definition that is solved for J_i as a function of φ^i. If we differentiate both sides of (8.28) with respect to φ^j, we have

$$\frac{\delta\Gamma}{\delta\varphi^j} = \frac{\delta W}{\delta\varphi^j} - \frac{\delta J_i}{\delta\varphi^j}\varphi^i - J_j, \tag{8.42}$$

[4] See Section 7.6 for the quantum mechanical version of this.

where we must regard W as a functional of φ through its dependence on J_i. Using the chain rule for differentiation, we have

$$\frac{\delta W}{\delta \varphi^j} = \frac{\delta W}{\delta J_i}\frac{\delta J_i}{\delta \varphi^j}. \tag{8.43}$$

With the definition (8.27) used for the first factor on the right-hand side of (8.42), it is easy to see that the first and second terms on the right-hand side cancel leaving us with

$$\frac{\delta \Gamma}{\delta \varphi^j} = -J_j. \tag{8.44}$$

This gives us an explicit result for J_i as a function of φ^i that we can use to remove all dependence on the external source J_i.

Starting with the definition (8.28) and using (8.9) for $W[J]$, we have

$$\exp\left(\frac{i}{\hbar}\Gamma[\varphi]\right) = \exp\left(-\frac{i}{\hbar}J_i\varphi^i\right)\langle \text{out}|\text{in}\rangle[J].$$

If we now use (8.41) and eliminate J_i using (8.44), we find

$$\exp\left(\frac{i}{\hbar}\Gamma[\varphi]\right) = \langle \text{out}|T\left\{\exp\left[\frac{i}{\hbar}S_1 - \frac{i}{\hbar}\frac{\delta\Gamma}{\delta\varphi^i}(\phi^i - \varphi^i)\right]\right\}|\text{in}\rangle_0. \tag{8.45}$$

Note that $\Gamma[\varphi]$ occurs on both sides of this equation, so this must be regarded as an implicit definition for the effective action. As a consequence, it appears at first sight as if this is not a particularly useful result; however, we will see that there is a very nice approximation scheme that we can use.

The formal expression (8.45) does not require any special choice to be made for S_0 and S_1; in other words, the result for $\Gamma[\varphi]$ is independent of how we make our split. Because of the occurrence of $\phi^i - \varphi^i$ in the exponential, it proves advantageous to expand $S[\phi]$ about $\phi^i = \varphi^i$, and moreover to define a new field ψ^i by[5]

$$\phi^i = \hbar^{1/2}\psi^i + \varphi^i. \tag{8.46}$$

We find

$$S[\phi] = S[\varphi] + \hbar^{1/2}S_{,i}[\varphi]\psi^i + \frac{\hbar}{2}S_{,ij}[\varphi]\psi^i\psi^j + S_{int}[\varphi,\psi]. \tag{8.47}$$

[5] The reason for the factor of $\hbar^{1/2}$ will become apparent later.

Here we are using the condensed notation $S_{,i}$ to stand for the functional derivative with respect to φ^i. $S_{,ij}$ stands for the second functional derivative with respect to φ^i and φ^j, and so on. By explicit construction, S_{int} involves only terms in ψ^i that are of cubic and higher orders; thus the leading power of $\hbar$ that occurs in S_{int} is $\hbar^{3/2}$. We will now make the choice

$$S_0 = S[\varphi] + \frac{\hbar}{2} S_{,ij}[\varphi]\psi^i\psi^j, \tag{8.48}$$

$$S_1 = \hbar^{1/2} S_{,i}[\varphi]\psi^i + S_{int}[\varphi, \psi]. \tag{8.49}$$

With this choice, the argument of the exponential in (8.45) involves

$$S_1 - \Gamma_{,i}[\varphi](\phi^i - \varphi^i) = \hbar^{1/2} \left(S_{,i}[\varphi] - \Gamma_{,i}[\varphi]\right) \psi^i + S_{int}[\varphi, \psi]. \tag{8.50}$$

The leading-order approximation to $\Gamma[\varphi]$ consists of disregarding the interaction and source terms altogether. This leads to

$$\exp\left(\frac{i}{\hbar}\Gamma[\varphi]\right) \simeq \langle \text{out}|\text{in}\rangle_0, \tag{8.51}$$

where on the right-hand side $\langle \text{out}|\text{in}\rangle_0$ is computed only using the theory generated by the action S_0 in (8.48). As a consequence, we can use our result for the free field found in Section 8.1. Using (8.32) it is easy to see that

$$\Gamma[\varphi] = S[\varphi] + \frac{i\hbar}{2} \ln\det(\ell^2 S_{,ij}[\varphi]) + \cdots. \tag{8.52}$$

If there are no cubic or higher-order terms in the fields, because S_{int} vanishes in this case, it is easy to see that all of the higher-order terms in (8.52) vanish (those indicated by $\cdots$) and the result recovers the free field result in Section 8.1.[6]

The form of (8.52) suggests that we regard $\Gamma[\varphi]$ as obtained perturbatively by expanding in powers of $\hbar$. Then (8.52) gives us the first two terms in the expansion. Although (8.50) would seem to indicate that fractional powers of $\hbar$ might occur, we will see that in fact this does not happen and only integral powers of $\hbar$ will be found. We will write

$$\Gamma[\varphi] = S[\varphi] + \sum_{n=1}^{\infty} \hbar^n \Gamma^{(n)}[\varphi] \tag{8.53}$$

[6] Note that $S_{,ij} = -A_{ij}$ if we compare with (8.1), but since we should strictly include an absolute value of the determinant inside the logarithm, the sign difference is not important here.

where we know

$$\Gamma^{(1)}[\varphi] = \frac{i}{2}\ln\det(\ell^2 S_{,ij}[\varphi]) \tag{8.54}$$

from (8.52). Our next concern will be the computation of $\Gamma^{(2)}[\varphi]$.

Returning to (8.50), using (8.53) for $\Gamma[\varphi]$ in the first term on the right-hand side shows that the expansion of the right-hand side of this result in powers of $\hbar$ begins with a term of order $\hbar^{3/2}$. (The classical action cancels with the first term in Γ coming from (8.53.) Suppose, for the purposes of counting powers of $\hbar$, we define

$$S_1 - \Gamma_{,i}(\phi^i - \varphi^i) = \hbar^{3/2}A_{3/2} + \hbar^2 A_2 + \hbar^{5/2}A_{5/2} + \cdots, \tag{8.55}$$

for some functionals $A_{n/2}$ that depend on both ψ^i and φ^i. Since S_{int} involves cubic and higher-order terms in the Taylor expansion of $S[\phi]$ in (8.47), it can be seen that

$$A_{3/2} = -\Gamma^{(1)}_{,i}[\varphi]\psi^i + \frac{1}{3!}S_{,ijk}[\varphi]\psi^i\psi^j\psi^k, \tag{8.56}$$

$$A_2 = \frac{1}{4!}S_{,ijkl}[\varphi]\psi^i\psi^j\psi^k\psi^l. \tag{8.57}$$

Higher-order terms may be evaluated in a straightforward manner. We now expand the exponential of (8.45) in powers of $\hbar$ to find

$$\exp\left[\frac{i}{\hbar}S_1 - \frac{i}{\hbar}\Gamma_{,i}(\phi^i - \varphi^i)\right] = 1 + i\hbar^{1/2}A_{3/2} + \hbar\left(iA_2 - \frac{1}{2}A_{3/2}^2\right) + \cdots \tag{8.58}$$

where the next term in the expansion is of order $\hbar^{3/2}$. To evaluate the right-hand side of (8.45) we need to know $\langle \text{out}|T(\psi^{i_1}\cdots\psi^{i_n})|\text{in}\rangle_0$ given the form of (8.56) and (8.57). Suppose that we define, as we did in (8.8),

$$\langle A[\psi]\rangle_0 = \frac{\langle \text{out}|T(A[\psi])|\text{in}\rangle_0}{\langle \text{out}|\text{in}\rangle_0}, \tag{8.59}$$

for any functional $A[\psi]$. Then from (8.45) we have

$$e^{(i/\hbar)\Gamma[\varphi]} = \langle \text{out}|\text{in}\rangle_0 \left\{1 + i\hbar^{1/2}\langle A_{3/2}\rangle_0 + \hbar\langle iA_2 - \frac{1}{2}A_{3/2}^2\rangle_0 + \cdots\right\}. \tag{8.60}$$

We can use (8.51) and (8.52) for $\langle \text{out}|\text{in}\rangle_0$, but we need to evaluate the expressions for all other terms in the expansion. To do this we will make

contact with the generating functional for a free theory coupled to an external source again.

We had the result in (8.39) for the action given in (8.1). The Green function G^{ij} was defined in (8.4). Furthermore, we know from the results of Section 7.6 that

$$\left.\frac{\delta^n \langle \text{out}|\text{in}\rangle[J]}{\delta J_{i_1}\cdots\delta J_{i_n}}\right|_{J=0} = \left(\frac{\hbar}{i}\right)^n \langle \text{out}|T(\phi^{i_1}\cdots\phi^{i_n})|\text{in}\rangle_0. \tag{8.61}$$

Thus,

$$\begin{aligned}\langle\phi^{i_1}\cdots\phi^{i_n}\rangle_0 &= \frac{\langle \text{out}|T(\phi^{i_1}\cdots\phi^{i_n})|\text{in}\rangle_0}{\langle \text{out}|\text{in}\rangle_0} \\ &= \left(\frac{\hbar}{i}\right)^n \frac{\delta^n}{\delta J_{i_1}\cdots\delta J_{i_n}} \left.\frac{\langle \text{out}|\text{in}\rangle[J]}{\langle \text{out}|\text{in}\rangle_0}\right|_{J=0} \\ &= \left(\frac{\hbar}{i}\right)^n \frac{\delta^n}{\delta J_{i_1}\cdots\delta J_{i_n}} \exp\left(\frac{i}{2\hbar}J_i G^{ij} J_j\right)\Bigg|_{J=0}. \end{aligned} \tag{8.62}$$

If we compare the action (8.1) with that in (8.48) it can be seen that we must set $\phi^i = \hbar^{1/2}\psi^i$ and scale $J_i \to \hbar^{1/2} J_i$ if we are to apply the results of Section 8.1. Doing this in (8.62), it can be observed that all factors of $\hbar$ cancel and we find

$$\langle\psi^{i_1}\cdots\psi^{i_n}\rangle_0 = \frac{1}{i^n}\frac{\delta^n}{\delta J_{i_1}\cdots\delta J_{i_n}} \exp\left(\frac{i}{2}J_i G^{ij} J_j\right)\Bigg|_{J=0}. \tag{8.63}$$

The cancellation of factors of $\hbar$ is a consequence of including the factor of $\hbar^{1/2}$ in (8.46); it is not necessary, but makes counting powers of $\hbar$ in our expansion easier. Since $A_{ij} = -S_{,ij}[\varphi]$ here, we have the Green function that occurs in (8.63) as the solution to

$$S_{,ij}[\varphi]G^{jk} = -\delta_i^k. \tag{8.64}$$

Because $S_{,ij}$ will have a dependence on φ in general, so will the Green function; the Green function is not identical to the free field result in this approach for an interacting theory. Again we emphasize that the Feynman Green function is to be chosen, a result that is guaranteed by the $i\epsilon$ prescription.

By expanding the exponential on the right-hand side of (8.63) in powers of the external source J_i, it is obvious that if n is odd $\langle\psi^{i_1}\cdots\psi^{i_n}\rangle_0 = 0$. (This is because the expansion of the exponential can only contain an even number of factors of J_i.) As a consequence, in the expansion of the effective action all terms on the right-hand side of (8.60) that

involve a fractional power of $\hbar$ (like $\hbar^{3/2}, \hbar^{5/2}, \ldots$) necessarily vanish. Only integral powers of $\hbar$ can occur as we claimed earlier and we have

$$e^{(i/\hbar)\Gamma[\varphi]} = \langle \text{out}|\text{in}\rangle_0 \left\{ 1 + \hbar\langle iA_2 - \frac{1}{2}A_{3/2}^2\rangle_0 + \cdots \right\}. \tag{8.65}$$

The next term in the expansion on the right-hand side of (8.65) will be of order $\hbar^2$. With (8.51) and (8.52) used for $\langle \text{out}|\text{in}\rangle_0$, we find

$$\begin{aligned}\Gamma[\varphi] &= S[\varphi] + \frac{i\hbar}{2}\ln\det\left(\ell^2 S_{,ij}[\varphi]\right) - i\hbar\ln\left\{1 + \hbar\langle iA_2 - \frac{1}{2}A_{3/2}^2\rangle_0 + \mathcal{O}(\hbar^2)\right\} \\ &= S[\varphi] + \frac{i\hbar}{2}\ln\det\left(\ell^2 S_{,ij}[\varphi]\right) + \hbar^2\langle A_2 + \frac{i}{2}A_{3/2}^2\rangle_0 + \mathcal{O}(\hbar^3). \end{aligned} \tag{8.66}$$

By continuing the expansion, higher-order terms in $\Gamma[\varphi]$ may be evaluated.

We now need to evaluate $\langle A_2\rangle_0$ and $\langle A_{3/2}^2\rangle_0$. This involves knowing the explicit results for expressions of the form $\langle \psi^{i_1}\cdots\psi^{i_n}\rangle_0$ as found using (8.63). We start with $\langle \psi^i\psi^j\rangle_0$ which is given by

$$\langle \psi^i\psi^j\rangle_0 = \frac{1}{i^2}\frac{\delta^2}{\delta J_i \delta J_j}\exp\left(\frac{i}{2}J_n G^{nm} J_m\right)\Big|_{J=0}. \tag{8.67}$$

Because we are setting $J_i = 0$, we can expand the exponential in its Taylor series. If this is done, it is clear that only the single term that involves two factors of J can possibly contribute. We have

$$\begin{aligned}\langle \psi^i\psi^j\rangle_0 &= -\frac{i}{2}G^{nm}\frac{\delta^2}{\delta J_i\delta J_j}(J_nJ_m) \\ &= -\frac{i}{2}G^{nm}(\delta_n^i\delta_m^j + \delta_m^i\delta_n^j) \\ &= -iG^{ij}, \end{aligned} \tag{8.68}$$

where in the last line we have used the symmetry of $G^{ij} = G^{ji}$.

Turn next to $\langle \psi^i\psi^j\psi^k\psi^l\rangle_0$. This time we have

$$\langle \psi^i\psi^j\psi^k\psi^l\rangle_0 = \frac{1}{i^4}\frac{\delta^4}{\delta J_i\delta J_j\delta J_k\delta J_l}\frac{1}{2!}\left(\frac{i}{2}J_nG^{nm}J_m\right)^2 \tag{8.69}$$

after expanding the exponential.[7] We find

$$\langle \psi^i\psi^j\psi^k\psi^l\rangle_0 = -\frac{1}{8}G^{nm}G^{pq}\frac{\delta^4(J_nJ_mJ_pJ_q)}{\delta J_i\delta J_j\delta J_k\delta J_l}. \tag{8.70}$$

[7] The only term in the expansion of the exponential that can contribute is the one that involves four factors of J.

If we perform the indicated differentiations we will end up with $4! = 24$ terms. It is not too difficult to write them down; however, it should be clear that proceeding like this will not be practical when more factors of ψ^i are present, since if there are $2n$ factors of ψ^i we will end up with $(2n)!$ possible terms. Instead, we can notice that we only need to know the result when the differentiations are contracted with products of Green functions that are symmetric in their indices. For the expression in (8.70) the order of the indices m and n does not matter, nor does the order of the indices p and q. Furthermore, since $G^{mn}G^{pq} = G^{pq}G^{mn}$, the order of the pair of indices (m, n) and the pair (p, q) does not matter. Of the 24 possible terms that arise, only $24/(2^2 2!) = 3$ will result in independent expressions.[8] We therefore find

$$\langle \psi^i \psi^j \psi^k \psi^l \rangle_0 = -G^{ij}G^{kl} - G^{ik}G^{jl} - G^{il}G^{jk}. \tag{8.71}$$

The next result we need is

$$\langle \psi^i \psi^j \psi^k \psi^l \psi^m \psi^n \rangle_0 = \frac{1}{i^6} \frac{\delta^6}{\delta J_i \delta J_j \delta J_k \delta J_l \delta J_m \delta J_n} \frac{1}{3!} \left(\frac{i}{2} J_a G^{ab} J_b \right)^3. \tag{8.72}$$

The differentiations with respect to J will give rise to $6! = 720$ terms this time. However the contraction with products of Green functions will reduce the number of independent terms considerably. Each Green function is symmetric in its indices, giving a factor of 2^3, one factor of 2 for each pair of indices. In addition, the order of the three Green functions in the product does not matter. Since there are 3! possible orderings, this means that of the 720 terms that arise, only $720/(2^3 3!) = 15$ will be independent. We have

$$\begin{aligned} \langle \psi^i \psi^j \psi^k \psi^l \psi^m \psi^n \rangle_0 = i[&G^{ij}G^{kl}G^{mn} + G^{ij}G^{lm}G^{nk} + G^{ij}G^{mn}G^{kl} \\ &+ (j \leftrightarrow k) + (j \leftrightarrow l) + (j \leftrightarrow m) + (j \leftrightarrow n)] \end{aligned} \tag{8.73}$$

where $(j \leftrightarrow k)$ means to write down the same three terms in the first line but with the indices j and k switched.

The general rule should be apparent from the examples we have just done. In any expression like $\langle \psi^{i_1} \cdots \psi^{i_{2n}} \rangle_0$ write down all possible pairings of terms:

$$\langle \psi^{i_1} \cdots \psi^{i_{2n}} \rangle_0 = \langle \psi^{i_1} \psi^{i_2} \rangle_0 \cdots \langle \psi^{i_{2n-1}} \psi^{i_{2n}} \rangle_0 + \text{ all possible pairs.} \tag{8.74}$$

[8] There is a factor of 2 for the symmetry of each of the two Green functions in its indices, and a factor of 2! for the fact that the order of the two Green functions is irrelevant.

For each pair, $\langle\psi^i\psi^j\rangle_0$, use $-iG^{ij}$. This gives the result. All of the numerical factors that arise from the Taylor expansion of the exponential will cancel due to the symmetry of the Green functions and the indifference of the result to the order of the Green functions in the product. The result in (8.74) is usually known as Wick's theorem after its formal elucidation by G. C. Wick (1950).

We are now in a position to evaluate $\langle A_2\rangle_0$ and $\langle A_{3/2}^2\rangle_0$. For $\langle A_2\rangle_0$ we use (8.57) to find

$$\langle A_2\rangle_0 = \frac{1}{4!}S_{,ijkl}[\varphi]\langle\psi^i\psi^j\psi^k\psi^l\rangle_0. \tag{8.75}$$

The result in (8.71) may now be used. It is seen that the result is contracted with $S_{,ijkl}$ which is symmetric in all of its indices since the order of differentiation does not matter. Each of the three terms coming from (8.71) gives an identical expression when contracted with $S_{,ijkl}$ upon a suitable relabelling of indices, and we are left with the single term

$$\langle A_2\rangle_0 = -\frac{1}{8}S_{,ijkl}[\varphi]G^{ij}G^{kl}. \tag{8.76}$$

The evaluation of $\langle A_{3/2}^2\rangle_0$ is a bit more involved. From (8.56) we find

$$\begin{aligned}\langle A_{3/2}^2\rangle_0 = {}&\Gamma^{(1)}_{,i}\Gamma^{(1)}_{,j}\langle\psi^i\psi^j\rangle_0 - \frac{1}{3}\Gamma^{(1)}_{,l}S_{,ijk}\langle\psi^i\psi^j\psi^k\psi^l\rangle_0\\ &+\frac{1}{(3!)^2}S_{,ijk}S_{,lmn}\langle\psi^i\psi^j\psi^k\psi^l\psi^m\psi^n\rangle_0.\end{aligned} \tag{8.77}$$

We will evaluate each of the three terms on the right-hand side separately.

The first term on the right-hand side of (8.77) is easy since we can simply use (8.68). We find

$$\Gamma^{(1)}_{,i}\Gamma^{(1)}_{,j}\langle\psi^i\psi^j\rangle_0 = -i\Gamma^{(1)}_{,i}\Gamma^{(1)}_{,j}G^{ij}. \tag{8.78}$$

The second term can be found using (8.71). The result is contracted with $S_{,ijk}$ that is symmetric in its indices; thus all three terms lead to an identical expression upon appropriate relabelling of indices. We obtain

$$\frac{1}{3}\Gamma^{(1)}_{,l}S_{,ijk}\langle\psi^i\psi^j\psi^k\psi^l\rangle_0 = -\Gamma^{(1)}_{,l}S_{,ijk}G^{ij}G^{kl}. \tag{8.79}$$

At this stage we can simplify the two terms we have obtained in (8.78) and (8.79) using the result for $\Gamma^{(1)}$ found in (8.54). Writing $\Gamma^{(1)}$ in the equivalent form

$$\Gamma^{(1)} = \frac{i}{2}\mathrm{tr}\ln\left(\ell^2 S_{,ij}\right), \tag{8.80}$$

we differentiate with respect to φ^i to find [9]

$$\Gamma^{(1)}_{,i} = -\frac{i}{2} S_{,ijk} G^{jk}. \tag{8.81}$$

Using (8.81) to simplify (8.78) and (8.79) results in

$$\frac{1}{3}\Gamma^{(1)}_{,l} S_{,ijk} \langle \psi^i \psi^j \psi^k \psi^l \rangle_0 = \frac{i}{2} S_{,ijk} S_{,lmn} G^{ij} G^{kl} G^{mn}, \tag{8.82}$$

and

$$\begin{aligned} \Gamma^{(1)}_{,i} \Gamma^{(1)}_{,j} \langle \psi^i \psi^j \rangle_0 &= \frac{i}{4} S_{,ikl} S_{,jmn} G^{ij} G^{kl} G^{mn} \\ &= \frac{i}{4} S_{,ijk} S_{,lmn} G^{ij} G^{kl} G^{mn} \end{aligned} \tag{8.83}$$

where in the second line of (8.83) we have relabelled the indices to make the result look like that in (8.82).

For the last term on the right-hand side of (8.77) we need to use (8.73). The result is contracted with $S_{,ijk}$ and $S_{,lmn}$ and upon an appropriate relabelling of indices we find only two independent terms:

$$\begin{aligned} \frac{1}{(3!)^2} S_{,ijk} S_{,lmn} \langle \psi^i \psi^j \psi^k \psi^l \psi^m \psi^n \rangle_0 = &\frac{i}{4} S_{,ijk} S_{,lmn} G^{ij} G^{kl} G^{mn} \\ &+ \frac{i}{6} S_{,ijk} S_{,lmn} G^{il} G^{jm} G^{kn}. \end{aligned} \tag{8.84}$$

We can now combine the results of (8.82)–(8.84) to find from (8.77) that

$$\langle A^2_{3/2} \rangle_0 = \frac{i}{6} S_{,ijk} S_{,lmn} G^{il} G^{jm} G^{kn}. \tag{8.85}$$

Note that the first two terms that occur on the right-hand side of (8.77) have led to expressions that cancel with the first term on the right-hand side of (8.84). We will return to this cancellation when we discuss Feynman diagrams in the next section. Our result for $\Gamma^{(2)}[\varphi]$ reads

$$\Gamma^{(2)}[\varphi] = -\frac{1}{8} S_{,ijkl}[\varphi] G^{ij} G^{kl} - \frac{1}{12} S_{,ijk} S_{,lmn} G^{il} G^{jm} G^{kn}. \tag{8.86}$$

It should be clear from our description how, in principle, you could evaluate terms in the expansion of $\Gamma[\varphi]$ to any order in $\hbar$.

[9] We have used the matrix identity $\delta(\mathrm{tr} \ln A) = \mathrm{tr}(A^{-1}\delta A)$, see (8.21), and noted that $-G^{ij}$ is the inverse of $S_{,ij}$ by virtue of (8.64).

8.3 Feynman diagrams

There is a very useful way of interpreting the terms in the perturbative expansion of the effective action that makes use of diagrams. This method was originally devised by Feynman (1949b), with the resulting diagrams now referred to as 'Feynman diagrams'.

The basic idea is to interpret the cubic and higher-order terms that arise in the expansion of the action functional about φ as vertices in the diagram. So for example we will interpret $S_{,ijk}$ as a three-point vertex, $S_{,ijkl}$ as a four-point vertex, and so on. The pictures we can draw for these vertices are illustrated in Fig. 8.1.

The contraction of the vertices with Green functions is indicated by joining together the lines emanating from the vertices to form closed loops. For example, $S_{,ijk}G^{ij}$ would be represented by the diagram shown in (a) of Fig. 8.2 and $S_{,ijkl}G^{ij}$ would be represented by the diagram in (b) of Fig. 8.2. The results that we found for the effective action in Section 8.2 do not involve any indices that are not summed. In this case we join up the relevant lines from the vertices according to the way they are connected by Green functions. For example, $S_{,ijkl}G^{ij}G^{kl}$ is represented by diagram (a) of Fig. 8.3, $S_{,ijk}S_{,lmn}G^{il}G^{jm}G^{kn}$ is represented by diagram (b) of Fig. 8.3, and $S_{,ijk}S_{,lmn}G^{ij}G^{kl}G^{mn}$ is represented by diagram (c) of Fig. 8.3. Because there are no lines coming out from the diagrams in Fig. 8.3, these are sometimes called 'vacuum diagrams'.

The expression for $\Gamma^{(2)}[\varphi]$ is made up solely from the Feynman diagrams (sometimes simply called 'graphs') corresponding to (a) and (b) of Fig. 8.3; the diagram in (c) does not occur. In the evaluation of $\langle A^2_{3/2}\rangle_0$ in

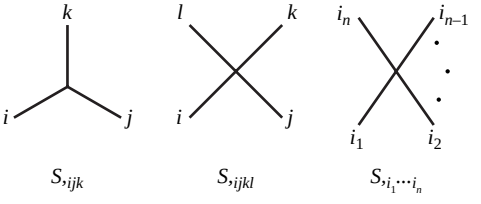

Fig. 8.1 The vertices that can occur in Feynman diagrams.

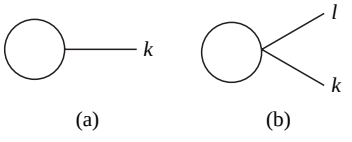

Fig. 8.2 The Feynman diagrams that correspond to $S_{,ijk}G^{ij}$ and $S_{,ijkl}G^{ij}$.

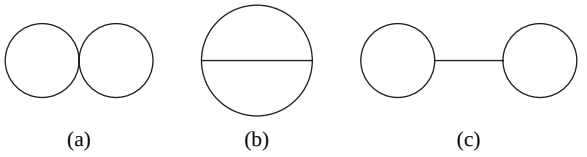

Fig. 8.3 Feynman diagram (a) corresponds to $S_{,ijkl}G^{ij}G^{kl}$, diagram (b) to $S_{,ijk}S_{,lmn}G^{il}G^{jm}G^{kn}$, and diagram (c) to $S_{,ijk}S_{,lmn}G^{ij}G^{kl}G^{mn}$.

Section 8.2 we did encounter terms that would have the graphical interpretation of (c) in Fig. 8.3. However, these terms ended up cancelling out of the final expression. A graph like that in (c) of Fig. 8.3, which can end up as two separate pieces by cutting one of the internal lines, is called 'one-particle reducible'. Graphs like those of (a) or (b) of Fig. 8.3, which do not have this property, are called 'one-particle irreducible'. One-particle irreducible graphs remain in one piece (called 'connected') when any single internal line is cut. What we have shown in Section 8.2 is that to order $\hbar^2$ the effective action is comprised of one-particle irreducible vacuum diagrams. This turns out to be true to all orders in $\hbar$.[10]

One other piece of terminology that is used concerns the number of loops in a diagram. Graphs like those in Fig. 8.3 are called 'two-loop diagrams' for a fairly obvious reason. Examples of three-loop diagrams are those in Fig. 8.4. By introducing $\hbar$ as we did earlier, the power of $\hbar$ that occurs in $\Gamma[\varphi]$ counts the number of loops. For this reason, the expansion we have described in Section 8.2 is called the 'loop expansion'. Before giving a proof that the $\hbar$ expansion is the same as expanding in the number of loops in a Feynman diagram, we will show how the use of Feynman diagrams shortens the calculation of the effective action. A recipe for the construction of $\Gamma[\varphi]$ is given below.

We have argued that $\Gamma[\varphi]$ contains only one-particle irreducible graphs. We only need to consider the vertices that arise from the expansion of $S[\phi]$ about $\phi = \varphi$. The two-loop effective action can contain two three-point vertices or one four-point vertex. Consider the two three-point vertices

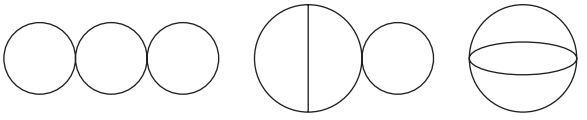

Fig. 8.4 Possible vacuum diagrams of three-loop order that can contribute to the effective action. They are one-particle irreducible.

[10] See Jackiw (1974) for a proof.

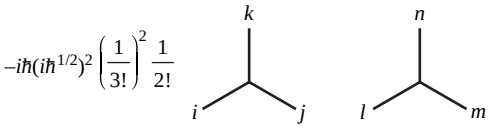

Fig. 8.5 Three-point vertices that when paired off can contribute to the two-loop effective action. The factor of $\hbar$ and the appropriate combinatorial factor is indicated.

first. Before pairing off the lines on the vertices according to Wick's theorem, we have the situation in Fig. 8.5. The numerical factor comes about as follows. There is a factor of $1/2!$ coming from the Taylor expansion of the exponential to second order to give rise to the two vertices, as well as a factor of $(i\hbar^{1/2})^2$. (Recall that the factor of $\hbar$ in the exponent is $\hbar^{-1} \times \hbar^{3/2}$ after scaling the fields $\psi^i \to \hbar^{1/2}\psi^i$.) Each vertex has a factor of $1/3!$ from the Taylor expansion of $S[\phi]$. Finally, there is a factor of $-i\hbar$ coming from that outside the logarithm in the definition of $\Gamma[\varphi]$ in the line above (8.66). Multiplication of these factors gives the coefficient indicated in Fig. 8.5.

We now pair off the lines on the vertices in Fig. 8.5 in all possible ways to give one-particle irreducible graphs. If we consider the line labelled i on the first vertex it can only join with the lines labelled l, m, or n on the second vertex.[11] Regardless of which of l, m, n is chosen for i to pair with we end up with the same result because of the symmetry of the vertex: $S_{,lmn} = S_{,mnl}$ etc. We therefore end up with the situation shown in Fig. 8.6 by choosing i to pair with l. The factor of 3 that has appeared in passing between Fig. 8.5 and Fig. 8.6 accounts for the three possible lines we can pair with i. (We chose to pair i with l, but we could equally well have chosen to pair with m or n giving an identical result.) In Fig. 8.6 we can now pair the line j with either m or n, each of which gives the same result.[12] This gives the result in Fig. 8.7 with the extra factor of 2 accounting for the two ways to pair j. There is only one possible pairing of the lines left, so simplifying the numerical factor we find the result in Fig. 8.8. Associated with each pairing of the lines is a factor of $-i$ coming from the basic result $\langle\psi^i\psi^j\rangle_0 = -iG^{ij}$ from (8.68) used in Wick's theorem. This gives the overall coefficient of $S_{,ijk}S_{,lmn}G^{il}G^{jm}G^{kn}$ in $\Gamma^{(2)}$ as $(-i)^3 \times (i\hbar^2/12) = -(\hbar^2/12)$ in complete agreement with that found for this particular term in (8.86).

For the four-point vertex, there is a factor of $i\hbar$ coming from the expansion of the exponential (arising from $i\hbar^{-1} \times (\hbar^{1/2})^4$) and a factor of $1/4!$

[11] If i joins with j or k, we will necessarily end up with a one-particle reducible graph.
[12] If j pairs with k the graph is one-particle reducible.

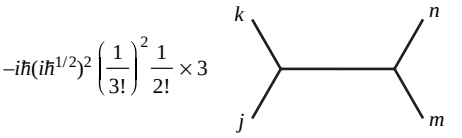

Fig. 8.6 We have paired off i with l in Fig. 8.6 to obtain this diagram. The factor of 3 comes about because we could choose to pair i with l, m, or n, and all such pairings give rise to the same expression.

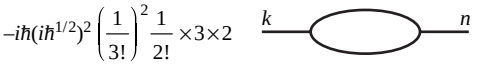

Fig. 8.7 We have paired off j with m in Fig. 8.6 to obtain this diagram. The additional factor of 2 comes about because we could have chosen to pair off j with n to give an identical diagram.

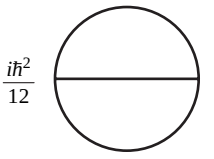

Fig. 8.8 We pair off k with n in Fig. 8.7 to obtain this diagram. There is only one possible pairing. The numerical factor that multiplies the diagram has been simplified.

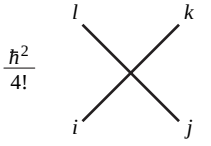

Fig. 8.9 The four-point vertex that can contribute to the two-loop effective action. The lines must be paired off in all possible ways.

Fig. 8.10 The two-loop diagram that results from pairing off the lines in Fig. 8.9.

coming from the Taylor expansion of $S[\phi]$ to give the vertex. If we multiply by the overall factor of $-i\hbar$ from outside the logarithm as before, we find the result in Fig. 8.9. If we consider the line i, there are three possible lines to pair with, each of which gives an identical result due to the symmetry of the vertex $S_{,ijkl}$. After this pairing there is only one possible pairing left. This results in the diagram of Fig. 8.10. Again there

is a factor of $-i$ coming from each Green function on the paired lines, resulting in $(-i)^2$ in this case. The coefficient of $S_{,ijkl}G^{ij}G^{kl}$ in $\Gamma^{(2)}$ is therefore $(-i)^2 \times \hbar^2/8 = -\hbar^2/8$ again in agreement with the result in (8.86). Hopefully it is clear how the general procedure may be used for other terms in $\Gamma[\varphi]$.

To finish this discussion we will now prove our earlier assertion that the number of loops in a given Feynman diagram that contributes to $\Gamma[\varphi]$ is identical to the power of $\hbar$ that occurs in our expansion. To do this, note that a general diagram consists of a number of different n-point vertices. Let v_n be the number of n-point vertices in some graph. (For example in Fig. 8.3 for diagram (a) we have $v_4 = 1$; for diagrams (b) and (c) we have $v_3 = 2$.) Let I be the number of Green functions that occur. Because each Green function corresponds to a line, this is also the number of lines that connect the vertices, called 'internal lines'. Each pairing of the lines in the different vertices connects up two lines from the complete set of lines coming from all the vertices. This means that we must have

$$2I = \sum_{n=3}^{\infty} n v_n. \tag{8.87}$$

The number of loops is given by the topological relation

$$L = I - \sum_{n=3}^{\infty} v_n + 1, \tag{8.88}$$

that can be recognized as Euler's theorem for planar graphs.[13] If we combine (8.87) and (8.88) we find

$$L = \sum_{n=3}^{\infty} \left(\frac{n}{2} - 1\right) v_n + 1. \tag{8.89}$$

We now argue that L is the power of $\hbar$ that occurs in the expansion of $\Gamma[\varphi]$. Each n-point vertex carries a power of $\hbar^{n/2}$ due to our scaling of $\psi^i \to \hbar^{1/2}\psi^i$ described above. There is a factor of $\hbar^{-1}$ in the argument of the exponential, therefore each n-point vertex gives us a factor of $\hbar^{(n/2-1)}$. Since there are v_n such vertices we find the factor $\hbar^{(n/2-1)v_n}$. Considering all possible vertices results in the factor of $\hbar$ being

$$\prod_{n=3}^{\infty} \hbar^{[n/2-1]v_n} = \hbar^{\sum_{n=3}^{\infty}[n/2-1]v_n}.$$

[13] See Rouse Ball and Coxeter (1974) for example.

Finally there is an overall factor of $-i\hbar$ in the definition of $\Gamma[\varphi]$ outside the logarithm, resulting in the final power being $\hbar^L$ with L given by (8.89) as claimed.

8.4 One-loop effective potential for a real scalar field

As an application of the general formalism, we will study a real scalar field with a $\lambda\phi^4$ self-interaction in four-dimensional spacetime. We will calculate the effective potential and compare the result with that found earlier using the simpler energy ζ-function method of Chapter 4. The benefit of the present approach is that it gives us a systematic way to go beyond lowest order in perturbation theory, which we will study in Section 8.6.

The classical action functional will be chosen to be

$$S[\phi] = \int dv_x \left(\frac{1}{2}\partial^\mu \phi \partial_\mu \phi - \frac{1}{2}m^2\phi^2 - \frac{\lambda}{4!}\phi^4 - c \right), \tag{8.90}$$

and we will be interested in only four-dimensional spacetime. With the insights gained from the simpler calculations of Chapter 4, the formal results that we have obtained for the effective action will be expected to be divergent and require regularization and renormalization to be carried out.

The key ingredients needed for $\Gamma[\varphi]$ are the terms that occur in the expansion of $S[\phi]$ about $\phi = \varphi$. If we let $\phi = \varphi + \hbar^{1/2}\psi$ as in (8.46), we find

$$\begin{aligned} S[\phi] = S[\varphi] &+ \hbar^{1/2} \int dv_x \left(\partial^\mu \varphi \partial_\mu \psi - m^2 \varphi\psi - \frac{\lambda}{6}\varphi^3\psi \right) \\ &+ \hbar \int dv_x \left(\frac{1}{2}\partial^\mu \psi \partial_\mu \psi - \frac{1}{2}m^2\psi^2 - \frac{\lambda}{4}\varphi^2\psi^2 \right) \\ &- \hbar^{3/2} \int dv_x \frac{\lambda}{6}\varphi\psi^3 - \hbar^2 \int dv_x \frac{\lambda}{4!}\psi^4. \end{aligned} \tag{8.91}$$

It is easy to identify $S_{,ijk}$ and $S_{,ijkl}$ in the last two terms of (8.91). We could have obtained them directly by repeated functional differentiation of (8.90) if we wished. The term in the middle line of (8.91) corresponds to $(\hbar/2)S_{,ij}\psi^i\psi^j$ in condensed notation. If we integrate $\partial^\mu\psi\partial_\mu\psi$ by parts, it can be seen that

$$S_{,ij} = -\left[\Box_x + m^2 + \frac{\lambda}{2}\varphi^2(x) \right] \delta(x, x'). \tag{8.92}$$

The Feynman Green's function is therefore defined by (see (8.64))

$$\left[\Box_x + m^2 + \frac{\lambda}{2}\varphi^2(x)\right] G(x,x') = \delta(x,x') \tag{8.93}$$

with m^2 understood to be $m^2 - i\epsilon$ here.

The calculation of the effective action, even at one-loop order, relies on an evaluation of $G(x,x')$. When $\varphi(x) = 0$, or more generally when the background field is constant, it is easy to calculate $G(x,x')$ by Fourier transforms. We will concentrate on constant background fields in this section. Suppose that we consider

$$\left(\Box_x + M^2 - i\epsilon\right) G(x,x') = \delta(x,x') \tag{8.94}$$

where $M^2 = m^2 + (\lambda/2)\varphi^2$ is constant. Let

$$G(x,x') = \int \frac{d^4k}{(2\pi)^4}\, e^{ik_\mu(x^\mu - x'^\mu)} G(k). \tag{8.95}$$

Because

$$\delta(x,x') = \int \frac{d^4k}{(2\pi)^4}\, e^{ik_\mu(x^\mu - x'^\mu)}, \tag{8.96}$$

we find

$$G(k) = \frac{-1}{k^2 - M^2 + i\epsilon}. \tag{8.97}$$

It is now possible to carry out the integration over k in (8.95) to obtain an explicit result for $G(x,x')$.[14] Instead of doing this we will perform a Wick rotation to imaginary time and evaluate the Euclidean Green function $G^E(x,x')$ that we define by

$$G^E(x,x') = \int \frac{d^4k}{(2\pi)^4}\, e^{ik_\mu(x^\mu - x'^\mu)} (k^2 + M^2)^{-1}. \tag{8.98}$$

The Euclidean Green function is easier to calculate, and we can always recover the original Green function by analytic continuation. Transform to spherical polar coordinates in (8.98) is defined by

$$\begin{aligned} k_1 &= k \sin\chi \sin\theta \cos\phi, \\ k_2 &= k \sin\chi \sin\theta \sin\phi, \\ k_3 &= k \sin\chi \cos\theta, \\ k_4 &= k \cos\chi, \end{aligned}$$

[14] See Bogoliubov and Shirkov (1959) for example.

and let

$$k_\mu(x^\mu - x'^\mu) = kr\cos\chi,$$

where $r = |x - x'|$. The integrations over θ and ϕ in (8.98) are easily performed leaving

$$G^E(x,x') = \frac{1}{4\pi^3}\int_0^\infty dk \frac{k^3}{k^2+M^2}\int_0^\pi d\chi \sin^2\chi\, e^{-ikr\cos\chi}. \tag{8.99}$$

The integration over χ in (8.99) results in a Bessel function:[15]

$$G^E(x,x') = \frac{1}{4\pi^3 r}\int_0^\infty dk\, \frac{k^2 J_1(kr)}{k^2+M^2}. \tag{8.100}$$

This last integral can also be done[16] to yield

$$G^E(x,x') = \frac{M}{4\pi^2 r}K_1(Mr), \tag{8.101}$$

with K_1 a Bessel function of the third kind. So long as $r \neq 0$ this result is perfectly finite; however, when $r \to 0$ we find

$$G^E(x,x') \simeq \frac{1}{4\pi^2 r^2} + \frac{M^2}{8\pi^2}\ln\left(\frac{Mr}{2}\right) + \cdots \tag{8.102}$$

by expanding the Bessel function. The divergences found in our earlier approach (described in Chapter 4) show up when we let $x \to x'$ in the Green function. In the expression for the one-loop effective action (8.54) the trace (since $\ln\det = \mathrm{tr}\ln$) involves setting two of the condensed notation indices i and j equal to each other and summing. In the normal notation this will involve two spacetime coordinates set equal to each other and integrating, a procedure that may lead to a divergent expression.

We can relate $\Gamma^{(1)}$ directly to $G(x,x')$ by varying both sides of (8.54), noting first that $\ln\det = \mathrm{tr}\ln$, with respect to M^2:

$$\begin{aligned}\frac{\partial}{\partial M^2}\Gamma^{(1)} &= \frac{i}{2}\mathrm{tr}\left(-G^{ij}\frac{\partial}{\partial M^2}S_{,jk}\right)\\ &= \frac{i}{2}\int dv_x G(x,x).\end{aligned} \tag{8.103}$$

[15] See #3.771.8 on page 427 of Gradsteyn and Ryzhik (1965).
[16] See #6.566.2 on page 687 of Gradsteyn and Ryzhik (1965).

In obtaining the second line we have used

$$\frac{\partial}{\partial M^2} S_{,jk} = -\delta_{jk}$$

as follows from (8.92). Thus, $G(x,x)$, which we have just seen to be infinite, appears. There are many different ways of dealing with $G(x,x)$ that have been developed. We will discuss one method here and an alternative method in the next section.

One of the oldest ways to deal with the divergences that arise is to note that because they are associated with high energies there may be some new physics that occurs at high energy. Our existing theory is then just a low energy approximation to this 'better' theory. This motivates the introduction of a cut-off in the momentum space integration. We will define

$$G(x,x) = -\int^{\Lambda} \frac{d^4k}{(2\pi)^4} (k^2 - M^2 + i\epsilon)^{-1}, \tag{8.104}$$

where the presence of Λ denotes that the integration only extends over values of k with $|k| \leq \Lambda$. If we regard the integration over k^0 in (8.104) as along a contour in the complex plane, we can rotate the contour of integration from the real axis to lie along the imaginary axis extending from $-i\infty$ to $+i\infty$. Making the change of variable (Wick rotation)

$$k^0 = ik^4, \tag{8.105}$$

and then switching to spherical polar coordinates as defined earlier we have the general result

$$\int^{\Lambda} f(k^2) d^4k = 2\pi^2 i \int_0^{\Lambda} \kappa^3 f(-\kappa^2) d\kappa, \tag{8.106}$$

where

$$\begin{aligned} \kappa^2 &= -(k^0)^2 + (k^1)^2 + (k^2)^2 + (k^3)^2 \\ &= (k^4)^2 + (k^1)^2 + (k^2)^2 + (k^3)^2. \end{aligned} \tag{8.107}$$

When applied to (8.104) we find

$$\begin{aligned} G(x,x) &= \frac{i}{8\pi^2} \int_0^{\Lambda} \frac{\kappa^3}{\kappa^2 + M^2}\, d\kappa \\ &= \frac{i}{16\pi^2} \left[\Lambda^2 - M^2 \ln\left(1 + \frac{\Lambda^2}{M^2}\right) \right]. \end{aligned} \tag{8.108}$$

It is clear how the divergence that is present in the original expression appears when we try to take $\Lambda \to \infty$. There is both a quadratic and a logarithmic dependence on Λ.

We return to the result for $G(x,x)$ before the integration in the first line of (8.108). As in (4.3) we may define the one-loop effective potential by

$$\Gamma^{(1)}[\varphi] = -\int dv_x V^{(1)}(\varphi). \tag{8.109}$$

We have, noting the relationship in (8.103),

$$V^{(1)} = \frac{1}{16\pi^2}\int_0^\Lambda d\kappa\, \kappa^3 \ln\left[(\kappa^2 + M^2)\ell^2\right] \tag{8.110}$$

where we introduce the arbitrary length scale ℓ to keep the argument of the logarithm dimensionless. Regardless of the value for ℓ, we can recover

$$\frac{\partial}{\partial M^2}V^{(1)} = -\frac{i}{2}G(x,x)$$

from (8.110). The integral in (8.110) can be done with the result

$$\begin{aligned} V^{(1)} &= \frac{1}{64\pi^2}\left[\Lambda^4 \ln\left(1+\frac{\Lambda^2}{M^2}\right) - M^4 \ln\left(1+\frac{\Lambda^2}{M^2}\right)\right. \\ &\quad \left. -\frac{1}{2}\Lambda^4 + \Lambda^2 M^2 + \Lambda^4 \ln(\ell^2 M^2)\right] \\ &\simeq \frac{1}{64\pi^2}\left[\Lambda^4 \ln(\ell^2\Lambda^2) - M^4 \ln\left(\frac{\Lambda^2}{M^2}\right)\right. \\ &\quad \left. -\frac{1}{2}\Lambda^4 + 2\Lambda^2 M^2 - \frac{1}{2}M^4\right]. \end{aligned} \tag{8.111}$$

In the second equality above we have taken $\Lambda \gg M$, expanded the logarithms, and kept only those terms that do not vanish in the limit $\Lambda \to \infty$. We can combine this with the classical part of the effective action, remembering that we have treated φ as constant here, to find

$$V_{\text{eff}} = c + \frac{1}{2}m^2\varphi^2 + \frac{\lambda}{4!}\varphi^4 + \hbar\, V^{(1)}(\varphi). \tag{8.112}$$

We have $V^{(1)}$ given in (8.111) with $M^2 = m^2 + (\lambda/2)\varphi^2$.

The physical parameters of the theory must be defined by adopting some set of renormalization conditions as discussed in Section 4.6. We will impose the same set of renormalization conditions as we did before (see (4.145)–(4.147)). The parameters that occur in the original action

(8.90) are treated as bare quantities. Because the difference between the bare and renormalized quantities only arises at one-loop order, we may write

$$c = c_R + \hbar\,\delta c^{(1)} + \hbar^2 \delta c^{(2)} + \cdots, \tag{8.113}$$

$$m^2 = m_R^2 + \hbar\,\delta m^{2(1)} + \hbar^2 \delta m^{2(2)} + \cdots, \tag{8.114}$$

$$\lambda = \lambda_R + \hbar\,\delta\lambda^{(1)} + \hbar^2 \delta\lambda^{(2)} + \cdots. \tag{8.115}$$

Here δ denotes a counterterm, with the superscript in brackets denoting the order of the counterterm in the loop expansion. So far we have only discussed one-loop order, but we expect there to be counterterms at all orders in the loop expansion necessary for renormalization. In addition, we have ignored a possible renormalization of the background field φ. We will verify that this is allowed at one-loop order in the next section when we discuss background fields that are not constant. In Section 8.6 we will consider what happens at two-loop order.

If we work only to order $\hbar$, then because $V^{(1)}$ is multiplied by $\hbar$ in (8.112), we can simply replace m^2, λ in (8.111) with their renormalized values m_R^2, λ_R. The renormalization conditions (4.145)–(4.147) fix the counterterms of order $\hbar$ to be

$$\delta c^{(1)} = -\frac{1}{64\pi^2}\Big[\Lambda^4 \ln(\ell^2\Lambda^2) - m_R^4 \ln\left(\frac{\Lambda^2}{m_R^2}\right) - \frac{1}{2}\Lambda^4 + 2\Lambda^2 m_R^2 - \frac{1}{2}m_R^2\Big], \tag{8.116}$$

$$\delta m^{2(1)} = -\frac{\lambda_R}{32\pi^2}\left[\Lambda^2 - m_R^2 \ln\left(\frac{\Lambda^2}{m_R^2}\right)\right], \tag{8.117}$$

$$\delta\lambda^{(1)} = \frac{3\lambda_R^2}{32\pi^2}\left[\ln\left(\frac{\Lambda^2}{m_R^2}\right) - 1\right]. \tag{8.118}$$

Using these counterterms back in the effective potential shows that we recover exactly the same expression as we found earlier in (4.151) using a completely different approach. There is no dependence in the final expression on the cut-off Λ that we may now safely take to infinity. The crucial feature that resulted in the disappearance of Λ from our final result is that all of the terms in $V^{(1)}$ that became infinite as we took $\Lambda \to \infty$ had the same form as those that appeared in the classical action (or potential). If, for example, we had ended up with a term in $V^{(1)}$ like $\Lambda^3 M$ that is allowed on dimensional grounds, we could not have removed the Λ dependence by using the renormalization counterterms in (8.116)–(8.118). We would then be forced to conclude that the theory was not renormalizable.

8.5 Dimensional regularization and the derivative expansion

8.5.1 Dimensional regularization

An alternative method of regularization to the cut-off scheme described in Section 8.4 makes use of dimensional regularization ('t Hooft and Veltman, 1972). Here we treat the spacetime dimension n initially as a complex variable and try to perform the analytic continuation to $n = 4$. For example, from Section 8.4 we have

$$G(x,x) = -\int \frac{d^n k}{(2\pi)^n}(k^2 - M^2 + i\epsilon)^{-1}. \tag{8.119}$$

Perform the Wick rotation of the k^0 contour as in (8.105) to find

$$G(x,x) = i\int \frac{d^n \kappa}{(2\pi)^n}(\kappa^2 + M^2)^{-1}. \tag{8.120}$$

with κ^2 defined as in (8.107), but extended to n spacetime dimensions. In order to examine the convergence of this integral, look at the behaviour of the integrand for large and small values of κ. The volume element contains κ^{n-1} and the integrand has a factor of κ^{-2} leading to the asymptotic behaviour of κ^{n-3} for large κ. We therefore take $\mathcal{R}(n) < 2$ to ensure convergence of the integrand for large κ. At the lower end of the integration, for small κ the integrand behaves like κ^{n-1} (assuming that $M \neq 0$), so we take $\mathcal{R}(n) > 0$ to ensure that the integral converges when $\kappa \to 0$. Combining these two results suggests that we work initially in the strip $0 < \mathcal{R}(n) < 2$ in the complex n-plane where we expect $G(x,x)$ as defined by (8.120) to be an analytic function of n. The aim is to evaluate this function and then to explore the analytic continuation back to the physical spacetime dimension (e.g. $n = 4$).

The integration in (8.120) may be performed using exactly the same procedure as we introduced in Section 4.2. We first write

$$(\kappa^2 + M^2)^{-1} = \int_0^\infty dt\, e^{-t(\kappa^2 + M^2)},$$

then do the integration over κ noting that this just involves a product of Gaussians, and finally make use of the integral representation of the Γ-function in (A1.1) of Appendix 1 to find

$$G(x,x) = i(4\pi)^{-n/2}\Gamma\left(1 - \frac{n}{2}\right)(M^2)^{n/2-1}. \tag{8.121}$$

This result is an analytic function of n in the strip $0 < \mathcal{R}(n) < 2$ as expected from the discussion above; however, it can now be defined

throughout the complex n-plane by analytic continuation of the Γ-function. The procedure is virtually the same as the energy ζ-function method we used earlier in the book, although of course the parameter that is being analytically continued is totally different here. In fact we could have used dimensional regularization in previous chapters had we wished. The result in (8.121) is seen to contain a simple pole at $n = 4$, and this is where the original divergence that is present in the coincidence limit of the Green function shows up.

The underlying approach of dimensional regularization suggests the following. Regard our original quantum fields ϕ^i as fields in an n-dimensional spacetime, with n viewed as a complex variable chosen in a suitable region of the complex plane to ensure that the expressions that we deal with are well defined (assuming this is possible). We are interested in analytic continuation back to $n = 4$. (Other spacetime dimensions are easily accommodated.) We can regard our n-dimensional 'regulating' spacetime as $M_n = M_4 \times V_{n-4}$ where M_4 is four-dimensional Minkowski spacetime, and V_{n-4} represents the additional dimensions whose volume we will call ℓ^{n-4} with ℓ an arbitrary unit of length. Only the quantum part of the field needs to depend on the coordinates of the extra dimensions for V_{n-4} because all we require is that the momentum integrals are n-dimensional. We can take the background field φ^i to only have a dependence on the physical four-dimensional coordinates. Using dimensional analysis it is easily seen from the action that the results in the following table are obtained.

Quantity	Dimension (units of length)
ϕ, φ	$1 - n/2$
m^2	-2
c	$-n$
λ	$n - 4$

In addition, $d^n x = \ell^{n-4} d^4 x$ when occurring in an expression that only involves the coordinates on four-dimensional Minkowski spacetime.

Because renormalized expressions may be related to physically measurable quantities, following 't Hooft (1971) we will choose renormalized quantities to have the same dimensions for all n as they do for $n = 4$. This means that we can write

$$m^2 = m_R^2 + \delta m^2, \tag{8.122}$$

$$c = \ell^{4-n} \left[c_R + \delta c \right], \tag{8.123}$$

$$\lambda = \ell^{n-4}\left[\lambda_R + \delta\lambda\right], \tag{8.124}$$

$$\varphi(x) = \ell^{2-n/2} Z^{1/2} \varphi_R(x). \tag{8.125}$$

The last result requires a brief explanation. We have written $\phi^i = \varphi^i + \hbar^{1/2}\psi^i$, so that our background field has dimensions of $1 - n/2$ (in units of length) according to the above table. We want the renormalized background field to have length units of -1 (corresponding to $n = 4$ in $1-n/2$), so that a factor of $\ell^{2-n/2}$ is introduced to balance the dimensions on both sides of (8.125). In addition, rather than writing a field counterterm, it is conventional to use a field renormalization factor $Z^{1/2}$. We can write

$$Z = 1 + \delta Z. \tag{8.126}$$

All of the counterterms in (8.122)–(8.126) may be expressed in terms of the loop expansion like

$$\delta q = \hbar\, \delta q^{(1)} + \hbar^2 \delta q^{(2)} + \cdots, \tag{8.127}$$

with q representing any relevant quantity (m^2, c, λ, Z). As before, the superscript (n) indicates the order in the loop expansion. In dimensional regularization, each $\delta q^{(n)}$ is expressed in terms of the poles that occur at $n = 4$ (plus possibly some additional finite parts depending upon how we define our renormalization conditions).

The one-loop effective potential in n dimensions $V_n^{(1)}$ is defined in terms of the one-loop effective action by $\Gamma^{(1)} = -\int d^n x\, V_n^{(1)}$. It is clear that since $d^n x = \ell^{n-4} d^4 x$ we should define the effective potential in four spacetime dimensions as

$$V^{(1)} = \ell^{n-4} V_n^{(1)}. \tag{8.128}$$

Using (8.103) we have

$$\begin{aligned} \frac{\partial}{\partial M^2} V^{(1)} &= -\frac{i}{2}\ell^{n-4} G(x,x) \\ &= \frac{1}{2}(4\pi)^{-n/2}\ell^{n-4}\Gamma\left(1 - \frac{n}{2}\right)(M^2)^{n/2-1}. \end{aligned} \tag{8.129}$$

We can integrate this result using the boundary condition $V^{(1)} = 0$ when $M^2 = 0$, and make use of the recurrence relation (A1.2) for the Γ-function in Appendix 1 to find

$$V^{(1)} = -\frac{1}{2}\ell^{n-4}(4\pi)^{-n/2}\ell^{n-4}\Gamma\left(-\frac{n}{2}\right)(M^2)^{n/2}. \tag{8.130}$$

This result may be analytically continued throughout the entire complex n-plane. There is a simple pole at the physical spacetime dimension of

$n = 4$. Making use of the Laurent expansion of the Γ-function described in Appendix 1 it can be shown that

$$V^{(1)} = \frac{M^4}{32\pi^2}\left[\frac{1}{n-4} + \frac{1}{2}\ln\left(\frac{M^2\ell^2}{4\pi}\right) - \frac{3}{4} + \frac{1}{2}\gamma + \cdots\right]. \tag{8.131}$$

Note that

$$\begin{aligned} M^2 &= m^2 + \frac{\lambda}{2}\varphi^2 \\ &= m_R^2 + \frac{\lambda_R}{2}\varphi_R^2 + \mathcal{O}(\hbar), \end{aligned} \tag{8.132}$$

if we make use of (8.122), (8.124), and (8.125). As in the earlier calculation of the effective potential, we can take the quantities that occur inside $V^{(1)}$ as renormalized to the order we are working.

With (8.122)–(8.125) used along with $d^n x = \ell^{n-4} d^4 x$ we have the classical, or zero-loop, potential given by

$$\begin{aligned} V^{(0)} = c_R + \hbar\delta c^{(1)} + \frac{1}{2}m_R^2\varphi_R^2 + \frac{\hbar}{2}\delta m^{2(1)}\varphi_R^2 \\ + \frac{\lambda_R}{4!}\varphi_R^4 + \hbar\frac{\delta\lambda^{(1)}}{4!}\varphi_R^4. \end{aligned} \tag{8.133}$$

Note that introducing ℓ as we have done has resulted in the factor of ℓ^{n-4} coming from the n-dimensional volume element cancelling with the factors of ℓ coming from the definition of the counterterms and renormalized quantities in (8.122)–(8.125). If we concentrate on simply removing the pole terms, so that we can take the $n \to 4$ limit, it can be seen that we must choose

$$\delta c^{(1)} = -\frac{m_R^4}{32\pi^2}(n-4)^{-1}, \tag{8.134}$$

$$\delta m^{2(1)} = -\frac{\lambda_R m_R^2}{16\pi^2}(n-4)^{-1}, \tag{8.135}$$

$$\delta\lambda^{(1)} = -\frac{3\lambda_R^2}{16\pi^2}(n-4)^{-1}. \tag{8.136}$$

It is easy to show that if we impose the same renormalization conditions we used earlier in (4.145)–(4.147), then in addition to the pole terms indicated in (8.134)–(8.136) there are additional finite terms present. The full renormalized result for the effective potential is identical to that found by the previous methods.

The main advantage of using dimensional regularization in place of the energy ζ-function method is that it extends in a straightforward way to

higher orders in the loop expansion. The main advantage that dimensional regularization has over the use of a cut-off is that it is manifestly gauge-invariant; gauge symmetry is independent of the spacetime dimension. A cut-off on the other hand introduces a mass scale into the theory that breaks gauge invariance unless special care is taken.

8.5.2 Non-constant background fields

In order to present a complete analysis of the renormalization of $\lambda\phi^4$ theory even at one-loop order it is necessary to remove the restriction to constant background fields. We must therefore solve (8.93) for an arbitrary value of $\varphi^2(x)$. We will study the more general equation

$$\left[\Box_x + m^2 + V(x)\right] G(x,x') = \delta(x,x') \tag{8.137}$$

where m^2 is understood to be $m^2 - i\epsilon$ as before. Here $V(x)$ is an arbitrary function of x. (For example, we might be interested in $V(x) = \lambda\varphi^2(x)/2$.)

The singular behaviour of $G(x,x')$ shows up as $x \to x'$. In addition, to calculate the one-loop effective action we only require $G(x,x)$. We can therefore concentrate on the behaviour of $G(x,x')$ when x and x' are close. To this end, let

$$x^\mu = x'^\mu + y^\mu, \tag{8.138}$$

with x'^μ regarded as fixed. The aim is to substitute this into (8.137), expand in powers of y^μ and then solve the resulting equations order by order in y^μ. This is a method that was introduced to study the short distance behaviour of the Green's function in curved spacetime by Bunch and Parker (1979), and first used in the present context in Moss *et al.* (1992).

Expanding $V(x)$ in a Taylor series about $x^\mu = x'^\mu$ gives

$$V(x) = V(x') + \sum_{j=1}^{\infty} \frac{1}{j!} y^{\mu_1} \cdots y^{\mu_j} V_{\mu_1 \cdots \mu_j}, \tag{8.139}$$

where

$$V_{\mu_1 \cdots \mu_j} = \left. \frac{\partial^n V(x)}{\partial x^{\mu_1} \cdots \partial x^{\mu_j}} \right|_{x=x'}. \tag{8.140}$$

Since $\Box_x = \Box_y = \eta^{\mu\nu} \dfrac{\partial^2}{\partial y^\mu \partial y^\nu}$ and $\delta(x,x') = \delta(y)$, we find that (8.137) can be written as

$$\left(\Box_y + M^2 + \sum_{j=1}^{\infty} \frac{1}{j!} y^{\mu_1} \cdots y^{\mu_j} V_{\mu_1 \cdots \mu_j}\right) G(x,x') = \delta(y), \tag{8.141}$$

where

$$M^2 = m^2 - i\epsilon + V(x'). \tag{8.142}$$

In order to solve (8.141), we Fourier transform $G(x, x')$ just as we did for the case of constant $V(x)$ with one slight difference:

$$G(x, x') = \int \frac{d^n k}{(2\pi)^n} e^{ik\cdot y}\, G(k; x'). \tag{8.143}$$

This time the Fourier transform $G(k; x')$ will depend on the fixed point x' that we choose to expand about. As we will see, this allows us to obtain an expansion for the effective action in terms of derivatives of the background field. The result is given in n spacetime dimensions because we will adopt dimensional regularization here.

The next step is to substitute (8.143) for $G(x, x')$ into (8.141). Before doing this, note that

$$\Box_y G(x, x') = \int \frac{d^n k}{(2\pi)^n} e^{ik\cdot y}\, (-k^2) G(k; x'), \tag{8.144}$$

and that

$$\begin{aligned} y^{\mu_1} \cdots y^{\mu_j} G(x, x') &= \int \frac{d^n k}{(2\pi)^n} (-i)^j \frac{\partial^j e^{ik\cdot y}}{\partial k_{\mu_1} \cdots \partial k_{\mu_j}}\, G(k; x') \\ &= \int \frac{d^n k}{(2\pi)^n} e^{ik\cdot y}\, i^j \frac{\partial^j G(k; x')}{\partial k_{\mu_1} \cdots \partial k_{\mu_j}}, \end{aligned} \tag{8.145}$$

if we integrate by parts to obtain (8.145) from the result of the previous line. The Fourier transform $G(k; x')$ must then satisfy

$$\left[(-k^2 + M^2) + \sum_{j=1}^{\infty} \frac{i^j}{j!} V_{\mu_1 \cdots \mu_j} \frac{\partial^j}{\partial k_{\mu_1} \cdots \partial k_{\mu_j}} \right] G(k; x') = 1. \tag{8.146}$$

We can solve this equation in terms of the number of derivatives of V that occur by letting

$$G(k; x') = \sum_{l=0}^{\infty} G_l(k, x'), \tag{8.147}$$

with l counting the number of derivatives.

When (8.147) is used in (8.146) by equating terms on each side that have no derivatives (i.e. ignore the terms coming from the sum over j since they involve at least one derivative) we find

$$G_0(k; x') = \frac{-1}{k^2 - M^2}. \tag{8.148}$$

This is exactly what we found for the case of constant V in Section 8.4.

Substitution of (8.147) into (8.146), and using the result in (8.148), leads to

$$\sum_{l=1}^{\infty} G_l(k;x') - (k^2-M^2)^{-1}\sum_{j=1}^{\infty}\sum_{l=0}^{\infty}\frac{i^j}{j!}V_{\mu_1\cdots\mu_j}\frac{\partial^j G_l(k;x')}{\partial k_{\mu_1}\cdots\partial k_{\mu_j}} = 0. \quad (8.149)$$

The first term can be clearly identified as an expansion in powers of the derivatives of V, but the second term is more complicated since it is really $j+l$ that counts the number of derivatives there. To deal with this we may relabel the summation indices using

$$\sum_{l=0}^{\infty}\sum_{j=1}^{\infty} f(l,j) = \sum_{n=1}^{\infty}\sum_{j=1}^{n} f(n-j,j). \quad (8.150)$$

(This is deduced by setting $n = j+l$, so that $l = n-j$. Because $l = 0, 1, \ldots$ we can only have $j = 1, 2, \ldots, n$. The range of n is $1, 2, \ldots$.) If we relabel $n \to l$ in (8.150) we obtain

$$\sum_{l=1}^{\infty} G_l(k;x') - (k^2-M^2)^{-1}\sum_{l=1}^{\infty}\sum_{j=1}^{l}\frac{i^j}{j!}V_{\mu_1\cdots\mu_j}\frac{\partial^j G_{l-j}(k;x')}{\partial k_{\mu_1}\cdots\partial k_{\mu_j}} = 0. \quad (8.151)$$

Now l counts the number of derivatives in both of the two terms, and we can conclude that

$$G_l(k;x') = (k^2-M^2)^{-1}\sum_{j=1}^{l}\frac{i^j}{j!}V_{\mu_1\cdots\mu_j}\frac{\partial^j G_{l-j}(k;x')}{\partial k_{\mu_1}\cdots\partial k_{\mu_j}}. \quad (8.152)$$

This result fully determines all of the $G_l(k;x')$ in an iterative manner beginning with $l = 1$.

Setting $l = 1$ in (8.152) and using the result for $G_0(k;x')$ in (8.148) it is found that

$$G_1(k;x') = 2iV_\mu k^\mu (k^2-M^2)^{-3}. \quad (8.153)$$

With $l = 2$ in (8.152), and making use of the results for $l = 0, 1$ it can be shown that

$$\begin{aligned} G_2(k;x') = {} & -\eta^{\mu\nu}V_{\mu\nu}(k^2-M^2)^{-3} + 4k^\mu k^\nu V_{\mu\nu}(k^2-M^2)^{-4} \\ & -2V_\mu V^\mu (k^2-M^2)^{-4} + 12k^\mu k^\nu V_\mu V_\nu (k^2-M^2)^{-5}. \end{aligned} \quad (8.154)$$

Higher-order terms may be evaluated in a similar, although increasingly more complicated, way.[17] The nature of the expansion is that the higher-order terms start to fall off with larger powers of k. This makes the

[17] The next two terms are given in Moss *et al.* (1992).

expansion useful for the purposes of discussing renormalization because eventually after a finite number of terms we will have an expression that converges as we take $n \to 4$ even for $x = x'$. Another feature that can be noticed is that for l odd, $G_l(k; x')$ is an odd function of k. This means that when we take $x \to x'$ in $G(x, x')$ the terms with l odd will make no contribution.

If we now work out $G(x', x')$, the expression that we need to determine $\Gamma^{(1)}$, we find

$$G(x', x') = \int \frac{d^n k}{(2\pi)^n} \left[G_0(k; x') + G_1(k; x') + G_2(k; x') + \cdots \right]. \quad (8.155)$$

By using dimensional regularization, all of the momentum integrals that occur in this result can be made convergent in an appropriate region of the complex n-plane. The basic structure that we need to evaluate is (restoring the factor of $i\epsilon$)

$$\begin{aligned} I(p) &= \int \frac{d^n k}{(2\pi)^n} (k^2 - M^2 + i\epsilon)^{-p} \\ &= i(-1)^p \int \frac{d^n \kappa}{(2\pi)^n} (\kappa^2 + M^2)^{-p} \end{aligned} \quad (8.156)$$

where we have performed the Wick rotation (8.105, 8.107) in the second equality. Following the same steps as we used in going from (8.120) to (8.121), it can be shown that

$$I(p) = i \frac{(-1)^p}{(4\pi)^{n/2}} \frac{\Gamma(p - n/2)}{\Gamma(p)} \, (M^2)^{n/2 - p}. \quad (8.157)$$

We also require

$$I_\mu(p) = \int \frac{d^n k}{(2\pi)^n} \, k_\mu (k^2 - M^2 + i\epsilon)^{-p}, \quad (8.158)$$

$$I_{\mu\nu}(p) = \int \frac{d^n k}{(2\pi)^n} \, k_\mu k_\nu (k^2 - M^2 + i\epsilon)^{-p}. \quad (8.159)$$

The evaluation of $I_\mu(p)$ is easy. Because the integrand is an odd function of k, the result must be zero:

$$I_\mu(p) = 0. \quad (8.160)$$

For $I_{\mu\nu}(p)$, we first note that $I_{\mu\nu}(p) = I_{\nu\mu}(p)$. The only symmetric object that we have at our disposal is the metric tensor $\eta_{\mu\nu}$; thus, we must have

$$I_{\mu\nu} = A(p) \eta_{\mu\nu}, \quad (8.161)$$

for some function $A(p)$.[18] To calculate $A(p)$ in (8.161), contract both sides with $\eta^{\mu\nu}$ and use $\eta^{\mu\nu}\eta_{\mu\nu} = n$ and $\eta^{\mu\nu}k_\mu k_\nu = k^2$ to find

$$A(p) = \frac{1}{n}\int \frac{d^n k}{(2\pi)^n}\; k^2(k^2 - M^2 + i\epsilon)^{-p}.$$

Writing $k^2 = (k^2 - M^2 + i\epsilon) + (M^2 - i\epsilon)$ allows us to evaluate $A(p)$ in terms of $I(p)$ defined in (8.156) and use (8.157) to find

$$\begin{aligned} A(p) &= \frac{1}{n}\left[I(p-1) + (M^2 - i\epsilon)I(p)\right] \\ &= \frac{i}{2}(4\pi)^{-n/2}(-1)^{p-1}\frac{\Gamma(p-1-n/2)}{\Gamma(p)}(M^2)^{n/2+1-p}. \end{aligned} \tag{8.162}$$

We have taken $\epsilon \to 0$ and simplified the Γ-functions using the recursion relation (A1.2).

Higher-order terms that arise in the expansion of $G(x', x')$ all will involve integrals of the form we have been considering, but with more factors of k_μ in the integrands. Terms with an odd number of factors will integrate to zero, just as we found for $I_\mu(p)$ above. This means that in the expression for $G(x', x')$ only terms of the form $G_{2l}(k; x')$ with $l = 0, 1, 2, \ldots$ will be non-zero.[19]

Returning to the expansion for $G(x', x')$ in (8.155), using the results for G_0, G_1, and G_2 found in (8.148, 8.153, 8.154), and performing the momentum integrals as just described leads to

$$\begin{aligned} G(x', x') = &-I(1) + \eta^{\mu\nu}V_{\mu\nu}\left[4A(4) - I(3)\right] \\ &+2V^\mu V_\mu\left[6A(5) - I(4)\right] + \cdots \\ = &\, i(4\pi)^{-n/2}\Gamma\left(1 - \frac{n}{2}\right)(M^2)^{n/2-1} \\ &+\frac{i}{6}(4\pi)^{-n/2}\Gamma\left(3 - \frac{n}{2}\right)(M^2)^{n/2-3}\eta^{\mu\nu}V_{\mu\nu} \\ &-\frac{i}{12}(4\pi)^{-n/2}\Gamma\left(4 - \frac{n}{2}\right)(M^2)^{n/2-4}V^\mu V_\mu. \end{aligned} \tag{8.163}$$

Although the last two terms in (8.163) are finite as we take $n \to 4$, some care must be taken here because we are really after $\Gamma^{(1)}$ given by

$$\frac{\partial}{\partial M^2}\Gamma^{(1)} = \frac{i}{2}\int dv_{x'}\, G(x', x').$$

[18] This result can also be deduced by noting that for $\mu \neq \nu$ in (8.159) the integrand involves odd functions of k and so must vanish, and that the results for $\mu = \nu = 0$ and $\mu = \nu = 1$ are opposite in sign, but equal in magnitude by symmetry.

[19] The odd terms will of course contribute to $G(x, x')$ for $x \neq x'$.

We should integrate with respect to M^2 first before taking the limit $n \to 4$. If we are not interested in terms of $G(x', x')$ that give rise to total derivatives in the integrand of the effective action, we may drop $\eta^{\mu\nu}V_{\mu\nu} = \Box_{x'}V(x')$. The first term in (8.163) clearly gives rise to the effective potential that we have already calculated. Call this contribution $\Gamma_0^{(1)}$. Upon integration with respect to M^2 we find

$$\Gamma^{(1)} \simeq \Gamma_0^{(1)} - \frac{1}{24}(4\pi)^{-n/2}\Gamma\left(3 - \frac{n}{2}\right)\int dv_{x'}(M^2)^{n/2-3}V_\mu V^\mu \quad (8.164)$$

$$= \Gamma_0^{(1)} - \frac{1}{384\pi^2}\int dv_{x'}\frac{V_\mu V^\mu}{M^2}. \quad (8.165)$$

In the second equality we have taken the limit $n \to 4$ noting that the result is finite. The second term in (8.165) therefore represents the first correction to the effective potential for a non-constant $V(x)$.

We can apply this straight away to the case of $\lambda\phi^4$ theory with a non-constant background field by taking $V(x) = (\lambda_R/2)\varphi_R^2(x)$ and $M^2 = m_R^2 + (\lambda_R/2)\varphi_R^2(x)$. The result is

$$\Gamma^{(1)} = \Gamma_0^{(1)} - \frac{\lambda_R^2}{384\pi^2}\int dv_x \frac{\varphi_R^2(x)}{m_R^2 + (\lambda_R/2)\varphi_R^2(x)}\partial^\mu\varphi_R(x)\partial_\mu\varphi_R(x). \quad (8.166)$$

There is no pole term present in the one-loop effective action involving derivatives of the field that requires renormalization. As we claimed earlier, to one-loop order no infinite field renormalization is needed. The result that we found here agrees with that first obtained in Iliopoulos *et al.* (1975) by a different method. The next term in the derivative expansion of the effective action contains four derivatives and can be found using the method that we have just described in Moss *et al.* (1992).

8.6 Renormalization of $\lambda\phi^4$ theory

To round off our discussion of renormalization we will consider what happens in $\lambda\phi^4$ theory at two-loop order. We will use dimensional regularization as described in the last section. The renormalization at one-loop order has already been considered, so we proceed directly to the next order in the loop expansion.

We had $\Gamma^{(2)}$ given by (8.86). With the action functional (8.91) it is clear that when we write the result in normal (uncondensed) notation,

$$\Gamma^{(2)} = \frac{\lambda}{8}\int d^n x G^2(x,x) - \frac{\lambda^2}{12}\int d^n x \int d^n x' \varphi(x)\varphi(x')G^3(x,x'). \quad (8.167)$$

In terms of Feynman diagrams, the first term corresponds to the graph in Fig. 8.10 and the second term to that in Fig. 8.8.

We are interested in the divergent part of $\Gamma^{(2)}$. The first term is easy to evaluate since it is the square of the one-loop term that we have already found. However, squaring the one-loop expression $\Gamma^{(1)}$ will end up with a double pole at $n = 4$, as well as a simple pole whose residue will involve the finite part of $G(x, x)$. For general background fields it is impossible to calculate the finite part of $G(x, x)$ exactly. A crucial part of the calculation will be to show that all such non-local pole terms cancel out of the divergent part of $\Gamma^{(2)}$ to leave a relatively simple structure that can be dealt with by the same type of counterterms as we used at one-loop order.

We will write

$$G(x, x') = G_s(x, x') + G_{ns}(x, x'), \tag{8.168}$$

where we require $G_{ns}(x, x')$ to be non-singular and finite as $n \to 4$ even when $x = x'$. The singular part of $G(x, x')$ and terms that contain poles as $n \to 4$ will therefore be found in $G_s(x, x')$. This split of the Green function is always possible because our expansion of $G(x, x')$ in Section 8.5.2 in powers of derivatives of the background field $\varphi(x)$ beyond G_0 all lead to finite expressions at $n = 4$. We are free to define $G_s(x, x')$ to be the result of including the first few terms in the derivative expansion of $G(x, x')$ with all of the higher-order terms (that lead to finite expressions even for $n = 4$) included in $G_{ns}(x, x')$. Any contributions to $G(x, x')$ coming from x nowhere close to x' can also be included in $G_{ns}(x, x')$. $G_{ns}(x, x')$ is therefore a very complicated function that we are unable to calculate for general background fields. We will prove that whatever we choose for $G_{ns}(x, x')$ does not affect the divergent part of $\Gamma^{(2)}$.

The simplest choice we can make is to define $G_s(x, x')$ to contain only the term G_0 in the derivative expansion:

$$G_s(x, x') = -\int \frac{d^n k}{(2\pi)^n}\, e^{ik\cdot(x-x')}\, (k^2 - M^2)^{-1}. \tag{8.169}$$

This will turn out to be sufficient for the later analysis as well. The result of performing the integration in $G_s(x, x)$ was given in (8.121). Expanding about the pole at $n = 4$ results in

$$G_s(x, x) = \frac{iM^2}{8\pi^2(n-4)} + \frac{iM^2}{16\pi^2}\left[\ln\left(\frac{M^2}{4\pi}\right) + \gamma - 1\right], \tag{8.170}$$

if we drop terms that vanish when $n \to 4$. From (8.168) we then find

$$\ell^{n-4} G(x, x) = \frac{iM^2}{8\pi^2(n-4)} + G_{reg}(x), \tag{8.171}$$

where

$$G_{reg}(x) = G_{ns}(x,x) + \frac{iM^2}{16\pi^2}\left[\ln\left(\frac{M^2\ell^2}{4\pi}\right) + \gamma - 1\right]. \tag{8.172}$$

$G_{reg}(x)$ is a regular finite function of x.

If we let $\Gamma_1^{(2)}$ denote the first term in the two-loop effective action in (8.167), we have

$$\begin{aligned}\Gamma_1^{(2)} &= \frac{\lambda}{8}\int d^n x G^2(x,x) \\ &= \frac{\lambda_R}{8}\int d^4x \left[\ell^{n-4}G(x,x)\right]^2 \qquad (8.173)\\ &= \int d^4x\left[-\frac{\lambda_R M^4}{512\pi^4(n-4)^2} + \frac{i\lambda_R M^2}{32\pi^2(n-4)}\,G_{reg}(x) + \cdots\right]. \qquad (8.174)\end{aligned}$$

In the second line above we have used $d^n x = \ell^{n-4}d^4x$ and (8.124), noting that we are only working to order $\hbar^2$ and that $\Gamma^{(2)}$ is already multiplied by $\hbar^2$. The last line in (8.174) has resulted from the use of (8.171) with only pole terms kept.

Up to now we have encountered divergences when we take the coincidence limit $x = x'$ in a Green function. Another source of divergences comes about when we multiply Green functions together even with $x \neq x'$. The second term of $\Gamma^{(2)}$ in (8.167) involves $G^3(x,x')$ and we need to see if this expression is divergent. We will first consider the easier problem of the evaluation of the divergent part of $G^2(x,x')$ for $x \neq x'$, since it will turn out that we need to know this anyway. We can use our decomposition (8.168) to obtain

$$G^2(x,x') = G_s^2(x,x') + 2G_s(x,x')G_{ns}(x,x') + G_{ns}^2(x,x'). \tag{8.175}$$

$G_{ns}(x,x')$ should be finite as $n \to 4$ whether we take $x \to x'$ or not by our assumption when making the split (8.168). The last term is then finite at $n = 4$. For the middle term, because of our assumption on $G_{ns}(x,x')$, any divergences can come only from $G_s(x,x')$. But $G_s(x,x')$ is not singular even for $n = 4$ unless $x = x'$ which is not the case here.[20] We conclude that any divergences that are present in $G^2(x,x')$ can come only from $G_s^2(x,x')$.

[20] The most divergent part of $G_s(x,x')$ was evaluated in terms of a Bessel function in (8.101).

Write $G_s(x,x')$ as in (8.143). We then find

$$G_s^2(x,x') = \int \frac{d^nk}{(2\pi)^n} \int \frac{d^np}{(2\pi)^n}\, e^{i(k+p)\cdot y}\, G(k;x')G(p;x') \\ = \int \frac{d^np}{(2\pi)^n}\, e^{ip\cdot y} \int \frac{d^nk}{(2\pi)^n} G(k;x')G(p-k;x'). \tag{8.176}$$

In the second equality we have changed variables from p to $p-k$. We only require the pole part of this expression. The first term in the derivative expansion of $G(k;x')$ is $G_0(k;x')$ and it behaves like k^{-2} for large k. This means that the leading behaviour of $G(k;x')G(p-k;x')$ for large k is k^{-4}, and that higher-order terms in the derivative expansion will lead to momentum integrals that converge at $n=4$ because they fall off at least as fast as k^{-6} for large k. The pole part of $G_s^2(x,x')$ comes only from using $G_0(k;x')$ for $G(k;x')$. If we let $\mathrm{PP}\{\cdots\}$ denote the pole part of any expression, we then have

$$\mathrm{PP}\left\{G^2(x,x')\right\} = \mathrm{PP}\left\{G_s^2(x,x')\right\} \\ = \int \frac{d^np}{(2\pi)^n}\, e^{ip\cdot y}\, \mathrm{PP}\left\{J_2(p)\right\}. \tag{8.177}$$

with

$$J_2(p) = \int \frac{d^nk}{(2\pi)^n} (k^2 - M^2 + i\epsilon)^{-1} \left[(p-k)^2 - M^2 + i\epsilon\right]^{-1}. \tag{8.178}$$

The easiest procedure now is to notice that the pole term of $J_2(p)$ is found by setting $p=0$, in which case we have $J_2(p=0) = I(2)$ where $I(2)$ was found in (8.157).[21] However, in order to introduce a more general approach we will proceed differently.

Combine the two denominators in $J_2(p)$ using the identity

$$\frac{1}{a_1a_2} = \int_0^1 dz\, \left[a_1z + a_2(1-z)\right]^{-2}. \tag{8.179}$$

This first appears in Feynman (1949b) although a similar idea was used by Schwinger.[22] Using (8.179) for $J_2(p)$ leads to

$$J_2(p) = \int_0^1 dz \int \frac{d^nk}{(2\pi)^n}\, \left[(k-zp)^2 + z(1-z)p^2 - M^2 + i\epsilon\right]^{-2}. \tag{8.180}$$

[21] This can be seen by expanding $J_2(p)$ about $p=0$ and noting that all terms beyond that for $J_2(0)$ lead to convergent integrals at $n=4$.

[22] See the parenthetical remark below Eq. (14a) in Feynman (1949b).

The integration over k may be done by first translating the variable of integration $k \to k + zp$, and then recognizing that the result is simply $I(2)$ of (8.157) with $M^2 \to M^2 - z(1-z)p^2$. This gives

$$J_2(p) = i(4\pi)^{-n/2}\Gamma\left(2 - \frac{n}{2}\right)\int_0^1 dz\left[M^2 - z(1-z)p^2\right]^{n/2-2}. \quad (8.181)$$

We can now expand about the pole at $n = 4$ to obtain

$$\mathrm{PP}\left\{J_2(p)\right\} = -\frac{i}{8\pi^2(n-4)}. \quad (8.182)$$

Using this back in (8.177) shows that

$$\mathrm{PP}\left\{G^2(x,x')\right\} = -\frac{i}{8\pi^2(n-4)}\delta(x,x') \quad (8.183)$$

since $\int [d^n p/(2\pi)^n]\, e^{ip\cdot y} = \delta(y)$.

We now turn to the more complicated case of $G^3(x,x')$. Using (8.168) we obtain

$$\begin{aligned} G^3(x,x') = {} & G_s^3(x,x') + 3G_s^2(x,x')G_{ns}(x,x') \\ & + 3G_s(x,x')G_{ns}^2(x,x') + G_{ns}^3(x,x'). \end{aligned} \quad (8.184)$$

The last two terms are finite for $n \to 4$ for $x \neq x'$ by our definition of $G_{ns}(x,x')$ and the result for $G_s(x,x')$ found earlier. Therefore any divergences can come only from the first two terms in (8.184). We have already shown that $\mathrm{PP}\left\{G_s^2(x,x')\right\}$ is given by (8.183); thus,

$$\mathrm{PP}\left\{G_s^2(x,x')G_{ns}(x,x')\right\} = -\frac{i}{8\pi^2(n-4)}\delta(x,x')G_{ns}(x',x'). \quad (8.185)$$

We have used the Dirac δ-distribution to set $x = x'$ in the factor of $G_{ns}(x,x')$. We know that $G_{ns}(x',x')$ is finite even at $n = 4$, so we have extracted the pole part of the second term in (8.184). This pole term can be observed to be a very complicated non-local expression.

The hard part is the evaluation of $\mathrm{PP}\left\{G_s^3(x,x')\right\}$. Proceed as we did leading up to (8.176) to find

$$\begin{aligned} G_s^3(x,x') &= \int \frac{d^n k}{(2\pi)^n}\int \frac{d^n p}{(2\pi)^n}\int \frac{d^n q}{(2\pi)^n}\, e^{i(k+p+q)\cdot y}G(k;x')G(p;x')G(q;x') \\ &= \int \frac{d^n p}{(2\pi)^n}\, e^{ip\cdot y}J_3(p) \end{aligned} \quad (8.186)$$

where

$$J_3(p) = \int \frac{d^n k}{(2\pi)^n} \int \frac{d^n q}{(2\pi)^n} G(k;x')G(q;x')G(p-k-q;x'). \qquad (8.187)$$

We now must deal with a double integral over momenta. If each of the two integrals (one over k and one over q) when considered separately converge as $n \to 4$ then $J_3(p)$ will be finite. We know from our derivative expansion of $G(k;x')$ that $G(k;x') = G_0(k;x') + \mathcal{O}(k^{-5})$ for large k. This allows us to conclude by counting powers of k and q that if we are interested in just the divergent part of $J_3(p)$, then we only need to use $G_0(k;x')$ for $G(k;x')$.[23] We have, using (8.148) for $G_0(k;x')$ and dropping the explicit $i\epsilon$ for brevity,

$$\mathrm{PP}\,\{J_3(p)\} = -\mathrm{PP}\Big\{ \int \frac{d^n k}{(2\pi)^n} \int \frac{d^n q}{(2\pi)^n} (k^2 - M^2)^{-1}(q^2 - M^2)^{-1} \times \left[(p-k-q)^2 - M^2\right]^{-1} \Big\}. \qquad (8.188)$$

Evaluating even the divergent part of $J_3(p)$ is a bit daunting. Fortunately, Collins (1974) has presented an elegant method that we can use. It begins with a generalization of the identity (8.179),

$$\frac{1}{a_1 a_2 a_3} = 2 \int_0^1 d^3 z\, \delta\Big(1 - \sum_{i=1}^3 z_i\Big)(a_1 z_1 + a_2 z_2 + a_3 z_3)^{-3} \qquad (8.189)$$

that introduces three Feynman parameters, although only two of them are independent because of the Dirac δ. We now use (8.189) for the three terms that occur in (8.188) in an obvious way. The resulting expression can be simplified by completing the square first on k and then on q, followed by a translation of the variables of integration. After some algebra the following result is obtained

$$\mathrm{PP}\,\{J_3(p)\} = -2 \int_0^1 d^3 z\, \delta\Big(1 - \sum_{i=1}^3 z_i\Big) \mathrm{PP}\Big\{ \int \frac{d^n k}{(2\pi)^n} \int \frac{d^n q}{(2\pi)^n} \times \Big[(z_1 + z_3)k^2 + \frac{z_1 z_2 + z_2 z_3 + z_3 z_1}{z_1 + z_3} q^2 + \frac{z_1 z_2 z_3}{z_1 z_2 + z_2 z_3 + z_3 z_1} p^2 - M^2 \Big]^{-3} \Big\}. \qquad (8.190)$$

[23] Higher-order terms in the derivative expansion will not diverge at $n = 4$.

The integration over k can be done using (8.156) with $p = 3$ taken there. Then the integral over q can be done using the same integral but with $p = 3 - n/2$ taken in (8.156). After some simplifications it can be shown that

$$\mathrm{PP}\left\{J_3(p)\right\} = -\mathrm{PP}\left\{(4\pi)^{-n}\Gamma(3-n)(M^2)^{n-3}K(p)\right\} \tag{8.191}$$

where

$$K(p) = \int_0^1 d^3z\ \delta\Big(1 - \sum_{i=1}^{3} z_i\Big)(z_1z_2 + z_2z_3 + z_3z_1)^{-n/2} \times \left(1 - \frac{z_1z_2z_3}{z_1z_2 + z_2z_3 + z_3z_1}\frac{p^2}{M^2}\right)^{n-3}. \tag{8.192}$$

The function $K(p)$ has poles coming from points where $z_1z_2+z_2z_3+z_3z_1 = 0$. The δ-function restricts the integration to a triangular region in the first quadrant of $\mathbb{R}^3$ cut off by the coordinate planes $z_1 = 0, z_2 = 0$, and $z_3 = 0$. This is pictured in Fig. 8.11. If we keep away from the edges of the triangular region, all of z_1, z_2, z_3 are non-zero and the integrand of (8.192) is finite at $n = 4$. The only way that $z_1z_2 + z_2z_3 + z_3z_1$ can vanish is if two of the z_i vanish with the third constrained to be 1. This means that the divergences at $n = 4$ in (8.192) come only from the vertices of the triangular region pictured in Fig. 8.11. Because the integrand of (8.192) is a symmetric function of z_1, z_2, z_3, the contribution to the pole at $n = 4$ must be the same for each vertex. We can therefore evaluate the contribution from one of the vertices and then multiply the result by 3 to obtain the complete pole contribution.

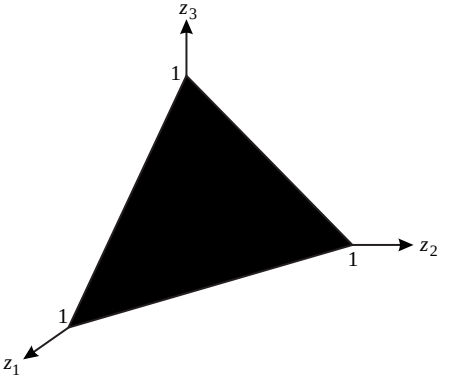

Fig. 8.11 The region of integration for (8.192) is shown by the shaded triangle.

Consider the pole coming from $z_1 = 1, z_2 + z_3 = 0$. Make the change of variable

$$z_1 = 1 - \alpha, \qquad z_2 = \alpha\beta, \qquad z_3 = \alpha(1 - \beta). \tag{8.193}$$

(Note that $z_1 + z_2 + z_3 = 1$.) The divergence at $n = 4$ should show up as $\alpha \to 0$ since $z_2 + z_3 = \alpha$ here. Use the δ-function to integrate out z_1 in (8.192), and then note that $dz_2 dz_3 = \alpha d\alpha d\beta$. It follows that[24]

$$\mathrm{PP}\,\{K(p)\} = 3\,\mathrm{PP}\Bigg\{ \int_0^1 d\alpha \int_0^1 d\beta\, \alpha^{1-n/2}\,[1 - \alpha + \alpha(1-\beta)]^{-n/2} \times \left[1 - \frac{\alpha\beta(1-\alpha)(1-\beta)}{1-\alpha+\alpha(1-\beta)}\,\frac{p^2}{M^2}\right]^{n-3} \Bigg\}. \tag{8.194}$$

The pole shows up as $\alpha \to 0$, so if we expand the integrand in powers of α it can be seen that only the leading term gives rise to a pole.[25] We have

$$\begin{aligned} \mathrm{PP}\,\{K(p)\} &= 3\,\mathrm{PP}\Bigg\{ \int_0^1 d\alpha \int_0^1 d\beta\, \alpha^{1-n/2} \Bigg\} \\ &= -\frac{6}{n-4}, \end{aligned} \tag{8.195}$$

and can conclude that

$$K(p) = -\frac{6}{n-4} + K_0(p) + \cdots, \tag{8.196}$$

where $K_0(p)$ is finite as $n \to 4$. The remaining terms indicated by $\cdots$ in (8.196) vanish as $n \to 4$ and are of no interest to us.

Looking back at (8.191), because $\Gamma(3 - n)$ has a simple pole at $n = 4$, it can be seen that we need to know what $K_0(p)$ is if we are to obtain the complete pole part of $J_3(p)$. We can get this by returning to the expression (8.192) for $K(p)$, subtracting off that part of the integrand that gave rise to the pole term in (8.195), and then letting $n \to 4$ knowing that the result will be finite. The pole came from the three vertices of the triangular region of integration at $z_1 + z_2 = 0$, $z_2 + z_3 = 0$, and $z_3 + z_1 = 0$

[24] The factor of 3 accounts for the contributions of the three vertices of the triangle as explained above.

[25] The second term in the expansion in powers of α behaves like $\alpha^{2-n/2}$ which does not integrate to give a pole as $n \to 4$.

and from the behaviour $(z_1+z_2)^{-2}$, $(z_2+z_3)^{-2}$, and $(z_3+z_1)^{-2}$ of the integrand. This means that we have

$$K_0(p) = \int_0^1 d^3z\ \delta\Big(1-\sum_{i=1}^3 z_i\Big)\Bigg[(z_1z_2+z_2z_3+z_3z_1)^{-2} \times\left(1-\frac{z_1z_2z_3}{z_1z_2+z_2z_3+z_3z_1}\frac{p^2}{M^2}\right) -(z_1+z_2)^{-2}-(z_2+z_3)^{-2}-(z_3+z_1)^{-2}\Bigg]. \tag{8.197}$$

Integrate out z_1 using the δ-function and make the change of variable (8.193) as before to find

$$K_0(p) = \int_0^1 d\alpha \int_0^1 d\beta\ \alpha\Big\{\alpha^{-2}\left[1-\alpha+\alpha\beta(1-\beta)\right]^{-2} \times\left[1-\frac{\alpha\beta(1-\alpha)(1-\beta)}{1-\alpha+\alpha(1-\beta)}\ \frac{p^2}{M^2}\right] -\alpha^{-2}-(1-\alpha+\alpha\beta)^{-2}-(1-\alpha\beta)^{-2}\Big\}. \tag{8.198}$$

The integrals are now elementary and easily done. It is best to evaluate the result as an indefinite integral and then work out the definite integral by taking the limit at the end since taken separately some of the definite integrals diverge. The result, after a bit of calculation, turns out to be

$$K_0(p) = 3-\frac{p^2}{2M^2}. \tag{8.199}$$

We can now evaluate (8.191) to find

$$\mathrm{PP}\,\{J_3(p)\} = -\frac{M^2}{(4\pi)^4}\Bigg\{-\frac{6}{(n-4)^2}+\frac{1}{n-4}\Bigg[9-\frac{p^2}{2M^2} -6\gamma-6\ln\left(\frac{M^2}{4\pi}\right)\Bigg]\Bigg\}. \tag{8.200}$$

If we note that

$$\int\frac{d^np}{(2\pi)^n}e^{ip\cdot y}\,p^2 = -\Box_y\delta(y),$$

then from (8.186) we have

$$\mathrm{PP}\left\{G_s^3(x,x')\right\} = \frac{M^2}{(4\pi)^4}\left\{\frac{6}{(n-4)^2} + \frac{1}{n-4}\left[6\gamma - 9 + 6\ln\left(\frac{M^2}{4\pi}\right) - \frac{1}{2M^2}\Box_x\right]\right\}\delta(x,x'). \tag{8.201}$$

We now combine the results of (8.185) and (8.201) to find $\mathrm{PP}\{G^3(x,x')\}$. The answer can be written in terms of $G_{reg}(x)$ defined in (8.172) and is

$$\mathrm{PP}\left\{G^3(x,x')\right\} = \left[\frac{3M^2}{128\pi^4(n-4)^2} - \frac{3M^2}{256\pi^4(n-4)}(1+2\ln\ell^2) - \frac{1}{512\pi^4(n-4)}\Box_x - \frac{3i}{8\pi^2(n-4)}G_{reg}(x)\right]\delta(x,x'). \tag{8.202}$$

If we call $\Gamma_2^{(2)}$ the second term in (8.167), then when we use (8.202) the integration over x' may be done using the δ-function that is present. Furthermore, we may use $\lambda = \ell^{n-4}\lambda_R$, $m^2 = m_R^2$, and $\varphi(x) = \ell^{2-n/2}\varphi_R(x)$, all valid to order $\hbar^0$ (that is all we need because $\Gamma_2^{(2)}$ is multiplied by $\hbar^2$ and we are only working to order $\hbar^2$), along with $d^nx = \ell^{n-4}d^4x$ to find

$$\mathrm{PP}\left\{\Gamma_2^{(2)}\right\} = -\frac{\lambda_R^2}{12}\int d^4x\,\varphi_R(x)\left[\frac{3M^2}{128\pi^4(n-4)^2} - \frac{3M^2}{256\pi^4(n-4)} - \frac{1}{512\pi^4(n-4)}\Box_x - \frac{3i}{8\pi^2(n-4)}G_{reg}(x)\right]\varphi_R(x). \tag{8.203}$$

This may now be combined with $\Gamma_1^{(2)}$ in (8.174) to find that the complete pole part of the two-loop effective action is

$$\mathrm{PP}\left\{\Gamma^{(2)}\right\} = \int d^4x\left[-\frac{\lambda_R}{512\pi^4(n-4)^2}\left(m_R^4 + 2\lambda_R m_R^2\varphi_R^2 + \frac{3}{4}\lambda_R^2\varphi_R^4\right) + \frac{\lambda_R^2}{1024\pi^4(n-4)}\left(m_R^2\varphi_R^2 + \frac{\lambda_R}{2}\varphi_R^4\right) + \frac{\lambda_R^2}{6144\pi^4(n-4)}\varphi_R\Box_x\varphi_R + \frac{i\lambda_R^2}{32\pi^2(n-4)}\left(m_R^2 + \frac{3}{2}\lambda_R\varphi_R^2\right)G_{reg}(x)\right]. \tag{8.204}$$

The pole part of $\Gamma^{(2)}$ can be seen to have a dependence on the complicated non-local part of the Green function $G_{reg}(x)$ present in the last

term in (8.204). If this was the complete contribution to the effective action of order $\hbar^2$ then the renormalization program would fail because to cancel the non-local pole term we would be forced to consider a non-local Lagrangian. However, there is a subtlety hidden in our loop expansion. We assumed in our counting in powers of $\hbar$ that all of the terms in the expansion of the classical action functional had no explicit factors of $\hbar$ associated with them; yet, the masses, coupling constants, and fields that entered the classical action were bare and we had to express them in terms of renormalized ones plus counterterms. The counterterms are necessary to remove the divergences in the effective action order by order in the loop expansion; thus, there is an $\hbar$ expansion hidden inside our formal expression for the effective action because we have obtained the expansion in terms of bare quantities only. A bit of care must be exercised if we want to work consistently to a given order in $\hbar$.

We are after $\Gamma[\varphi]$ to order $\hbar^2$. Because $\Gamma^{(2)}[\varphi]$ is multiplied by $\hbar^2$ it makes no difference in our result (8.167) if we take all masses, coupling constants, and fields to be renormalized. In contrast, the formal expression for $\Gamma^{(1)}[\varphi]$ is only multiplied by $\hbar$. Therefore when we replace m^2, λ, φ with their renormalized values plus counterterms, the counterterms of one-loop order (order $\hbar$) will affect the final result to order $\hbar^2$. This must be taken into account if we wish to obtain the complete contribution to the effective action that is of order $\hbar^2$. We had from (8.80)

$$\Gamma^{(1)} = \frac{i\hbar}{2}\mathrm{tr}\ln\left(\ell^2 S_{,ij}\right).$$

By expressing $S_{,ij}$ in terms of the renormalized values and counterterms we will find

$$S_{,ij} = S^{(0)}_{,ij} + \hbar S^{(1)}_{,ij} + \cdots \tag{8.205}$$

where $S^{(0)}_{,ij}$ is given as in (8.92) but with renormalized values, and

$$S^{(1)}_{,ij} = -\left[\delta m^{2(1)} + \frac{\delta\lambda^{(1)}}{2}\varphi_R^2(x)\right]\delta(x,x') \tag{8.206}$$

arises from the one-loop counterterms. Note that $\varphi = \varphi_R$ to order $\hbar$ because we did not need to perform any infinite field renormalization to this order. If we take

$$S^{(0)}_{,ij}G^{jk} = -\delta^k_i, \tag{8.207}$$

then our Green function will not involve $\hbar$. We may expand the logarithm to find

$$\Gamma^{(1)} = \frac{i\hbar}{2}\,\mathrm{tr}\ln\left[\ell^2 S^{(0)}_{,ij}\left(\delta^j_l - \hbar G^{jk}S^{(1)}_{,kl} + \cdots\right)\right]$$
$$= \frac{i\hbar}{2}\,\mathrm{tr}\ln\left[\ell^2 S^{(0)}_{,ij}\right] - \frac{i\hbar^2}{2}G^{ij}S^{(1)}_{,ij} + \cdots . \tag{8.208}$$

When we return from condensed notation to normal notation, the second term in (8.208) may be seen to make an order $\hbar^2$ contribution to the effective action that is

$$\Gamma^{(1)}_{2-loop} = \frac{i\hbar^2}{2}\int d^n x\left[\delta m^{2(1)} + \frac{\delta\lambda^{(1)}}{2}\varphi_R^2(x)\right]G(x,x). \tag{8.209}$$

To obtain the complete contribution to order $\hbar^2$ it is necessary to add the result in (8.209) to our earlier one in (8.204) for $\Gamma^{(2)}[\varphi]$. We can use the one-loop counterterms found in (8.135) and (8.136), and the expression for $G(x,x)$ in (8.171) to see that

$$\mathrm{PP}\left\{\Gamma^{(1)}_{2-loop}\right\} = \frac{i}{2}\hbar^2\int d^4x\left[\delta m^{2(1)} + \frac{1}{2}\delta\lambda^{(1)}\varphi_R^2(x)\right]\ell^{n-4}G(x,x)$$
$$= \hbar^2\int d^4x\left[\frac{\lambda_R}{256\pi^4(n-4)}\left(m_R^4 + 2\lambda_R m_R^2\varphi_R^2 + \frac{3}{4}\lambda_R^2\varphi_R^4\right)\right.$$
$$\left. -\frac{i\lambda_R}{32\pi^2(n-4)}\left(m_R^2 + \frac{3}{2}\lambda_R\varphi_R^2\right)G_{reg}(x)\right]. \tag{8.210}$$

When this result is added to that found in (8.204) we find the complete, and final, pole part of the effective action at two-loop order to be

$$\mathrm{PP}\left\{\Gamma_{2-loop}\right\} = \hbar^2\int d^4x\left[\frac{\lambda_R}{512\pi^4(n-4)^2}\left(m_R^4 + 2\lambda_R m_R^2\varphi_R^2 + \frac{3}{4}\lambda_R^2\varphi_R^4\right)\right.$$
$$+\frac{\lambda_R^2}{1024\pi^4(n-4)}\left(m_R^2\varphi_R^2 + \frac{1}{2}\lambda_R\varphi_R^4\right)$$
$$\left. +\frac{\lambda_R^2}{6144\pi^4(n-4)}\varphi_R\Box_x\varphi_R\right]. \tag{8.211}$$

The potentially damaging non-local pole term that involved $G_{reg}(x)$ at intermediate steps in the calculation has cancelled out of the final result. The appearance of $G_{reg}(x)$ in (8.210) coming from the one-loop counterterms in the effective action was exactly what was needed to remove the dependence on $G_{reg}(x)$ from (8.204). The pole terms that remain are all of a form that can be dealt with by local counterterms in the classical action. We make use of (8.122)–(8.126) with (8.127) to find that the order $\hbar^2$ part of the classical action is

$$S^{(2)} = \hbar^2 \int d^4x \Big\{ -\frac{1}{2}\delta Z^{(2)} \varphi_R \Box_x \varphi_R - \frac{1}{2}\left[\delta m^{2(2)} + m_R^2 \delta Z^{(2)}\right] \varphi_R^2 - \frac{1}{4!}\left[\delta\lambda^{(2)} + 2\lambda_R \delta Z^{(2)}\right] \varphi_R^4 - \delta c^{(2)} \Big\}. \tag{8.212}$$

The two-loop counterterms in (8.212) are now fixed by the requirement that $S^{(2)}$ cancels the pole terms in (8.208). A short calculation shows that

$$\delta Z^{(2)} = \frac{\lambda_R^2}{3072\pi^4(n-4)}, \tag{8.213}$$

$$\delta m^{2(2)} = \frac{\lambda_R^2 m_R^2}{128\pi^4(n-4)^2} + \frac{5\lambda_R^2 m_R^2}{3072\pi^4(n-4)}, \tag{8.214}$$

$$\delta\lambda^{(2)} = \frac{9\lambda_R^3}{256\pi^4(n-4)^2} + \frac{17\lambda_R^3}{1536\pi^4(n-4)}, \tag{8.215}$$

$$\delta c^{(2)} = \frac{\lambda_R m_R^4}{512\pi^4(n-4)^2}. \tag{8.216}$$

This completes the renormalization of the theory to two-loop order.

After all this, a modification of our previous loop expansion suggests itself. We have seen that due to the renormalization process we must express bare quantities in terms of renormalized ones plus counterterms with the counterterms having an expansion in powers of the loop counting parameter $\hbar$. This $\hbar$-dependence is hidden inside every term in the perturbative expansion that we have obtained, rendering the extraction of the complete part of the effective action of a given order in $\hbar$ a bit cumbersome.[26] A better approach is to acknowledge from the start that the bare terms in the classical action will contain an expansion in powers of $\hbar$ through the necessary counterterms, and to treat the counterterms as part of the interaction by a suitable modification of the A_n defined in (8.55). This organizes the $\hbar$ expansion in a better manner and obviates the need to consider expansions within expansions.[27]

8.7 Finite temperature

In Chapter 5 we obtained results for the effective action at finite temperature to lowest order in perturbation theory. We now want to discuss how the more general perturbative approach of the previous sections of the

[26] It has been seen to involve expansions within expansions in our two-loop calculation.
[27] See the calculation in Toms (1982) for example.

present chapter may be generalized to include finite temperature. The expansion of the effective action at zero temperature was built around the Green function; therefore, we will first study the Green function at finite temperature.

8.7.1 Real scalar field

The natural replacement for the vacuum expectation value of any operator $A[\phi]$, defined as in (8.8), is the statistical, ensemble, or thermal, average:

$$\langle A \rangle = \mathrm{tr}(\rho A). \tag{8.217}$$

Here ρ is the density operator: $\rho = Z^{-1}e^{-\beta H}$, with Z the partition function (see Section 5.1). In particular, we will define the finite temperature, or thermal, Green function by

$$G(x,x') = i\left\langle T\left(\phi(t,\mathbf{x})\phi(t',\mathbf{x}')\right)\right\rangle. \tag{8.218}$$

(Compare this to (8.19). The angle brackets now mean the thermal average as in (8.217). We will set $\hbar = 1$ here since it is not needed to count loops; we have already done this.) It proves convenient to deal with $G^{>}(x,x')$ and $G^{<}(x,x')$ defined by

$$G^{>}(x,x') = i\left\langle \phi(t,\mathbf{x})\phi(t',\mathbf{x}')\right\rangle, \tag{8.219}$$

$$G^{<}(x,x') = i\left\langle \phi(t',\mathbf{x}')\phi(t,\mathbf{x})\right\rangle, \tag{8.220}$$

so that

$$G(x,x') = \theta(t-t')G^{>}(x,x') + \theta(t'-t)G^{<}(x,x'). \tag{8.221}$$

Note that with these definitions we have

$$G^{<}(x,x') = G^{>}(x',x). \tag{8.222}$$

This means that we may concentrate on $G^{>}$ and obtain $G^{<}$ by (8.222).

Making use of the expansion (3.187) of the field in terms of creation and annihilation operators, we can express $G^{>}(x,x')$ and $G^{<}(x,x')$ in terms of $\langle a_n a_{n'}\rangle$, $\langle a_n a_{n'}^{\dagger}\rangle$, $\langle a_n^{\dagger} a_{n'}\rangle$, and $\langle a_n^{\dagger} a_{n'}^{\dagger}\rangle$. These thermal averages were already calculated in Section 5.2 with the results (see (5.55) and (5.56) with $\mu = 0$)

$$\langle a_n a_{n'}^{\dagger}\rangle = F(E_n)\delta_{nn'}, \tag{8.223}$$

$$\langle a_n^{\dagger} a_{n'}\rangle = \left[1 + F(E_n)\right]\delta_{nn'}, \tag{8.224}$$

and $\langle a_n a_{n'} \rangle = 0 = \langle a_n^\dagger a_{n'}^\dagger \rangle$. Here $F(E)$ is the Bose–Einstein distribution function defined by

$$F(E) = \left(e^{\beta E} - 1\right)^{-1}. \tag{8.225}$$

A short calculation shows that

$$G^>(x,x') = i \sum_n (2E_n)^{-1} \Big\{ f_n(\mathbf{x}) f_n^*(\mathbf{x}') e^{-iE_n(t-t')} \left[1 + F(E_n)\right] + f_n^*(\mathbf{x}) f_n(\mathbf{x}') e^{iE_n(t-t')} F(E_n) \Big\}. \tag{8.226}$$

This result can be simplified by making use of the results of Section 3.6, beginning with (3.174) and using the properties of the $C_{nn'}$.

Let $G(E_n)$ be any function. Then

$$\begin{aligned} \sum_n G(E_n) f_n^*(\mathbf{x}) f_n(\mathbf{x}') &= \sum_{n,n',n''} G(E_n) C_{nn'} C_{nn''}^* f_{n'}(\mathbf{x}) f_{n''}^*(\mathbf{x}') \\ &= \sum_{n,n',n''} G(E_{n'}) C_{nn'} C_{nn''}^* f_{n'}(\mathbf{x}) f_{n''}^*(\mathbf{x}') \\ &= \sum_{n'} G(E_{n'}) f_{n'}(\mathbf{x}) f_{n'}^*(\mathbf{x}'). \end{aligned} \tag{8.227}$$

In the first line we have used (3.174) along with its complex conjugate. In the second line we have used the property (3.179). In the final line we have used the symmetry of $C_{nn'}$ along with the unitary property (3.180).

By using (8.227) for the second term in (8.226), we find

$$G^>(x,x') = i \sum_n \frac{f_n(\mathbf{x}) f_n^*(\mathbf{x}')}{2E_n} \, G_n^>(t-t') \tag{8.228}$$

where

$$G_n^>(t-t') = e^{-iE_n(t-t')} \left[1 + F(E_n)\right] + e^{iE_n(t-t')} F(E_n). \tag{8.229}$$

From (8.222) we obtain immediately that

$$G^<(x,x') = i \sum_n \frac{f_n(\mathbf{x}) f_n^*(\mathbf{x}')}{2E_n} \, G_n^<(t-t') \tag{8.230}$$

where

$$G_n^<(t-t') = e^{iE_n(t-t')} \left[1 + F(E_n)\right] + e^{-iE_n(t-t')} F(E_n). \tag{8.231}$$

At this stage we can note a remarkable feature that starts with the simple identity

$$1 + F(E) = e^{\beta E} F(E) \tag{8.232}$$

obeyed by the Bose–Einstein distribution function (8.225). If we now allow the time to be viewed as a complex variable, then from (8.229) we have

$$\begin{aligned} G_n^{>}(t - t' - i\beta) &= e^{-iE_n(t-t')} e^{-\beta E_n} \left[1 + F(E_n)\right] + e^{iE_n(t-t')} e^{\beta E_n} F(E_n) \\ &= e^{-iE_n(t-t')} F(E_n) + e^{iE_n(t-t')} \left[1 + F(E_n)\right] \\ &= G_n^{<}(t - t'). \end{aligned} \tag{8.233}$$

We have used (8.232) in the middle line, and (8.231) to obtain the result in terms of $G_n^{<}(t - t')$.

Because of the behaviour in (8.233) involving a shift along the imaginary axis, this suggests performing a Wick rotation to imaginary time. Define

$$\tau = it, \qquad \tau' = it'. \tag{8.234}$$

with $0 \leq \tau, \tau' \leq \beta$, so that $-\beta \leq \tau - \tau' \leq \beta$. The Feynman Green function (8.218) obeys

$$\left(\Box_x + M^2 - i\epsilon\right) G(x, x') = \delta(x, x'). \tag{8.235}$$

Using (8.234) we have

$$\Box_x = \frac{\partial}{\partial t^2} - \nabla^2 = -\frac{\partial}{\partial \tau^2} - \nabla^2 = -\tilde{\Box}_x, \tag{8.236}$$

where the tilde denotes that a positive definite Euclidean metric, resulting from the Wick rotation of the time coordinate, has been used. We also have $\delta(t - t')$ that occurs on the right-hand side of (8.235), becoming

$$\delta(t - t') = \delta[-i(\tau - \tau')] = i\delta(\tau - \tau') \tag{8.237}$$

if we make use of the property $\delta(ax) = (1/a)\delta(x)$, assumed to be true for a complex. We will therefore define

$$G(t, \mathbf{x}; t', \mathbf{x}') = i\tilde{G}(\tau, \mathbf{x}; \tau', \mathbf{x}') \tag{8.238}$$

with

$$\left(-\tilde{\Box}_x + M^2\right) \tilde{G}(x, x') = \tilde{\delta}(x, x'). \tag{8.239}$$

When occurring inside an expression with a tilde, like $\tilde{G}$ or $\tilde{\delta}$, we regard $x^\mu = (\tau, \mathbf{x})$. Note that the $i\epsilon$ is not necessary after a Wick rotation, as discussed in Section 8.4.

We can write

$$\tilde{G}(x,x') = \left\langle T_\tau \left(\tilde{\phi}(\tau,\mathbf{x})\tilde{\phi}(\tau',\mathbf{x}') \right) \right\rangle \tag{8.240}$$

$$= \theta(\tau-\tau')\tilde{G}^{>}(x,x') + \theta(\tau'-\tau)\tilde{G}^{<}(x,x') \tag{8.241}$$

with T_τ denoting time-ordering with respect to imaginary time τ. $\tilde{G}^{>}(x,x')$ and $\tilde{G}^{<}(x,x')$ are related to $G^{>}(x,x')$ and $G^{<}(x,x')$ exactly as in (8.238). If we define

$$\tilde{G}^{>}(x,x') = \sum_n \frac{f_n(\mathbf{x})f_n^*(\mathbf{x}')}{2E_n}\, \tilde{G}_n^{>}(\tau-\tau'), \tag{8.242}$$

$$\tilde{G}^{<}(x,x') = \sum_n \frac{f_n(\mathbf{x})f_n^*(\mathbf{x}')}{2E_n}\, \tilde{G}_n^{<}(\tau-\tau'), \tag{8.243}$$

then

$$\tilde{G}_n^{>}(\tau-\tau') = -iG_n^{>}[-i(t-t')], \tag{8.244}$$

$$\tilde{G}_n^{<}(\tau-\tau') = -iG_n^{<}[-i(t-t')]. \tag{8.245}$$

Using (8.233) it is easy to show that

$$\tilde{G}_n^{>}(\tau-\tau'+\beta) = \tilde{G}_n^{<}(\tau-\tau'). \tag{8.246}$$

By taking $\tau = 0$, (8.241) shows that

$$\begin{aligned}\tilde{G}(\tau=0,\mathbf{x};\tau',\mathbf{x}') &= \tilde{G}^{<}(\tau=0,\mathbf{x};\tau',\mathbf{x}') \\ &= \tilde{G}^{>}(\tau=\beta,\mathbf{x};\tau',\mathbf{x}') \\ &= \tilde{G}(\tau=\beta,\mathbf{x};\tau',\mathbf{x}').\end{aligned} \tag{8.247}$$

(The first equality follows because if $\tau = 0$, since $0 \le \tau' \le \beta$, we have $\tau' \ge \tau$. The second equality follows using (8.246). The final result follows because with $\tau = \beta$ we have $\tau \ge \tau'$.) This establishes the important result that the imaginary time Green function is periodic in imaginary time with period β. (A similar conclusion holds for τ'.) We can therefore regard the Green function $\tilde{G}(x,x')$ as the solution to (8.239) that is subject to periodic boundary conditions in imaginary times τ, τ' with period β.

A consequence of the periodicity in imaginary time is that we can expand the Green function $\tilde{G}(x,x')$ in a Fourier series

$$\tilde{G}(x,x') = \frac{1}{\beta}\sum_{j=-\infty}^{\infty} e^{i\omega_j(\tau-\tau')}\tilde{G}_j(\mathbf{x},\mathbf{x}') \tag{8.248}$$

where

$$\omega_j = \frac{2\pi j}{\beta} \tag{8.249}$$

are called the 'Matsubara frequencies'. From (8.239) the Fourier 'coefficients' $\tilde{G}_j(\mathbf{x}, \mathbf{x}')$ obey

$$\left(-\nabla^2 + M^2 + \omega_j^2\right) \tilde{G}_j(\mathbf{x}, \mathbf{x}') = \delta(\mathbf{x}, \mathbf{x}'). \tag{8.250}$$

The solution to this is

$$\tilde{G}_j(\mathbf{x}, \mathbf{x}') = \sum_n \frac{f_n(\mathbf{x}) f_n^*(\mathbf{x}')}{\omega_j^2 + \sigma_n + M^2} \tag{8.251}$$

where σ_n are the eigenvalues of $-\nabla^2$ as defined in (3.171) and $f_n(\mathbf{x})$ are the associated eigenfunctions.

We can write the imaginary time Green function in a form that looks more like the real-time result by performing the sum over j in (8.248). This can be done by using

$$\sum_{j=-\infty}^{\infty} \frac{e^{ija}}{j^2 + b^2} = \frac{\pi}{b} e^{-ab} + \frac{\pi}{b} (e^{2\pi b} - 1)^{-1} (e^{ab} + e^{-ab}), \tag{8.252}$$

and can be derived by making use of the method described in Section A1.3. (Here $a \geq 0, b > 0$ are assumed.) It is easy to show that

$$\tilde{G}(x, x') = \sum_n \frac{f_n(\mathbf{x}) f_n^*(\mathbf{x}')}{(2E_n)} \left\{ e^{-E_n(\tau - \tau')} [1 + F(E_n)] + e^{E_n(\tau - \tau')} F(E_n) \right\}. \tag{8.253}$$

Here $E_n = \sqrt{\sigma_n + M^2}$ as in (3.185). For $0 \leq \tau - \tau' \leq \beta$ this agrees with $\tilde{G}^>(x, x')$ obtained using (8.229) and (8.244). For $-\beta \leq \tau - \tau' \leq 0$ this agrees with $\tilde{G}^<(x, x')$ obtained using (8.231) and (8.244).

We have discussed what we need to concerning the Green functions. Our consideration now turns to the effective action at finite temperature. Bearing in mind the generalization (8.217), we take the mean, or background, field φ^i to now involve a thermal average,

$$\varphi^i = \langle \phi^i \rangle = \frac{\delta W[J]}{\delta J_i}. \tag{8.254}$$

(This is identical to (8.27) with the angle brackets now interpreted as a thermal average as in (8.217).) The only difference with what we did before is that in place of the zero temperature Green function we use the

thermal, finite temperature one. All of our formal perturbative results for the effective action follow as before, but with

$$G^{jk} \to i\tilde{G}^{jk} \tag{8.255}$$

where $\tilde{G}^{jk}$ is the imaginary time Green function just discussed (see (8.238)).

In order to see that this agrees with the simple one-loop approach adopted in Chapter 5, we will consider the one-loop effective potential at finite temperature. We had, at $T = 0$,

$$\frac{\partial}{\partial M^2} V^{(1)} = -\frac{i}{2} \ell^{n-4} G(x, x). \tag{8.256}$$

Making the replacement (8.255) leads to

$$\frac{\partial}{\partial M^2} V^{(1)} = \frac{1}{2} \ell^{n-4} \tilde{G}(x, x). \tag{8.257}$$

For Minkowski space-time, (8.248) and (8.251) give the imaginary time Green function as

$$\tilde{G}(x, x') = \frac{1}{\beta} \sum_{j=-\infty}^{\infty} e^{i\omega_j(\tau - \tau')} \int \frac{d^{n-1}k}{(2\pi)^{n-1}} \frac{e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')}}{\omega_j^2 + k^2 + M^2}. \tag{8.258}$$

We therefore find,

$$\tilde{G}(x, x) = \int \frac{d^{n-1}k}{(2\pi)^{n-1}} \frac{1}{2E_k} [1 + 2F(E_n)], \tag{8.259}$$

where $E_k = \sqrt{k^2 + M^2}$. Noting that

$$\frac{\partial}{\partial M^2} E_k = \frac{1}{2E_k}, \tag{8.260}$$

and

$$\frac{\beta F(E_k)}{2E_k} = \frac{\partial}{\partial M^2} \ln(1 - e^{-\beta E_k}), \tag{8.261}$$

we find

$$V^{(1)} = \ell^{n-4} \int \frac{d^{n-1}k}{(2\pi)^{n-1}} \frac{1}{2} E_k + \frac{1}{\beta} \int \frac{d^3k}{(2\pi)^3} \ln(1 - e^{-\beta E_k}). \tag{8.262}$$

The second term is finite as $n \to 4$, so we have taken the limit there. The first term is the sum over zero-point energies that arises at $T = 0$. This result agrees with that for the thermodynamic potential in (5.58).

8.7.2 Charged scalar field

In the case of the charged scalar field we can still make the replacement in (8.217), but this time $\rho = \mathcal{Z}^{-1} e^{-\beta(H-\mu Q)}$ with $\mathcal{Z}$ the grand canonical partition function. The Feynman Green function will be defined by

$$G(x,x') = i\left\langle T\left(\Phi(t,\mathbf{x})\Phi^\dagger(t',\mathbf{x}')\right)\right\rangle \tag{8.263}$$

with

$$G^>(x,x') = i\left\langle \Phi(t,\mathbf{x})\Phi^\dagger(t',\mathbf{x}')\right\rangle \tag{8.264}$$

and

$$G^<(x,x') = i\left\langle \Phi^\dagger(t',\mathbf{x}')\Phi(t,\mathbf{x})\right\rangle. \tag{8.265}$$

We now follow the same procedure as that which led to (8.230) and (8.231) in the real field case. Use the field expansion (3.206) and its Hermitian conjugate, then evaluate the thermal averages of the creation and annihilation operators with (5.83) and (5.84). The result can be simplified by making use of the identity (8.227) to find

$$G^>(x,x') = i\sum_n \frac{f_n(\mathbf{x})f_n^*(\mathbf{x}')}{2E_n} G_n^>(t-t'), \tag{8.266}$$

where

$$G_n^>(t-t') = e^{-iE_n(t-t')}[1+F_-(E_n)] + e^{iE_n(t-t')}F_+(E_n) \tag{8.267}$$

and

$$G^<(x,x') = i\sum_n \frac{f_n(\mathbf{x})f_n^*(\mathbf{x}')}{2E_n} G_n^<(t-t'), \tag{8.268}$$

with

$$G_n^<(t-t') = e^{-iE_n(t-t')}F_-(E_n) + e^{iE_n(t-t')}[1+F_+(E_n)]. \tag{8.269}$$

Here

$$F_\pm(E) = [e^{\beta(E\pm e\mu)}-1]^{-1} \tag{8.270}$$

gives the distribution function for charged particles and antiparticles. The analogue of (8.232) is

$$1+F_\pm(E) = e^{\beta(E\pm e\mu)}F_\pm(E). \tag{8.271}$$

If we again allow time to become complex, we find

$$G_n^>(t-t'-i\beta) = e^{-\beta e\mu}G_n^<(t-t'). \tag{8.272}$$

For $\mu = 0$ this agrees with what we found in (8.233).

As in the real scalar field case, it proves advantageous to perform a Wick rotation to imaginary time, and to define the imaginary time Green function by (8.238). $\tilde{G}^{>}(\tau - \tau)$ and $\tilde{G}^{<}(\tau - \tau)$ are given by (8.267) and (8.269) respectively by replacing $t = -i\tau$ and $t' = -i\tau'$ in these equations. In terms of the imaginary time Green functions (8.272) becomes

$$\tilde{G}_n^{>}(\tau - \tau' + \beta) = e^{-\beta e\mu}\tilde{G}_n^{<}(\tau - \tau'). \tag{8.273}$$

This time, unlike the real scalar field case, the imaginary time Green function is not periodic in imaginary time with period β. However it is easy to relate it to a function that is periodic and therefore to make use of a Fourier expansion again.

Suppose that

$$f(\tau + \beta) = e^{-k\beta}f(\tau), \tag{8.274}$$

for some constant k. Simply define

$$\bar{f}(\tau) = e^{k\tau}f(\tau), \tag{8.275}$$

and it is obvious that

$$\bar{f}(\tau + \beta) = \bar{f}(\tau). \tag{8.276}$$

Because $\bar{f}(\tau)$ is a periodic function, we can expand it in a normal Fourier series,

$$\bar{f}(\tau) = \frac{1}{\beta}\sum_{j=-\infty}^{\infty} c_j\, e^{i\omega_j\tau} \tag{8.277}$$

for expansion coefficients c_j with ω_j given by (8.249). From (8.275) we can see that the expansion for $f(\tau)$ is just

$$f(\tau) = \frac{1}{\beta}\sum_{j=-\infty}^{\infty} c_j\, e^{(i\omega_j - k)\tau}. \tag{8.278}$$

We can view the imaginary time Green function as the solution to (8.239) subject to the boundary condition that results from (8.273). Write

$$\tilde{G}(x, x') = \sum_n \frac{f_n(\mathbf{x})f_n^*(\mathbf{x}')}{2E_n}\tilde{G}_n(\tau - \tau'). \tag{8.279}$$

It is easy to show that $e^{e\mu(\tau-\tau')}\tilde{G}_n(\tau-\tau')$ is periodic in $\tau-\tau'$ with period β. We therefore express

$$\tilde{G}_n(\tau - \tau') = \frac{1}{\beta}\sum_{j=-\infty}^{\infty} e^{i\omega_j(\tau-\tau') - e\mu(\tau-\tau')}G_{nj} \tag{8.280}$$

for some coefficients G_{nj}. (This is similar to (8.278).) Requiring that $\tilde{G}(x,x')$ solve (8.239) determines the coefficients G_{nj} to be

$$G_{nj} = \frac{2E_n}{(\omega_j + ie\mu)^2 + \sigma_n + M^2}. \tag{8.281}$$

We therefore have

$$\tilde{G}(x,x') = \frac{1}{\beta}\sum_{j=-\infty}^{\infty}\sum_n \frac{f_n(\mathbf{x})f_n^*(\mathbf{x}')e^{(i\omega_j - e\mu)(\tau-\tau')}}{[(\omega_j + ie\mu)^2 + \sigma_n + M^2]} \tag{8.282}$$

as the imaginary time Green function.

We will now show how (8.282) leads to the result for the thermodynamic potential given for the free complex scalar field in (5.82). The grand partition function is defined by

$$\mathcal{Z} = \mathrm{tr}\left[e^{-\beta(H-\mu Q)}\right] \tag{8.283}$$

and is related to the thermodynamic potential Ω by

$$\mathcal{Z} = e^{-\beta\Omega}. \tag{8.284}$$

By differentiation with respect to m^2 we have

$$\frac{\partial\Omega}{\partial m^2} = \left\langle \frac{\partial H}{\partial m^2} \right\rangle. \tag{8.285}$$

But

$$\frac{\partial H}{\partial m^2} = \int d\sigma_x |\Phi(t,\mathbf{x})|^2, \tag{8.286}$$

so we find

$$\begin{aligned}\frac{\partial\Omega}{\partial m^2} &= \int d\sigma_x \left\langle |\Phi(t,\mathbf{x})|^2 \right\rangle \\ &= -i\int d\sigma_x G(x,x) \\ &= \int d\sigma_x \tilde{G}(x,x) \\ &= \frac{1}{\beta}\sum_{j=-\infty}^{\infty}\sum_n [(\omega_j + ie\mu)^2 + \sigma_n + M^2]^{-1}\end{aligned} \tag{8.287}$$

making use of (8.238), (8.263), and (8.282). (Recall that $E_n^2 = \sigma_n + m^2$ as in (3.185).) To do the sum over j, we make use of

$$\sum_{j=-\infty}^{\infty}[(j+ia)^2+b^2]^{-1} = \frac{\pi}{b}\left\{1 + \left[e^{2\pi(b-a)} - 1\right]^{-1} + \left[e^{2\pi(b+a)} - 1\right]^{-1}\right\} \tag{8.288}$$

that is easily established by the contour integral method described in Section A1.3, assuming $b > a \geq 0$. This results in

$$\frac{\partial \Omega}{\partial m^2} = \frac{1}{2E_n}\big[1 + F_-(E_n) + F_+(E_n)\big]. \tag{8.289}$$

After integration with respect to m^2 we recover (5.82).

We close this section with some comments. It is possible to establish the much more general results that the full Green function for an interacting theory obeys the periodic boundary conditions in imaginary time that we only established for the free Green functions. The details can be found in the standard references Kadanoff and Baym (1962), Abrikosov *et al.* (1975), and Fetter and Walecka (2003). Because of the way μ entered in Section 8.7.2, the time development is often taken using $\bar{H} = H - \mu Q$ rather than simply H. This is done in Abrikosov *et al.* (1975) and Fetter and Walecka (2003) for example; however, this is just a convenience. Obviously this short section has merely introduced the area of finite temperature field theory. The interested reader can find much more detail in Kadanoff and Baym (1962), Abrikosov *et al.* (1975), Fetter and Walecka (2003), Kapusta (1989), and Le Bellac (1996) for example.

8.8 Generalized CJT effective action

We have already discussed how when the perturbative expansion for the effective action is interpreted in terms of Feynman diagrams it only contains those diagrams that are one-particle irreducible; that is, only those diagrams that remain connected (in one piece) when any internal line is cut are contained. It is possible to generalize the effective action to obtain a result that is two-particle irreducible; that is, only diagrams that remain connected when any two lines are cut are contained in the perturbative expansion. The general formalism for this was described using the path integral method in Cornwall *et al.* (1974). We will refer to the result as the generalized CJT effective action. This section will contain the basic formalism for calculating the generalized CJT effective action obtained using the Schwinger action principle. In the next section we will apply the formalism to the interacting Bose gas.

In order to define the effective action, at the start of this chapter, we introduced a coupling of the field ϕ^i to an external source J_i. (See (8.1) for the free field case.) This led to the replacement of the action functional $S[\phi]$ with $S[\phi, J]$ where

$$S[\phi, J] = S[\phi] + J_i \phi^i. \tag{8.290}$$

The perturbative expansion of the effective action began with the division of $S[\phi]$ into two parts $S_0 + S_1$ in (8.40) with S_1 viewed as an interaction. We had

$$e^{(i/\hbar)W[J]} = \langle \text{out}|T\left\{\exp\left(\frac{i}{\hbar}S_1 + \frac{i}{\hbar}J_i\phi^i\right)\right\}|\text{in}\rangle_0 \tag{8.291}$$

as in (8.41). The background, or mean, field φ^i was defined by (8.27) and is used to eliminate the dependence of $W[J]$ on the external source using (8.28). The perturbative expansion of $\Gamma[\varphi]$ was the subject of Section 8.2.

In order to obtain the generalized effective action, in addition to the linear field coupling $J_i\phi^i$, we introduce a second independent source K_{ij} and adopt

$$S_{JK} = S[\phi] + J_i\phi^i + \frac{1}{2}K_{ij}\phi^i\phi^j. \tag{8.292}$$

The source $K_{ij} = K_{ji}$ is taken to be symmetric. We will define, in analogy with (8.291), $W[J,K]$ by

$$e^{(i/\hbar)W[J,K]} = \langle \text{out}|T\left\{\exp\left(\frac{i}{\hbar}S_1 + \frac{i}{\hbar}J_i\phi^i + \frac{i}{2\hbar}K_{ij}\phi^i\phi^j\right)\right\}|\text{in}\rangle_0. \tag{8.293}$$

It is clear from this definition that $W[J, K = 0] = W[J]$ corresponds to the generating functional that we studied earlier in this chapter as obtained from (8.291). The aim now is to remove dependence on both source terms J_i and K_{ij} from $W[J,K]$ and to obtain the generalized effective action. We will do this in two stages, dealing first with the dependence on J_i.

The two sources J_i and K_{ij} are independent of each other, so we are free to vary them independently. Differentiation of both sides of (8.293) with respect to J_i keeping K_{ij} fixed gives

$$\left.\frac{\delta W[J,K]}{\delta J_i}\right|_K = \frac{\langle \text{out}|T\left\{\phi^i \exp\left[(i/\hbar)S_1 + (i/\hbar)J_i\phi^i + (i/2\hbar)K_{ij}\phi^i\phi^j\right]\right\}|\text{in}\rangle_0}{e^{(i/\hbar)W[J,K]}} = \varphi^i \tag{8.294}$$

with φ^i background field. As in (8.28) we define

$$\Gamma_K[\varphi] = W[J,K] - J_i\varphi^i. \tag{8.295}$$

Then $\Gamma_K[\varphi]$ has no dependence on J_i, but still depends on the source K_{ij} since we have not done anything with this source yet. Differentiation of both sides of (8.295) with respect to φ^i while keeping K_{ij} fixed results in

$$\frac{\delta\Gamma_K[\varphi]}{\delta\varphi^i} = -J_i \tag{8.296}$$

exactly as in (8.44).

It should be obvious from (8.293) that $\Gamma_K[\varphi]$ is the normal effective action that we have already discussed, with the difference that the theory is now governed by the action functional

$$S_K[\phi] = S[\phi] + \frac{1}{2}K_{ij}\phi^i\phi^j \tag{8.297}$$

in place of simply $S[\phi]$. This means that all the results found for the effective action earlier in this chapter may be applied to $\Gamma_K[\varphi]$ with the replacement of $S[\phi]$ with $S_K[\phi]$. In particular, from Section 8.2 we find the perturbative expansion of $\Gamma_K[\varphi]$ to two-loop order as

$$\begin{aligned}\Gamma_K[\varphi] = S_K[\varphi] + \frac{i\hbar}{2}\mathrm{tr}\ln\left(\ell^2 S_{K,ij}[\varphi]\right) - \frac{\hbar^2}{8}S_{,ijkl}G_K^{ij}G_K^{kl} \\ -\frac{\hbar^2}{12}S_{,ijk}S_{,lmn}G_K^{il}G_K^{jm}G_K^{kn} + \mathcal{O}(\hbar^3).\end{aligned} \tag{8.298}$$

Here we have defined G_K^{ij} by

$$S_{K,ij}G_K^{jk} = -\delta_i^k \tag{8.299}$$

as follows from (8.64). Note that by virtue of (8.297), cubic and higher-order derivatives of S_K agree with those of S; thus, we can drop the subscript K on the derivatives of S appearing in the two-loop (and higher) order parts of $\Gamma_K[\varphi]$. Obviously, if we set $K_{ij} = 0$, then $\Gamma_K[\varphi]$ reduces to the effective action that we had earlier.

We now want to remove the dependence of $\Gamma_K[\varphi]$ on the source K_{ij}. To do this, note first of all that (8.296) defines J_i as a functional of φ^i and K_{ij}. If we differentiate both sides of (8.295) with respect to K_{ij} keeping φ^i fixed, we find

$$\begin{aligned}\left.\frac{\delta\Gamma_K[\varphi]}{\delta K_{ij}}\right|_\varphi &= \left.\frac{\delta W[J,K]}{\delta K_{ij}}\right|_\varphi - \left.\frac{\delta J_k}{\delta K_{ij}}\right|_\varphi \varphi^k \\ &= \left.\frac{\delta W[J,K]}{\delta K_{ij}}\right|_J + \left.\frac{\delta W[J,K]}{\delta J_k}\right|_K \left.\frac{\delta J_k}{\delta K_{ij}}\right|_\varphi - \left.\frac{\delta J_k}{\delta K_{ij}}\right|_\varphi \varphi^k \\ &= \left.\frac{\delta W[J,K]}{\delta K_{ij}}\right|_J .\end{aligned} \tag{8.300}$$

(The last two terms in the middle line cancel if we use (8.294).) From (8.293) we find

$$\left.\frac{\delta W[J,K]}{\delta K_{ij}}\right|_J = \frac{\langle \mathrm{out}|T\left\{\phi^i\phi^j \exp\left[(i/\hbar)S_1 + (i/\hbar)J_i\phi^i + (i/2\hbar)K_{ij}\phi^i\phi^j\right]\right\}|\mathrm{in}\rangle_0}{2\,e^{(i/\hbar)W[J,K]}} \tag{8.301}$$

Differentiation of the first line in (8.294) with respect to J_j, holding K_{ij} fixed, gives us

$$\left.\frac{\delta^2 W[J,K]}{\delta J_j \delta J_i}\right|_K = \frac{i}{\hbar}\frac{\langle \text{out}|T\left\{\phi^i\phi^j \exp\left[(i/\hbar)S_1 + (i/\hbar)J_i\phi^i + (i/2\hbar)K_{ij}\phi^i\phi^j\right]\right\}|\text{in}\rangle_0}{e^{(i/\hbar)W[J,K]}}$$
$$- \frac{i}{\hbar}\left.\frac{\delta W[J,K]}{\delta J_j}\right|_K \frac{\langle \text{out}|T\left\{\phi^i \exp\left[(i/\hbar)S_1 + (i/\hbar)J_i\phi^i + (i/2\hbar)K_{ij}\phi^i\right]\right\}|\text{in}\rangle_0}{e^{(i/\hbar)W[J,K]}}$$
$$= \frac{i}{\hbar}\frac{\langle \text{out}|T\left\{\phi^i\phi^j \exp\left[(i/\hbar)S_1 + (i/\hbar)J_i\phi^i + (i/2\hbar)K_{ij}\phi^i\phi^j\right]\right\}|\text{in}\rangle_0}{e^{(i/\hbar)W[J,K]}}$$
$$-\frac{i}{\hbar}\varphi^i\varphi^j. \tag{8.302}$$

We will define

$$\left.\frac{\delta^2 W[J,K]}{\delta J_j \delta J_i}\right|_K = \Delta^{ij}. \tag{8.303}$$

From (8.301) and (8.302) we find

$$\left.\frac{\delta W[J,K]}{\delta K_{ij}}\right|_J = \frac{1}{2}(\varphi^i\varphi^j - i\hbar\Delta^{ij}). \tag{8.304}$$

We can use this in (8.300) to obtain

$$\left.\frac{\delta \Gamma_K[\varphi]}{\delta K_{ij}}\right|_\varphi = \frac{1}{2}(\varphi^i\varphi^j - i\hbar\Delta^{ij}). \tag{8.305}$$

At this stage we can perform a Legendre transformation of $\Gamma_K[\varphi]$ to eliminate the dependence on K_{ij} in favour of a dependence on Δ^{ij} by defining

$$\Gamma[\varphi,\Delta] = \Gamma_K[\varphi] - \frac{1}{2}K_{ij}(\varphi^i\varphi^j - i\hbar\Delta^{ij}). \tag{8.306}$$

$\Gamma[\varphi,\Delta]$ is the generalized CJT effective action and is regarded as a functional of independent variables φ^i and Δ^{ij}. If we differentiate both sides of (8.306) with respect to φ^i holding Δ^{ij} fixed we find

$$\left.\frac{\delta\Gamma[\varphi,\Delta]}{\delta\varphi^i}\right|_\Delta = \left.\frac{\delta\Gamma_K[\varphi]}{\delta\varphi^i}\right|_\Delta - \frac{1}{2}\left.\frac{\delta K_{kl}}{\delta\varphi^i}\right|_\Delta (\varphi^k\varphi^l - i\hbar\Delta^{kl}) - K_{ij}\varphi^j. \tag{8.307}$$

Note that because we are viewing φ^i and Δ^{ij} as the independent variables we must regard the source K_{ij} as a functional of them; hence, the middle term above. For the first term on the right-hand side of (8.307) we use

$$\left.\frac{\delta\Gamma_K[\varphi]}{\delta\varphi^i}\right|_\Delta = \left.\frac{\delta\Gamma_K[\varphi]}{\delta\varphi^i}\right|_K + \left.\frac{\delta\Gamma_K[\varphi]}{\delta K_{kl}}\right|_\varphi \left.\frac{\delta K_{kl}}{\delta\varphi^i}\right|_\Delta. \tag{8.308}$$

For the first term on the right-hand side of (8.308) we may use (8.296). For the second term on the right-hand side of (8.308) we use (8.305) and notice that it cancels the middle term of (8.307). This leaves us with

$$\left.\frac{\delta\Gamma[\varphi,\Delta]}{\delta\varphi^i}\right|_{\Delta} = -J_i - K_{ij}\varphi^j. \tag{8.309}$$

If we differentiate both sides of (8.306) with respect to Δ^{ij} holding φ^i fixed, we have

$$\left.\frac{\delta\Gamma[\varphi,\Delta]}{\delta\Delta^{ij}}\right|_{\varphi} = \left.\frac{\delta\Gamma_K[\varphi]}{\delta\Delta^{ij}}\right|_{\varphi} - \frac{1}{2}\left.\frac{\delta K_{kl}}{\delta\Delta^{ij}}\right|_{\varphi}(\varphi^k\varphi^l - i\hbar\Delta^{kl}) + \frac{i\hbar}{2}K_{ij}. \tag{8.310}$$

For the first term on the right-hand side of (8.310), because φ is held fixed, we have

$$\left.\frac{\delta\Gamma_K[\varphi]}{\delta\Delta^{ij}}\right|_{\varphi} = \left.\frac{\delta\Gamma_K[\varphi]}{\delta K_{kl}}\right|_{\varphi}\left.\frac{\delta K_{kl}}{\delta\Delta^{ij}}\right|_{\varphi}.$$

Making use of (8.305), it is seen that the first two terms in (8.310) cancel leaving us with

$$\left.\frac{\delta\Gamma[\varphi,\Delta]}{\delta\Delta^{ij}}\right|_{\varphi} = \frac{i\hbar}{2}K_{ij}. \tag{8.311}$$

The physical theory is governed by setting both of the external sources J_i and K_{ij} to zero. From (8.309) and (8.311) we obtain

$$\left.\frac{\delta\Gamma[\varphi,\Delta]}{\delta\Delta^{ij}}\right|_{\varphi} = 0, \tag{8.312}$$

$$\left.\frac{\delta\Gamma[\varphi,\Delta]}{\delta\varphi^i}\right|_{\Delta} = 0. \tag{8.313}$$

We can regard the first equation as defining Δ^{ij} in terms of φ^i. When this result is used in (8.313) we end up with the field equation for the background field φ^i.

The perturbative evaluation of $\Gamma[\varphi,\Delta]$ can be obtained from our knowledge of the result for $\Gamma_K[\varphi]$. Substitution for $\Gamma_K[\varphi]$ and $S_K[\varphi]$ into (8.306) results in

$$\begin{aligned}\Gamma[\varphi,\Delta] = S[\varphi] + \frac{i\hbar}{2}K_{ij}\Delta^{ij} + \frac{i\hbar}{2}\mathrm{tr}\ln\left(\ell^2 S_{K,ij}[\varphi]\right)\\ -\hbar^2\left(\frac{1}{8}S_{,ijkl}G_K^{ij}G_K^{kl} + \frac{1}{12}S_{,ijk}S_{,lmn}G_K^{il}G_K^{jm}G_K^{kn}\right) + \cdots .\end{aligned} \tag{8.314}$$

We need to eliminate all dependence on K_{ij} from this expression. The aim is to use (8.305) with (8.306) for $\Gamma_K[\varphi]$ and to solve for K_{ij}. Differentiation of (8.306) with respect to K_{ij} holding φ^i fixed gives us

$$\left.\frac{\delta\Gamma_K[\varphi]}{\delta K_{ij}}\right|_\varphi = \frac{1}{2}\varphi^i\varphi^j + \frac{i\hbar}{2}\frac{\delta}{\delta K_{ij}}\mathrm{tr}\ln\left(\ell^2 S_{K,ij}[\varphi]\right) - \frac{\hbar^2}{4}S_{,klmn}\frac{\delta G_K^{kl}}{\delta K_{ij}}G_K^{mn} - \frac{\hbar^2}{4}S_{,klm}S_{,npq}\frac{\delta G_K^{kn}}{\delta K_{ij}}G_K^{lp}G_K^{mq} + \cdots . \tag{8.315}$$

Because $-G_K^{ij}$ is the inverse of $S_{K,ij}$ according to (8.299), we have

$$\frac{\delta}{\delta K_{ij}}\mathrm{tr}\ln\left(\ell^2 S_{K,ij}\right) = -G_K^{kl}\,\frac{\delta S_{K,kl}}{\delta K_{ij}}. \tag{8.316}$$

To evaluate $\delta S_{K,kl}/\delta K_{ij}$ we use (8.297) to find

$$\frac{\delta S_{K,kl}}{\delta K_{ij}} = \frac{\delta K_{kl}}{\delta K_{ij}} = \frac{1}{2}\left(\delta_k^i\delta_l^j + \delta_l^i\delta_k^j\right). \tag{8.317}$$

Because $G_K^{ij} = G_K^{ji}$ is symmetric, upon using (8.317) in (8.316) we find

$$\frac{\delta}{\delta K_{ij}}\mathrm{tr}\ln\left(\ell^2 S_{K,ij}\right) = -G_K^{ij}. \tag{8.318}$$

To eliminate the K_{ij} dependence in the remaining terms of (8.315) we need $\delta G_K^{kl}/\delta K_{ij}$. The necessary expression can be found by differentiating both sides of (8.299) with respect to K_{ij}:

$$\begin{aligned} 0 &= \frac{\delta}{\delta K_{ij}}\left(S_{K,kl}G_K^{lm}\right) \\ &= \frac{1}{2}\left(\delta_k^i\delta_l^j + \delta_l^i\delta_k^j\right)G_K^{lm} + S_{K,kl}\,\frac{\delta G_K^{lm}}{\delta K_{ij}}. \end{aligned} \tag{8.319}$$

Again noting that $-G_K^{ij}$ is the inverse of $S_{K,ij}$, we obtain

$$\begin{aligned} \frac{\delta G_K^{nm}}{\delta K_{ij}} &= \frac{1}{2}G_K^{nk}\left(\delta_k^i\delta_l^j + \delta_l^i\delta_k^j\right)G_K^{lm} \\ &= \frac{1}{2}\left(G_K^{ni}G_K^{jm} + G_K^{nj}G_K^{im}\right) \end{aligned} \tag{8.320}$$

if we solve for $\delta G_K^{nm}/\delta K_{ij}$ using (8.319). The results in (8.318) and (8.320) can be used in (8.315) to find

$$\left.\frac{\delta\Gamma_K[\varphi]}{\delta K_{ij}}\right|_\varphi = \frac{1}{2}\varphi^i\varphi^j - \frac{i\hbar}{2}G_K^{ij} - \frac{\hbar^2}{4}S_{,klmn}G_K^{ik}G_K^{jl}G_K^{mn} - \frac{\hbar^2}{4}S_{,klm}S_{,npq}G_K^{ik}G_K^{jn}G_K^{lp}G_K^{mq} + \cdots . \tag{8.321}$$

Comparison with (8.305) shows that

$$\Delta^{ij} = G_K^{ij} - \frac{i\hbar}{2} S_{,klmn} G_K^{ik} G_K^{jl} G_K^{mn} - \frac{i\hbar}{2} S_{,klm} S_{npq} G_K^{ik} G_K^{jn} G_K^{lp} G_K^{mq} + \mathcal{O}(\hbar^2). \tag{8.322}$$

We can invert this quite simply to order $\hbar$ to find

$$G_K^{ij} = \Delta^{ij} + \frac{i\hbar}{2} S_{,klmn} \Delta^{ik} \Delta^{jl} \Delta^{mn} + \frac{i\hbar}{2} S_{,klm} S_{npq} \Delta^{ik} \Delta^{jn} \Delta^{lp} \Delta^{mq} + \mathcal{O}(\hbar^2). \tag{8.323}$$

This allows us to eliminate all of the dependence on K_{ij} that occurs through G_K^{ij} in (8.314). There is still the explicit dependence on K_{ij} that must be dealt with. Begin with (8.299) using (8.297) for S_K:

$$(S_{,ij} + K_{ij})\, G_K^{jk} = -\delta_i^k. \tag{8.324}$$

This allows us to solve for

$$K_{ij} = -(G_K^{-1})_{ij} - S_{,ij}. \tag{8.325}$$

From (8.323) we can write, in matrix form,

$$G_K = \Delta + \hbar\, G^{(1)} + \cdots \tag{8.326}$$

where

$$\big[G^{(1)}\big]^{mn} = \frac{i}{2} \Delta^{mp} \Delta^{nq} \big(S_{,pqkl} \Delta^{kl} + S_{,pkl} S_{,qrs} \Delta^{kr} \Delta^{ls} \big). \tag{8.327}$$

Inverting the expansion in (8.326) to order $\hbar$ results in the following steps:

$$\begin{aligned} G_K^{-1} &= \big[\Delta + \hbar\, G^{(1)} + \cdots\big]^{-1} \\ &= \big[\Delta\big(I + \hbar \Delta^{-1} G^{(1)} + \cdots\big)\big]^{-1} \\ &= \big[I + \hbar \Delta^{-1} G^{(1)} + \cdots\big]^{-1} \Delta^{-1} \\ &= \Delta^{-1} - \hbar \Delta^{-1} G^{(1)} \Delta^{-1} + \cdots . \end{aligned} \tag{8.328}$$

Taking the matrix element of (8.328) and using (8.327) for $G^{(1)}$ gives us

$$K_{ij} = -(\Delta^{-1})_{ij} - S_{,ij} + \frac{i\hbar}{2} S_{,ijkl} \Delta^{kl} + \frac{i\hbar}{2} S_{,ikl} S_{,jmn} \Delta^{km} \Delta^{ln} + \cdots \tag{8.329}$$

when used in (8.325). We then find, upon contraction of K_{ij} with Δ^{ij},

$$K_{ij}\Delta^{ij} = -\delta_i^i - S_{,ij}\Delta^{ij} + \frac{i\hbar}{2}S_{,ijkl}\Delta^{ij}\Delta^{kl} + \frac{i\hbar}{2}S_{,ikl}S_{,jmn}\Delta^{ij}\Delta^{km}\Delta^{ln} + \cdots . \tag{8.330}$$

The final term we need is $\mathrm{tr}\ln(\ell^2 S_{K,ij})$. This is easy to evaluate using[28]

$$\begin{aligned}\mathrm{tr}\ln(\ell^2 S_{K,ij}) &= \mathrm{tr}\ln\bigl[\ell^2 (G_K^{-1})_{ij}\bigr] \\ &= -\mathrm{tr}\ln(\ell^{-2} G_K^{ij}).\end{aligned} \tag{8.331}$$

We can use (8.323) for G_K^{ij} noting that

$$G_K^{ij} = \Delta^{ik}\left(\delta_k^j + \frac{i\hbar}{2}S_{,klmn}\Delta^{jl}\Delta^{mn} + \frac{i\hbar}{2}S_{,klm}S_{,npq}\Delta^{jn}\Delta^{lp}\Delta^{nq}\right) + \cdots$$

and using

$$\mathrm{tr}\ln(I + \hbar M) \simeq \hbar\ \mathrm{tr}(M) + \cdots . \tag{8.332}$$

This results in

$$\begin{aligned}\mathrm{tr}\ln(\ell^2 S_{K,ij}) = -\mathrm{tr}\ln(\ell^{-2}\Delta^{ij}) &- \frac{i\hbar}{2}S_{,ijkl}\Delta^{ij}\Delta^{kl} \\ &- \frac{i\hbar}{2}S_{,ijk}S_{,lmn}\Delta^{il}\Delta^{jm}\Delta^{kn} + \cdots .\end{aligned} \tag{8.333}$$

Finally, we return to (8.314) and use (8.330) for the second term on the right-hand side, (8.333) for the third term on the right-hand side, and (8.323) for the last term on the right-hand side. Because we are only working to order $\hbar^2$, we find[29]

$$\begin{aligned}\Gamma[\varphi,\Delta] = S[\varphi] &- \frac{i\hbar}{2}\ \mathrm{tr}(I) - \frac{i\hbar}{2}S_{,ij}\Delta^{ij} - \frac{i\hbar}{2}\ \mathrm{tr}\ln(\ell^{-2}\Delta^{ij}) \\ &- \hbar^2\left(\frac{1}{8}S_{,ijkl}\Delta^{ij}\Delta^{kl} + \frac{1}{12}S_{,ijk}S_{,lmn}\Delta^{il}\Delta^{jm}\Delta^{kn}\right) + \cdots .\end{aligned} \tag{8.334}$$

The two-loop part of $\Gamma[\varphi,\Delta]$ is seen to consist of the same two terms as those that occurred in $\Gamma[\varphi]$, but with the replacement of G^{ij} there with Δ^{ij} here. The Feynman diagrams that correspond to these terms are both two-particle irreducible. A proof that only two-particle irreducible diagrams are contained in higher-order terms can be found in Cornwall *et al.* (1974). We will not proceed beyond two-loop order here.

[28] We may be cavalier about the sign of the argument of the logarithm since it should really involve an absolute value to keep the result real.

[29] We have written δ_i^i that occurs in (8.330) as $\mathrm{tr}(I)$ here.

8.9 CJT approach to Bose–Einstein condensation

The aim of this section is to study the application of the generalized CJT effective action to the interacting non-relativistic Bose gas. Although we only considered the zero temperature quantum field theory in Section 8.8, we can obtain the results at finite temperature by using the appropriate finite temperature Green functions similarly to what was done in Section 8.7. We will initially work with the real time formalism and go over to imaginary time later.

The interacting non-relativistic Bose gas is described by the Hamiltonian

$$H = \int_\Sigma d\sigma_x \left(\frac{1}{2m} |\nabla \Psi|^2 + \frac{\lambda}{6} |\Psi|^4 \right). \tag{8.335}$$

Here Σ is the spatial region that we will take to be $\mathbb{R}^3$ at the end. As usual, it is convenient to initially consider a finite box. At finite density, we use a chemical potential with the particle number being

$$N = \int_\Sigma d\sigma_x |\Psi|^2. \tag{8.336}$$

As described at the end of Section 8.7, it is convenient to define $\bar{H}$ by

$$\bar{H} = H - \mu N, \tag{8.337}$$

and to use $\bar{H}$ as the Hamiltonian (instead of simply H). When we consider the effects of finite temperature this will allow us to deal with periodic boundary conditions in imaginary time. The action corresponding to the Hamiltonian $\bar{H}$ here is

$$S[\Psi, \Psi^\dagger] = \int dt \int_\Sigma d\sigma_x \left[\frac{i}{2} (\Psi^\dagger \dot{\Psi} - \dot{\Psi}^\dagger \Psi) - \frac{1}{2m} |\nabla \Psi|^2 + \mu |\Psi|^2 - \frac{\lambda}{6} |\Psi|^4 \right]. \tag{8.338}$$

The formalism of Section 8.8 has been based around the use of real, as opposed to complex, fields. To avoid going through the analysis again we will write

$$\Psi = \frac{1}{\sqrt{2}} (\phi_1 + i\phi_2), \tag{8.339}$$

where ϕ_1 and ϕ_2 are both real. The action (8.338) becomes

$$\begin{aligned} S[\phi_1, \phi_2] = - \int dt \int_\Sigma d\sigma_x \Big[& \frac{1}{2} (\phi_1 \dot{\phi}_2 - \phi_2 \dot{\phi}_1) + \frac{1}{4m} (|\nabla \phi_1|^2 + |\nabla \phi_2|^2) \\ & - \frac{1}{2} \mu (\phi_1^2 + \phi_2^2) + \frac{\lambda}{4!} (\phi_1^2 + \phi_2^2)^2 \Big] \end{aligned} \tag{8.340}$$

when written in terms of the real fields.

The generalized CJT effective action requires a knowledge of $S_{,i_1,\ldots,i_n}$. We may vary (8.340) with respect to ϕ_1 to find

$$S_{,1} = -\dot{\phi}_2 + \frac{1}{2m}\nabla^2\phi_1 + \mu\phi_1 - \frac{\lambda}{6}(\phi_1^2 + \phi_2^2)\phi_1. \tag{8.341}$$

Similarly,

$$S_{,2} = \dot{\phi}_1 + \frac{1}{2m}\nabla^2\phi_2 + \mu\phi_2 - \frac{\lambda}{6}(\phi_1^2 + \phi_2^2)\phi_2. \tag{8.342}$$

Calculating the functional derivatives of these last two expressions with respect to $\phi_1(x')$ and $\phi_2(x')$ gives us

$$S_{,11'} = \left(\frac{1}{2m}\nabla^2 + \mu - \frac{\lambda}{2}\phi_1^2 - \frac{\lambda}{6}\phi_2^2\right)\delta(x,x'), \tag{8.343}$$

$$S_{,12'} = \left(-\frac{\partial}{\partial t} - \frac{\lambda}{3}\phi_1\phi_2\right)\delta(x,x'), \tag{8.344}$$

$$S_{,21'} = \left(\frac{\partial}{\partial t} - \frac{\lambda}{3}\phi_1\phi_2\right)\delta(x,x'), \tag{8.345}$$

$$S_{,22'} = \left(\frac{1}{2m}\nabla^2 + \mu - \frac{\lambda}{2}\phi_2^2 - \frac{\lambda}{6}\phi_1^2\right)\delta(x,x'). \tag{8.346}$$

Here $\delta(x,x') = \delta(t-t')\delta(\mathbf{x},\mathbf{x}')$ and $S_{,11'} = \delta^2 S/\delta\phi_1(x')\delta\phi_1(x)$, and so on for the other derivatives that are indicated. Performing further functional derivatives of (8.343)–(8.346) with respect to $\phi_1(x'')$ and $\phi_2(x'')$ results in

$$S_{,11'1''} = -\lambda\phi_1\,\delta(x,x')\delta(x,x''), \tag{8.347}$$

$$S_{,11'2''} = -\frac{\lambda}{3}\phi_2\,\delta(x,x')\delta(x,x''), \tag{8.348}$$

$$S_{,12'2''} = -\frac{\lambda}{3}\phi_1\,\delta(x,x')\delta(x,x''), \tag{8.349}$$

$$S_{,22'2''} = -\lambda\phi_2\,\delta(x,x')\delta(x,x''). \tag{8.350}$$

We have not written out all the terms that are equivalent to those given here by a permutation of labels (such as $S_{,21'2''} = S_{,1'22''}$, etc.). Finally, the fourth derivatives are found from (8.347)–(8.350) after further functional differentiation to be

$$S_{,11'1''1'''} = -\lambda\delta(x,x')\delta(x,x'')\delta(x,x'''), \tag{8.351}$$

$$S_{,11'2''2'''} = -\frac{\lambda}{3}\delta(x,x')\delta(x,x''')\delta(x,x''), \tag{8.352}$$

$$S_{,22'2''2'''} = -\lambda\delta(x,x')\delta(x,x'')\delta(x,x'''). \tag{8.353}$$

The only other non-zero fourth derivatives consist of those found by permuting labels on the middle term.

Because the effective action should only depend on $|\Psi|^2 = \phi_1^2 + \phi_2^2$, we can simplify the calculation by taking the background field to be

$$\varphi_1 = \varphi, \qquad \varphi_2 = 0. \tag{8.354}$$

The background field φ representing the ground state will also be chosen to be constant. This gives us the only non-zero derivatives

$$S_{,11'}[\varphi] = \left(\frac{1}{2m}\nabla^2 + \mu - \frac{\lambda}{2}\varphi^2\right)\delta(x,x'), \tag{8.355}$$

$$S_{,12'}[\varphi] = -\frac{\partial}{\partial t}\delta(x,x'), \tag{8.356}$$

$$S_{,21'}[\varphi] = \frac{\partial}{\partial t}\delta(x,x'), \tag{8.357}$$

$$S_{,22'}[\varphi] = \left(\frac{1}{2m}\nabla^2 + \mu - \frac{\lambda}{6}\varphi^2\right)\delta(x,x'), \tag{8.358}$$

$$S_{,11'1''}[\varphi] = -\lambda\varphi\,\delta(x,x')\delta(x,x''), \tag{8.359}$$

$$S_{,12'2''}[\varphi] = S_{21'2''}[\varphi] = S_{22'1''}[\varphi] = -\frac{\lambda}{3}\varphi\,\delta(x,x')\delta(x,x''), \tag{8.360}$$

in addition to (8.351)–(8.353) that are unaffected by the background field. From (8.340),

$$S[\varphi] = \int dt \int_\Sigma d\sigma_x \left(\frac{1}{2}\mu\varphi^2 - \frac{\lambda}{24}\varphi^4\right). \tag{8.361}$$

We also require $S_{,ij}[\varphi]\Delta^{ij}$. In order to evaluate this, we will first calculate $S_{,ij}[\varphi]\Delta^{jk}$ and then contract on $k = i$. Because of this contraction, we only need to know the terms with $i = 1, k = 1$ and $i = 2, k = 2$. Recall that the repeated condensed index j involves an integration over the corresponding spacetime coordinate. We have

$$\begin{aligned} S_{11'}\Delta^{1'1''} &= \int dv_{x'}\left(\frac{1}{2m}\nabla^2 + \mu - \frac{\lambda}{2}\varphi^2\right)\delta(x,x')\Delta^{11}(x',x'') \\ &= \left(\frac{1}{2m}\nabla^2 + \mu - \frac{\lambda}{2}\varphi^2\right)\Delta^{11}(x,x'') \end{aligned} \tag{8.362}$$

when the indices are uncondensed on the right-hand side. (Here $dv_{x'} = dt'd\sigma_{x'}$ is the spacetime volume element.) In a similar way,

$$S_{,12'}\Delta^{2'1''} = -\frac{\partial}{\partial t}\Delta^{21}(x,x''), \tag{8.363}$$

$$S_{,21'}\Delta^{1'2''} = \frac{\partial}{\partial t}\Delta^{12}(x,x''), \tag{8.364}$$

$$S_{,22'}\Delta^{2'2''} = \left(\frac{1}{2m}\nabla^2 + \mu - \frac{\lambda}{6}\varphi^2\right)\Delta^{22}(x,x''). \tag{8.365}$$

Before going further we will evaluate the other terms of $\Gamma[\varphi,\Delta]$.

We have

$$\begin{aligned} S_{,11'1''1'''}\Delta^{1''1'''} &= \int dv_{x''}dv_{x'''}(-\lambda)\delta(x,x')\delta(x,x'')\delta(x,x''')\Delta^{11}(x'',x''') \\ &= -\lambda\delta(x,x')\Delta^{11}(x,x). \end{aligned} \tag{8.366}$$

Remaining terms can be evaluated in a similar manner leading to

$$\begin{aligned} S_{,ijkl}\Delta^{ij}\Delta^{kl} = -\lambda\int dv_x \Big\{ &\left[\Delta^{11}(x,x)\right]^2 + \left[\Delta^{22}(x,x)\right]^2 \\ &+\frac{2}{3}\Delta^{11}(x,x)\Delta^{22}(x,x) + \frac{1}{3}\left[\Delta^{12}(x,x) + \Delta^{21}(x,x)\right]^2 \Big\} \end{aligned} \tag{8.367}$$

after a short calculation.

The term that involves $S_{,ijk}S_{,lmn}\Delta^{il}\Delta^{jm}\Delta^{kn}$ can be seen to be multiplied by $\lambda^2\varphi^2$ from (8.359, 8.360). This means that if we have a normal phase, characterized by $\varphi = 0$, this term will make no contribution to Γ. Furthermore, even if $\varphi \neq 0$, the term is down by a factor of λ compared with the contribution of the first two-loop term written explicitly in (8.367). If we only work to leading order in λ, then we can ignore the second part of the two-loop contribution in (8.334) and approximate the generalized effective action by

$$\Gamma[\varphi,\Delta] \simeq S[\varphi] - \frac{i\hbar}{2}S_{,ij}\Delta^{ij} - \frac{i\hbar}{2}\mathrm{tr}\ln(\ell^{-2}\Delta^{ij}) - \frac{\hbar^2}{8}S_{,ijkl}\Delta^{ij}\Delta^{kl}. \tag{8.368}$$

At this stage we will proceed to the imaginary time formalism. We take $t = -i\tau$ where $0 \leq \tau \leq \beta$. The fields, and Green functions, will be periodic in τ with period β. We interpret $\int dt = -i\int_0^\beta d\tau = -i\beta$. From (8.361) we find

$$S = -i\beta V\left(\frac{1}{2}\mu\varphi^2 - \frac{\lambda}{24}\varphi^4\right). \tag{8.369}$$

In addition, we write

$$\begin{aligned} \Delta^{ik}(x,x') &= i\tilde{\Delta}^{ik}(x,x') \\ &= i\sum_{j=-\infty}^{\infty}\frac{1}{\beta}\sum_n f_n(\mathbf{x})f_n^*(\mathbf{x}')e^{i\omega_j(\tau-\tau')}\Delta^{ik}_{jn}, \end{aligned} \tag{8.370}$$

for some expansion coefficients Δ^{ik}_{jn}. Here $\omega_j = 2\pi j/\beta$. Note that

$$\tilde{\delta}(x,x') = \sum_{j=-\infty}^{\infty} \frac{1}{\beta} \sum_n f_n(\mathbf{x}) f_n^*(\mathbf{x}') e^{i\omega_j(\tau-\tau')} \tag{8.371}$$

where $f_n(\mathbf{x})$ is the eigenfunction of $-\nabla^2$ with eigenvalue σ_n. The thermodynamic potential, Ω, is defined in terms of the effective action by

$$\Gamma = \int dt(-\Omega) = i\beta\Omega. \tag{8.372}$$

Because $\Delta^{ij}(x,x)$ has no dependence on τ, we have

$$\begin{aligned} S_{,ijkl}\Delta^{ij}\Delta^{kl} = -i\beta\lambda \int_\Sigma d\sigma_x \Big\{ &\left[\tilde{\Delta}^{11}(x,x)\right]^2 + \left[\tilde{\Delta}^{22}(x,x)\right]^2 \\ &+ \frac{2}{3}\tilde{\Delta}^{11}(x,x)\tilde{\Delta}^{22}(x,x) + \frac{1}{3}\left[\tilde{\Delta}^{12}(x,x) + \tilde{\Delta}^{21}(x,x)\right]^2 \Big\} \end{aligned} \tag{8.373}$$

from (8.367). We can use the expansion (8.370) to evaluate expressions like (8.362)–(8.365). For example, from (8.362) we find

$$S_{,11'}\Delta^{1'1''} = \frac{i}{\beta} \sum_{j,n} f_n(\mathbf{x}) f_n^*(\mathbf{x}'') \left(-\frac{\sigma_n}{2m} + \mu - \frac{\lambda}{2}\varphi^2 \right) e^{i\omega_j(\tau-\tau'')} \Delta^{11}_{jn}. \tag{8.374}$$

To obtain $S_{,ij}\Delta^{ij}$ using the results found from (8.362)–(8.365) we must set $\mathbf{x}'' = \mathbf{x}$ and $t'' = t$ with integrations over $\mathbf{x}$ and over t performed. Because the functions $f_n(\mathbf{x})$ are orthonormal, and $\int dt = -i\beta$ since $t = -i\tau$ where $0 \le \tau \le \beta$, we find

$$S_{,11'}\Delta^{1'1} = \sum_{j,n} \left(-\frac{\sigma_n}{2m} + \mu - \frac{\lambda}{2}\varphi^2 \right) \Delta^{11}_{jn}. \tag{8.375}$$

In a similar way,

$$S_{,12'}\Delta^{2'1} = \sum_{j,n} \omega_j \, \Delta^{21}_{jn}, \tag{8.376}$$

$$S_{,21'}\Delta^{1'2} = \sum_{j,n} (-\omega_j) \, \Delta^{12}_{jn}, \tag{8.377}$$

$$S_{,22'}\Delta^{2'2} = \sum_{j,n} \left(-\frac{\sigma_n}{2m} + \mu - \frac{\lambda}{6}\varphi^2 \right) \Delta^{22}_{jn}. \tag{8.378}$$

We then find

$$S_{,ij}\Delta^{ij} = \sum_{j,n}\left[\left(-\frac{\sigma_n}{2m}+\mu-\frac{\lambda}{2}\varphi^2\right)\Delta^{11}_{jn}+\omega_j\,\Delta^{21}_{jn}\right.$$
$$\left.-\omega_j\Delta^{12}_{jn}+\left(-\frac{\sigma_n}{2m}+\mu-\frac{\lambda}{6}\varphi^2\right)\Delta^{22}_{jn}\right]. \tag{8.379}$$

We can now work out the field equation (8.313) for the background field using our approximation (8.368). To the order we are working, the only background field dependence occurs in $S[\varphi]$ in (8.369) and $S_{,ij}\Delta^{ij}$ in (8.379). It is readily seen that

$$0=\varphi\left[\frac{\lambda}{6}\varphi^2-\mu+\frac{\lambda\hbar}{2\beta V}\sum_{j,n}\left(\Delta^{11}_{jn}+\frac{1}{3}\Delta^{22}_{jn}\right)\right]. \tag{8.380}$$

We can solve this equation in two ways. The first is if $\varphi=0$. This does not correspond to symmetry-breaking and there will be no Bose–Einstein condensation. The second possibility occurs if

$$\mu=\frac{\lambda}{6}\varphi^2+\frac{\lambda\hbar}{2\beta V}\sum_{j,n}\left(\Delta^{11}_{jn}+\frac{1}{3}\Delta^{22}_{jn}\right). \tag{8.381}$$

This can result in $\varphi\neq 0$ and corresponds to symmetry-breaking and Bose–Einstein condensation. Notice that if we ignore the loop correction, we obtain simply $\mu=(\lambda/6)\varphi^2$ in agreement with what we found earlier in (6.221) using the simpler approach.

In order to proceed further, we need to know something about Δ^{11}_{jn}. Because $\Delta^{ij}=G^{ij}+\cdots$, we will look first at G^{ij} then adopt a simple form for Δ^{ij} based on our result. We have

$$S_{,ij}G^{jk}=-\delta^k_i. \tag{8.382}$$

The Green functions can be expanded the same way as Δ^{ij} in (8.370) in terms of expansion coefficients G^{ik}_{jn}. When uncondensed, $\delta^k_i\to\delta^k_i\delta(x,x')$ using (8.237) to relate $\delta(t-t')=i\delta(\tau-\tau')$. Because,

$$\tilde{\delta}(x,x')=\sum_{j,n}\frac{1}{\beta}\,e^{i\omega_j(\tau-\tau')}f_n(\mathbf{x})f^*_n(\mathbf{x}'),$$

it can be shown that the expansion coefficients for the Green function satisfying (8.382) are given by the solution to

$$\begin{pmatrix} -\frac{\sigma_n}{2m}+\mu-\frac{\lambda}{2}\varphi^2 & \omega_j \\ -\omega_j & -\frac{\sigma_n}{2m}+\mu-\frac{\lambda}{6}\varphi^2 \end{pmatrix} \begin{pmatrix} G^{11}_{jn} & G^{12}_{jn} \\ G^{21}_{jn} & G^{22}_{jn} \end{pmatrix} = -\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{8.383}$$

The matrix occurring on the left-hand side is easily inverted to give

$$\begin{pmatrix} G^{11}_{jn} & G^{12}_{jn} \\ G^{21}_{jn} & G^{22}_{jn} \end{pmatrix} = \frac{1}{\omega_j^2+E_n^2} \begin{pmatrix} \frac{\sigma_n}{2m}-\mu+\frac{\lambda}{2}\varphi^2 & \omega_j \\ -\omega_j & \frac{\sigma_n}{2m}-\mu+\frac{\lambda}{6}\varphi^2 \end{pmatrix} \tag{8.384}$$

where

$$E_n = \left(\frac{\sigma_n}{2m}-\mu+\frac{\lambda}{2}\varphi^2\right)^{1/2}\left(\frac{\sigma_n}{2m}-\mu+\frac{\lambda}{6}\varphi^2\right)^{1/2} \tag{8.385}$$

may be recognized as the excitation energy from the simpler approach (see (6.208)).

At this stage we can adopt an ansatz for Δ^{ij}. Because $\Delta^{ij} = G^{ij} + \cdots$, we will define

$$\begin{pmatrix} \Delta^{11}_{jn} & \Delta^{12}_{jn} \\ \Delta^{21}_{jn} & \Delta^{22}_{jn} \end{pmatrix} = \frac{1}{(\omega_j^2+\bar{E}_n^2)} \begin{pmatrix} \frac{\sigma_n}{2m}-\bar{\mu}+\frac{\lambda}{2}\varphi^2 & \omega_j \\ -\omega_j & \frac{\sigma_n}{2m}-\bar{\mu}+\frac{\lambda}{6}\varphi^2 \end{pmatrix} \tag{8.386}$$

where $\bar{E}_n$ is given as in (8.385) but with $\bar{\mu}$ in place of μ. $\bar{\mu}$ is to be determined by the equation (8.312). For later use, we note that

$$\det\Delta^{ik}_{jn} = (\omega_j^2+\bar{E}_n^2)^{-1}. \tag{8.387}$$

We hold φ fixed when varying Γ with respect to Δ^{ij} in (8.312). From (8.368) we compute

$$\delta\Gamma|_\varphi = -\frac{i\hbar}{2}S_{,ij}\delta\Delta^{ij} - \frac{i\hbar}{2}(\Delta^{-1})_{ij}\delta\Delta^{ij} - \frac{\hbar^2}{4}S_{,ijkl}\,\delta\Delta^{ij}\Delta^{kl} + \cdots .$$

This allows us to see that (8.312) results in

$$(\Delta^{-1})_{ij} = -S_{,ij} + \frac{i\hbar}{2}S_{,ijkl}\Delta^{kl} \tag{8.388}$$

within our approximation scheme. We will evaluate the second term on the right-hand side of (8.388) first using (8.351)–(8.353). It is straightforward to show that

$$\begin{aligned} S_{,11'kl}\Delta^{kl} &= S_{,11'1''1'''}\Delta^{1''1'''} + S_{,11'2''2'''}\Delta^{2''2'''} \\ &= -\lambda\delta(x,x')\left[\Delta^{11}(x,x) + \frac{1}{3}\Delta^{22}(x,x)\right], \qquad (8.389) \\ S_{,12'kl}\Delta^{kl} &= S_{,12'1''2'''}\Delta^{1''2'''} + S_{,12'2''1'''}\Delta^{2''1'''} \\ &= -\frac{\lambda}{3}\delta(x,x')\left[\Delta^{12}(x,x) + \Delta^{21}(x,x)\right] \\ &= 0, \qquad (8.390) \end{aligned}$$

$$S_{,21'kl}\Delta^{kl} = 0, \qquad (8.391)$$

$$\begin{aligned} S_{,22'kl}\Delta^{kl} &= S_{,22'1''1'''}\Delta^{1''1'''} + S_{,22'2''2'''}\Delta^{2''2'''} \\ &= -\lambda\delta(x,x')\left[\frac{1}{3}\Delta^{11}(x,x) + \Delta^{22}(x,x)\right], \qquad (8.392) \end{aligned}$$

where we have noted that $\Delta^{12}_{jn} = -\Delta^{21}_{jn}$ from (8.386) resulting in the zeros in (8.390) and (8.391). With (8.355)–(8.358) we find that (8.388) requires

$$\begin{aligned} (\Delta^{-1})_{11}(x,x') &= \left\{-\left(\frac{1}{2m}\nabla^2 + \mu - \frac{\lambda}{2}\varphi^2\right)\right. \\ &\quad \left. -\frac{i\hbar\lambda}{2}\left[\Delta^{11}(x,x) + \frac{1}{3}\Delta^{22}(x,x)\right]\right\}\delta(x,x'), \qquad (8.393) \\ (\Delta^{-1})_{12}(x,x') &= \frac{\partial}{\partial t}\,\delta(x,x'), \qquad (8.394) \\ (\Delta^{-1})_{21}(x,x') &= -\frac{\partial}{\partial t}\,\delta(x,x'), \qquad (8.395) \\ (\Delta^{-1})_{22}(x,x') &= \left\{-\left(\frac{1}{2m}\nabla^2 + \mu - \frac{\lambda}{6}\varphi^2\right)\right. \\ &\quad \left. -\frac{i\hbar\lambda}{2}\left[\frac{1}{3}\Delta^{11}(x,x) + \Delta^{22}(x,x)\right]\right\}\delta(x,x'). \qquad (8.396) \end{aligned}$$

Because our ansatz for Δ^{ij} is simply G^{ij} with μ replaced by $\bar{\mu}$, it follows that $(\Delta^{-1})_{ij}$ is simply $-S_{,ij}$ with this same replacement.[30] The off-diagonal equations (8.394, 8.395) are identically satisfied. The first equation (8.393) gives us

$$\bar{\mu} = \mu + \frac{i\hbar\lambda}{2}\left[\Delta^{11}(x,x) + \frac{1}{3}\Delta^{22}(x,x)\right], \qquad (8.397)$$

[30] This can be verified by inverting (8.386) if required.

while the last equation (8.396) results in

$$\bar{\mu} = \mu + \frac{i\hbar\lambda}{2}\left[\frac{1}{3}\Delta^{11}(x,x) + \Delta^{22}(x,x)\right]. \tag{8.398}$$

As it stands, these two results for $\bar{\mu}$ are not consistent. However we are only interested in the leading order term in λ. Making use of (8.370) we find

$$\Delta^{11}(x,x) + \frac{1}{3}\Delta^{22}(x,x) = \frac{i}{\beta}\sum_{j,n} |f_n(\mathbf{x})|^2 \left(\Delta^{11}_{jn} + \frac{1}{3}\Delta^{22}_{jn}\right), \tag{8.399}$$

and

$$\frac{1}{3}\Delta^{11}(x,x) + \Delta^{22}(x,x) = \frac{i}{\beta}\sum_{j,n} |f_n(\mathbf{x})|^2 \left(\frac{1}{3}\Delta^{11}_{jn} + \Delta^{22}_{jn}\right). \tag{8.400}$$

Using the ansatz (8.386) shows that

$$\Delta^{11}_{jn} + \frac{1}{3}\Delta^{22}_{jn} = \frac{1}{(\omega_j^2 + \bar{E}_n^2)}\left[\frac{4}{3}\left(\frac{\sigma_n}{2m} - \bar{\mu}\right) + \frac{\lambda}{3}\varphi^2\right], \tag{8.401}$$

$$\frac{1}{3}\Delta^{11}_{jn} + \Delta^{22}_{jn} = \frac{1}{(\omega_j^2 + \bar{E}_n^2)}\left[\frac{4}{3}\left(\frac{\sigma_n}{2m} - \bar{\mu}\right) + \frac{5\lambda}{9}\varphi^2\right]. \tag{8.402}$$

The difference between (8.397) and (8.398) is seen using (8.399)–(8.402) to be of order $\lambda^2\varphi^2$. This is the same order as the two-loop term we dropped in our approximation (8.368). For consistency of our approximation we must also drop it here and therefore (8.397) is now consistent with (8.398) within our approximation. By passing to the large volume limit, $f_n(\mathbf{x}) = V^{-1/2}e^{i\mathbf{k}\cdot\mathbf{x}}$ may be assumed, leading to $|f_n(\mathbf{x})|^2 = 1/V$ in (8.399) and (8.400). Adopting (8.397) we find

$$\bar{\mu} \simeq \mu - \frac{\hbar\lambda}{2\beta V}\sum_{j,n}\left(\Delta^{11}_{jn} + \frac{1}{3}\Delta^{22}_{jn}\right). \tag{8.403}$$

Combining this with (8.381) shows that

$$\bar{\mu} \simeq \frac{\lambda}{6}\varphi^2. \tag{8.404}$$

This is exactly the same result as we found in the classical theory but with the replacement of μ there with $\bar{\mu}$ here. The transition temperature between the normal phase, characterized by $\varphi = 0$, and the condensed phase, characterized by $\varphi \neq 0$, is determined by the condition $\bar{\mu} = 0$

(within our approximations). $\bar{\mu}$ plays the role of an effective chemical potential.

At this stage we can use our results to evaluate the particle number and energy density, or other thermodynamic quantities. The particle number is

$$N = -\left(\frac{\partial\Omega}{\partial\mu}\right)\Big|_{T,V,\varphi,\Delta}, \tag{8.405}$$

and the internal energy is

$$U = -\left[\frac{\partial(\beta\Omega)}{\partial\beta}\right]\Big|_{\beta\mu,V,\varphi,\Delta}, \tag{8.406}$$

where $\Gamma = i\beta\Omega$ (see Section 5.1).

Because there is no μ-dependence in $S_{,i_1\cdots i_n}$ for $n \geq 3$, there is no explicit μ-dependence in the higher-loop terms. From (8.368) and (8.369) we find

$$N \simeq \frac{1}{2}V\varphi^2 + \frac{\hbar}{2\beta}\sum_{j,n}(\Delta^{11}_{jn} + \Delta^{22}_{jn}), \tag{8.407}$$

$$U \simeq \frac{\lambda}{24}V\varphi^4 - \frac{\hbar}{2}\left[\frac{\partial}{\partial\beta}(S_{,ij}\Delta^{ij})\right]\Big|_{\beta\mu,V,\varphi,\Delta}. \tag{8.408}$$

With $\beta\mu$ fixed, we regard μ as a function of β. We have

$$d(\beta\mu) = 0 = d\beta\,\mu + \beta\,d\mu,$$

from which

$$\left(\frac{\partial\mu}{\partial\beta}\right)\Big|_{\beta\mu} = -\frac{\mu}{\beta}.$$

The β-dependence in (8.379) occurs through μ as well as through $\omega_j = 2\pi j/\beta$. (Remember that Δ^{ik}_{jn} and φ are fixed.) It is obvious that

$$\frac{\partial\omega_j}{\partial\beta} = -\frac{\omega_j}{\beta},$$

so we find

$$U \simeq \frac{\lambda}{24}V\varphi^4 + \frac{\hbar\mu}{2\beta}\sum_{j,n}(\Delta^{11}_{jn} + \Delta^{22}_{jn}) - \frac{\hbar}{2\beta}\sum_{j,n}\omega_j(\Delta^{12}_{jn} - \Delta^{21}_{jn}).$$

By eliminating the middle term using (8.407) we obtain the energy density

$$\rho = \frac{U}{V} \simeq \frac{\lambda}{24}\varphi^4 - \frac{1}{2}\mu\varphi^2 + \frac{\mu N}{V} - \frac{\hbar}{2\beta V}\sum_{j,n}\omega_j(\Delta^{12}_{jn} - \Delta^{21}_{jn}). \tag{8.409}$$

We can now use our ansatz for Δ^{ik}_{jn} in (8.386) to evaluate the relevant expressions (8.407) and (8.409). First of all we have

$$\begin{aligned}\sum_{j,n}(\Delta^{11}_{jn}+\Delta^{22}_{jn}) &= \sum_{j,n}\frac{1}{\left(\omega_j^2+\bar{E}_n^2\right)}\left[2\left(\frac{\sigma_n}{2m}-\bar{\mu}\right)+\frac{2}{3}\lambda\varphi^2\right],\\ &= \sum_{j,n}\frac{2}{\left(\omega_j^2+\bar{E}_n^2\right)}\left[\frac{\sigma_n}{2m}+\frac{\lambda}{6}\varphi^2\right], \end{aligned} \tag{8.410}$$

if we eliminate $\bar{\mu}$ using (8.404). Using (8.385) with μ replaced by $\bar{\mu}$ to give $\bar{E}_n$, and the eliminating $\bar{\mu}$ with (8.404), we find

$$\begin{aligned}\bar{E}_n^2 &= \left(\frac{\sigma_n}{2m}-\bar{\mu}+\frac{\lambda}{2}\varphi^2\right)\left(\frac{\sigma_n}{2m}-\bar{\mu}+\frac{\lambda}{6}\varphi^2\right)\\ &= \frac{\sigma_n}{2m}\left(\frac{\sigma_n}{2m}+\frac{\lambda}{3}\varphi^2\right). \end{aligned} \tag{8.411}$$

The particle number density $n = N/V$ follows from (8.407) as

$$n \simeq \frac{1}{2}\varphi^2 + \hbar I\left(\frac{1}{6}\right), \tag{8.412}$$

where we define

$$I(\kappa) = \frac{1}{\beta V}\sum_{j,n}\left(\omega_j^2+\bar{E}_n^2\right)^{-1}\left(\frac{\sigma_n}{2m}+\kappa\lambda\varphi^2\right) \tag{8.413}$$

for constant κ. In the large volume limit, $\sigma_n \to k^2$ and $\sum_n \to V\int d^Dk/(2\pi)^D$ with D the spatial dimension. We can conveniently use D as a regulating parameter by adopting dimensional regularization with $D \to 3$ taken at the end.

To evaluate $I(\kappa)$ we first perform the sum over j. The result has been quoted previously in (8.252), and using the result given there we find

$$I(\kappa) = I_1(\kappa) + I_2(\kappa) \tag{8.414}$$

where

$$I_1(\kappa) = \frac{1}{2}\int\frac{d^Dk}{(2\pi)^D}\bar{E}_n^{-1}\left(\frac{k^2}{2m}+\kappa\lambda\varphi^2\right), \tag{8.415}$$

$$I_2(\kappa) = \int\frac{d^Dk}{(2\pi)^D}\,\frac{\left[k^2/(2m)+\kappa\lambda\varphi^2\right]}{\bar{E}_n\left(e^{\beta\bar{E}_n}-1\right)}. \tag{8.416}$$

($\bar{E}_n$ is given by (8.411) with $\sigma_n \to k^2$.) Clearly, $I_2(\kappa)$ contains the finite temperature contribution. $I_1(\kappa)$ may be evaluated exactly just as we evaluated the energy ζ-function in Section 6.7.2. The result for $I_1(\kappa)$ is, after analytic continuation to $D = 3$,

$$I_1(\kappa) = \frac{1}{6\pi^2}\left(1 - \frac{9}{2}\kappa\right)\left(\frac{2\lambda}{3}m\varphi^2\right)^{3/2}. \tag{8.417}$$

For $I_2(\kappa)$, the analysis is similar to the evaluation of $\rho^{(1)}_{T\neq 0}$ in Section 6.7.2. After rescaling $k \to (2m/\beta)^{1/2}k$, it is found that

$$\begin{aligned} I_2(\kappa) =& \frac{2\,(2mT)^{D/2}}{(4\pi)^{D/2}\Gamma(D/2)}\int_0^\infty dk \frac{k^{D-2}(k^2 + \kappa\beta\lambda\varphi^2)}{[k^2 + (1/3)\beta\lambda\varphi^2]} \\ & \left\{e^{k[k^2+(1/3)\beta\lambda\varphi^2]^{1/2}} - 1\right\}^{-1}. \end{aligned} \tag{8.418}$$

The remaining integral depends on the dimensionless ratio $\beta\lambda\varphi^2$. For low temperatures, $\beta\lambda\varphi^2 >> 1$. Following the same analysis as in Section 6.7.2, it can be shown that (with $D \to 3$ taken)

$$\begin{aligned} I_2(\kappa) \simeq & \frac{\kappa}{4}(2m)^{3/2}\left(\frac{\lambda}{3}\varphi^2\right)^{-1/2} T^2 \\ & + \frac{\pi^2}{30}(2m)^{3/2}\left(1 - \frac{15}{2}\kappa\right) T^4 \left(\frac{\lambda}{3}\varphi^2\right)^{-5/2} + \cdots. \end{aligned} \tag{8.419}$$

For $\beta\lambda\varphi^2 \ll 1$ we can expand the integrand of (8.418) in powers of $\beta\lambda\varphi^2$ to find (with $D \to 3$ taken)

$$I_2(\kappa) \simeq \left(\frac{m}{2\pi\beta}\right)^{3/2}\left[\zeta_R\left(\frac{3}{2}\right) + \left(2\kappa - \frac{1}{2}\right)\zeta_R\left(\frac{1}{2}\right)\beta\lambda\varphi^2 + \cdots\right]. \tag{8.420}$$

Because the first-order correction to the classical result $n \simeq (1/2)\varphi^2$ in (8.412) is of order $\hbar$, we may substitute $\varphi^2 \simeq 2n$ in the results for $I(1/6)$ (because it is already multiplied by $\hbar$). At low temperature, using (8.419) we find

$$\varphi^2 \simeq 2n - \frac{2\hbar}{3\pi^2}\left(\frac{\lambda}{3}mn\right)^{3/2} - \frac{\hbar T^2}{12}(2m)^{3/2}\left(\frac{2\lambda}{3}n\right)^{-1/2} + \cdots. \tag{8.421}$$

This gives us the behaviour of φ as a function of T for fixed n.

To evaluate the energy density, we use (8.386) along with (8.411) for $\bar{E}_n$ to find

$$\sum_{j,n}\omega_j\left(\Delta^{12}_{jn} - \Delta^{21}_{jn}\right) = 2\sum_{j,n}\omega_j^2\left(\omega_j^2 + \bar{E}_n^2\right)^{-1}. \tag{8.422}$$

This must be regarded as a formal expression in need of regularization, since the sum over j is divergent. To deal with the regularization we will consider

$$\tilde{\zeta}(s) = \sum_{j,n} \omega_j^2 \left(\omega_j^2 + \bar{E}_n^2\right)^{-s} \tag{8.423}$$

with the right-hand side of (8.422) defined as $2\tilde{\zeta}(1)$ by analytic continuation. Making use of the summation formula given in Section A1.3 (see (A1.58) there), it can be seen that

$$\begin{aligned}\tilde{\zeta}(s) = &\frac{\beta\Gamma(s-3/2)}{4\pi^{1/2}\Gamma(s)}\,\bar{E}(2s-2)\\ &+2\left(\frac{2\pi}{\beta}\right)^{2-2s}\sum_n \int_{-\infty+i\epsilon}^{\infty+i\epsilon} dz\left(e^{-2\pi i z}-1\right)^{-1} z^2\left(z^2+\frac{\beta^2\bar{E}_n^2}{4\pi^2}\right)^{-s},\end{aligned}$$

with $\bar{E}(2s-2)$ the energy ζ-function defined in (6.229) and found in (6.232). By taking $s=1$ in this expression it follows that

$$\tilde{\zeta}(1) = -\frac{1}{2}\beta\bar{E}(0) - \beta\sum_n \bar{E}_n(e^{\beta\bar{E}_n}-1)^{-1}.$$

Using (8.409) the energy density becomes

$$\rho \simeq \frac{\lambda}{24}\varphi^4 - \frac{1}{2}\mu\varphi^2 + \mu n + \frac{\hbar}{2V}\bar{E}(0) + \frac{\hbar}{V}\sum_n \bar{E}_n(e^{\beta\bar{E}_n}-1)^{-1}.$$

The last term is the same as $\rho^{(1)}_{T\neq 0}$ found in (6.235) and the second last term was evaluated in (6.233). If we work to order $\hbar$, then from (8.403) and (8.404) we have $\mu \simeq \lambda\varphi^2/6 + \cdots \simeq \lambda n/3 + \cdots$. Thus $\mu(n-\varphi^2/2) \simeq (\lambda/3)n\hbar I(1/6)$ from (8.412). Finally, we find

$$\begin{aligned}\frac{\lambda}{24}\varphi^4 - \frac{1}{2}\mu\varphi^2 + \mu n &\simeq \frac{\lambda}{24}\left[2n - 2\hbar I\left(\frac{1}{6}\right)\right]^2 + \frac{\lambda}{3}n\hbar I\left(\frac{1}{6}\right)\\ &\simeq \frac{\lambda}{6}n^2 + \cdots\end{aligned}$$

to order $\hbar$. This gives (using (6.233))

$$\rho \simeq \frac{\lambda}{6}n^2 + \frac{\hbar}{30\pi^2}(2m)^{3/2}\left(\frac{2\lambda}{3}n\right)^{5/2} + \rho^{(1)}_{T\neq 0}.$$

The result is in complete agreement with the simpler approach of Section 6.7.2.

In this section we have seen how the generalized CJT effective action can be used to study the interacting Bose gas and to recover the results found using the simpler approach of Section 6.7.[31] The main advantage of using the effective action approach is that it is a completely general treatment that can be generalized to arbitrary orders in perturbation theory (at least in principle).

Notes

This chapter was strongly influenced by the work of DeWitt (1965) and the discussion in Jackiw (1974). A generalization of the renormalization of $\lambda\phi^4$ theory to curved spacetime can be found in Parker and Toms (2008). The review of Abers and Lee (1973) and the papers of 't Hooft (1971) and Collins (1974) were also very influential.

[31] It is possible to perform an analysis of the pressure as in Section 6.7.3 as well; however, we will omit this somewhat lengthy calculation here.

Appendix 1
Mathematical appendices

A1.1 Gamma function

Here we summarize some of the properties of the Γ-function which are needed. If $\mathcal{R}(z) > 0$ we define $\Gamma(z)$ by[1]

$$\Gamma(z) = \int_0^\infty dt\, t^{z-1} e^{-t}. \tag{A1.1}$$

An integration by parts in (A1.1) shows that $\Gamma(z)$ satisfies the recursion relation

$$\Gamma(z+1) = z\Gamma(z). \tag{A1.2}$$

By putting $z = 1$ in (A1.1) it is seen that

$$\Gamma(1) = 1. \tag{A1.3}$$

The results in (A1.2) and (A1.3) are sufficient to establish that $\Gamma(1+z) = z!$ if z is a non-negative integer.

As we try to let z become close to 0 the integral representation (A1.1) diverges; however we can define the analytic continuation of $\Gamma(z)$ from the region of the complex plane where $\mathcal{R}(z) > 0$ to $\mathcal{R}(z) < 0$ using the recursion relation (A1.2). By taking z close to 0 in (A1.2) and using (A1.3) it can be seen that

$$\Gamma(z) = \frac{1}{z} + \cdots. \tag{A1.4}$$

Thus $\Gamma(z)$ has a simple pole with residue 1 at $z = 0$. It is now easy to see by repeated application of (A1.2) that $\Gamma(z)$ is analytic everywhere

[1] $\mathcal{R}(z)$ denotes the real part of z.

except at $z = -n$ for $n = 0, 1, 2, \ldots$ where a simple pole occurs. Define the Laurent expansion of $\Gamma(z)$ about $z = -n$ by

$$\Gamma(z) = \frac{a_{-1}(n)}{z+n} + a_0(n) + \cdots. \tag{A1.5}$$

The recursion relation (A1.2) may be used to show that the coefficients defined in (A1.5) satisfy

$$a_{-1}(n) = -\frac{1}{n} a_{-1}(n-1), \tag{A1.6}$$

$$a_0(n) = -\frac{1}{n} a_0(n-1) - \frac{1}{n^2} a_{-1}(n-1). \tag{A1.7}$$

Given that $a_0(1) = 1$ from (A1.4), it follows that (A1.6) results in

$$a_{-1}(n) = \frac{(-1)^n}{n!}. \tag{A1.8}$$

The relation (A1.7) is most easily solved if we define

$$a_0(n) = \frac{(-1)^n}{n!} b_0(n). \tag{A1.9}$$

Substitution of this definition into (A1.7) shows that

$$b_0(n) = b_0(n-1) + \frac{1}{n}. \tag{A1.10}$$

This is easily solved with the result

$$b_0(n) = b_0(0) + \sum_{k=1}^{n} \frac{1}{k}. \tag{A1.11}$$

We therefore have

$$a_0(n) = \frac{(-1)^n}{n!} \left\{ a_0(0) + \sum_{k=1}^{n} \frac{1}{k} \right\}. \tag{A1.12}$$

To complete this result we need to know $a_0(0)$. Using (A1.2) and (A1.5) with $n = 0$ we have

$$\Gamma(1+z) = 1 + z a_0(0) + \ldots, \tag{A1.13}$$

for z in a neighbourhood of $z = 0$. It then follows that

$$a_0(0) = \Gamma'(1) \tag{A1.14}$$

$$= \int_0^\infty dt\, e^{-t} \ln t \tag{A1.15}$$

if we use (A1.1) to evaluate $\Gamma'(1)$. The integral in (A1.15) is a mathematical constant which can be identified as the negative of the Euler constant γ. We therefore have

$$a_0(0) = -\gamma, \tag{A1.16}$$

and the evaluation of $a_0(n)$ is complete.[2]

The Γ-function may be evaluated in a simple way at other special values of z. Putting $z = 1/2$ in (A1.1) leads to[3]

$$\begin{aligned}\Gamma\left(\frac{1}{2}\right) &= \int_0^\infty dt\, t^{-1/2} e^{-t} \\ &= 2\int_0^\infty e^{-t} dt^{1/2} \\ &= \sqrt{\pi}.\end{aligned} \tag{A1.17}$$

The recursion relation (A1.2) then shows that

$$\begin{aligned}\Gamma\left(n+\frac{1}{2}\right) &= \left(n-\frac{1}{2}\right)\left(n-\frac{3}{2}\right)\cdots\left(\frac{3}{2}\right)\left(\frac{1}{2}\right)\Gamma\left(\frac{1}{2}\right) \\ &= \frac{1\cdot 3\cdot 5\cdot \ldots \cdot (2n-1)}{2^n}\sqrt{\pi}\end{aligned} \tag{A1.18}$$

for $n = 1, 2, \ldots$.

Other useful results require more work using either the Hankel contour integral representation for $\Gamma(z)$ or the expression as the Weierstrass infinite product.[4] One useful result is the reflection formula

$$\Gamma(z)\Gamma(1-z) = \frac{\pi}{\sin \pi z}. \tag{A1.19}$$

By putting $z = (1/2) + n$ in (A1.19) and using (A1.18) it follows that

$$\Gamma\left(\frac{1}{2} - n\right) = \frac{(-2)^n \sqrt{\pi}}{1\cdot 3\cdot 5\cdot \ldots \cdot (2n-1)}, \tag{A1.20}$$

for $n = 1, 2, \ldots$. Another useful result is the duplication formula

$$\Gamma(2z) = (4\pi)^{-1/2} 2^{2z} \Gamma(z)\Gamma\left(z+\frac{1}{2}\right). \tag{A1.21}$$

[2] Numerically, it is found that $\gamma \simeq 0.5772156649$.

[3] We have used the result $\int_0^\infty du\, e^{-u^2} = (1/2)\sqrt{\pi}$ here.

[4] See Whittaker and Watson (1928) for example.

It is useful to define the logarithmic derivative of the Γ-function by

$$\psi(z) = \frac{d}{dz} \ln \Gamma(z) = \frac{\Gamma'(z)}{\Gamma(z)}. \tag{A1.22}$$

From (A1.14) and (A1.16) we see that

$$\psi(1) = -\gamma. \tag{A1.23}$$

For any positive integer n if we use the recursion relation (A1.2) it can be seen that

$$\begin{aligned} \psi(z+n) &= \frac{d}{dz} \ln \Gamma(z+n) \\ &= \frac{d}{dz} \ln \left[(z+n-1)(z+n-2)\cdots z\Gamma(z)\right] \\ &= \psi(z) + \frac{d}{dz} \sum_{k=0}^{n-1} \ln(z+k) \\ &= \psi(z) + \sum_{k=1}^{n} \frac{1}{z+k-1}. \end{aligned} \tag{A1.24}$$

Thus

$$\psi(1+n) = -\gamma + \sum_{k=1}^{n} \frac{1}{k}. \tag{A1.25}$$

Finally we quote

$$\psi\left(\frac{1}{2}\right) = -\gamma - \ln 4. \tag{A1.26}$$

A1.2 Riemann and Hurwitz zeta functions

We will summarize some of the properties of the Riemann and Hurwitz ζ-functions here. The basic reference is Whittaker and Watson (1928).

For $\mathcal{R}(z) > 1$ and $\mathcal{R}(a) > 0$ the Hurwitz ζ-function is defined by

$$\zeta(z, a) = \sum_{n=0}^{\infty} (n+a)^{-z}. \tag{A1.27}$$

The Riemann ζ-function is the special case

$$\zeta(z) = \zeta(z, 1). \tag{A1.28}$$

An integral representation for $\zeta(z,a)$ may be obtained by making use of the definition (A1.1) for the Γ-function. We may write (A1.27) as

$$\begin{aligned}\zeta(z,a) &= \sum_{n=0}^{\infty} \frac{1}{\Gamma(z)} \int_0^\infty dt\, t^{z-1} e^{-(n+a)t} \\ &= \frac{1}{\Gamma(z)} \int_0^\infty dt\, t^{z-1} e^{-at} (1-e^{-t})^{-1}. \end{aligned} \tag{A1.29}$$

The integrand in (A1.29) is well behaved for large values of t, so that any poles come only from the $t=0$ limit. If we expand $(1-e^{-t})^{-1}$ in powers of t we find

$$(1-e^{-t})^{-1} = \frac{1}{t} + \frac{1}{2} + \frac{t}{12} + \ldots. \tag{A1.30}$$

We can write (A1.29) as

$$\begin{aligned}\zeta(z,a) &= \frac{1}{\Gamma(z)} \int_0^\infty dt\, t^{z-1} e^{-at} \left[(1-e^{-t})^{-1} - \frac{1}{t} \right] + \frac{1}{\Gamma(z)} \int_0^\infty dt\, t^{z-2} e^{-at} \\ &= \frac{a^{1-z}}{z-1} + \frac{1}{\Gamma(z)} \int_0^\infty dt\, t^{z-1} e^{-at} \left[(1-e^{-t})^{-1} - \frac{1}{t} \right]. \end{aligned} \tag{A1.31}$$

The integral in (A1.31) now converges for $z=1$ and we see that $\zeta(z,a)$ has a simple pole at $z=1$ with residue 1. It is possible to relate the remaining terms in (A1.31) to $\psi(a)$ with the result

$$\zeta(z,a) = \frac{1}{z-1} - \psi(a) + \cdots. \tag{A1.32}$$

For special values of z it is possible to evaluate $\zeta(z,a)$ in terms of simple functions. We have

$$\zeta(-n,a) = -\frac{B_{n+1}(a)}{n+1} \tag{A1.33}$$

where $B_{n+1}(a)$ is a Bernoulli polynomial. Here $n = 0, 1, 2, \ldots$. A list of Bernoulli polynomials appears in Abramowitz and Stegun (1965). We list the first few results for the convenience of the reader.

$$\zeta(0,a) = \frac{1}{2} - a, \tag{A1.34}$$

$$\zeta(-1,a) = -\frac{1}{12} + \frac{1}{2}a - \frac{1}{2}a^2, \tag{A1.35}$$

$$\zeta(-2,a) = -\frac{1}{6}a + \frac{1}{2}a^2 - \frac{1}{3}a^3, \tag{A1.36}$$

$$\zeta(-3,a) = \frac{1}{120} - \frac{1}{4}a^2 + \frac{1}{2}a^3 - \frac{1}{4}a^4. \tag{A1.37}$$

By taking $a = 1$ in (A1.33) we obtain

$$\zeta(-2n) = 0 \quad \text{for } n = 1, 2, \ldots, \tag{A1.38}$$

$$\zeta(0) = -\frac{1}{2}, \tag{A1.39}$$

$$\zeta(1-2n) = (-1)^n \frac{B_{2n}}{2n} \quad \text{for } n = 1, 2, \ldots. \tag{A1.40}$$

Here B_n are the Bernoulli numbers defined in terms of the Bernoulli polynomials by

$$B_n = B_n(a = 1). \tag{A1.41}$$

The first few non-zero Bernoulli numbers are given by[5]

$$B_0 = 1, \quad B_1 = -\frac{1}{2}, \quad B_2 = \frac{1}{6}, \quad B_4 = -\frac{1}{30}, \quad B_6 = \frac{1}{42}.$$

All of $B_{2n+1} = 0$ for $n = 1, 2, 3, \ldots$, which is easily verified from the definition of the generating function for Bernoulli polynomials:

$$e^{at}(e^t - 1)^{-1} = \sum_{n=0}^{\infty} \frac{t^{n-1}}{n!} B_n(a). \tag{A1.42}$$

It can be shown (Whittaker and Watson, 1928) that the Riemann ζ-function satisfies the reflection formula

$$\zeta(1-z) = 2(2\pi)^{-z}\Gamma(z)\cos\left(\frac{\pi}{2}z\right)\zeta(z). \tag{A1.43}$$

From this it is possible to deduce (A1.39) as well as

$$\zeta'(0) = -\frac{1}{2}\ln(2\pi). \tag{A1.44}$$

The derivative of $\zeta(z)$ at negative integral values of z can be obtained in a similar manner.

If we set $a = m$ where m is an integer, it is clear from (A1.27) that

$$\zeta(z, m) = \zeta(z) - \sum_{n=1}^{m-1} n^{-z}. \tag{A1.45}$$

[5] Again an extensive list of the Bernoulli numbers, which are related to the coefficients of the Bernoulli polynomials, is found in Abramowitz and Stegun (1965).

Another case where $\zeta(z,a)$ can be evaluated in terms of the Riemann ζ-function occurs if $a = 1/2$. In this case we have

$$\begin{aligned}\zeta\left(z,\frac{1}{2}\right) &= 2^z \sum_{n=0}^{\infty}(2n+1)^{-z} \\ &= 2^z\left[\sum_{n=1}^{\infty} n^{-z} - \sum_{n=1}^{\infty}(2n)^{-z}\right] \\ &= (2^z-1)\zeta(z). \end{aligned} \tag{A1.46}$$

We also require the asymptotic expansion of $\zeta(z,a)$ for both large and small values of a. For small a we may simply use the binomial expansion in (A1.27) to obtain

$$\begin{aligned}\zeta(z,a) &= a^{-z} + \sum_{n=1}^{\infty} n^{-z}\left(1+\frac{a}{n}\right)^{-z} \\ &\simeq a^{-z} + \sum_{n=1}^{\infty} n^{-z}\left[1 - z\frac{a}{n} + \frac{z(z+1)}{2}\frac{a^2}{n^2}\right. \\ &\quad - \frac{z(z+1)(z+2)}{3!}\frac{a^3}{n^3} \\ &\quad \left. + \frac{z(z+1)(z+2)(z+3)}{4!}\frac{a^4}{n^4} + \cdots\right]\end{aligned}$$

The sums over n may be done in terms of the simpler Riemann ζ-function and we find

$$\begin{aligned}\zeta(z,a) \simeq a^{-z} &+ \zeta(z) - az\zeta(1+z) + \frac{a^2}{2}z(z+1)\zeta(2+z) \\ &- \frac{a^3}{6}z(z+1)(z+2)\zeta(3+z) + \ldots. \end{aligned} \tag{A1.47}$$

It can be verified that (A1.47) reproduces (A1.33) if we take $z = -n$ since the infinite expansion in (A1.47) terminates in this case.

For large values of a we can use (A1.29). Because of the presence of e^{-at} in the integrand, the dominant contribution to the integral should come from near $t = 0$. Using (A1.41) and (A1.42) we have

$$(1-e^{-t})^{-1} = \sum_{n=0}^{\infty}(-1)^n\frac{B_n}{n!}t^{n-1}, \tag{A1.48}$$

and we find

$$\zeta(z,a) \simeq \sum_{n=0}^{\infty}(-1)^n\frac{B_n}{n!}\frac{\Gamma(z+n-1)}{\Gamma(z)}a^{1-n-z}$$

$$\simeq \frac{a^{1-z}}{z-1} + \frac{1}{2}a^{-z} + \frac{z}{12}a^{-1-z} + \frac{1}{720}z(z+1)(z+2)a^{-3-z} + \cdots . \tag{A1.49}$$

Once again if we take z to be a negative integer the infinite expansion in (A1.49) terminates and we reproduce the result in (A1.33) which is exact.

We also have occasion to expand $\zeta(z, a)$ about certain values of a. This can be done easily if it is noted that

$$\frac{\partial}{\partial a}\zeta(z, a) = -z\zeta(z+1, a). \tag{A1.50}$$

This result follows from differentiating (A1.27) for $\mathcal{R}(z) > 1$ and extending the result to $\mathcal{R}(z) < 1$ by analytic continuation.

One final result we need is the contour integral representation of the Hurwitz ζ-function. This is described in Whittaker and Watson (1928). Here we will choose a different branch cut to make contact with the result needed in Section 6.10.

If we consider the integrand as a function of a complex variable t, then the integrand of (A1.29) is analytic except at $t = 0$ which is a branch point. We will take the branch cut along the negative real axis as shown in Fig. A1.1. Above the branch cut we have $t = e^{i\pi}\tau$ where $\tau \in [\infty, 0]$, and below the branch cut we have $t = e^{-i\pi}\tau$ where $\tau \in [0, \infty]$. (The phases are determined by restricting $|\arg t| \leq \pi$, and considering the direction of rotation with respect to the positive real axis.) By shrinking the portion of the contour around the origin to zero, we have[6]

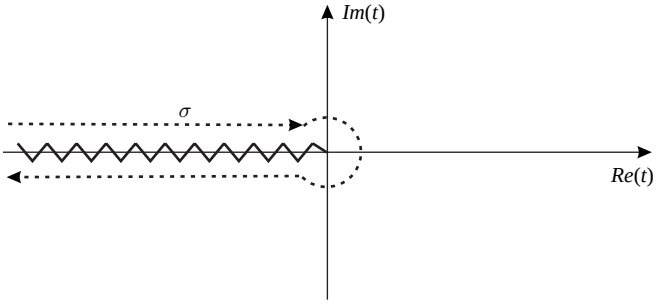

Fig. A1.1 This shows the contour σ used in the evaluation of the Hurwitz ζ-function. The branch cut is taken along the negative real axis as shown by the jagged line.

[6] The first term is the contribution of that portion of σ above the negative real axis, and the second term comes from the portion of σ below the negative real axis.

$$\int_\sigma \frac{t^{z-1}e^{-at}}{(1-e^{-t})}\,dt = \int_\infty^0 \frac{e^{i\pi z}\tau^{z-1}e^{a\tau}}{(1-e^{\tau})}\,d\tau + \int_0^\infty \frac{e^{-i\pi z}\tau^{z-1}e^{a\tau}}{(1-e^{\tau})}\,d\tau. \quad \text{(A1.51)}$$

It follows very simply from this result that[7]

$$\zeta(z,a) = \frac{1}{2i\sin\pi z\,\Gamma(z)} \int_\sigma \frac{t^{z-1}e^{(a-1)t}}{(1-e^{-t})}\,dt.$$

By making use of the Γ-function identity (A1.19) we can see that

$$\zeta(z,a) = \frac{\Gamma(1-z)}{2\pi i} \int_\sigma \frac{t^{z-1}e^{at}}{(e^t-1)}\,dt. \quad \text{(A1.52)}$$

This is completely equivalent to the expression given by Whittaker and Watson (1928), with the difference explained by our different handling of the branch cut. This contour integral representation for the Hurwitz ζ-function can be used to derive (A1.33).

A1.3 Summation of series

It is often convenient to convert an infinite sum into a contour integral which then allows the result to be extended to the entire complex plane by analytic continuation of some parameters entering the sum. There are many ways to do this (Whittaker and Watson, 1928; Lindelöf, 1905), and we will describe one simple way here.

Let $f(z)$ be a function which is analytic inside and on the contour $\mathcal{C}$ as shown in Fig. A1.2. Here $\epsilon > 0$ is an arbitrary small real number and N is a positive integer. In particular we will assume that $f(z)$ has no singularities on the real axis. We will also require that $f(x+iy) \to 0$ as $|x| \to \infty$ for $-\epsilon \le y \le \epsilon$.

Consider the contour integral $\int_{\mathcal{C}} (\cot \pi z/2i) f(z)\,dz$. The integrand has simple poles at $z = 0, \pm 1, \ldots, \pm N$ arising from $\cot \pi z$. By the residue theorem we have

$$\sum_{n=-N}^{n=N} f(n) = \int_{\mathcal{C}} \frac{\cot \pi z}{2i} f(z)\,dz. \quad \text{(A1.53)}$$

Let $\mathcal{C}_+$ ($\mathcal{C}_-$) denote that part of the contour above (below) the real axis. On $\mathcal{C}_+$ use

$$\cot \pi z = -i - 2i(e^{-2\pi i z} - 1)^{-1}. \quad \text{(A1.54)}$$

[7] Each of the two terms in (A1.51) is related to the Hurwitz ζ-function in (A1.29) by a simple factor.

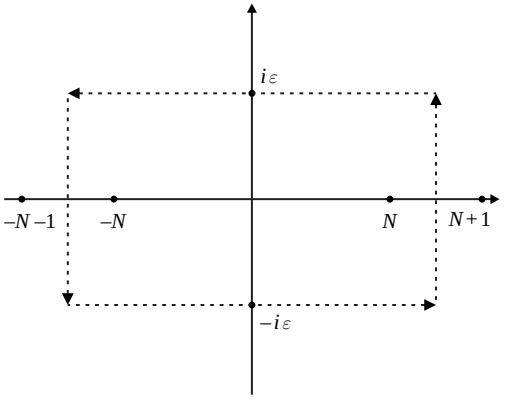

Fig. A1.2 The integration contour in the complex z-plane for the derivation of the summation formula.

On $\mathcal{C}_-$ use

$$\cot \pi z = i + 2i(e^{2\pi iz} - 1)^{-1}. \tag{A1.55}$$

Because $f(z)$ is analytic inside and on $\mathcal{C}$ we have

$$\int_{\mathcal{C}_+} f(z)\,dz = -\int_{\mathcal{C}_-} f(z)\,dz. \tag{A1.56}$$

By splitting the integral over $\mathcal{C}$ in (A1.53) into a sum over $\mathcal{C}_+$ and $\mathcal{C}_-$, and using (A1.54)–(A1.56) it is easy to see that

$$\sum_{n=-N}^{n=N} f(n) = \int_{\mathcal{C}_-} f(z)\,dz + \int_{\mathcal{C}_-} (e^{2\pi iz} - 1)^{-1} f(z)\,dz - \int_{\mathcal{C}_+} (e^{-2\pi iz} - 1)^{-1} f(z)\,dz. \tag{A1.57}$$

Because of our assumption that $f(x+iy) \to 0$ as $|x| \to \infty$ for $-\epsilon \le y \le \epsilon$, as we take the limit $N \to \infty$, the contributions from the vertical parts of the contours $\mathcal{C}_+$ and $\mathcal{C}_-$ in (A1.57) will vanish leaving us with[8]

$$\sum_{n=-\infty}^{n=\infty} f(n) = \int_{-\infty}^{\infty} f(x)\,dx + \int_{-\infty+i\epsilon}^{\infty+i\epsilon} (e^{-2\pi iz} - 1)^{-1} f(z)\,dz + \int_{-\infty-i\epsilon}^{\infty-i\epsilon} (e^{2\pi iz} - 1)^{-1} f(z)\,dz. \tag{A1.58}$$

[8] In the first term the integration contour can be deformed to lie along the real axis since $f(z)$ is analytic.

This is our basic summation formula.

One case of interest to us in Section 4.4 was

$$f(z) = [(z+a)^2 + b^2]^{-\lambda}, \tag{A1.59}$$

with $\mathcal{R}(\lambda) > 1/2$ and a, b real. Let

$$F(\lambda; a, b) = \sum_{n=-\infty}^{\infty} [(n+a)^2 + b^2]^{-\lambda}, \tag{A1.60}$$

where the sum converges if $\mathcal{R}(\lambda) > 1/2$. The function $f(z)$ in (A1.59) has branch points at $z = -a \pm ib$. Take branch cuts parallel to the imaginary axis to satisfy our assumption that $f(z)$ has no singularities on the real axis. The summation formula (A1.58) can be applied to find (for $\mathcal{R}(\lambda) > 1/2$)

$$\begin{aligned} F(\lambda; a, b) = \sqrt{\pi}\frac{\Gamma(\lambda - 1/2)}{\Gamma(\lambda)} b^{1-2\lambda} + \int_{-\infty+i\epsilon}^{\infty+i\epsilon} (e^{-2\pi i z} - 1)^{-1} f(z)\, dz \\ + \int_{-\infty-i\epsilon}^{\infty-i\epsilon} (e^{2\pi i z} - 1)^{-1} f(z)\, dz. \end{aligned} \tag{A1.61}$$

The first term in (A1.58) with $f(x)$ given by (A1.59) may be done in terms of the Γ-function as shown if we use results from Section A1.1. It now remains to manipulate the second and third terms of (A1.61) into a more manageable form. If we call the integration contours in (A1.61) $\mathcal{C}_+$ and $\mathcal{C}_-$ as we did earlier, then the picture in the complex plane is shown in Fig. A1.3.

Because $f(z)$ is analytic everywhere except along the two branch cuts we can deform the contours $\mathcal{C}_+$ and $\mathcal{C}_-$ as shown in Fig. A1.4. For $\mathcal{C}_+$ we can take

$$(z+a)^2 + b^2 = b^2 - y^2,$$

if we let $z = -a + iy$ where y varies between b and ∞. $b^2 - y^2$ is negative, and its argument changes by 2π as we circle the branch point. If we define its argument to be $-\pi$ on the left-hand side of the branch cut, then its argument on the right-hand side will be π. We then have

$$(z+a)^2 + b^2 = e^{-i\pi}(y^2 - b^2),$$

on the left-hand side of the branch cut, and

$$(z+a)^2 + b^2 = e^{i\pi}(y^2 - b^2),$$

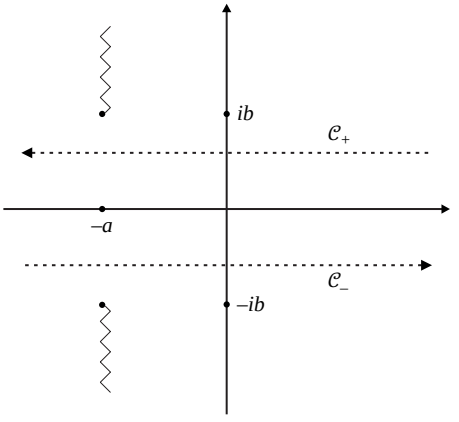

Fig. A1.3 The integration contour for (A1.61) with branch cuts parallel to the imaginary axis.

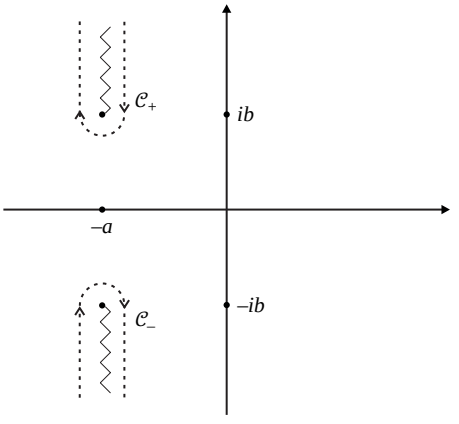

Fig. A1.4 The contour shown in Fig. A1.3 can be deformed around the two branch cuts as shown here.

on the right-hand side. Thus, we can write

$$\begin{aligned}\int_{\mathcal{C}_+} \frac{f(z)dz}{(e^{-2\pi iz}-1)} &= -i\int_b^\infty dy\, e^{i\pi\lambda}(y^2-b^2)^{-\lambda}[e^{2\pi(y+ia)}-1]^{-1} \\ &\quad +i\int_b^\infty dy\, e^{-i\pi\lambda}(y^2-b^2)^{-\lambda}[e^{2\pi(y+ia)}-1]^{-1} \\ &= 2\sin\pi\lambda\int_b^\infty dx\,(x^2-b^2)^{-\lambda}[e^{2\pi(x+ia)}-1]^{-1}. \quad \text{(A1.62)}\end{aligned}$$

A similar analysis for $\mathcal{C}_-$ (or more simply note that we can just replace a with $-a$ in the result for $\mathcal{C}_+$) results in

$$\int_{\mathcal{C}_-} \frac{f(z)dz}{(e^{2\pi iz}-1)} = 2\sin\pi\lambda \int_b^\infty dx\,(x^2-b^2)^{-\lambda}\,[e^{2\pi(x-ia)}-1]^{-1}. \quad \text{(A1.63)}$$

The net result is that (A1.61) becomes

$$F(\lambda;a,b) = \sqrt{\pi}\,\frac{\Gamma(\lambda-1/2)}{\Gamma(\lambda)}\,b^{1-2\lambda} + f_\lambda(a,b), \quad \text{(A1.64)}$$

where we have defined

$$f_\lambda(a,b) = 4\sin\pi\lambda \int_b^\infty dx\,(x^2-b^2)^{-\lambda}\,\mathcal{R}[e^{2\pi(x+ia)}-1]^{-1}. \quad \text{(A1.65)}$$

This result was first given by Ford (1980).

A1.4 The polylogarithm

The polylogarithm function is defined by

$$Li_p(z) = \sum_{n=1}^{\infty} \frac{z^n}{n^p} \quad \text{(A1.66)}$$

for all p if $|z|<1$. If we let $z\to 1$ then the sum in (A1.66) only converges if $\mathcal{R}(p)>1$ in which case

$$Li_p(1) = \zeta(p) \quad [\mathcal{R}(p)>1]. \quad \text{(A1.67)}$$

For special values of p, $Li_p(z)$ can be evaluated in closed form. In particular, if $p=0$ (A1.66) is just the geometrical series which can be summed to give

$$Li_0(z) = \frac{z}{1-z}. \quad \text{(A1.68)}$$

For $p=1$ (A1.66) is related to the Taylor series expansion of $\ln(1-z)$ by

$$Li_1(z) = -\ln(1-z). \quad \text{(A1.69)}$$

By differentiating (A1.66) with respect to z it is easy to see that

$$\frac{\partial}{\partial z} Li_p(z) = z^{-1} Li_{p-1}(z). \quad \text{(A1.70)}$$

This allows $Li_p(z)$ to be obtained recursively for $p = -1, -2, \ldots$ from a knowledge of $Li_0(z)$ in (A1.69).

It is also possible to obtain a simple integral representation for $Li_p(z)$ when $\mathcal{R}(p) > 1$ by making use of that for the Γ-function in (A1.1). From (A1.66) we have

$$Li_p(z) = \sum_{n=1}^{\infty} z^n \frac{1}{\Gamma(p)} \int_0^{\infty} dt\ t^{p-1} e^{-nt}.$$

If we write $z^n = e^{n \ln z}$ and interchange the order of summation and integration, the sum over n can be performed with the result

$$Li_p(z) = \frac{1}{\Gamma(p)} \int_0^{\infty} dt\ t^{p-1} (e^{t - \ln z} - 1)^{-1}. \tag{A1.71}$$

We often require an asymptotic expansion of $Li_p(z)$ for z close to 1. To obtain this we will set $z = e^{-\theta}$ and look at what happens as $\theta \to 0$. The method for obtaining the desired expansion makes use of the Mellin–Barnes integral representation in (5.62).[9] From (A1.66) we have

$$\begin{aligned} Li_p(e^{-\theta}) &= \sum_{n=1}^{\infty} n^{-p} e^{-n\theta} \\ &= \sum_{n=1}^{\infty} n^{-p} \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} d\alpha\ \Gamma(\alpha)(n\theta)^{-\alpha} \\ &= \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} d\alpha\ \Gamma(\alpha)\theta^{-\alpha}\zeta(p+\alpha). \end{aligned} \tag{A1.72}$$

(In the middle line we have used (5.62), and in the last line we have interchanged the order of summation and integration and made use of the definition of the Riemann ζ-function.) We will take c greater than the largest of 0 and $\mathcal{R}(1-p)$ so that the integration contour in (A1.72) lies to the right of all of the poles in the integrand. It is now a straightforward matter of closing the contour in the left-hand side of the complex plane and using the residue theorem. $\zeta(p+\alpha)$ has a simple pole at $\alpha = 1-p$ with residue 1 (see Section A1.2). $\Gamma(\alpha)$ has simple poles at $\alpha = -n$ where $n = 0, -1, -2, \ldots$ with residue $(-1)^n/n!$ (see Section A1.1). Providing that $p \neq 1, 2, 3, \ldots$ the poles of the Γ-function are distinct from the pole of the ζ-function and we find

[9] This was first given by Robinson (1951).

$$Li_p(e^{-\theta}) \simeq \Gamma(1-p)\theta^{p-1} + \sum_{n=0}^{\infty} \frac{(-1)^n}{n!}\theta^n \zeta(p-n) \quad (p \neq 1, 2, 3, \ldots). \tag{A1.73}$$

For $p = m + 1$ where $m = 0, 1, 2, \ldots$ the integrand has a double pole at $\alpha = -m$. A short calculation using the results of Section A1.1 and A1.2 gives

$$Li_p(e^{-\theta}) \simeq \frac{(-1)^m}{m!}\theta^m \left(\sum_{k=1}^{m} \frac{1}{k} - \ln\theta \right) + \sum_{\substack{n=0 \\ n \neq m}}^{\infty} \frac{(-1)^n}{n!}\theta^n \zeta(m+1-n) \quad (m = 0, 1, 2, \ldots). \tag{A1.74}$$

(For $m = 0$ we define $\sum_{k=1}^{m}(1/k) = 0$. It is easy to show that (A1.74) agrees with the direct expansion of (A1.69).)

Appendix 2
Review of special relativity

This appendix contains a very brief review of the basic concepts of special relativity needed to understand relativistic quantum field theory. The reader should already have studied this subject in some depth, and this appendix is intended merely as a refresher, not a first introduction. If you have never studied special relativity before, the book of French (1968) provides a nice introduction. Chapter 2 of Weinberg (1972) is also recommended.

Einstein's theory of special relativity is based on two basic postulates:

1. The laws of physics are the same for all inertial observers.
2. The speed of light in a vacuum is a universal constant, c, irrespective of the motion of the source or observer.

Here inertial observers are those that are in motion with respect to each other at a constant velocity. The theory of special relativity holds in an idealized world where there are no gravitational interactions, and in the real world to a good approximation provided that the gravitational interactions can be neglected in comparison with other (e.g. electromagnetic) interactions.

The Lorentz transformations relate the time and spatial coordinates used by two different inertial observers. Suppose that observer $\mathcal{O}$ uses time coordinate t and rectangular Cartesian coordinates x, y, z to describe the location of some point particle. A different inertial observer $\mathcal{O}'$ will use a different time coordinate t', and different spatial coordinates x', y', z' to describe the same point particle. The only allowed motion for inertial observers is relative motion at constant velocity. We may choose the

direction of the relative motion to be x and call the constant speed v. The equations relating the coordinates used by the two observers are[1]

$$\begin{aligned} t' &= \gamma\left(t - \frac{v}{c^2}x\right), \\ x' &= \gamma\left(x - vt\right), \\ y' &= y, \\ z' &= z, \end{aligned} \tag{A2.1}$$

where $\gamma = \left[1 - (v^2/c^2)\right]^{-1/2}$. These are the Lorentz transformations which lie at the heart of special relativity. In the non-relativistic limit, which is characterized by $v << c$, the first transformations reduce to

$$\begin{aligned} t' &\simeq t, \\ x' &\simeq x - vt, \end{aligned} \tag{A2.2}$$

which are the Galilean transformations of Newtonian physics.[2]

The physical consequences of the distinction between (A2.1) and (A2.2) are substantial. From (A2.2) it is easy to see that different inertial observers in Newtonian physics agree on time intervals (i.e. $\Delta t' = \Delta t$) and on length measurements made at a given time (i.e. $\Delta x' = \Delta x$). The first of (A2.1) shows that a clock which is fixed relative to $\mathcal{O}$ ($\Delta x = 0$) and which measures a time interval Δt as recorded by $\mathcal{O}$ measures a different time interval $\Delta t' = \gamma \Delta t$ according to $\mathcal{O}'$. This is the phenomenon of time dilation: a clock appears to run more slowly when it is moving than when it is at rest. If $\mathcal{O}$ measures the length of an object at a given instant ($\Delta t = 0$) to be Δx (in the x-direction), then if $\mathcal{O}'$ measures the length of the same object at a given instant ($\Delta t' = 0$) the result is[3] $\Delta x' = \Delta x/\gamma$. Both observers agree that $\Delta y' = \Delta y$ and $\Delta z' = \Delta z$. This is the phenomenon of length contraction: an object appears shorter in its direction of motion relative to its length at rest, whereas lengths orthogonal to the direction of motion are unaffected.

The discussion given in the previous paragraph shows how neither time intervals nor spatial intervals have absolute meaning in special relativity. This is a drastic change from Newtonian physics. However there is an object that does have an invariant meaning in special relativity. We

[1] We will not take conventional relativistic units with $c = 1$ in this appendix.

[2] In Newtonian physics $\simeq$ becomes $=$.

[3] To see this it is necessary to use both of the first two equations because $\mathcal{O}'$ makes the length measurement with $\Delta t' = 0$. Details are left to the reader.

define[4] the line element by

$$ds^2 = c^2(dt)^2 - (dx)^2 - (dy)^2 - (dz)^2. \tag{A2.3}$$

Using the Lorentz transformations (A2.1) it is an exercise in simple algebra to show that if $\mathcal{O}'$ forms ds'^2 by using t', x', y', z' in place of t, x, y, z in (A2.3), then $ds'^2 = ds^2$. All observers agree on the value of the line element. The line element is said to be Lorentz-invariant.

To proceed further with special relativity it is helpful to introduce a type of index notation. First of all we define $x^0 = !ct$ and let $x^1 = x, x^2 = y, x^3 = z$. This has the advantage that $x^0, \ldots, x^3$ all have equal dimensions of length. If (A2.1) are rewritten in terms of $x^0 = ct$ and $x'^0 = ct'$, we find that the first two equations become

$$\begin{aligned} x'^0 &= \gamma\left(x^0 - \frac{v}{c}x^1\right) \\ x'^1 &= \gamma\left(x^1 - \frac{v}{c}x^0\right). \end{aligned} \tag{A2.4}$$

There is an obvious symmetry between the way x^0 and x^1 enter that is obscured in the original form of the Lorentz transformations in (A2.1). We now use the convention that Greek letters (like $\mu, \nu, \alpha, \beta, \ldots$) take values 0, 1, 2, 3. This is a direct extension of using an index $i = 1, 2, 3$ to label the three coordinates in Euclidean space. We can therefore refer to the four spacetime coordinates x^0, x^1, x^2, x^3 by the collective name x^μ, since our convention is that $\mu = 0, 1, 2, 3$.

The next piece of notation is the one that causes the most difficulty for students meeting it for the first time: the Einstein summation convention. We will introduce this by returning to the line element (A2.3) and first of all noting that because we have defined $x^0 = ct$ we can write

$$\begin{aligned} ds^2 &= (dx^0)^2 - (dx^1)^2 - (dx^2)^2 - (dx^3)^2 \\ &= \sum_{\mu=0}^{3}\sum_{\nu=0}^{3} \eta_{\mu\nu} dx^\mu dx^\nu \end{aligned} \tag{A2.5}$$

where $\eta_{\mu\nu}$ is defined by

$$\eta_{\mu\nu} = \begin{cases} +1, \mu = \nu = 0; \\ -1, \mu = \nu = 1, 2, 3; \\ \ \ 0, \mu \neq \nu. \end{cases} \tag{A2.6}$$

[4] We could equally well adopt $ds^2 = -c^2(dt)^2 + (dx)^2 + (dy)^2 + (dz)^2$ in place of (A2.3).

This object $\eta_{\mu\nu}$ is called the 'Minkowski metric tensor'.[5] $\eta_{\mu\nu}$ may be thought of as the 4×4 matrix

$$\eta_{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}. \tag{A2.7}$$

Because professional relativists like to write as little as possible, the Einstein summation convention states that (A2.5) can be expressed simply as

$$ds^2 = \eta_{\mu\nu} dx^\mu dx^\nu \tag{A2.8}$$

without any summation signs being written. We obviously need some way of knowing when a given expression contains a summation sign or not. The understanding is that whenever the same index occurs twice in an expression this means that this repeated index is summed over $0, 1, 2, 3$. In the case of (A2.8) the index μ occurs once in $\eta_{\mu\nu}$ and once in dx^μ so it must be summed. Furthermore the index ν occurs once in $\eta_{\mu\nu}$ and once in dx^ν so it must also be summed. Hence (A2.8) contains a double summation and is identical to the long expression in (A2.5).

This might not appear too difficult to get used to, but the difficulty is in realizing that any repeated index can have any name we like. For example, we have

$$\eta_{\mu\nu} dx^\mu dx^\nu = \eta_{\alpha\beta} dx^\alpha dx^\beta = \eta_{\mu\lambda} dx^\mu dx^\lambda = \dots.$$

The reason for this is that repeated indices are simply 'dummy labels' in a summation, so for example it is clear that

$$\sum_{\mu=0}^{3} \sum_{\nu=0}^{3} \eta_{\mu\nu} dx^\mu dx^\nu = \sum_{\alpha=0}^{3} \sum_{\beta=0}^{3} \eta_{\alpha\beta} dx^\alpha dx^\beta.$$

(Both expressions stand for the top line in (A2.5).) It is the confusion of dummy indices that leads to mistakes, and the solution only comes with experience.

Having introduced x^μ, we can write the Lorentz transformations in the simple form

$$x'^\mu = L^\mu{}_\nu x^\nu \tag{A2.9}$$

where $L^0{}_0 = \gamma, L^0{}_1 = -\gamma v/c, L^1{}_0 = -\gamma v/c, L^1{}_1 = \gamma, L^2{}_2 = L^3{}_3 = 1$ and all other components vanish. (Remember our summation convention

[5] More about tensors later.

which means that ν is summed over $0, 1, 2, 3$ on the right-hand side.) More formally, we can define a Lorentz transformation as any transformation of the form (A2.9) for which the line element (A2.8) is invariant. This restricts ${L^\mu}_\nu$ to satisfy

$$\eta_{\alpha\beta} = \eta_{\mu\nu} {L^\mu}_\alpha {L^\nu}_\beta. \tag{A2.10}$$

The general definition of a Lorentz transformation is a set of 16 numbers ${L^\mu}_\nu$ which satisfies (A2.10).

A contravariant 4-vector A^μ is a set of four numbers that satisfies the same transformation (A2.9) as x^μ:

$$A'^\mu = {L^\mu}_\nu A^\nu. \tag{A2.11}$$

The invariant product of two 4-vectors is defined by $\eta_{\mu\nu} A^\mu A^\nu$ and is seen to obey $\eta_{\mu\nu} A^\mu A^\nu = \eta_{\mu\nu} A'^\mu A'^\nu$ by virtue of (A2.10).

Associated with the Lorentz transformation is the inverse transformation. In the original form (A2.1) we have

$$\begin{aligned} t &= \gamma \left(t' + \frac{v}{c^2} x' \right) \\ x &= \gamma \left(x' + v t' \right) \\ y &= y' \\ z &= z'. \end{aligned} \tag{A2.12}$$

This follows from (A2.1) upon interchanging the roles of the primed and unprimed coordinates and reversing the sign of v. On physical grounds this inverse transformation follows because if $\mathcal{O}$ sees $\mathcal{O}'$ move in the positive x-direction at speed v, then $\mathcal{O}'$ sees $\mathcal{O}$ move in the negative x-direction at the same speed. In terms of the index notation, we distinguish a 4-vector which transforms under the Lorentz transformation from one which transforms under the inverse transformation by writing the index as a subscript, rather than a superscript. If ${\left(L^{-1}\right)^\mu}_\nu$ represents the inverse of ${L^\mu}_\nu$, then

$${\left(L^{-1}\right)^\mu}_\nu {L^\nu}_\lambda = \delta^\mu_\lambda = {L^\mu}_\nu {\left(L^{-1}\right)^\nu}_\lambda, \tag{A2.13}$$

where δ^μ_λ is the Kronecker delta defined by

$$\delta^\mu_\lambda = \begin{cases} 1, \mu = \lambda; \\ 0, \mu \neq \lambda. \end{cases} \tag{A2.14}$$

We call B_μ a covariant 4-vector if

$$B'_\mu = B_\nu {\left(L^{-1}\right)^\nu}_\mu. \tag{A2.15}$$

The invariant product between a covariant 4-vector B_μ and a contravariant 4-vector A^μ is

$$B_\mu A^\mu = B'_\mu A'^\mu.$$

Given any contravariant 4-vector A^μ we can define a covariant 4-vector A_μ by

$$A_\mu = \eta_{\mu\nu} A^\nu. \tag{A2.16}$$

(It is easy to show that this definition satisfies (A2.15) if we use (A2.10) and (A2.13).) This is called 'lowering an index'. Conversely we can raise an index to form a contravariant vector from a covariant vector. To do this, note that the matrix (A2.7) is its own inverse. To keep the index assignments right we will define

$$\eta^{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \tag{A2.17}$$

so that

$$\eta^{\mu\nu}\eta_{\nu\lambda} = \eta_{\lambda\nu}\eta^{\nu\mu} = \delta^\mu_\lambda. \tag{A2.18}$$

This leads to

$$A^\mu = \eta^{\mu\nu} A_\nu \tag{A2.19}$$

from (A2.16). A deeper understanding of why the distinction between contravariant and covariant 4-vectors is important requires the understanding of vector spaces and their duals.[6]

Because the laws of physics are usually expressed in the form of differential equations it is advantageous to pursue the index notation for partial derivatives. The set of three partial derivatives $(\partial/\partial x, \partial/\partial y, \partial/\partial z)$ forms the gradient operator ∇ in normal vector calculus. With the addition of $(\partial/\partial x^0) = (1/c)(\partial/\partial t)$ we obtain a 4-vector $(\partial/\partial x^0, \partial/\partial x^1, \partial/\partial x^2, \partial/\partial x^3)$ denoted by ∂_μ or ∇_μ in index notation. The lower index position indicates that $\nabla_\mu = \partial_\mu$ is a covariant 4-vector. This is easy to verify using

$$\begin{aligned} \nabla'_\mu = \frac{\partial}{\partial x'^\mu} &= \frac{\partial x^\nu}{\partial x'^\mu}\frac{\partial}{\partial x^\nu} \\ &= \left(L^{-1}\right)^\nu{}_\mu \frac{\partial}{\partial x^\nu}, \end{aligned} \tag{A2.20}$$

[6] See Choquet-Bruhat *et al.* (1977) or Misner *et al.* (1973) for a comprehensive treatment.

where we used the chain rule in the first line, and the inverse of (A2.9) to obtain the second line. The contravariant components are given by $\nabla^\mu = [\partial/\partial x^0, -(\partial/\partial x^1), -(\partial/\partial x^2), -(\partial/\partial x^3)]$ and follow from (A2.19). Finally we define

$$\begin{aligned} \Box = \nabla^\mu \nabla_\mu &= \eta^{\mu\nu} \nabla_\mu \nabla_\nu \\ &= \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} - \frac{\partial^2}{\partial z^2} \end{aligned} \tag{A2.21}$$

which is recognized as the wave operator. $\Box$ is easily seen to be invariant under Lorentz transformations.

The last concept we wish to mention is tensors. A tensor is simply a generalization of a 4-vector to include an object with more than one index. For example $T^{\mu\nu}$ is called a tensor if

$$T'^{\mu\nu} = L^\mu{}_\alpha L^\nu{}_\beta T^{\alpha\beta} \tag{A2.22}$$

when the coordinates undergo the transformation (A2.9). The rank of the tensor is the number of factors of $L^\mu{}_\nu$ which occur in the transformation law. In the case of (A2.22) the rank is 2. Indices may be raised and lowered on tensors exactly as on 4-vectors in (A2.16) and (A2.19). An example of a second-rank tensor is the electromagnetic field strength tensor $F_{\mu\nu}$.

Appendix 3
Interaction picture

Suppose that the Hamiltonian H is expressed as

$$H = H_0 + V(t), \tag{A3.1}$$

where the operator H_0 has no explicit time dependence.[1] Let $|\alpha, t\rangle_S$ be the state vector in the Schrödinger picture with $|\alpha, t = t_0\rangle_S = |\alpha\rangle_S$ the initial state. The time development operator $U(t, t_0)$ was defined in (3.16) and satisfies the Schrödinger equation (3.20) with the boundary condition $U(t_0, t_0) = \mathrm{I}$. The Heisenberg picture also makes use of $U(t, t_0)$ to give the time development of the operators representing observables. In some cases, such as the simple harmonic oscillator, it may be possible to evaluate $U(t, t_0)$ exactly, or equivalently to solve the Heisenberg equations of motion. However, in general this will not be possible. In such cases other methods must be resorted to. It may be that $V(t)$ can be treated as a small perturbation. An approach for dealing with this was originated by Dirac (1926, 1927). The utility of this method in quantum field theory was shown by Tomonaga (1946) and Schwinger (1949).

Suppose that $V(t)$ is only non-zero for $t_- \leq t \leq t_+$ for some times t_- and t_+. Then for $t \leq t_-$ the state vector obeys the Schrödinger equation with the Hamiltonian H_0. If we choose $t_0 < t_-$, then

$$U(t, t_0) = \exp\left[-\frac{i}{\hbar}(t - t_0)H_0\right]$$

gives the time development operator for times $t \leq t_-$. If $V(t)$ was identically equal to zero then this would describe the time development for all

[1] We are in the Schrödinger picture here.

time. The key idea behind the interaction picture is to define a new state vector $|\alpha, t\rangle_I$ by

$$|\alpha, t\rangle_I = \exp\left[\frac{i}{\hbar}(t - t_-)H_0\right]|\alpha, t\rangle_S. \tag{A3.2}$$

The interaction picture and Schrödinger state vectors are chosen to coincide at the time t_- when $V(t)$ becomes non-zero. It should be noted that the time development of the state defined in (A3.2) is opposite to the time development of the state in the Schrödinger picture. This means that if $V(t)$ was identically zero, the state $|\alpha, t\rangle_I$ would be independent of time. This suggests that in the case where $V(t)$ is not identically zero, the time development of the state is governed by $V(t)$ rather than the full Hamiltonian. Since $|\alpha, t\rangle_S$ obeys the Schrödinger equation with the full Hamiltonian H in (A3.1), it is easy to show that

$$i\hbar\frac{\partial}{\partial t}|\alpha, t\rangle_I = V_I(t)|\alpha, t\rangle_I, \tag{A3.3}$$

where[2]

$$V_I(t) = \exp\left[\frac{i}{\hbar}(t - t_-)H_0\right]V_S(t)\exp\left[-\frac{i}{\hbar}(t - t_-)H_0\right]. \tag{A3.4}$$

The result in (A3.3) shows that $V(t)$ governs the dynamics in the interaction picture.

We can define a time development operator $U_I(t, t_0)$ in the interaction picture by

$$|\alpha, t'\rangle_I = U_I(t', t)|\alpha, t\rangle_I \tag{A3.5}$$

with $t' > t$. From (A3.3) it follows that

$$i\hbar\frac{\partial}{\partial t'}U_I(t', t) = V_I(t')U_I(t', t), \tag{A3.6}$$

with the boundary condition

$$U_I(t, t) = \mathrm{I}. \tag{A3.7}$$

We can relate $U_I(t, t_0)$ to $U(t, t_0)$ defined earlier. First of all, from (3.16) we know that

$$|\alpha, t\rangle_S = U(t, t_0)|\alpha, t_0\rangle_S.$$

[2] We have appended the subscript S to $V(t)$ which occurs in (A3.1) to clarify that it is taken in the Schrödinger picture.

Equation (A3.2) gives

$$|\alpha, t\rangle_I = \exp\left[\frac{i}{\hbar}(t - t_-)H_0\right] U(t, t_0)|\alpha, t_0\rangle_S. \tag{A3.8}$$

From (A3.5),

$$\begin{aligned}|\alpha, t\rangle_I &= U_I(t, t_0)|\alpha, t_0\rangle_I \\ &= U_I(t, t_0) \exp\left[-\frac{i}{\hbar}(t_- - t_0)H_0\right] |\alpha, t_0\rangle_S\end{aligned} \tag{A3.9}$$

using (A3.2) with $t = t_0$. Comparing (A3.8) with (A3.9) results in the identification

$$U(t, t_0) = \exp\left[-\frac{i}{\hbar}(t - t_-)H_0\right] U_I(t, t_0) \exp\left[-\frac{i}{\hbar}(t_- - t_0)H_0\right]. \tag{A3.10}$$

We can obtain a solution to (A3.6) in the same way as we did for $U(t, t_0)$ in Section 3.1.2. First of all we can convert (A3.6) into the integral equation

$$U_I(t, t_0) = \mathrm{I} - \frac{i}{\hbar}\int_{t_0}^{t} dt'\, U_I(t', t_0)V_I(t'). \tag{A3.11}$$

The solution now follows as

$$U_I(t, t_0) = \mathrm{I} + \sum_{n=1}^{\infty} \frac{1}{n!}\Big(-\frac{i}{\hbar}\Big)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \cdots \int_{t_0}^{t} dt_n \mathrm{T}\left[V_I(t_1) \cdots V_I(t_n)\right] \tag{A3.12}$$

where T is the time-ordered product defined in (3.27). As before, this can be written in the shorthand form as

$$U_I(t, t_0) = \mathrm{T} \exp\left[-\frac{i}{\hbar}\int_{t_0}^{t} dt' V_I(t')\right]. \tag{A3.13}$$

We will now show how the interaction picture can be used to study the forced harmonic oscillator, and make contact with what we obtained in Section 7.4 using the Schwinger action principle. From (7.59) we see that we may choose

$$V_S(t) = -J(t)x_S, \tag{A3.14}$$

with H_0 the Hamiltonian operator for the simple harmonic oscillator. From (A3.4) we have

$$V_I(t) = -J(t) \exp\left[\frac{i}{\hbar}(t - t_-)H_0\right] x_S \exp\left[-\frac{i}{\hbar}(t - t_-)H_0\right]. \tag{A3.15}$$

Let

$$x_I(t) = \exp\left[\frac{i}{\hbar}(t-t_-)H_0\right] x_S \exp\left[-\frac{i}{\hbar}(t-t_-)H_0\right]. \tag{A3.16}$$

Then by differentiation of (A3.16) it follows that

$$\begin{aligned} i\hbar\frac{d}{dt}x_I(t) &= [x_I(t), H_0] \\ &= \exp\left[\frac{i}{\hbar}(t-t_-)H_0\right][x_S, H_0]\exp\left[-\frac{i}{\hbar}(t-t_-)H_0\right] \\ &= \frac{i\hbar}{m}\exp\left[\frac{i}{\hbar}(t-t_-)H_0\right] p_S \exp\left[-\frac{i}{\hbar}(t-t_-)H_0\right], \end{aligned}$$

where p_S is the momentum operator in the Schrödinger picture. Define

$$p_I(t) = \exp\left[\frac{i}{\hbar}(t-t_-)H_0\right] p_S \exp\left[-\frac{i}{\hbar}(t-t_-)H_0\right] \tag{A3.17}$$

analogously to (A3.16). We then have

$$\frac{d}{dt}x_I(t) = \frac{1}{m}p_I(t). \tag{A3.18}$$

Differentiation of (A3.17) leads to

$$\frac{d}{dt}p_I(t) = -m\omega^2 x_I(t). \tag{A3.19}$$

The operator $x_I(t)$ therefore satisfies

$$\frac{d^2}{dt^2}x_I(t) + \omega^2 x_I(t) = 0, \tag{A3.20}$$

which is just the equation of motion for the simple harmonic oscillator with no forcing term.

The general solution to (A3.20) can be written as

$$x_I(t) = \left(\frac{\hbar}{2m\omega}\right)^{1/2}\left\{a e^{-i\omega(t-t_-)} + a^\dagger e^{i\omega(t-t_-)}\right\} \tag{A3.21}$$

for some constant operators a and $a^\dagger$. From (A3.16) we have

$$x_I(t_-) = x_S = \left(\frac{\hbar}{2m\omega}\right)^{1/2}\left(a + a^\dagger\right). \tag{A3.22}$$

Using (A3.17), (A3.18), and (A3.21) we find

$$p_I(t_-) = p_S = m\left(\frac{\hbar}{2m\omega}\right)^{1/2}(-i\omega a + i\omega a^\dagger). \tag{A3.23}$$

Using the fact that $[x_S, p_S] = i\hbar$, it is easy to show that the operators a and $a^\dagger$ obey

$$[a, a^\dagger] = 1. \tag{A3.24}$$

It should be clear from our earlier discussion in Section 3.5 that a and $a^\dagger$ may be interpreted as the annihilation and creation operators for the free (i.e. unforced) simple harmonic oscillator.

If we define

$$a(t) = ae^{-i\omega(t-t_-)}, \tag{A3.25}$$

$$a^\dagger(t) = a^\dagger e^{i\omega(t-t_-)}, \tag{A3.26}$$

then $x_I(t)$ in (A3.21) may be written as

$$x_I(t) = \left(\frac{\hbar}{2m\omega}\right)^{1/2}\Big\{a(t) + a^\dagger(t)\Big\}. \tag{A3.27}$$

If we borrow the language used in quantum field theory, (A3.27) represents the decomposition of $x_I(t)$ into a sum of positive and negative frequency parts. For later use we record that

$$[a(t), a^\dagger(t)] = e^{-i\omega(t-t_-)}. \tag{A3.28}$$

This result follows immediately from using (A3.24)–(A3.26). From (A3.15) and (A3.27) we have

$$V_I(t) = -\left(\frac{\hbar}{2m\omega}\right)^{1/2} J(t)\Big\{a(t) + a^\dagger(t)\Big\}, \tag{A3.29}$$

as the perturbation expressed in the interaction picture.

If the system at the initial time t_0 is in the state $|\alpha, t_0\rangle_I$ where $t_0 < t_-$, and at some final time $t_f > t_+$ is in the state $|\alpha, t_f\rangle_I$, we will define

$$|\alpha, t_f\rangle_I = S_I|\alpha, t_0\rangle_I, \tag{A3.30}$$

where S_I is called the 'scattering operator' in the interaction picture. Comparison of this result with (A3.5) shows that

$$S_I = U_I(t_f, t_0). \tag{A3.31}$$

(Normally in quantum field theory, one imagines that the interaction is turned off in the remote past and the remote future, so that $t_0 \to -\infty$ and $t_f \to \infty$ in (A3.31).) The scattering operator transforms the state before the interaction is turned on into the state that occurs after the interaction is turned off. If the system is prepared in the state $|\alpha, t_0\rangle_I$, the probability that it is found in the state $|\beta, t_f\rangle_I$ at the final time is obtained by squaring the modulus of the transformation function

$$ {}_I\langle\beta, t_f|\alpha, t_f\rangle_I = {}_I\langle\beta, t_f|S_I|\alpha, t_0\rangle_I. \tag{A3.32}$$

As an example, suppose that we try to evaluate the transformation function for the transition from an energy eigenstate at time t_0 to a different energy eigenstate at time t_f. As in Section 3.5, let

$$ H_0|n'\rangle = \hbar\omega_{n'}|n'\rangle \tag{A3.33}$$

where $\omega_{n'} = (n' + 1/2)\omega$. Then if $|n', t_0\rangle_S = |n'\rangle$, we have

$$ |n', t\rangle_I = e^{-i\omega_{n'}(t-t_0)}|n'\rangle. \tag{A3.34}$$

The state in the interaction picture has no time dependence in this case, as in the Heisenberg picture. The transformation function between two energy eigenstates becomes

$$ {}_I\langle n'', t_f|n', t_f\rangle_I = e^{i(\omega_{n''}-\omega_{n'})(t_- - t_0)}\langle n''|S_I|n'\rangle \tag{A3.35}$$

using (A3.32) and (A3.34). We must now use (A3.12) and (A3.31) to evaluate $\langle n''|S_I|n'\rangle$. The simplest case occurs when we concentrate on the vacuum-to-vacuum transition amplitude. Then

$$ {}_I\langle 0, t_f|0, t_f\rangle_I = \langle 0|S_I|0\rangle \tag{A3.36}$$

$$ = 1 + \sum_{n=1}^{\infty} \frac{1}{n!}\Big(-\frac{i}{\hbar}\Big)^n \times \int_{t_-}^{t_+} dt_1 \cdots \int_{t_-}^{t_+} dt_n \langle 0|\mathrm{T}\Big[V_I(t_1)\cdots V_I(t_n)\Big]|0\rangle. \tag{A3.37}$$

Note that because $V(t) = 0$ if $t < t_-$ or $t > t_+$, we can take the integration limits in (A3.12) as shown, or equivalently replace t_- with $-\infty$ and t_+ with $+\infty$.

There are several ways to evaluate $\langle 0|S_I|0\rangle$. The most widely used method makes use of Wick's theorem. Instead of using this method, which involves some complicated combinatorics, we will make use of a method developed by Schwinger (1949). Following Schwinger, define

$$ \overline{|\alpha, t\rangle} = e^{(i/\hbar)F(t)}|\alpha, t\rangle_I, \tag{A3.38}$$

for some operator $F(t)$. Because the interaction picture state satisfies the equation (A3.3), if we substitute for $|\alpha, t\rangle_I$ from (A3.38) we have

$$i\hbar\frac{\partial}{\partial t}\overline{|\alpha,t\rangle} = e^{(i/\hbar)F(t)}\left\{V_I(t)e^{-(i/\hbar)F(t)} - i\hbar\left[\frac{\partial}{\partial t}e^{-(i/\hbar)F(t)}\right]\right\}\overline{|\alpha,t\rangle} \tag{A3.39}$$

The aim now is to choose $F(t)$ so that the factor enclosed by braces in (A3.39) becomes a function rather than an operator. This will result in the transformed state $\overline{|\alpha,t\rangle}$ satisfying an ordinary differential equation, rather than one that has an operator on the right-hand side, and the solution may be easily obtained.

The factors which occur on the right-hand side of (A3.39) can be evaluated using the following identity,

$$\exp(A+B) = \exp\left(\frac{1}{2}[A,B]\right)\exp(B)\exp(A), \tag{A3.40}$$

that is true provided $[A,[A,B]] = 0$ and $[B,[A,B]] = 0$. In order to prove this, define

$$G(\lambda) = \exp\left[\lambda(A+B)\right]\exp(-\lambda A)\exp(-\lambda B). \tag{A3.41}$$

By differentiation of $G(\lambda)$ with respect to λ it is easy to show that

$$G'(\lambda) = AG(\lambda) + [B, G(\lambda)] - G(\lambda)\exp(\lambda B)A\exp(-\lambda B). \tag{A3.42}$$

The last term on the right-hand side may be simplified by using the identity (3.165) resulting in

$$G'(\lambda) = [A+B, G(\lambda)] + \lambda G(\lambda)[A,B]. \tag{A3.43}$$

It is now straightforward to show that the first term on the right-hand side vanishes.[3] We end up with

$$G'(\lambda) = \lambda[A,B]G(\lambda). \tag{A3.44}$$

This can be regarded as a differential equation for $G(\lambda)$ that is easily solved using the boundary condition $G(0) = \mathrm{I}$ following from (A3.41). The solution to (A3.44) with this boundary condition is

$$G(\lambda) = \exp\left(\frac{1}{2}\lambda^2[A,B]\right)\mathrm{I},$$

proving (A3.40).

[3] The identity (3.165) is useful here.

We must be extremely careful about computing $(\partial/\partial t)e^{-(i/\hbar)F(t)}$. It is not true in general that $(\partial/\partial t)e^{-(i/\hbar)F(t)} = -(i/\hbar)\dot{F}(t)e^{-(i/\hbar)F(t)}$ when $F(t)$ is an operator. This result only holds in the special case that $[F, \dot{F}] = 0$. In order to compute $(\partial/\partial t)e^{-(i/\hbar)F(t)}$ correctly, we must use the basic definition of the derivative:

$$\frac{\partial}{\partial t}e^{-(i/\hbar)F(t)} = \lim_{\epsilon\to 0}\frac{1}{\epsilon}\Big\{e^{-(i/\hbar)F(t+\epsilon)} - e^{-(i/\hbar)F(t)}\Big\}. \tag{A3.45}$$

We now need an expansion of the quantity enclosed in braces that is correct to order ϵ. We can use the first two terms of the Taylor expansion of $F(t+\epsilon)$ about $\epsilon = 0$ to obtain

$$\frac{\partial}{\partial t}e^{-(i/\hbar)F(t)} = \lim_{\epsilon\to 0}\frac{1}{\epsilon}\Big\{e^{-(i/\hbar)F(t)-(i/\hbar)\epsilon\dot{F}(t)} - e^{-(i/\hbar)F(t)}\Big\}. \tag{A3.46}$$

If we now make the assumption that $[F, \dot{F}]$ is a function, rather than an operator, then we can use the identity (A3.40) to obtain

$$\frac{\partial}{\partial t}e^{-(i/\hbar)F(t)} = \lim_{\epsilon\to 0}\frac{1}{\epsilon}\Big\{e^{-(\epsilon/2\hbar^2)[F(t),\dot{F}(t)]}e^{-(i/\hbar)\epsilon\dot{F}(t)} - 1\Big\}e^{-(i/\hbar)F(t)}. \tag{A3.47}$$

Expanding the exponentials on the right-hand side, and taking the limit $\epsilon \to 0$ results in

$$\frac{\partial}{\partial t}e^{-(i/\hbar)F(t)} = \Big\{-\frac{i}{\hbar}\dot{F}(t) - \frac{1}{2\hbar^2}[F(t), \dot{F}(t)]\Big\}e^{-(i/\hbar)F(t)}. \tag{A3.48}$$

It is important to note that this result was derived under the assumption that $[F, \dot{F}]$ was a function and therefore commuted with F and $\dot{F}$. If this is not true, then the result is much more complicated. It can be seen in the simplest possible case where $[F, \dot{F}] = 0$, the result that one would naively write down if $F(t)$ was an ordinary function is correct.

We will now choose

$$F(t) = \int_{t_-}^{t} dt' V_I(t'), \tag{A3.49}$$

so that

$$\dot{F}(t) = V_I(t). \tag{A3.50}$$

Using (A3.28) and (A3.29) we have

$$[V_I(t), V_I(t')] = -\frac{i\hbar}{m\omega}J(t)J(t')\sin\omega(t-t'). \tag{A3.51}$$

For $F(t)$ chosen as in (A3.49) we find

$$[F(t), \dot{F}(t)] = \frac{i\hbar}{m\omega} \int_{t_-}^{t} dt' J(t) J(t') \sin \omega(t - t'), \tag{A3.52}$$

which is just a function as assumed in our derivation above.

We can now return to simplify (A3.39). It is easily shown that

$$e^{(i/\hbar)F(t)} V_I(t) e^{-(i/\hbar)F(t)} = V_I(t) - \frac{1}{m\omega} \int_{t_-}^{t} dt' J(t) J(t') \sin \omega(t - t') \tag{A3.53}$$

and

$$e^{(i/\hbar)F(t)} \left[i\hbar \frac{\partial}{\partial t} e^{-(i/\hbar)F(t)} \right] = V_I(t) - \frac{1}{2m\omega} \int_{t_-}^{t} dt' J(t) J(t') \sin \omega(t - t'). \tag{A3.54}$$

It is again necessary to use the fact that $[F, \dot{F}]$ is a function, not an operator here. (A3.39) then becomes

$$i\hbar \frac{\partial}{\partial t} \overline{|\alpha, t_-; t\rangle} = -\frac{1}{2m\omega} \int_{t_-}^{t} dt' J(t) J(t') \sin \omega(t - t') \; \overline{|\alpha, t_-; t\rangle}. \tag{A3.55}$$

The solution to this equation is

$$\begin{aligned} \overline{|\alpha, t_-; t\rangle} = \exp \Big\{ \frac{i}{2\hbar m\omega} \int_{t_-}^{t} dt' \int_{t_-}^{t'} dt'' J(t') J(t'') \sin \omega(t' - t'') \Big\} \\ \times \overline{|\alpha, t_-; t_-\rangle}. \end{aligned} \tag{A3.56}$$

Returning to (A3.38), and using the definition of $U_I(t, t_-)$ which follows from (A3.6), we have

$$\begin{aligned} U_I(t, t_-) = \exp \Big\{ -\frac{i}{\hbar} \int_{t_-}^{t} dt' V_I(t') \\ + \frac{i}{2\hbar m\omega} \int_{t_-}^{t} dt' \int_{t_-}^{t'} dt'' J(t') J(t'') \sin \omega(t' - t'') \Big\}. \end{aligned} \tag{A3.57}$$

This form is noteworthy because no time-ordering operation occurs. Making use of (A3.31) we find

$$\begin{aligned} \langle 0 | S_I | 0 \rangle = \exp \Big\{ \frac{i}{2\hbar m\omega} \int_{t_-}^{t_+} dt' \int_{t_-}^{t'} dt'' J(t') J(t'') \sin \omega(t' - t'') \Big\} \\ \times \langle 0 | \exp \left[-\frac{i}{\hbar} \int_{t_-}^{t_+} dt' V_I(t') \right] | 0 \rangle. \end{aligned} \tag{A3.58}$$

The remaining matrix element in (A3.58) can be easily evaluated if we note the expression (A3.29) for $V_I(t)$, and make use of the identity

$$e^{\lambda a - \lambda^* a^\dagger} = e^{-(1/2)|\lambda|^2} e^{-\lambda^* a^\dagger} e^{\lambda a}, \tag{A3.59}$$

which follows from (A3.40) with $[a, a^\dagger] = 1$.[4] From (A3.59) we find (using $a|0\rangle = 0 = \langle 0|a^\dagger$)

$$\langle 0|e^{\lambda a - \lambda^* a^\dagger}|0\rangle = e^{-(1/2)|\lambda|^2}. \tag{A3.60}$$

The net result for $\langle 0|S_I|0\rangle$ now becomes

$$\begin{aligned}\langle 0|S_I|0\rangle = \exp\Big\{\frac{i}{2\hbar m\omega}\int_{t_-}^{t_+} dt \int_{t_-}^{t} dt' J(t)J(t')\sin\omega(t-t')\Big\} \\ \times \exp\Big\{-\frac{1}{4\hbar m\omega}\int_{t_-}^{t_+} dt \int_{t_-}^{t_+} dt' J(t)J(t')\cos\omega(t-t')\Big\}.\end{aligned} \tag{A3.61}$$

This can be written in a simpler form by noting first of all that due to the symmetry of the integrand,

$$\int_{t_-}^{t_+} dt \int_{t_-}^{t} dt' J(t)J(t')\sin\omega(t-t') = \frac{1}{2}\int_{t_-}^{t_+} dt \int_{t_-}^{t_+} dt' J(t)J(t')\sin\omega|t-t'|.$$

Because $\cos\omega(t-t') = \cos\omega|t-t'|$, we find the more symmetrical looking expression

$$\langle 0|S_I|0\rangle = \exp\Big\{-\frac{1}{4\hbar m\omega}\int_{t_-}^{t_+} dt \int_{t_-}^{t_+} dt' J(t)J(t')e^{-i\omega|t-t'|}\Big\}. \tag{A3.62}$$

This result was first given in this form by Feynman (1950).

[4] λ is any complex number in (A3.59).

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