**Physics 851**, www.nscl.msu.edu/ pratt/phy851

Scott Pratt, pratt@nscl.msu.edu

# 1 States and Operators

## 1.1 States

Quantum mechanics consists of states and operators. All systems can be described by being in a state $|\psi\rangle$, which can be written as a linear superposition of states in an orthonormal basis $|i\rangle$,

$$\langle i|j\rangle = \delta_{ij} \tag{1}$$

Any physical system can be described by a state $\psi$ which is a linear combination of basis states.

$$\begin{aligned} |\psi\rangle &= \sum_i a_{\psi,i}|i\rangle & (2)\\ \langle\psi| &= = \sum_i a^*_{\psi,i}\langle i|, & (3) \end{aligned}$$

where $a_{i,\psi}$ is a complex number. By taking the product of $|\psi\rangle$ with $|i\rangle$, one sees that

$$a_{i,\psi} = \langle i|\Psi\rangle. \tag{4}$$

Furthermore, by taking the overlap of $\psi$ with itself (the norm)

$$\begin{aligned} \langle\psi|\psi\rangle &= \sum_i \langle\psi|i\rangle\langle i|\psi\rangle & (5)\\ &= |\sum\langle\psi|i\rangle|^2, & (6) \end{aligned}$$

one can see that the square of the overlap can be considered as a probability. That is, if $\psi$ is normalized to unity, that $|\langle\psi|i\rangle|^2$ is a positive real number, and that summing over $i$ yields unity. This allows $|\langle\psi|i\rangle|^2$ to be interpreted as a probability, i.e. if one prepares a state $\psi$ the chance one finds that one is in a state $i$ is $|\langle\psi|i\rangle|^2$. Of course, once finds that one is in the state $i$, the state $\psi$ no longer exists.

All states can be written as vectors. For instance, if a basis has two states, the two states might be defined in terms of vectors as,

$$|\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{7}$$

The choice of these two vectors is arbitrary. As long as the two vectors are orthonormal, the system may be fully described.

## 1.2 Operators

Operators operate on vectors and return another vector. All operators may be described in terms of bras and kets,

$$\mathcal{A} = \sum_{ij} a_{ij} |i\rangle\langle j|. \tag{8}$$

Just as any state can be equivalently expressed as a vector, any operator can be defined by a matrix. Just as a state's definition in terms of a matrix depends on the basis, so does the definition of an operator in terms of a matrix. Knowing the coeficients $a_{ij}$ is sufficient to define the matrix. In fact if the basis is defined by

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \\ \vdots \end{pmatrix}, \quad |2\rangle = \begin{pmatrix} 0 \\ 1 \\ \vdots \end{pmatrix}, \quad \cdots, \tag{9}$$

the matix and the coefficients are synonymous $A_{ij} = a_{ij}$. Otherwise,

$$A_{ij} = \sum_{mn} a_{mn} v(m)_i v^*(n)_j, \tag{10}$$

where $v(m)_i$ is the $i^{th}$ component of the state vector $m$.

**Hermitian Conjugate:**
Consider a matrix element, $\langle\phi|\mathcal{A}|\psi\rangle$. Expressing the operators as matrices and the states as vectors, then taking the complex conjugate one sees that,

$$\begin{aligned} \langle\phi|\mathcal{A}|\psi\rangle^* &= (\phi_i^* a_{ij} \psi_j)^* && (11) \\ &= \psi_j^* a_{ij}^* \phi_j && (12) \end{aligned}$$

Thus, if one wishes to define an operator $\mathcal{A}^\dagger$ such that

$$\langle\phi|\mathcal{A}|\psi\rangle^* = \langle\psi|\mathcal{A}^\dagger|\phi\rangle, \tag{13}$$

the operator $\mathcal{A}^\dagger$ must be represented by the complex-conjugate of the matrix that represents $\mathcal{A}$, then transposed.

$$a_{ij}^\dagger = a_{ji}^* \tag{14}$$

The operator $\mathcal{A}^\dagger$ is known as the Hermitian conjugate of $\mathcal{A}$.

A Hermitian operator is one that obeys the relation,

$$\mathcal{K} = \mathcal{K}^\dagger. \tag{15}$$

Hermitian operators are important for two reasons.

1. They yield real numbers as expectations, $\langle\psi|\mathcal{K}|\psi\rangle^* = \langle\psi|\mathcal{K}|\psi\rangle$.
2. They can be used to generate unitary transformations, $e^{iK\theta}$. This will be discussed in the next section.

**Unitary Operators**

One type of operator of particular interest is one that corresponds to a change of basis, while keeping the new basis orthonormal. Consider a transformation operator $\mathcal{R}$,

$$\begin{aligned} \mathcal{R} &= \sum_{i,i'} R_{i',i} |i'\rangle\langle i| && (16) \\ |i'\rangle &= \sum_i R_{i'i} |i\rangle. && (17) \end{aligned}$$

The coefficients must retain the orthormality properties, which puts a constraint on the coefficients.

$$\begin{aligned} \langle i'|j'\rangle &= \delta_{i'j'} && (18) \\ &= \sum_i R^*_{j'i} R_{ii'} && (19) \\ &= (R^\dagger R)_{j'i'} && (20) \end{aligned}$$

Here, the † superscript refers to taking the Hermitian conjugate of the matrix and reflecting the coefficient about the diagonal. In bra and ket language,

$$\begin{aligned} \mathcal{A} &= \sum_{ij} a_{ij} |i\rangle\langle j| && (21) \\ \mathcal{A}^\dagger &= \sum_{ij} a^*_{ji} |i\rangle\langle j|. && (22) \end{aligned}$$

If an operator $\mathcal{R}$ is to behave like a transformation, we demand that $\mathcal{R}^\dagger\mathcal{R} = \mathbf{1}$, or equivalently, $R^{-1} = R^\dagger$. This conditions means the operator $\mathcal{R}$ is *unitary.* The word unitary follows from the fact that a state $U|\psi\rangle$ has the same norm as $|\psi\rangle$, implying that the net probability is unchanged by the unitary transformation $U$. Changes of basis and other rotations are represented by unitary transformations, as are evolution operators which we study later.

Hermitian operators satisfy the condition

$$\mathcal{K}^\dagger = K. \qquad (23)$$

Hermitian operators are often used to generate unitary transformations,

$$U = e^{iK\theta}. \qquad (24)$$

For instance, if $\mathcal{K}$ is the Hamiltonian, $U$ is the evolution operator that develops states through time.

Both operators and states are rotated by a transformation $U$. If both operators and states are transformed identically the resulting matrix element is unaffected.

$$\begin{aligned} |\psi'\rangle &= U|\psi\rangle && (25) \\ \langle\psi'| &= \langle\psi|U^\dagger && (26) \\ \mathcal{K}' &= U\mathcal{K}U^\dagger && (27) \\ <\psi'|\mathcal{K}'|\psi'\rangle &= \langle\psi|\mathcal{K}|\psi\rangle && (28) \end{aligned}$$

**Density Matrices**:

First, we stop and consider what forms of matrix elements might be considered as an observable. Observables must be real and independent of the basis, i.e. all unitary transformations that act on the bras, kets and operators should leave the observable unchanged. All observables can be expressed in one of two forms:

$$\langle\psi|\mathcal{K}|\psi\rangle, \tag{29}$$

where $\mathcal{K}$ is Hermitian, or

$$|\langle\phi|\psi\rangle|^2. \tag{30}$$

Instead of describing a state $\psi$ by a vector, one could describe it by a density matrix,

$$\rho_\psi = |\psi\rangle\langle\psi|. \tag{31}$$

From the definition of the density matrix, one can see that

$$\langle\psi|\mathcal{K}|\psi\rangle = \mathrm{Tr}\rho_\psi K, \tag{32}$$

and that

$$|\langle\phi|\psi\rangle|^2 = \mathrm{Tr}\rho_\psi\rho_\phi. \tag{33}$$

Thus, the density matrices are sufficient to give all observables. The trace of a density matix is invariant under unitary transformations. Thus, one should always be able to pick a basis such that when $\rho_\psi$ is diagonalized it has the form,

$$\rho_\psi = \begin{pmatrix} 1,0, & \cdots, & 0 \\ 0, & \cdots, & 0 \\ & \vdots & \\ 0, & \cdots, & 0 \end{pmatrix} \tag{34}$$

A density matrix that diagonalizes in such a way is known as a **pure** state A projection operator is a density matrix corresponding to a pure state. The reason that it is often called a projection operator is that

$$P\psi^2 = P_\psi,\ \mathrm{Tr}P_\psi. \tag{35}$$

Projection operators can also play the role of a filter, e.g. a polarization filter. since it can be described by a single state $\psi$.

However, density matrices can be more general. If one has a density matrix which is an incoherent sum over several states, the resulting diagonalized density matrix could have more than one non-zero element, though the trace would have to remain equal to unity. Thus, density matrices can be used to express non-pure states such as unpolarized beams. For instance, one can define the following density matrix,

$$\rho = \frac{1}{2}|1\rangle\langle 1| + \frac{1}{2}|2\rangle\langle 1|. \tag{36}$$

This density matrix describes being in state $|1\rangle$ 50% of the time and in state $|2\rangle$ 50% of the time. If one were to write a state that was described by this density matrix, it would like like

$$\frac{1}{\sqrt{2}}|1\rangle + e^{i\phi}\frac{1}{\sqrt{2}}|2\rangle, \tag{37}$$

with $\phi$ being treated as a random phase. When performing calculations with such a state, one would have to ignore all terms with a leftover phase in order to account for the randomness of the phase.

Density matrices also play an essential part in thermodynamics. In that case, one considers incoherent sums over many states weighted by the energy. If one is in a basis where the Hamiltonian is diagonalized, the density matrix takes the form

$$\rho_{\text{thermal}} = \frac{1}{Z}\begin{pmatrix} e^{-\beta E_1} & 0 & \cdots & 0 \\ 0 & e^{-\beta E_2} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & e^{-\beta E_N} & 0 \end{pmatrix} \tag{38}$$

with $Z$ serving as a normalization constant.

### Rotations of Two-Component Systems

In a two-component system, all operators can be written as a linear combination of the Pauli $\sigma$ matrices and the unit matrix.

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}. \tag{39}$$

As we will see later, these matrices behave like 3-dimensional rotations. For now, we only notice that each matrix is Hermitian and that when squared gives the unit matrix.

A rotation of a photon's polarization about the $z$ axis in the basis described above can be written as

$$\mathcal{R}(\theta) = e^{i\theta\sigma_y}, \tag{40}$$

while for rotating a spin 1/2 particle about the $y$ axis is

$$\mathcal{R}(\theta) = e^{i\theta\sigma_y/2}. \tag{41}$$

Furthermore, it is easy to see that

$$e^{i\theta\sigma_y} = \cos\theta + i\sin\theta\sigma_y \tag{42}$$

This trick comes in handy for a large number of physics examples, not just rotations.

**Examples**:

1. Photons, travelling along the $z$ axis can be polarized either linearly along the $x$ or $y$ axis, or a linear combination of the two states. Write the operator that rotates the states by 45° about the $z$ axis in terms of $|x\rangle$ and $|y\rangle$.

2. Choosing the basis,
$$|x\rangle \to \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |y\rangle \to \begin{pmatrix} 0 \\ 1 \end{pmatrix},$$
write the matrix that rotates the states by $\theta$.

3. Right-hand circularly polarized (RCP) light is made of a linear combination of $x$ and $y$ polarized light.
$$|R\rangle = \frac{1}{\sqrt{2}}\left(|x\rangle + i|y\rangle\right).$$
Light travelling along the $z$ axis passes through a thin slab of thickness $t$ whose index of refraction, $k = n\omega/c$, is different for light polarized in the $x$ and $y$ directions. In terms of $n_x$, $n_y$ and $t$ find the polarization of light which entered the slab as right-circularly polarized.

4. Find the density matrix for right-circularly polarized light in the basis defined above.

5. Using the basis described above, write the density matrix for light that is an incoherent mixture, 50% polarized along the $x$ direction and 50% along the $y$ direction.

6. Given that the $\sigma$ matrices satisfy anticommutation relations,
$$\{\sigma_i, \sigma_j\} = 2i\epsilon_{ijk}\sigma_k,$$
Show that for any unit vector $\hat{n}$,
$$|\vec{\sigma} \cdot \hat{n}|^2 = 1,$$
and that
$$e^{i\theta\sigma\cdot\hat{n}} = \cos(\theta) + i\sin\theta\sigma\cdot\hat{n}.$$

7. Considering a photon's polarization, calculate $\langle x|\mathcal{R}(\theta)|x\rangle$ for $\theta{=}\pi/2, \pi, 2\pi$, where the rotation is about the $z$ axis.

8. For a spin 1/2 particle, calculate $\langle z, +|\mathcal{R}(\theta)|z, +\rangle$, for the same angles when the rotation is about the $y$ axis.

# 1 Evolution in time

States evolve in time as

$$|\psi(t')\rangle = U(t,t')|\psi(t)\rangle, \tag{1}$$

where $U$ is a unitary matrix known as the evolution operator. The unitarity is necessary to preserve probability throughout time. In order for $U$ to be unitary, the state must evolve as

$$\frac{\partial}{\partial t}|\psi(t)\rangle = -iH(t)|\psi(t)\rangle, \tag{2}$$

or equivalently,

$$\frac{\partial}{\partial t}U(t,t') = -iH(t)U(t,t'), \tag{3}$$

where $H(t)$ is a Hermitian matrix, referred to as the Hamiltonian. Either of these equations could be referred to as Schroedinger's equation. One can see that the restriction that $H$ is Hermitian is necessary to ensure unitarity by integrating $U$ forward in time by a small amount, $\Delta t$.

$$U(t+\Delta t,t') = U(t,t') - iH(t)\Delta t U(t,t'). \tag{4}$$

The product $U^\dagger U$ only gives unity if $H$ is Hermitian. Thus, Schrödinger's equation is merely a statement that states must evolve in such a way as to preserve probability.

## 1.1 Two-component problems

Many problems in quantum mechanics can be reduced to two-state problems. Aside from the "spin-up spin-down" problem, the two-kaon problem (see Baym), the solar neutrino problem along with many other examples are really simple manifestations of the two-state problem.

The two-state problem is especially nice because all two-by-two matrices can be written in terms of the unit matrix and the three sigma matrices,

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} , \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} , \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} . \tag{5}$$

These matrices are Hermitian, traceless, and obey simple commutation relations,

$$[\sigma_i, \sigma_j] = 2i\epsilon_{ijk}\sigma_k. \tag{6}$$

In fact, as we will see later, the matrices $\vec{\sigma}/2$ obey the same commutation rules as angular momentum. Additionally, the square of any $\sigma$ matrix is unity,

$$(\vec{\sigma}\cdot\hat{n})^2 = \mathbf{1} \tag{7}$$

The evolution of states under a Hamiltonian,

$$H = \beta\vec{\sigma}\cdot\hat{n}, \tag{8}$$

is especially simple. In this case the evolution operator is

$$\begin{aligned} U(t) &= e^{-iHt/\hbar} && (9)\\ &= 1 - i\beta t\vec{\sigma}\cdot\hat{n} + \left(-i\beta t\vec{\sigma}\cdot\hat{n}\right)^2/2! + \left(i\beta t\vec{\sigma}\cdot\hat{n}\right)^3/3! + \cdots && (10)\\ &= \cos(\beta t) - i\vec{\sigma}\cdot\hat{n}\sin(\beta t) && (11)\end{aligned}$$

**Example Problem:**
A spin-up(along the z-axis) particle is placed in an environment at $t=0$ where it interacts with a magnetic field pointed along the $x$ axis,

$$H = \beta\sigma_x. \tag{12}$$

Find the probability of being in the "up" state as a function of time.

**Solution**:

$$\begin{aligned} \psi(t) &= e^{-iHt/\hbar}\psi(0) && (13)\\ &= \left(\cos(\beta t) - i\sin(\beta t)\sigma_x\right)\begin{pmatrix}1\\0\end{pmatrix} && (14)\\ &= \begin{pmatrix}\cos(\beta t)\\ -i\sin(\beta t)\end{pmatrix}. && (15)\end{aligned}$$

Thus the probability of being in the "up" state is $\cos^2(\beta t)$.

**Another Example:**
Two species of neutrinos, the $\nu_\mu$ and $\nu_\tau$ have masses $m_\mu$ and $m_\tau$. The Hamiltonian that describes these masses could be written:

$$H_0 = \begin{pmatrix} m_\mu c^2 & 0\\ 0 & m_\tau c^2\end{pmatrix}. \tag{16}$$

Now, we consider an extra term added to the Hamiltonian that mixes the two flavors of neutrinos,

$$H_{\text{mix}} = \begin{pmatrix} 0 & \alpha c^2\\ \alpha c^2 & 0\end{pmatrix}. \tag{17}$$

First, let us find the energy of two new states. We do this by first writing the Hamiltonian in terms of the sigma matrices.

$$\begin{aligned} H &= \frac{1}{2}(m_\mu + m_\tau)c^2\mathbf{1} + \frac{1}{2}(m_\mu - m_\tau)c^2\sigma_z + \alpha c^2\sigma_x && (18)\\ &= \frac{1}{2}(m_\mu + m_\tau)c^2\mathbf{1} + \beta c^2\vec{\sigma}\cdot\hat{n}. && (19)\end{aligned}$$

Here, $\beta$ is the "magnitude" of the two terms that multiply sigma matrices,

$$\beta = \sqrt{\alpha^2 + (m_\tau - m_\mu)^2}, \tag{20}$$

and $\hat{n}$ is a unit vector pointing in the direction,

$$\hat{n} = \hat{z}\cos\theta + \hat{x}\sin\theta \tag{21}$$

$$\sin\theta = \frac{\alpha}{\beta} \tag{22}$$

Finding the eigenvalues is simply a matter of rotating the $\sigma$ matrices such that $\hat{n}$ is in the $z$ direction. The two energies are then,

$$E_{\pm} = \frac{1}{2}(m_\mu + m_\tau)c^2\mathbf{1} \pm \beta c^2. \tag{23}$$

**Heisenberg and Schrödinger representations:**

Usually, one wishes to caculate expectations of operators, e.g. $\langle\phi|AB\cdots C|\psi\rangle$, where the states evolve as a function of time, but the states are considered independent of time. Considering an evolution operator, $U = e^{-iHt/\hbar}$, one can express the time development of the expectation of $AB\cdots C$ in either of two equivalent representations,

$$\langle\phi(t)|AB\cdots C|\psi(t)\rangle = \langle\phi(0)|U^\dagger AB\cdots CU|\psi(0)\rangle \tag{24}$$

$$= \langle\phi(0)|\ U^\dagger AU\ U^\dagger BU\ \cdots U^\dagger CU\ |\psi(0)\rangle. \tag{25}$$

The upper line, Eq. (**??**), known as the Schrödinger representation, with the states evolving while the operators are fixed.

In the Heisenberg representation, the time development of the operators can be written as a differential equation, where the rate of change of the operator is given by the commutation of the Hamiltonian with $A$.

$$A_H(t) \equiv U^\dagger A_S(t)U(t) \tag{26}$$

$$\frac{\partial A_H(t)}{\partial t} = \frac{\partial}{\partial t}U^\dagger(t,t')A_S(t)U(t,t') \tag{27}$$

$$= iU^\dagger(t,t')[H(t),A_S]U(t,t') + U^\dagger(t,t')\left(\frac{\partial}{\partial t}A_S(t)\right)U(t,t'). \tag{28}$$

Here, the subscripts $S$ and $H$ refer to Schrödinger and Heisenberg representations respectfully. If there is no explicit time dependence in $A_S$, then any operator that commutes with the Hamiltonian represents a constant of the motion. The most obvious such operator is $H$ itself. Thus, if the Hamiltonian has no explicit time dependence, the expectation of $H$, a.k.a. the energy, is a constant of the motion.

The spin-precession example from above could also have been written as a differential equation. In that case, the time development of $\sigma_z$ and $\sigma_y$ could be written as,

$$\frac{\partial}{\partial t}\sigma_z(t) = i\beta U^\dagger[\sigma_x,\sigma_z]U = 2\beta\sigma_y(t) \tag{29}$$

$$\frac{\partial}{\partial t}\sigma_y(t) = i\beta U^\dagger[\sigma_x,\sigma_y]U = -2\beta\sigma_z(t), \tag{30}$$

or equivalently,

$$\frac{\partial^2}{\partial t^2}\sigma_z(t) = -4\beta\sigma_z(t). \tag{31}$$

Thus,

$$\langle \sigma_z(t) \rangle = \cos 2\beta t, \tag{32}$$

if the initial spin is along the $z$ axis. This is the same result as seen above in Eq. (**??**).

Finally, we should point out that for any two Hermitian operators $\mathcal{A}$ and $\mathcal{B}$ that commute, a set of states can be found that are eigenstates of both $\mathcal{A}$ and $\mathcal{B}$. To see this, consider eigenstates of $\mathcal{B}$,

$$\mathcal{B}|b\rangle = b|b\rangle. \tag{33}$$

If $\mathcal{A}$ and $\mathcal{B}$ commute,

$$\langle b'|\,[\mathcal{A},\mathcal{B}]\,|b\rangle = 0 = (b - b')\langle b'|\mathcal{A}|b\rangle. \tag{34}$$

Thus the operator $\mathcal{A}$ does not mix states with different eigenvalues of $\mathcal{B}$. Or in other words, one can take the subset of states which have a given eigenvalue $b$, and this set should provide a basis for simultaneously diagonalizing $\mathcal{A}$.

The implications of this simple statement are profound. For example if the angular momentum operator operator $\mathcal{L}_z$ commutes with the Hamiltonian, the subset of states with the same eigenvalue of $\mathcal{L}_z$, usually denoted by $m$, can be considered by themselves while diagonalizing the Hamiltonian.

# 1 Coordinate and momentum space

One of the most famous equations in physics is Schrödinger's wave equation.

$$i\frac{\partial}{\partial t}\psi(x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) + V(x)\psi(x). \tag{1}$$

Rather than thinking of $\psi(x)$ as a wave function, it is more revealing to recognize it as overlap of the state $\psi\rangle$ with the state $|x\rangle$.

$$\psi(x) = \langle x|\psi\rangle. \tag{2}$$

The only difference between a label in coordinate space and a label that denotes a discrete variable such as spin, is that since the $x$ label is continuous, the normalization has to be changed.

$$\langle x'|x\rangle = \delta(x - x'). \tag{3}$$

This infers that $|x\rangle$ has dimensions of inverse length to the one-half power. The completenes relation becomes

$$\int \langle\phi|x\rangle\langle x|\psi\rangle dx = \langle\phi|\psi\rangle. \tag{4}$$

Next, we wish to show that the Schrödinger equation is merely the continuum limit of a matrix equation where $\psi_0, \psi_1 \cdots \psi_N$ will represent $\psi(x)$ at $x = 0, \delta x, 2\delta x \cdots$. To do this we write the second derivative as

$$\begin{aligned} \frac{\partial^2}{\partial x^2}\psi(x) &= \lim_{\delta x \to 0} \frac{\partial}{\partial x}\frac{\psi(x + \delta x/2) - \psi(x - \delta x/2)}{\delta x} && (5)\\ &= \lim_{\delta x \to 0} \frac{\psi(x + \delta x) - 2\psi(x) + \psi(x - \delta x)}{\delta x^2}. && (6) \end{aligned}$$

Thus, by making the substitution,

$$\psi(x) \to \psi_i \frac{1}{\sqrt{\delta x}}, \tag{7}$$

one may rewrite Schrödinger's equation in terms of discrete vectors,

$$i\frac{\partial}{\partial t}\psi_i = -\frac{\hbar^2}{2m\delta x^2}\psi_i + V(x)\psi_i. \tag{8}$$

The normalizations are:

$$\begin{aligned} \sum_i |\psi_i|^2 &= 1 && (9)\\ \int dx|\psi(x)|^2 &= 1. && (10) \end{aligned}$$

For the discrete case, one may also write the Hamiltonian as matrix.

$$H = -\frac{\hbar^2}{2m\delta x^2}\begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdots & -2 & 1 & \cdot & \cdots \\ \cdots & 1 & -2 & 1 & \cdots \\ \cdots & \cdot & 1 & -2 & \cdots \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix} + \begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdots & V(x_{i-1}) & 0 & 0 & \cdots \\ \cdots & 0 & V(x_i) & 0 & \cdots \\ \cdots & 0 & 0 & V(x_{i+1}) & \cdots \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}. \tag{11}$$

Here, the potential term is diagonal while the kinetic term is barely band diagonal.

**Momentum states:**

A momentum state is no more than a linear combination of coordinate-space states,

$$|p\rangle = \int dx e^{ipx/\hbar}|x\rangle. \tag{12}$$

With this definition of the state $|p\rangle$, the normalization becomes

$$\langle p'|p\rangle = 2\pi\hbar\delta(p-p'), \tag{13}$$

and the inverse transformation is

$$|x\rangle = \frac{1}{2\pi\hbar}\int dp e^{-ipx/\hbar}|p\rangle. \tag{14}$$

Expressed as a completeness relation,

$$\int \frac{dp}{(2\pi\hbar)}\langle\phi|p\rangle\langle p|\psi\rangle = \langle\phi|\psi\rangle. \tag{15}$$

Changing the problem to $n$ dimensions only affects the expressions here by changing $(2\pi\hbar)$ to $(2\pi\hbar)^n$.

The label $p$ here refers to a continuum of momentum states. If a system is confined, then no eigenstate of the momentum operator really exists. In that case discrete states are possible. Sometimes, the label $p$ is used for discrete states in which case the normalizations are different. It is the duty of the watchful reader to accurately interpret the notation.

**The momentum and position operators:**

The momentum and position operators can be expressed as,

$$\mathcal{X} = \int dx x|x\rangle\langle x| \tag{16}$$

$$\mathcal{P} = \int \frac{dp}{2\pi\hbar}p|p\rangle\langle p|. \tag{17}$$

From the definition of $\mathcal{X}$, one can see that

$$\langle\phi|\mathcal{X}|\psi\rangle = \int dx\phi^*(x)x\psi(x). \tag{18}$$

One can also perform a similar operation with the momentum operator.

$$\langle\phi|\mathcal{P}|\psi\rangle = \int \frac{dp}{2\pi\hbar}\phi^*(p)p\psi(p). \tag{19}$$

However, the customary way to view the momentum operator is not in momentum space, but as a derivative in coordinate space. Expanding $|p\rangle$ in terms of coordinate space states, one can see that

$$\langle\phi|\mathcal{P}|\psi\rangle = \int dxdy\frac{dp}{2\pi\hbar}\langle\phi|x\rangle e^{ip(x-y)/\hbar}p\langle y|\psi\rangle. \tag{20}$$

The factor $p$ can be changed into a derivative of the phase $e^{ipy/\hbar}$ with respect to y, then through integration by parts changed into a derivative of $\psi(y)$ with respect to $y$,

$$\begin{aligned} \langle\phi|\mathcal{P}|\psi\rangle &= \int dxdy\frac{dp}{2\pi\hbar}\langle\phi|x\rangle e^{ip(x-y)/\hbar} - i\hbar\frac{\partial}{\partial y}\langle y|\psi\rangle. && (21) \\ &= \int dx\phi^*(x)\left(-i\hbar\frac{\partial}{\partial x}\psi(x)\right) && (22) \\ &= \int dx\left(i\hbar\frac{\partial}{\partial x}\phi^*(x)\right)\psi(x), && (23) \end{aligned}$$

Thus the momentum operator can be thought of a $i\hbar\partial/\partial x$. One also sees that commuting $\mathcal{P}$ with $\mathcal{X}$ yields,

$$[\mathcal{P},\mathcal{X}] = -i\hbar. \tag{24}$$

# 1 Potential Problems in One Dimension

Consider Schrödinger's wave equation,

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

If $\Psi(x,t)$ is an eigenstate of the Hamiltonian, the solution becomes

$$\Psi(x,t)=e^{-iEt/\hbar}\psi(x), \tag{2}$$

and the time derivative $i\partial/\partial t$ can be replaced by $E$ in Schrödinger's wave equation. For the most part, we will consider the steady-state case where we look for eigenstates.

---

**Aside:**

Before we find solutions, we regress to consider the notation and vocabulary associated with Schrödinger's equation. One often refers to the Hamiltonian in this context,

$$H\psi(x)=E\psi(x), \quad H\psi(x)=\left\{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)\right\}psi(x). \tag{3}$$

This notation is actually incorrect, as it does not represent the fact that the Hamiltonian is an operator. More correctly the left hand side of the above equation should be replaced by

$$H\psi(x)\rightarrow\langle x|H|\psi\rangle. \tag{4}$$

However, this clumsiness usually does not cause problems and we will not go out of our way to avoid it.

---

To find solutions for problems where the potential is continuous, it is sufficient to find solutions to the wave equation that have the correct behavior at $x\rightarrow\pm\infty$. If the potential is discontinuous at certain points, boundary conditions must be enforce at every point where a discontinuity is formed.

If the discontinuity is finite (not a delta function), the boundary conditions at the discontinuity are that

1. $\psi(x)$ is continuous.
2. $\partial/\partial x\ \psi(x)$ is continuous.

If the first derivative were discontinuous at $y$, the second derivative would be infinite at that point. To understand the boundary conditions we integrate Schrödinger's equation from $x_a$ to $x_b$,

$$-\frac{\hbar^2}{2m}\left(\frac{\partial}{\partial x}\psi(x)|_{x_b}-\frac{\partial}{\partial x}\psi(x)|_{x_a}\right)=\int_{x_a}^{x_b}dx(E-V(x))\psi(x). \tag{5}$$

We now consider a discontinuity at $y$, and perform the integral over an infinitesimal range centered about $y$. If the potential is finite one obtains

$$-\frac{\hbar^2}{2m}\left(\frac{\partial}{\partial x}\psi(x)|_{y+\epsilon}-\frac{\partial}{\partial x}\psi(x)|_{y-\epsilon}\right)=0, \tag{6}$$

thus demonstrating the requirement that the derivative be continuous. However, if the potential is a delta function, integrating the right-hand side of Eq. (**??**) over the infinitesimal range can yield a finite value. Thus, if

$$V(x)=\beta\delta(x-y), \tag{7}$$

the boundary condition becomes

$$-\frac{\hbar^2}{2m}\left(\frac{\partial}{\partial x}\psi(x)|_{x+\epsilon}-\frac{\partial}{\partial x}\psi(x)|_{y-\epsilon}\right)=-\beta V(y)\psi(y). \tag{8}$$

For the remainder of this lecture, we merely consider a large number of potential examples.

**Square Well Example:**

Consider the potential,

$$V(x)=\left\{\begin{array}{cc}\infty, & x<0\\ -V_0, & 0<x<a\\ 0, & x>a\end{array}\right. \tag{9}$$

Solve for the binding energy and wave function of the lowest energy state:

**Solution:** Assume the energy is negative. In the region of the well solutions of Schrödinger's equation are sines and cosines with wave number, $k=\sqrt{(2m(V_0-B)/\hbar^2)}$, where $B$ is the binding energy (a positive number). The BC at the origin is that the wave function must go to zero due to the infinite potential. Thus, only the sine piece remains,

$$\psi_I(x)=\sin(kx). \tag{10}$$

We have chosen an arbitrary normalization constant of unity.

In the second region, exponentially growing/decaying solutions work with a decay constant of $q=\sqrt{(2mB/\hbar^2)}$. The exponentially growing piece can be thrown out as we wish to find a solution where some probability is near the origin.

$$\psi_{II}(x)=Ae^{-qr} \tag{11}$$

Thus far we have neglected the two BCs at $x=a$, which will be sufficient to determine the two unknowns, the binding energy $B$ and the normalization factor $A$. Writing the two BCs,

$$\begin{aligned}\sin(ka) &= Ae^{-qa} & (12)\\ k\cos(ka) &= -qAe^{-qa} & (13)\end{aligned}$$

Dividing the two BCs eliminates $A$ and gives the relation,

$$\tan(ka) = \frac{-k}{q}. \tag{14}$$

This is a transcendental equation for $B$ which can be solved graphically or on the computer.

One can see that the solution disappears if the depth, $V_0$ is too low or if the the width $a$ is too narrow. At this point the solution has binding energy zero and from the previous equation one can see that $\tan(ka) = \infty$, or $ka = \pi/2$, with $k = \sqrt{2mV_0/\hbar^2}$. One physical way to understand the constraint is that the wave function $\sin(kx)$ must turn over and have a negative slope at $x = a$ in order to match to an exponentially falling solution. Thus $ka$ must be larger than $\pi/2$.

It is worthwhile to note that if a potential remains below zero everywhere, that there is always at least one bound state. In this case, the potential is infinite for $x < 0$.

**Delta Function Example:**

Consider the potential,

$$V(x) = -\beta\delta(x), \quad \beta > 0. \tag{15}$$

Find the binding energy of the bound state.

**Solution:** Assume the existence of a bound state of binding energy $B$. The solutions are exponentials with decay constant $k = \sqrt{2mB/\hbar^2}$, and the requirement that they go to zero at $x = \pm\infty$ gives

$$\psi(x) = \begin{cases} \exp(-kx) & x > 0 \\ \exp(kx) & x < 0 \end{cases} \tag{16}$$

Plugging them into the BC at $x = 0$, Eq. (**??**), gives

$$\frac{\hbar^2 k}{m} = \beta. \tag{17}$$

Thus the binding energy is $m\beta^2/(2\hbar^2)$.

**Barrier Penetration:**

Consider a plane wave incident on a positive barrier,

$$V(x) = \begin{cases} 0, & x < 0 \\ V_0, & x > 0 \end{cases} \tag{18}$$

Find the reflection and transmission probabilities for a particle with energy $E$ which is greater than $V_0$.

**Solution:**

Solutions must be of the form,

$$\psi_I(x) = e^{ikx} + Ae^{-ikx}, \; k = \sqrt{2mE/\hbar^2} \tag{19}$$

$$\psi_{II}(x) = Be^{iqx}, \; q = \sqrt{2m(E - V_0)/\hbar^2} \tag{20}$$

The reflection probability is $|A|^2$. The transmission probability is $1-|A|^2$ which should equal the ratio of the fluxes, $(q/k)|B/A|^2$.

The BCs yield

$$\begin{aligned} 1+A &= B \quad (21)\\ k(1-A) &= qB \quad (22)\end{aligned}$$

Here, $k$ and $q$ are known, and the unknowns are $A$ and $B$. Solving for $A$ and $B$,

$$A = \frac{k-q}{k+q}, \quad B = \frac{2k}{k+q} \quad (23)$$

Thus, one quickly obtains the reflection and transmission probability. In order to check the answer, one can see that the outgoing fluxes sum to the incoming flux.

$$k|A|^2 + q|B|^2 = k. \quad (24)$$

### Expanding to more dimensions and Electro-Magnetic Couplings:

In more dimensions the look of Schrödinger's equation is similar, with the second derivative becoming $\nabla^2$. The wave packets then become $\exp(i\vec{p}\cdot\vec{r})$, and all is pretty simple, until a potential is added. Then one, must find a bag with a whole new set of tricks.

Adding the electromagnetic coupling to Schrödinger's wave equation is straight forward. One simply replaces $-i\hbar\nabla$ with $-i\hbar\nabla - e\mathbf{A}/c$ and $i\hbar\partial/\partial t$ with $i\hbar\partial/\partial t - e\Phi$. This is referred to as "minimal substitution" with $\mathbf{A}$ and $\Phi$ being the electromagnetic vector and scalar fields. The coupling $e$ must change sign if the charge of the particle is reversed.

Schrödinger's wave equation then becomes:

$$\frac{(-i\hbar\nabla - e\mathbf{A}(\mathbf{r},t)/c)^2}{2m}\psi(x,t) + V(\mathbf{r},t)\psi(\mathbf{r},t) + e\Phi(\mathbf{r},t)\psi(\mathbf{r},t) = i\hbar\partial/\partial t\psi(\mathbf{r},t) \quad (25)$$

We will consider the EM case in greater detail later in the course.

# 1 Wave Packets

A plane wave can be written as

$$\psi_k(x) = \frac{1}{\sqrt{V}} e^{ikx/\hbar}, \tag{1}$$

which is normalized in the volume $V$, but is not really an eigenstate of the momentum operator due to the sharp cutoff at the boundaries.

A more physical description is a wave packet, which is described by not just a momentum, as it represents a spread of momenta described by a function $g$.

$$\psi_k(x) = \int \frac{dp}{2\pi\hbar} e^{ipx/\hbar} g(p-k). \tag{2}$$

For our purposes we will consider $g$ to be of Gaussian shape,

$$g(p-k) = \alpha \exp\left(\frac{-(p-k)^2}{4\Delta^2}\right). \tag{3}$$

As an exercise, one should check that this resulting wave packet is properly normalized by

$$\alpha = (2\pi)^{1/4}\sqrt{\frac{\hbar}{\Delta}} \tag{4}$$

By inspection, one sees that the width of the wave packet in momentum space is $\Delta$. To understand the spatial shape of the packet, one can see that

$$|\psi(x)|^2 = \frac{1}{\sqrt{2\pi}} \frac{2\Delta}{\hbar} \exp - \frac{(2\Delta)^2}{\hbar^2} \frac{x^2}{2}, \tag{5}$$

which is also of Gaussian form, with the spread being $\hbar/(2\Delta)$.

Thus the product of the spread in momentum space multiplied by the spread in coordinate space is $\hbar/2$. If the packet had been described with $x - x_0$ instead of $x$, the packet would be centered at $x_0$ instead of the origin.

If we consider the wave packet at arbitrary times,

$$\psi_k(x,t) = \int \frac{dp}{2\pi\hbar} e^{-Et/\hbar + ipx/\hbar} g(p-k), \tag{6}$$

We expect the packet to move in time. The packet has contributions from all momenta which make differential additions with a wide variety of phases. At every time $t$ there is a point $x$ for which the phases are constant in the region near $k$. At this point, the differential contributions add in-phase and the wave function in coordinate space is a maximum. To find that point we take a derivative of the phase factor with respect to $p$ at $k$, and require it to be zero.

$$\frac{\partial}{\partial p}(-iE_p t + ipx)|p = k = 0. \tag{7}$$

Given that $dE/dp = v$, even for relativistic particles, one sees that

$$x = vt \tag{8}$$

which is not too surprising.

**Reflecting a wave packet and time delays:**

As an example where wave packets are involved, we will consider a packet as described above, incident on a potential barrier,

$$V(x) = \begin{cases} 0, & x > 0 \\ V_0, & x < 0 \end{cases} \tag{9}$$

We also assume that the packet is narrow and that $V_0$ is larger than $E_k$.

The incoming wave packet can have the form,

$$\psi_{\text{in}}(x,t) = -\frac{2\pi\hbar}{\Delta} \int dp e^{-iE_p t - ipx} e^{-2i\delta(p)} g(p-k). \tag{10}$$

Such a packet should have a reflection, with the reflected wave packet looking like

$$\psi_{\text{out}}(x,t) = -\frac{2\pi\hbar}{\Delta} \int dp e^{-iE_p t + ipx} e^{+2i\delta(p)} g(p-k). \tag{11}$$

The negative sign is chosen so that in the limit of an infinite potential $\delta(p) = 0$. The reflected packet has the same amplitude, but with a phase factor that might be momentum dependent. The factor of two in the phase is a convention which we will encounter again when we discuss scattering theory.

Looking for the point $x$ where the phase is stationary, one finds the expression

$$x = vt - 2\frac{d}{dp}\delta(p). \tag{12}$$

Thus the packet has a lag in space, or a delay in time, which may be expressed as

$$\Delta x = -2\hbar \frac{d}{dp}\delta(p) \qquad \Delta t = -2\hbar \frac{d}{dE}\delta(E). \tag{13}$$

This time delay is relative to the case where $V_0 = \infty$.

**The Uncertainty Principle:**

When two operators do not commute, one can not usually specify states which are eigenstates of both operators. An example of such operators are momentum and position.

Proof: Consider two operators, $\Delta A$ and $\Delta B$,

$$\Delta A = A - \langle\psi|A|\psi\rangle, \quad \Delta B = B - \langle\psi|B|\psi\rangle. \tag{14}$$

Now, we consider states $|\alpha\rangle$ and $|\beta\rangle$,

$$|\alpha\rangle = \Delta A|\psi\rangle, \quad |\beta\rangle = \Delta B|\psi\rangle. \tag{15}$$

The Schwarz inequality,

$$\langle\alpha|\alpha\rangle\langle\beta|\beta\rangle \geq |\langle\alpha|\beta\rangle|^2, \tag{16}$$

can then be applied to give

$$\langle\psi|(\Delta A)^2|\psi\rangle\langle\psi|(\Delta B)^2|\psi\rangle \geq |\langle\psi|\Delta A\Delta B|\psi\rangle|^2. \tag{17}$$

Furthermore, one may rewrite the product

$$\langle\phi|\Delta A\Delta B|\psi\rangle = \frac{1}{2}\langle\psi|[A,B]|\psi\rangle + \frac{1}{2}\langle\psi|\{\Delta A,\Delta B\}|\psi\rangle, \tag{18}$$

where the first term is purely imaginary while the second term is purely real, which means that it square can be written as the sum of the squares of each side and,

$$\langle\psi|\Delta A\Delta B|\psi\rangle|^2 = \frac{1}{4}\langle\psi|[A,B]|\psi\rangle|^2 + \frac{1}{4}|\langle\psi|\{\Delta A,\Delta B\}|\psi\rangle|^2. \tag{19}$$

The term with the anti-commutator is greater than zero, thus we only strengthen the uncertainty relation by ignoring it,

$$\langle\psi|(\Delta A)^2|\psi\rangle\langle\psi|(\Delta B)^2|\psi\rangle \geq \frac{1}{4}\langle\psi|[A,B]|\psi\rangle|^2. \tag{20}$$

For $P$ and $X$ operators this becomes

$$(\Delta p)^2(\Delta x)^2 \geq \left(\frac{\hbar}{2}\right)^2 \tag{21}$$

# 1 The Harmonic Oscillator

One of the most important problems in physics is the harmonic oscillator. In fact, quantum field theory considers every point in space to have it's own oscillator. We will start with a single oscillator with the Hamiltonian,

$$H = \frac{p^2}{2m} + \frac{m\omega^2}{2}x^2, \tag{1}$$

where the spring constant is expressed in terms of a frequency $\omega$. Here, $x$ and $p$ are operators.

Dirac's solution to the problem is to define two new operators,

$$a \equiv \sqrt{\frac{m\omega}{2\hbar}}x + i\sqrt{\frac{1}{2\hbar m\omega}}p, \quad a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}x - i\sqrt{\frac{1}{2\hbar m\omega}}p. \tag{2}$$

The operators are known as the annihilation (or destruction) and creation operators respectively for reasons to be seen below.

The operators satisfy simple commutation relations,

$$[a, a^\dagger] = 1, \tag{3}$$

which can be checked by substituting the expressions for $x$ and $p$ into the commutator. Furthermore, the Hamiltonian may be written as

$$H = \hbar\omega(a^\dagger a + \frac{1}{2}). \tag{4}$$

To see that the creation operator does exactly what is sounds like, consider an eigenstate of the Hamiltonian such that

$$a^\dagger a|n\rangle = n|n\rangle. \tag{5}$$

By using the commutation relations one can see that

$$a^\dagger a(a^\dagger|n\rangle) = (n+1)(a^\dagger|n\rangle) \tag{6}$$

by commuting the $a^\dagger$ to the far left. Performing the same trick with the state $a|n\rangle$ one finds

$$a^\dagger a(a|n\rangle) = (n-1)(a|n\rangle). \tag{7}$$

The operator $a^\dagger a$ is referred to as the number operator, and since the energy is expressed in terms of the number operator, and since that energy must not have negative values, one of the eigenstates must have eigenvalue $n = 0$. Otherwise, one could lower the number, and therefore the energy, to an arbitrarily low number by succesive operations of $a$.

Thus, one knows that eigenstates of the number operator are 0,1,2$\cdots$, but one does not yet know the normalization of the states.

To see the effect of the creation operators toward normalization, one considers the norm of the state $a^\dagger|n\rangle$, where $|n\rangle$ is a normalized state.

$$\langle n|aa^\dagger|n\rangle = n+1, \tag{8}$$

where one has commuted $a^\dagger$ past $a$. Therefore, one can see that the creation and destruction operators have the following effect on the normalization.

$$a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle, \quad a|n\rangle = \sqrt{n}|n-1\rangle \tag{9}$$

Note that the destruction operator returns zero when acting on the ground state, where $n=0$.

We will see later on that similar tricks are used with angular momentum raising and lowering operators.

Finally, it is straight-forward to find the ground state wave function if one is clever enough to guess that the form of the solution is a Gaussian.

$$\psi_0(x) = e^{-x^2/(2a^2)}. \tag{10}$$

For the moment, we neglect the normalization. To show that it is a solution we first take derivatives with respect to $x$.

$$\frac{d}{dx}\psi_0(x) = -\frac{x}{a^2}\psi_0(x), \quad \frac{d^2}{dx^2}\psi_0(x) = \frac{x^2}{z^4}\psi_0(x) - \frac{1}{a^2}\psi_0(x). \tag{11}$$

Plugging this into the Schrödinger equation,

$$-\frac{\hbar^2}{2m}\left[\frac{x^2}{a^4} - \frac{1}{a^2}\right]\psi_0(x) + \frac{m\omega^2}{2}\psi_0(x) = E\psi_0(x), \tag{12}$$

allows one to determine $a$ and $E$ by inspection.

$$a = \frac{\hbar}{m\omega}, \quad E = \frac{1}{2}\hbar\omega. \tag{13}$$

One may also calculate the normalization $Z$ by enforcing the constraint

$$\psi_0(x) = Z^{1/2}e^{-x^2/(2a^2)}, \quad 1 = Z\int_{-\infty}^{\infty} dx e^{-x^2/a^2}. \tag{14}$$

This gives $Z = 1/(\pi^{1/4}a^{1/2})$.

If one were to consider an $n$ dimensional problem,

$$H\Psi = -\frac{\hbar^2}{2m}\frac{d^2}{dx_1^2}\Psi - \frac{\hbar^2}{2m}\frac{d^2}{dx_2^2}\Psi \cdots - \frac{\hbar^2}{2m}\frac{d^2}{dx_n^2}\Psi + \frac{m\omega^2}{2}x_1^2\Psi + \frac{m\omega^2}{2}x_2^2\Psi \cdots + \frac{m\omega^2}{2}x_n^2\Psi, \tag{15}$$

one can write the solution as

$$\Psi(x_1, x_2, \cdots x_n) = \psi_1(x_1)\psi_2(x_2)\cdots\psi_n(x_n), \tag{16}$$

where $\psi_i$ are the solutions to the 1-d Schrödinger equation and

$$E = \frac{n}{2}\hbar\omega. \tag{17}$$

**Examples:**

1. Calculate $\langle 0|aaa^\dagger aa^\dagger a^\dagger|0\rangle$ and $\langle n|a^\dagger a^\dagger a^\dagger a|m\rangle$.
2. Find $\psi_1(x)$, the wave function of the first excited state by operating $a^\dagger$ on $\psi_0(x)$.

# 1 Interactions of a Charged Particle with the Electromagnetic Field

Electric and magnetic fields are determined by the vector potential **A** and scalar potential $\phi$,

$$\mathbf{E} = -\nabla\phi - \frac{1}{c}\frac{\partial \mathbf{A}}{\partial t}, \quad \mathbf{B} = \nabla \times \mathbf{A}. \tag{1}$$

The Hamiltonian for a charge $e$ (For a negative charge, $e < 0$) is written in terms of the vector and scalar potentials,

$$\begin{aligned} H &= \frac{1}{2m}\left(\mathbf{p} - \frac{e\mathbf{A}}{c}\right)^2 + e\phi \quad (2) \\ &= \frac{1}{2mi}\left[p^2 - \frac{e}{c}(\mathbf{p}\cdot\mathbf{A} + \mathbf{A}\cdot\mathbf{p}) + \left(\frac{e}{c}\right)^2 A^2\right] + e\phi \quad (3) \end{aligned}$$

Solving for the equations of motion,

$$\begin{aligned} \frac{d\mathbf{x}}{dt} &= \frac{[\mathbf{x}, H]}{i\hbar} \quad (4) \\ \frac{d}{dt}x_i &= \frac{1}{2mi\hbar}\left\{x_i(p_j - eA_j/c)(p_j - eA_j/c) - (p_j - eA_j/c)(p_j - eA_j/c)x_i\right\} \quad (5) \\ &= \frac{1}{2mi\hbar}\left\{x_i(p_j - eA_j/c)(p_j - eA_j/c) - (p_j - eA_j/c)x_i(p_j - eA_j/c) + (p_j - eA_j/c)(i\hbar\delta_{ij})\right\} \quad (6) \\ &= \frac{(p_i - eA_i/c)}{m}. \quad (7) \end{aligned}$$

As an exercise, one can solve for the "force" and find

$$m\frac{d^2\mathbf{x}}{dt^2} = e\left[\mathbf{E} + \frac{1}{2c}\left(\frac{d\mathbf{x}}{dt} \times \mathbf{B} - \mathbf{B} \times \frac{d\mathbf{x}}{dt}\right)\right]. \tag{8}$$

Note that since $dx/dt$ includes a derivative that the two similar terms in the brackets above can be different.

As was shown in a previous homework assignment, the density,

$$\rho(\mathbf{x}, t) = \psi^*(\mathbf{x}, t)\psi(\mathbf{x}, t), \tag{9}$$

and current density

$$\mathbf{j}(\mathbf{x}, t) \equiv \frac{-i\hbar}{2m}\left(\psi^*\nabla\psi - (\nabla\psi^*)\psi\right) - \left(\frac{e}{mc}\right)\mathbf{A}|\psi|^2 \tag{10}$$

satisfy the continuity equation,

$$\frac{\partial}{\partial t} + \nabla\cdot\mathbf{j} = 0. \tag{11}$$

Also, from the previous homework, remember that gauge transformations,

$$\mathbf{A} \rightarrow \mathbf{A} + \nabla\Lambda(\mathbf{x}, t), \quad \phi \rightarrow \phi - \frac{1}{c}\frac{\partial\Lambda(\mathbf{x}, t)}{\partial t}, \tag{12}$$

yield a new Hamiltonian, whose solutions are identical to the old Hamiltonians with an extra phase added

$$\psi(\mathbf{x}, t) \rightarrow \exp\left[\frac{ie\Lambda(\mathbf{x}, t)}{\hbar c}\right]\psi(\mathbf{x}, t) \tag{13}$$

### Circular Motion in a Magnetic Field

A constant magnetic field in the $z$ direction can be described with the vector potentials,

$$A_z = 0,\ A_\rho = 0,\ A_\phi = \rho B, \tag{14}$$

which has a nice symmetry as the vector potential winds around the $z$ axis, or through a gauge transformation,

$$A_y = Bx,\ A_x = 0, A_z = 0. \tag{15}$$

This appears to violate the symmetry but yields the identical magnetic field. The advantage is that it is easy to solve. The wave function can be written in the form

$$\psi(x, y, z) = e^{ik_z z + ik_y y}\phi(x) \tag{16}$$

because both $P_y$ and $P_z$ commute with the Hamiltonian.

The differential equation for $\phi$ then turns out to be

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\phi(x) + \frac{e^2B^2}{2mc^2}(x - x_0)^2\phi(x) = E_{xy}\phi(x), \tag{17}$$

where $E_{xy} = E - \hbar^2 k_z^2/(2m)$, and

$$x_0 \equiv \hbar k_y c/(eB) \tag{18}$$

But this is the harmonic oscillator Hamiltonian with

$$\omega = \frac{eB}{mc}, \tag{19}$$

the usual expression for a classical particle.

The solutions thus look like a particle whose $x$ position is centered about $x_0$, which is determined by $k_y$ and whose position in the $y$ and $z$ directions are simply uniform. Furthermore, it seems odd that a particle with circular motion would be an eigenstate of $P_y$.

The solution to the paradox is that if $P_y$ is constant, that means

$$mv_y + eBx/c = \text{constant}, \tag{20}$$

and in fact this does describe circular motion centered about a point $(x_c, y_c)$, where $x_c$ is determined by the constant but $y_c$ could be anything. Thus the solution is a linear combination of circular orbits, all centered about points with different $y$ values.

### Landau Levels

The motion in the $x - y$ plane has discrete solutions with eigenvalues,

$$E = \frac{\hbar^2 k_z^2}{2m} + (n + 1/2)\hbar\omega, \tag{21}$$

where $\omega$ is the cyclotron frequency described above.

These levels will play the central role in describing the integral quantum Hall effect which we will discuss next semester.

# 1 Path Integrals and the Aharanov-Bohm Effect

## 1.1 Path Integrals

One way to perform Quantum Mechanics is through path integrals. Path integrals are usually a rather inconvenient way to go, but sometimes come in handy. The name refers to the fact that a sum over all intermediate states can be thought of as a path. To get a better idea we consider the matrix element

$$\langle\psi_f|e^{-iHt}|\psi_i\rangle = \sum_{x_1\cdots x_{N-1}} \langle\psi_i|e^{-iH\delta t}|x_{N-1}\rangle\langle x_{N-1}|\cdots|x_2\rangle\langle x_2|e^{-iH\delta t}|x_1\rangle\langle x_1|e^{-iH\delta t}|\psi_i\rangle \tag{1}$$

$$\approx \sum_{x_1\cdots x_{N-1}} \langle\psi_f|(1-iH\delta t)|x_{N-1}\rangle\langle x_{N-1}|\cdots|x_2\rangle\langle x_2|(1-iH\delta t)|x_1\rangle\langle x_1|(1-iH\delta t)|\psi_i\rangle \tag{2}$$

Here, $\delta t = t/N$ and the approximation becomes exact in the limit of large $N$.

If the states $x_n$ correspond to positions in coordinate space arranged in a mesh of size $\delta x$, the succesive points in the path, $x_i$ and $x_{i+1}$, are constrained to be neighbors since $H$ is local. That means that each term in the sum can be thought of as a continuous trajectory where any at each step in time the trajectory either remains at the same position or moves by $\pm\delta x$. This motivates the name *path integral*, though one might more accurately state that one sums over all trajectories rather than over all paths.

The classical limit of quantum mechanics comes from the constraint of choosing the trajectory for which the phase becomes fixed with respect to small variations of the trajectory. We will not pursue this further.

In principle, all matrix elements can be considered in this fashion. Lattice gauge theory, which provides a powerful tool for numerically calculating the structure of the non-perturbative QCD vacuum, is built upon exactly such concepts. Path integral techniques are also often used in statistical mechanics by making the analagous decomposition,

$$e^{-\beta H} = \sum_{\alpha_1\cdots\alpha_{N-1}} e^{-\delta\beta H}|\alpha_{N-1}\rangle\langle\alpha_{N-1}|\cdots|\alpha_2\rangle\langle\alpha_2|e^{-\delta\beta H}|\alpha_1\rangle\langle\alpha_1|e^{-\delta\beta H} \tag{3}$$

## 1.2 Free particles and the Aharanov-Bohm Effect

When we studied the Hamiltonian for a free particle from the perspective that the space was described by discrete points in space separated by $\delta x$, we saw that the kinetic term of the Hamiltonian mixed states from neighboring sites,

$$\langle i|H|i+1\rangle = -\frac{\hbar^2}{2m\delta x^2}, \tag{4}$$

while the potential term, as well as the remainder of the kinetic term, was purely diagonal. If it were not for the off-diagonal piece, probability would not spread over space with time.

The interaction with an electromagnetic field $\mathbf{A}$ also contributes an off-diagnoal piece due to the presence of the term $(-ie\hbar/mc)\mathbf{A}\cdot\nabla$. The off-diagonal term to the Hamiltonian is then

$$\langle i|H|i+1\rangle = -\frac{\hbar^2}{2m\delta x^2} - \frac{ie\hbar}{2mc\delta x}A_i = -\frac{\hbar^2}{2m\delta x^2}\left(1+\frac{ie\delta x}{\hbar c}A_i\right). \tag{5}$$

Now, if we consider the evaluation of element $\langle x_i|e^{-iHt}|x_f\rangle$ as a sum over trajectories as described above. Each must include a series of links between neighboring sites. The effect of the vector potential is to add a product of the terms

$$\prod_{\text{links}}\left(1+\frac{ie\delta x}{\hbar c}A_i\right) \tag{6}$$

to each trajectory.

Thus the effect of the vector potential for propagation along a path from $x_1$ to $x_2$ is to modify the matrix element by a phase factor,

$$\langle \mathbf{x}_1|e^{-iHt}|\mathbf{x}_2\rangle \rightarrow \langle \mathbf{x}_1|e^{-iHt}|\mathbf{x}_2\rangle \exp\left[\frac{ie}{\hbar c}\int_{\text{path}} d\mathbf{x}\cdot\mathbf{A}\right], \tag{7}$$

where the path extends from $\mathbf{x}_1$ to $\mathbf{x}_2$. This added phase depends only on the path taken, but not the time-dependence of the trajectory. Note that we have taken the liberty to jump to three dimensions at this point.

Now, we consider a two-slit interference experiment, where between the slits lies a small magnetic solenoid. In the upper path, the particle goes above the solenoid, while in the lower path the particle travels below the solenoid. Neither path samples the region inside the solenoid where there is a magnetic field $B$ and a flux, $\Phi = BA$.

However, there is a vector potential ouside the solenoid which must satisfy Stoke's theorem,

$$\oint \mathbf{A}\cdot d\ell = \Phi. \tag{8}$$

Thus the two path's contributions to the amplitude have phases which differ by

$$\Delta\phi = \frac{e\Phi}{\hbar c} \tag{9}$$

due to the presence of the vector potential $\mathbf{A}$.

Thus altering the current through the solenoid shifts the inerfeence pattern, illustrating that it is $\mathbf{A}$ that is the fundamentail field, not $\mathbf{E}$ and $\mathbf{B}$. This phenomena has been observed with a thin magnetized iron filament called a *whisker*.

# 1 Propagators, Green's Functions and Integral Equations

A propagator is merely an incarnation of an evolution operator and is often confused with being the same as a Green's function, which it sometimes is. A propagator is defined as

$$K(\mathbf{x},t;\mathbf{x}',t') \equiv \langle \mathbf{x}| \exp\left[\frac{-iH(t-t')}{\hbar}\right] |\mathbf{x}'\rangle. \tag{1}$$

If the eigenstates, $|a\rangle$, of $H$ are known the propagator may be written as

$$K(\mathbf{x},t;\mathbf{x}',t') = \sum_a e^{-i\epsilon_a t/\hbar}\langle \mathbf{x}|a\rangle\langle a|\mathbf{x}'\rangle. \tag{2}$$

Since $K$ is the evolution operator, one sees that determining the propagator is equivalent to solving the Schrödinger equation,

$$\psi(x,t) = \int d^3x' K(\mathbf{x},t;\mathbf{x}',t')\psi(\mathbf{x}',t'). \tag{3}$$

In fact, the propagator is a solution of Schrödinger's equation for $t > t'$,

$$\left(-\frac{\hbar^2\nabla^2}{2m} + V(\mathbf{x})\right) K(\mathbf{x},t;\mathbf{x}',t') = i\hbar\frac{\partial}{\partial t}K(\mathbf{x},t;\mathbf{x}',t'), \tag{4}$$

while being zero for $t < t'$ and equal to $\delta^3(\mathbf{x}-\mathbf{x}')$ when $t = t_{0+}$.

We now consider the simple case of a free particle in one dimension. In that case the eigenstates of the Hamiltonian are momentum states and

$$\begin{aligned} K_0(x,t;x',t') &= \left(\frac{1}{2\pi\hbar}\right)\int dp \exp\left[\frac{i\mathbf{p}\cdot(x-x')}{\hbar} - \frac{ip^2(t-t')}{2m\hbar}\right] && (5)\\ &= \sqrt{\frac{m}{2\pi i\hbar(t-t')}}\exp\left[\frac{im(x-x')^2}{2\hbar(t-t')}\right]. && (6)\end{aligned}$$

The integral in the last step was performed by completing the square. Note that the phase in the exponential looks $(1/2)mv^2t/\hbar$, where the velocity is given by $\Delta x/\Delta t$. A similar expression can easily be found in higher dimension. To see that this form approaches $\delta(x-x')$ as $t \to 0$, one can check:

1. that $\int dx K(x,t;x',t') = 1$.
2. that at small time differences the phase oscillates quickly except when $x = x'$.

Adding a potential makes finding the propagator much more difficult. One can see that if the propagator is expressed as

$$K(x,t;x',t') = K_0(x,t;x',t') + \frac{1}{i\hbar}\int dt''dx'' K_0(x,t;x'',t'')V(x'',t'')K(x'',t'';x',t'), \tag{7}$$

the Schrödinger equation will be satisfied. This expression for the propagator can be viewed as the integral representation of Schrödinger's wave equation. Note that the second propagator in the right side is the "full" propagator which means that solving the equation is not simply a matter of performing an integral. Instead, one must find a self-consistent solution.

By replacing $K$ with $K_0$, one has found the "first-order perturbative corrections to the propagator". We will see this again later.

# 1 Angular Momentum

### Baker-Campbell-Hausdorff Lemma

Before we go further, let us step back and derive the Baker-Campbell-Hausdorff relation,

$$e^{A+B} = e^A e^B e^{-C/2}, \tag{1}$$

for the case the commuting $A$ and $B$ gives an operator $C$ that commutes with both $A$ and $B$, e.g. the unit matrix.

$$C \equiv [A, B] \tag{2}$$

To see that this is true, consider the expansion

$$e^{A+B} = \sum_N \frac{(A+B)^n}{n!}. \tag{3}$$

Expanding $(A+B)^n$ gives all terms with all orderings of the $n$ operators. For example, for $n = 5$ one of the terms is $ABBAB$. We wish to move all the $A$ operators to the left, which requires commuting them past the $B$ operators. Everytime an $A$ operator moves past a $B$ operator one must add a term where the $BA$ pair is replaced by $-C = [B, A]$. Using the binomial theorem, one can then write

$$\begin{aligned} \frac{(A+B)^n}{n!} &= \sum_{i+j=n} \frac{A^i B^j}{n!}\frac{n!}{i!j!} + (-C)\frac{A^{i-1}B^{j-1}}{n!}\frac{n!}{i!j!}\bar{N}_1(i,j) + (-C)^2\frac{A^{i-2}B^{j-2}}{n!}\frac{n!}{i!j!}\bar{N}_2(i,j) \\ &\quad + \cdots + (-C)^\ell \frac{A^{i-\ell}B^{j-\ell}}{n!}\frac{n!}{i!j!}\bar{N}_e ll(i,j) + \cdots \end{aligned} \tag{4}$$

where $\bar{N}_\ell$ is the average number of ways to pick $\ell$ $AB$ pairs from an order $n$ term, under the constraint that the $B$ operators in the pair were initially to the right of the $A$ terms. This number is simply the number of such independent pairs times $(1/2)^\ell$ to account for the fact that only half the time does a given pair start off with the $BA$ ordering,

$$\bar{N}_\ell = \left(\frac{1}{2}\right)^\ell \frac{i(i-1)\cdots(i-\ell+1)j(j-1)\cdots(j-\ell+1)}{\ell!}. \tag{5}$$

One can then factor the exponentials in the expression above to get Eq. (**??**).

### The rotation group

Without going into group theory we consider the rotation group which consists of unitary operators,

$$R(\vec{\alpha}) = e^{i\vec{L}\cdot\vec{\alpha}/\hbar}. \tag{6}$$

To understand why this a rotation, consider the case where $\vec{\alpha}$ is along the $z$ axis. One can then see that

$$L_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) = -i\hbar\frac{\partial}{\partial\phi}, \tag{7}$$

which means that

$$\begin{aligned} e^{iL_z\alpha/\hbar}f(\phi) &= \left(1+\alpha\frac{\partial}{\partial\phi}+\frac{\alpha^2}{2!}\frac{\partial^2}{\partial\phi^2}\cdots\right)f(\phi) && (8)\\ &= f(\phi+\alpha) && (9) \end{aligned}$$

What defines the rotation group is that the effect of subsequent rotations of $\vec{\alpha}$ and $\vec{\beta}$ result in a single rotation $\vec{\gamma}$.

$$e^{i\hbar\vec{L}\cdot\vec{\beta}}e^{i\hbar\vec{L}\cdot\vec{\alpha}} = e^{i\hbar\vec{L}\cdot\vec{\gamma}}. \tag{10}$$

Since the different components of $\vec{L}$ do not commute it is non-trivial to find the equivalent single rotation $\vec{\gamma}$ given $\vec{\alpha}$ and $\vec{\beta}$.

Given the definition $\vec{L}=\vec{r}\times\vec{p}$, it is straightforward to find the commutation relations,

$$[L_i, L_j] = i\hbar\epsilon_{ijk}L_k. \tag{11}$$

Our goal in this section is to discuss the requirement of using different operators, $S_x$, $S_y$ and $S_z$ to generate rotations, not in coordinate space but in a discrete vector space, meaning that $\vec{S}$ can be expressed as matrices. The important requirement for $S$ to be considered a rotation is that

$$e^{i\hbar\vec{S}\cdot\vec{\beta}}e^{i\hbar\vec{S}\cdot\vec{\alpha}} = e^{i\hbar\vec{S}\cdot\vec{\gamma}}, \tag{12}$$

where the same $\vec{\gamma}$ results from a given $\vec{\alpha}$ and $\vec{\beta}$ as would have resulted from using $\vec{L}$ instead of $\vec{S}$.

We wish to demonstrate that if the components of $\vec{S}$ obey the same commutation laws of the components of $\vec{L}$, the rotations will be identical. To see this we divide the two rotations into $N$ smaller rotations with $N\to\infty$.

$$e^{i\hbar\vec{S}\cdot\vec{\beta}}e^{i\hbar\vec{S}\cdot\vec{\alpha}} = e^{i\hbar\vec{S}\cdot\vec{\beta}/N}e^{i\hbar\vec{S}\cdot\vec{\beta}/N}\cdots e^{i\hbar\vec{S}\cdot\vec{\beta}/N}e^{i\hbar\vec{S}\cdot\vec{\alpha}/N}e^{i\hbar\vec{S}\cdot\vec{\alpha}/N}\cdots e^{i\hbar\vec{S}\cdot\vec{\alpha}/N}. \tag{13}$$

To find the equivalent single rotation, one must expand each exponential then commute them in a manner as was done for the Baker-Campbell-Hausdorff lemma earlier. There are of order $N^2$ such commutations.

For our purposes we wish to consider the inner two exponentials,

$$\begin{aligned} e^{i\hbar\vec{S}\cdot\vec{\beta}/N}e^{i\hbar\vec{S}\cdot\vec{\alpha}/N} &= 1+i\hbar\vec{S}\cdot(\vec{\alpha}+\vec{\beta})/N-\frac{\hbar^2}{2N^2}\left(\vec{S}\cdot(\vec{\alpha}+\vec{\beta})\right)^2+\frac{\hbar^2}{2N^2}[\vec{S}\cdot\vec{\alpha},\vec{S}\cdot\vec{\beta}]+\mathcal{O}\frac{1}{N^3} && (14)\\ &= \exp i\left(\hbar\vec{S}\cdot(\vec{\alpha}+\vec{\beta})/N+i\frac{\hbar^2}{2N^2}[\vec{S}\cdot\vec{\alpha},\vec{S}\cdot\vec{\beta}]\right)+\mathcal{O}\frac{1}{N^3}. && (15) \end{aligned}$$

Since there are of order $N^2$ such commutations we must perform to find $\vec{\gamma}$, we may throw away all terms of order $1/N^3$ or higher. One can then see that the final rotation is determined by knowing the commutation relations, i.e. if the commutation relations for the components for $\vec{S}$ are identical to the commutation relations for $\vec{L}$, that the equivalent angle $\vec{\gamma}$ will be the same in both cases.

In group theory the rotation matrices, $\exp(i\hbar\vec{S}\cdot\vec{\alpha})$ are the group elements and the components of $\vec{S}$ are referred to as generators of the group.

The simplest example of three operators, $S_x$, $S_y$ and $S_z$ which generate rotations is the $2\times 2$ representation,

$$S_x \equiv \frac{\hbar}{2}\sigma_x\ , \quad S_y \equiv \frac{\hbar}{2}\sigma_y\ , \quad S_z \equiv \frac{\hbar}{2}\sigma_z. \tag{16}$$

Many Lagrangians in physics have rotational symmetry, which would suggest that the angular momentum is conserved. This can be seen by commuting the rotation operator for an infinitesimal rotation with the Hamiltonian. If $L_z$ commutes with the Hamiltonian, then the eigenstates of $H$ can be simultaneously chosen as eigenstates of $L_z$. However, if the Hamiltonian has terms such as $\vec{L}\cdot\vec{S}$, neither $L_z$ nor $S_z$ commutes with the Hamiltonian. However, in that case the operator $J_z \equiv L_z + S_z$ does commute. We perform this as an example in class.

### $\mathcal{D}$ Matrices

This is for the most point an exercise in notation. Rather than expressing rotations as a function of $\alpha_x$, $\alpha_y$ and $\alpha_z$, one can express the rotation as a function of the three Euler angles, which represent subsequent rotations about the $z$, $y$ and the new $z$ axes.

$$\mathcal{D}^{\ell}_{mm'}(\alpha,\beta,\gamma) = \exp\left(\frac{-iJ_z\alpha}{\hbar}\right)\exp\left(\frac{-iJ_y\beta}{\hbar}\right)\exp\left(\frac{-iJ_z\gamma}{\hbar}\right). \tag{17}$$

The label $\ell$ refers to dimension of the matrices used to represent the rotations, e.g. for two component matrices $\ell = 1/2$, while $m$ and $m'$ refer to the components of the matrices, $-\ell \leq m \leq \ell$.

For instance, for $\ell = 1/2$,

$$\begin{aligned}\mathcal{D}^{1/2} &= \exp\left(\frac{-i\sigma_z\alpha}{2}\right)\exp\left(\frac{-i\sigma_y\beta}{2}\right)\exp\left(\frac{-i\sigma_z\gamma}{2}\right)\\ &= \begin{pmatrix} e^{-i(\alpha+\gamma)/2}\cos(\beta/2) & e^{-i(\alpha-\gamma)/2}\sin(\beta/2)\\ e^{i(\alpha-\gamma)/2}\sin(\beta/2) & e^{i(\alpha+\gamma)/2}\cos(\beta/2)\end{pmatrix}.\end{aligned}$$

**More Angular Momentum** The angular momentum operator $L_z = -i\hbar\partial/\partial\phi$ commutes with the Hamiltonian if the Hamiltonian is invariant to rotations about the $z$ axis. Furthermore, if the Hamiltonian is invariant to rotations about any axis, all three components of $\vec{L}$ commute with $H$. One may then define states which are simultaneously eigenstates of $H$ and $L_z$, or $L_x$ or $L_z$. But, one may not necessarily find states which are eigenstates of $L_x$, $L_y$ an d $L_z$ since these operators do not commute with one another.

However, the operator $L^2 = L_x^2 + L_y^2 + L_z^2$ is spherically symmetric and thus commutes with any of the three components of $\vec{L}$. One may there for define eigenstates of a spherically symmetric Hamiltonian that are also eigenstates of $L^2$ and $L_z$. We define the eigenvalues in terms of $m$ and $\ell$.

$$L_z|\ell,m\rangle = m\hbar|\ell,m\rangle\ , \quad L^2|\ell,m\rangle = \ell(\ell+1)\hbar^2|\ell,m\rangle. \tag{18}$$

The curious choice of $\ell(\ell+1)$ will become apparent below.

**Raising and Lowering operators** We define operators,

$$L_\pm \equiv L_x + i\text{Ł}_y. \tag{19}$$

These operators have the fortuitous property that

$$[L_z, L_\pm] = \pm L_\pm, \tag{20}$$

which means that

$$\begin{aligned} L_z\left(L_\pm|m\rangle\right) &= L_\pm L_z|m\rangle \pm L_\pm|m\rangle \qquad (21)\\ &= (m\pm 1)\hbar\left(L_\pm|m\rangle\right). \qquad (22)\end{aligned}$$

This means that $L_\pm$ effectively change an eigenstate of $L_z$ to a new eigenstate with the eigenvalue either raised or lowered by $\hbar$.

One can also find the normalization of the new states by noting that

$$\begin{aligned} \left(\langle m|L\mp\right)\left(L_\pm|m\rangle\right) &= \langle m|L_x^2 + L_y^2 \mp L_z|m\rangle \qquad (23)\\ &= \langle m|L^2 - L_z^2 \mp L_z|m\rangle \qquad (24)\\ &= \Big(\ell(\ell+1) - m^2 \mp m\Big)\,\hbar^2. \qquad (25)\end{aligned}$$

By inspection, one can see that if the sequence of $m$s is to be finite that they must begin at $-\ell$ and end at $\ell$. Since the $m$s must be separated by unit steps, $\ell$ and $m$ must therefore be either integer or half integer.

# 1 Spherical Harmonics

The kinetic energy term in Schrödinger's wave equation may be written

$$H_K = -\hbar^2 \frac{\nabla^2}{2m} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right) - \frac{\hbar^2}{2mr^2}\left(\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}\right). \tag{1}$$

Furthermore, the components of angular momentum may be written in terms of angular derivatives,

$$\begin{aligned} L_z &= -i\hbar\frac{\partial}{\partial\phi} && (2)\\ L_x &= -i\hbar\left(-\sin\phi\frac{\partial}{\partial\theta} - \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right) && (3)\\ L_y &= -i\hbar\left(\cos\phi\frac{\partial}{\partial\theta} - \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right) && (4)\\ L_\pm &= -i\hbar e^{\pm i\phi}\left(\pm i\frac{\partial}{\partial\theta} - \cot\theta\frac{\partial}{\partial\phi}\right). && (5)\end{aligned}$$

Using the relation, $L^2 = L_z^2 + L_+L_+ i\hbar L_z$, one can see that the $\nabla^2$ term for the kinetic energy may be written as

$$-\frac{\hbar^2}{2m}\nabla^2 = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right) + \frac{\mathbf{L}^2}{2mr^2}. \tag{6}$$

If the potential is spherically symmetric, the Hamiltonian commutes with all the components of $\mathbf{L}$ since they only involve angular derivatives, and each component of $\mathbf{L}$ commutes with $\mathbf{L}^2$. Thus we may write the solution as an eigenstate of $L_z$ and $\mathbf{L^2}$ denoted by $\ell$ and $m$,

$$\Psi(\mathbf{r}) = \phi_{\ell,m}(r)Y_{\ell,m}(\theta,\phi). \tag{7}$$

Schrödinger's equation may then be written as,

$$E\phi_{\ell,m}(r) = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right)\phi_{\ell,m}(r) + \hbar^2\ell(\ell+1)\phi_{\ell,m}(r). \tag{8}$$

Our immediate goal is to understand the angular functions $Y_{\ell,m}(\theta,\phi)$ which are eigenstates of $L_z$ and $\mathbf{L}^2$ and are refered to as spherical harmonics. In terms of bras and kets,

$$Y_{\ell,m}(\theta,\phi) = \langle\hat{n}|\ell,m\rangle, \tag{9}$$

which implies the normalization,

$$\int d\phi d\cos\theta |Y_{\ell,m}(\theta,\phi)|^2 = 1. \tag{10}$$

Given the requirement that the raising operator (see definition above) working on $Y_{\ell,\ell}$ gives zero, one can write the expression for $Y_{\ell,\ell}(\theta,\phi)$,

$$Y_{\ell,\ell}(\theta,\phi) = c_\ell e^{i\ell\phi}\sin^\ell\theta, \tag{11}$$

where the normalization is given by

$$c_\ell = \left[\frac{(-1)^\ell}{2^\ell \ell!}\right]\sqrt{\frac{(2\ell+1)(2\ell)!}{4\pi}}. \tag{12}$$

By operating on the known $Y_{\ell,m}$s with $L_-$ one may generate $Y_{\ell,m}$s for successively lower values of $m$. Since the $Y_{\ell,m}$s are eigenstates of $L_z$ the $m$ dependence is always trivial as it goes proportional to $e^{im\phi}$, but the $\theta$ dependence can be messy. Examples of a few spherical harmonics are

$$\begin{aligned}
Y_{0,0} &= \frac{1}{\sqrt{4\pi}} && (13)\\
Y_{1,0} &= \sqrt{\frac{3}{4\pi}}\cos\theta && (14)\\
Y_{1,\pm1} &= -\sqrt{\frac{3}{8\pi}}\sin\theta e^{i\pm\phi} && (15)\\
Y_{2,0} &= \sqrt{\frac{5}{16\pi}}(3\cos^2\theta - 1) && (16)\\
Y_{2,\pm1} &= -\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta e^{\pm i\phi} && (17)\\
Y_{2,\pm2} &= \sqrt{\frac{15}{32\pi}}\sin^2\theta e^{\pm 2i\phi} && (18)
\end{aligned}$$

One might ask why half integer values of $\ell$ are never mentioned for spherical harmonics. The problem is that the wave functions then become discontinuous as $\phi$ goes past $2\pi$. Thus half-integral angular momenta can only be used for intrinsic spins and not as labels for a spatial wave functin where the Hamiltonian includes spatial gradients.

Finally, Legendre polynomials are defined as

$$P_\ell(\cos\theta) \equiv \sqrt{\frac{4\pi}{(2\ell+1)}}Y_{\ell,m=0}(\theta). \tag{19}$$

### Parity

The $Y_{\ell,m}$s with odd $\ell$ have odd parity, i.e. under the transformation $(\theta \to \pi - \theta,\ \phi \to \phi + \phi)$ the $Y_{\ell,m}$s with odd $\ell$ switch sign. This will play an important role in determining that many matrix elements will be zero. Note that the radial wavefunction is always invariant under parity.

### Separating out relative and center-of-mass coordinates

Consider the Schrödinger equation for two particles interacting through a potential $V(\mathbf{r}_2-\mathbf{r}_1)$. The kinetic energy term,

$$H_K = -\frac{\hbar^2}{2m_1}\nabla_1^2 - \frac{\hbar^2}{2m_2}\nabla_2^2 \tag{1}$$

needs to be rewritten such that the derivates are with respect to center-of-mass and relative coordinates,

$$\mathbf{r} \equiv \mathbf{r_2} - \mathbf{r}_1 \ , \quad \mathbf{R} \equiv \frac{m_1\mathbf{r_1} + m_2\mathbf{r_2}}{m_1+m_2} \tag{2}$$

Using these definitions, one can show that that the kinetic energy becomes

$$H_K = -\frac{\hbar^2}{2M}\nabla_{\mathbf{R}}^2 - \frac{\hbar^2}{2\mu}\nabla_{\mathbf{r}}^2 \tag{3}$$

where $M \equiv m_1 + m_2$ and $\mu \equiv m_1m_2/(m_1+m_2)$.

The wave function may then be written as a product of center-of-mass and relative coordinates,

$$\Psi(\mathbf{R},\mathbf{r}) = e^{i\mathbf{K}\cdot\mathbf{R}}\phi_{\text{rel.}}(\mathbf{r}), \tag{4}$$

with the overall energy being a sum of the eigen-energy of the relative wave function plus $\hbar^2K^2/2M$.

Note that if one of the masses is much larger than the other that the reduced mass $\mu$ equals the smaller of the two masses. If both masses are equal, the reduced mass is half the mass of either of the two individual masses. For our purposes, we will solve problems such as the hydrogen atom assuming the potential is fixed. For the real case, one need only replace the mass with the reduced mass to include the effect that the source of the potential is itself mobile.

Separating the center of mass coordinates is convenient whenever one has a potential that is a function of $\mathbf{r}_1 - \mathbf{r}_2$ only. Writing Schrödinger's equation,

$$-\frac{\hbar^2}{2M}\nabla_{\mathbf{R}}^2 - \frac{\hbar^2}{2\mu}\nabla_{\mathbf{r}}^2 e^{i\mathbf{K}\cdot\mathbf{R}}\phi(\mathbf{r}) + V(r)e^{i\mathbf{K}\cdot\mathbf{R}}\phi(\mathbf{r}) = Ee^{i\mathbf{K}\cdot\mathbf{R}}\phi(\mathbf{r}), \tag{5}$$

One can factor out $e^{i\mathbf{K}\cdot\mathbf{R}}$ after operating with $\nabla_{\mathbf{R}}^2$ and get a simple equation for the relative wave function $\phi(\mathbf{r})$.

$$\begin{aligned} -\frac{\hbar^2}{2\mu}\nabla_{\mathbf{r}}^2\phi(\mathbf{r}) + V(r)\phi(\mathbf{r}) &= E_{\text{rel}}\phi(\mathbf{r}) && (6) \\ E &= \frac{\hbar^2K^2}{2M} + E_{\text{rel}} && (7) \end{aligned}$$

### Example: Three-dimensional Harmonic Oscillator – Cartesian Basis

This factorization works whenever the potential is a function of $\mathbf{r}$ and not $\mathbf{R}$. One especially easy example is the three-dimensional harmonic oscillator. In this case the problem is even more factorizable.

$$V(\mathbf{r}_1,\mathbf{r}_2)=\frac{1}{2}k|\mathbf{r}_1-\mathbf{r}_2|^2=\frac{1}{2}m\omega^2r^2=\frac{1}{2}k\left[x^2+y^2+z^2\right]. \tag{8}$$

Since this potential can be written as the sum of an $x$-dependent, a $y$-dependent and a $z$-dependent piece,

$$\phi(\mathbf{r})=\phi_x(x)\phi_y(y)\phi_z(z), \tag{9}$$

one can separate the Schrödinger equation for the three-dimensional relative wave function into three one-dimensional Schrödinger equations.

$$-\frac{\hbar^2}{2\mu}\partial_x^2\phi_x+\frac{1}{2}kx^2\phi_x(x) = E_x\phi_x(x) \tag{10}$$

$$-\frac{\hbar^2}{2\mu}\partial_y^2\phi_y+\frac{1}{2}ky^2\phi_y(y) = E_y\phi_y(y) \tag{11}$$

$$-\frac{\hbar^2}{2\mu}\partial_z^2\phi_z+\frac{1}{2}kz^2\phi_z(z) = E_z\phi_z(z) \tag{12}$$

Here, $E=E_x+E_y+E_z$. By multiplying the first equation by $\phi_y\phi_z$, the second equation by $\phi_x\phi_z$ and the third by $\phi_x\phi_y$, then adding the three equations, one finds that they provide a solution to the three-dimensional equation.

Thus, one is able to take a six-dimensional equation, factor out the center-of-mass motion, and recognize the factorizability, and reduce the problem to three trivial one-dimensional equations of motion. The energies are

$$E_x=(n_x+1/2)\hbar\omega,\ E_y=(n_y+1/2)\hbar\omega,\ E_z=(n_z+1/2)\hbar\omega, \tag{13}$$

where $\omega=\sqrt{k/\mu}$. The total energy is thus the sum

$$E=(n_x+n_y+n_z+3/2)\hbar\omega. \tag{14}$$

These solutions are known as the Cartesian-basis solutions to the harmonic oscillator. Since the harmonic oscillator has a spherically symmetric solution there also exist eigenstates of good angular momentum which can be expressed in terms of $Y_{\ell,m}$s.

One convenient aspect of harmonic oscillator potentials is that they can be solved form the $N-$ *body* case where $N$ particles of mass $m$ interact through mutual harmonic oscillator potentials. Consider the potential,

$$V(\mathbf{r}_1,\cdots\mathbf{r}_N)=\frac{1}{2}k\left(\sum_{i<j}|\mathbf{r}_i-\mathbf{r}_j|^2\right). \tag{15}$$

This potential is independent of the center-of-mass coordinates. That is, a translation of all coordinates does not affect the potential. One can therefore write the solution as a product of a center-of-mass wave function and a wave function that depends on $N-1$ relative coordinates.

The above problem would be intractable if not for a trick which is unique to the harmonic oscillator. One adds a fictitious potential that depends only on the center of mass coordinate.

$$V_f = \frac{1}{2}k|\mathbf{r}_1 + \mathbf{r}_2 + \cdots \mathbf{r}_N|^2 = \frac{1}{2}N^2 k|R_{cm}|^2. \tag{16}$$

The energies are thus equal to

$$E_{tot} = E_{\rm rel} + (n_f + 3/2)\hbar\sqrt{Nk/m}, \tag{17}$$

where $E_{\rm rel}$ is the energy of relative motion which is our ultimate goal. Here the term $(n_f + 3/2)\hbar\sqrt{Nk/m}$ replaces the usual kinetic energy of the center-of-mass.

The trick comes in noticing that the sum of the original potential and the fictious potential turns out to be the same as that of $N$ independent oscillators.

$$V_{tot} = V_f + V = \frac{1}{2}Nk\left(r_1^2 + r_2^2 + \cdots r_N^2\right). \tag{18}$$

Thus the energies are:

$$E_{tot} = (n_1 + n_2 \cdots n_N + 3N/2)\hbar\sqrt{Nk/m}. \tag{19}$$

The ground state energy we are interested in is thus $E_{tot}(n_i = 0)$ minus the energy of the center of mass, $(3/2)\hbar\sqrt{Nk/m}$. The wave function of the ground state can be written as the product of all the ground state wave functions, divided by the wave function of the center-of-mass.

### Solving the Radial Wave Equation for Spherically Symmetric Cases

Similar factorization ideas are applied any time one deals with a spherically symmetric potential. In that case one can write the wave function as a product of $\phi_\ell(r)$ and $Y_{\ell,m}(\theta,\phi)$ and reduce the problem to a one-dimensional problem of the radial coordinate. In that case the one-dimensional Schrödinger equation for $\phi_\ell(r)$ becomes

$$-\frac{\hbar^2}{2\mu}\left(\partial_r^2 + \frac{2}{r}\partial_r\right)\phi_\ell(r) + \left(\frac{\hbar^2\ell(\ell+1)}{2\mu r^2} + V(r)\right)\phi_\ell(r) = E\phi_\ell(r). \tag{20}$$

Although this is a one-dimensional differential equation, it is not a one-dimensional Schrödinger equation due to the extra derivative term $(2/r)\partial_r$. The Schrödinger form $\phi(r)$ can be regained by defining

$$u(r) \equiv r\phi(r). \tag{21}$$

The wave equation for $u$ looks like a 1-d Schrödinger equation with a centrifigul potential,

$$-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial r^2}u(r) + \left(\frac{\hbar^2\ell(\ell+1)}{2\mu r^2} + V(r)\right)u(r) = Eu(r). \tag{22}$$

The boundary condition on $u$ is that it must go to zero at the origin so that $\phi$ is finite at the origin.

The wave equation is particularly simple for $s$ waves ($\ell = 0$) as such solutions reduce to simple 1-d problems with an infinite potential when $r < 0$. Considering non-zero $\ell$ introduces a divergent potential at the origin. In the neighborhood of $r = 0$ the solution looks like either

$$u_\ell(r)\ r^{\ell+1}\left(1 + \mathcal{O}r + \mathcal{O}r^2 \cdots\right), \text{the regular solution,} \tag{23}$$

or

$$u_\ell(r)\ r^{-\ell}\left(1 + \mathcal{O}r + \mathcal{O}r^2 \cdots\right), \text{the irregular solution.} \tag{24}$$

Clearly, only the regular solution satisfies the boundary conditions. Even when a Coulomb potential is added, which is also divergent at the origin only less so, the behavior at the origin can be expanded as shown. If the potential is more strongly divergent, then there is a problem.

When the potential is zero the solutions are known as spherical bessel functions. The solution that behaves regularly at the origin is referred to as $j_\ell(kr)$, while the irregular solution is referred to as $n_\ell(kr)$. For the low $\ell$s,

$$j_0(x) = \frac{\sin x}{x} \quad , \quad n_0(x) = -\frac{\cos(x)}{x} \tag{25}$$

$$j_1(kr) = \frac{\sin x}{x^2} - \frac{\cos x}{x} \quad , \quad n_1(x) = -\frac{\cos x}{x^2} - \frac{\sin x}{x} \tag{26}$$

$$j_2(kr) = \left(\frac{3}{x^3} - \frac{1}{x}\right)\sin x - \frac{3}{x^2}\cos x \quad , \quad n_2(kr) = -\left(\frac{3}{x^3} - \frac{1}{x}\right)\cos x - \frac{3}{x^2}\sin x \tag{27}$$

$$\vdots \tag{28}$$

By taking a linear combination of $j_\ell$ and $n_\ell$, one can find a solution which behaves like an outgoing wave at large $r$,

$$h_\ell(kr) = j_\ell(kr) + i n_\ell(kr) \tag{29}$$

$$\approx (-i)^{\ell+1}\frac{e^{ikr}}{kr}\ , \text{ as } r \to \infty \tag{30}$$

As an example, we consider $\ell = 1$,

$$h_1(x) = \frac{e^{ix}}{x}\left(-1 - \frac{i}{x}\right) \tag{31}$$

**Examples:**

1. Solve for lowest $\ell = 0$ and $\ell = 1$ states of infinite spherical well of radius $R$. (Note that for the $\ell = 1$ solutions, a transcendental expression will remain.
2. Outline how one would solve for the boundstate of an $\ell = 1$ solution for a well of finite depth.

**Spherical Harmonic Oscillator – Spherical Basis**

The spherical harmonic oscillator can be approached either through cartesian coordinates as described in above or in a spherical basis. First, we review the Cartesian solutions. Since the potential can be written as

$$V(\mathbf{r}) = \frac{1}{2}kr^2 = \frac{1}{2}k\left(x^2+y^2+z^2\right), \tag{32}$$

the solutions factorize into $x$, $y$ and $z$-dependent functions,

$$\Psi(\mathbf{r}) = \psi_{n_x}(x)\psi_{n_y}(y)\psi_{n_z}(z). \tag{33}$$

Each piece is a solution of the 1-dimensional Schrödinger's equation and the total energy is

$$E = (N+3/2)\hbar\omega\ ,\quad N \equiv n_x+n_y+n_z,\ \omega\sqrt{k/\mu}. \tag{34}$$

The $N=0$ and $N=1$ eigenstates have the form

$$\begin{aligned}
\phi_{n_x=n_y=n_z=0}(\mathbf{r}) &\sim e^{-r^2/(2a^2)} && (35)\\
\phi_{n_x=1,n_y=n_z=0}(\mathbf{r}) &\sim xe^{-r^2/(2a^2)} && (36)\\
\phi_{n_x=0,n_y1,n_z=0}(\mathbf{r}) &\sim ye^{-r^2/(2a^2)} && (37)\\
\phi_{n_x=n_y=0,n_z=1}(\mathbf{r}) &\sim ze^{-r^2/(2a^2)} && (38)\\
& && (39)
\end{aligned}$$

By looking at the form of the $Y_{\ell,m}$s, one can see that the $N=0$ state has a $\ell=0, m=0$ angular dependence, and can therefore be written as a spherically symmetric function, $e^{-r^2/(2a_0^2)}$, multiplied by $Y_{0,0}$. The solution for the $n_x=n_y=0, n_z=1$ state can be written as a product of $Y_{1,0}$ and the radial function $re^{-r^2/(2a_0^2)}$. By taking linear combinations, $\phi_{n_x=1,n_y=n_z=0} \pm \phi_{n_x=0,n_y1,n_z=0}$, one finds solutions which can be written as the same radial wave function multiplied by $Y_{1,\pm 1}$.

In spherical coordinates the labels $n_x$, $n_y$ and $n_z$ are replaced by $N$, $\ell$ and $m$. Mapping the solutions for higher $N$ is a bit tricky. For $N \geq 2$, one can count the states from a Cartesian perspective. One needs to know the number of ways to get three integers to add to $N$. First, the number of ways, $d_\perp$ to get two integers to add to $N_\perp$ is

$$d_\perp(N_\perp) = \sum_{n_x=0,N_\perp} = N_\perp + 1. \tag{40}$$

Requiring that a third integer adds to $N$ gives the total degeneracy $d(N)$,

$$d(N) = \sum_{N_\perp=0,N} d_\perp(N_\perp) = \frac{(N+1)(N+2)}{2}. \tag{41}$$

Thus there is one way to get $N=0$, 3 ways to get $N=1$, six ways to get $N=2$, etc.

To determine which $\ell$ multiplets combine to create the $d_N$ Cartesian solutions with a given energy, $(N+3/2)\hbar\omega$, consider two pieces of evidence: First, creating the cartesian state with

$n_z = N, n_x = n_y = 0$ is represented by the spherical state $Y_{\ell=N,\ell=N}$, therefore there must be at least one $\ell = N$ multiplet. Secondly, all the multiplets for $N-2$ must have corresponding multiplets which are generatedy by operating on those states with the spherically symmetric operator $a_x^2 + a_y^2 + z_z^2$. We can now determine the multiplets by:

$$d(N) = \frac{(N+1)(N+2)}{2} = (2N+1) + d(N-2) + \textit{ any others.} \tag{42}$$

Solving for the number of *others*, one finds there are no others. Hence the excitation $N+2$ states have the same states, but with one more multiplet of $\ell = N+2$. Since one knows that for $N=0$ there is one $\ell = 0$ state and for $N=1$ there is one $\ell = 1$ multiplet, one can quickly find all the multiplets for any $N$.

As an example the $N=5$ states are covered by one $\ell = 5$ multiplet, one $\ell = 3$ multiplet and one $\ell = 1$ multiplet. Note that all states with even $N$ have even parity and all states with odd $N$ have odd parity.

## The Hydrogen Atom

There are three standard problems of spherically symmetric potentials where the solutions are analytic, the inifinite well, the harmonic oscillator and the Coulomb potential. Here, we consider the case where the potential is attractive,

$$V(r) = -\frac{e^2}{r}. \tag{43}$$

One may rewrite the Schrödinger equation,

$$\left(-\frac{\partial^2}{\partial r^2} + \frac{\ell(\ell+1)}{r^2} - \frac{Z_1 Z_2}{a_0 r}\right) u_\ell(r) = -k^2 u_\ell(r), \tag{44}$$

where the Bohr radius is defined $a_0 \equiv \hbar^2/(\mu e^2)$ and $k^2 = -2\mu E/\hbar^2$. For large $r$ the potential and centrifigal terms are negligible and the wave function must behave as $e^{-kr}$ multiplied by terms that vary more slowly in $r$.

The solutions to the Schrödinger equation can be written in terms of associated Laguerre plynomials.

$$R_{n,\ell}(r) = \frac{u_{n,\ell}}{r} = \left\{ \left(\frac{2}{na_0}\right)^3 \frac{(n-\ell-1)!}{2n[(n+\ell)!]^3} \right\}^{1/2} e^{-r/(na_0)} \left(\frac{2r}{na_0}\right)^\ell L_{n+\ell}^{2\ell+1}\left(\frac{2r}{na_0}\right). \tag{45}$$

For a given $\ell$ there are many solutions labeled by the integer $n > \ell$. The eigen-energies can be written simply as

$$E_n = -\frac{e^2}{2a_0}\frac{1}{n^2}. \tag{46}$$

If larger charges are used the above expressions are modified by scaling $a_0$ by $1/(Z_1 Z_2)$.

Writing a few solutions,

$$R_{1,0} = \frac{2}{a_0^{3/2}} e^{-r/a_0} \tag{47}$$

$$R_{2,0} = \frac{1}{(2a_0)^{3/2}}\left(2-\frac{r}{a_0}\right)e^{-r/(2a_0)} \tag{48}$$

$$R_{2,1} = \frac{1}{(2a_0)^{3/2}}\frac{r}{a_0\sqrt{3}}e^{-r/(2a_0)} \tag{49}$$

The degeneracy, where energies with different $\ell$ have the same energies seems accidental, but is related to the similar degeneracy in the harmonic oscillator. Both degeneracies can be explained by considering the Lenz vector, which commutes with the Hamiltonian for the special case of the Coulomb potential.

$$\mathbf{R} \equiv \frac{1}{2\mu}\left(\mathbf{p}\times\mathbf{L} - \mathbf{L}\times\mathbf{p}\right) - \frac{e^2}{r}\mathbf{r}. \tag{50}$$

This operator is Hermitian and, if the commutation between $\mathbf{p}$ and $\mathbf{L}$ is ignored, is identical to the classical expression for the Lenz vector.

One can also define a scaled operator,

$$\mathbf{K} \equiv \sqrt{\frac{-m}{2H}}\mathbf{R}, \tag{51}$$

which is a little odd since one is defining the square root of an operator. However, since we are considering only eigenstates with negative energies, this is not too sick.

One can show that the components of $\mathbf{K}$ and the components of the angular momentum $\mathbf{L}$ obey simple commutation relations,

$$[K_i, K_j] = i\hbar\epsilon_{ijk}L_k\ , \quad [K_i, L_j] = i\hbar\epsilon_{ijk}K_k \tag{52}$$

These commutation relations are reminiscent of angular momentum commutation relations, and in fact, if one defines two new operators,

$$\mathbf{M} \equiv \frac{\mathbf{L}+\mathbf{K}}{2} \tag{53}$$

$$\mathbf{N} \equiv \frac{\mathbf{L}-\mathbf{K}}{2}, \tag{54}$$

one can see that $\mathbf{M}$ and $\mathbf{N}$ obey the same commutation relations as $\mathbf{L}$,

$$[M_i, M_j] = i\hbar\epsilon_{ijk}M_k, \quad [N_i, N_j] = i\hbar\epsilon_{ijk}N_k, \quad [M_i, N_j] = 0 \tag{55}$$

Since $\mathbf{M}$ and $\mathbf{N}$ are linear combination of the $\mathbf{L}$ and $\mathbf{R}$, they commute with the Hamiltonian, and since they commute with one another they may simultaneously be defined.

Furthermore, some algebra reveals that the Hamiltonian may be written as

$$H = -\frac{me^4}{2(K^2+L^2+\hbar^2)} = \frac{me^4}{2(2M^2+2N^2+\hbar^2)} \tag{56}$$

Finally, note that the Lenz vector is always perpendicular to the angular momentum, which means that $\mathbf{R}\cdot\mathbf{L} = \mathbf{K}\cdot\mathbf{L} = 0$. From the definitions of $\mathbf{M}$ and $\mathbf{N}$, one then sees the constraint that

$$\mathcal{M} = \mathcal{N} \tag{57}$$

where $\mathcal{M}$ and $\mathcal{N}$ are the quantum numbers denoting the magnitude of the vectors $\mathbf{M}$ and $\mathbf{N}$ in the same way that $\ell$ denotes the magnitude of $\mathbf{L}$. The eigen-energies are thus,

$$E_{\mathcal{M}} = -\frac{me^4}{2\hbar^2(4\mathcal{M}(\mathcal{M}+1)+1)} = -\frac{me^4}{2\hbar^2(2\mathcal{M}+1)^2} \tag{58}$$

Since $\mathcal{M}$ could be either integral over half integral, the numbers

$$n \equiv 2\mathcal{M}+1 \tag{59}$$

are integral values.

These states are not eigenstates of $\mathbf{L}$, but given the fact that there must exist eigenstates of $\mathbf{L}$, one can conclude that several states of the same $\ell$ must be degenerate.

## Adding Angular Momentum

In a spherically symmetric potential, the orbital angular momentum, $\mathbf{L}$, commutes with the Hamiltonian and $\ell$ and $m_\ell$ are good quantum numbers as $\ell(\ell+1)$ and $m_\ell$ are the eigenvalues of $L^2$ and $L_z$ respectively. Many particles also have intrinsic spin, even those particles which are currently considered as point particles such as electrons and photons. Thus in addition to the orbital quantum numbers two more quantum numbers may be used to describe the eigenstates of a single particle in the potential, $s$ and $m_s$, which describe the magnitude and projection of the spin angular momentum.

Often a term exists in the Hamiltonian which couples the two types of spin,

$$H_{\text{s.o.}} = \alpha \mathbf{L} \cdot \mathbf{S}, \tag{1}$$

which is known as the spin-orbit term. This term originates from relativistic considerations which we will see later in the course. Since the term is written as a rotational scalar and does not involve an externa field, which would explicitly break the rotational symmetry, we expect that the overall angular momentum remains conserved. Indeed, one can see that the total anuglar momentum

$$\mathbf{J} \equiv \mathbf{L} + \mathbf{S} \tag{2}$$

commutes with the spin-orbit term, even though neither $\mathbf{L}$ or $\mathbf{S}$ commute with $H_{\text{s.o.}}$. Furthermore the total orbital and total spin angular momentum also commute with $H_{\text{s.o.}}$. Thus there are two new quantum numbers $j$ and $m_j$ which replace $m_\ell$ and $m_s$ as good quantum numbers, while $m_\ell$ and $m_s$ are no longer good quantum numbers.

A clearer insight into the spin-orbit term can be attained by rewriting it explicitly in terms of $j$, $\ell$ and $s$.

$$\begin{aligned} (\mathbf{L}+\mathbf{S})^2 &= \mathbf{L}^2 + \mathbf{S}^2 + 2\mathbf{L}\cdot\mathbf{S} & (3) \\ \mathbf{L}\cdot\mathbf{S} &= \frac{1}{2}\left(\mathbf{J}^2 - \mathbf{L}^2 - \mathbf{S}^2\right), & (4) \end{aligned}$$

which means that the spin-orbit term may be rewritten in terms of the eigenenstates of the $j, m-j$ basis,

$$H_{\text{s.o.}} = \frac{\alpha\hbar^2}{2}\left(j(j+1) - \ell(\ell+1) - s(s+1)\right). \tag{5}$$

The coupling of spins is a common occurence in all branches of physics. In nuclear physics, the spin-orbit term is surprisingly large, and is responsible for the basic scheme for nuclear shell structure. In describing hadron spectroscopy, a spin-spin interaction is largely responsible for the difference of the spin 3/2 delta baryon and the spin 1/2 proton which are comprised of quarks of the same flavor. The coupling of angular momentum in physics is thus really a study of changing bases from the $m_\ell, m_s$ basis to the $j, m_j$ basis.

When changing bases, the number of states involved is $(2s+1)(2\ell+1)$ as can be determined by considering the number of combinations of $m_\ell$ and $m_s$. However, changing to the $j, m_j$ basis only mixes states with identical $m_j - m_\ell + m_s$. Since the states in a multiplet described by $j$ must be complete, running from $-j$ to $j$, we see that the maximum value of $j$ is

$$j \leq \ell + s. \tag{6}$$

Since there is only one state with $m_\ell = \ell$ and $m_s = s$, there is only one state with $m_j = \ell + s$ and thus only one $j$ multiplet with $j = \ell + s$. Counting the number of pairs of $m_\ell$ and $m_s$ that add up to a specific value of $m_j$, and realizing that every $j$ multiplet must be complete lets one see that the values of $j$ involved are

$$\begin{aligned} j_{\max} &= \ell + s && (7)\\ j_{\min} &= |\ell - s|. && (8) \end{aligned}$$

These are known as the triangle relations, as they can be considered as constraints involved in adding vectors. One can not add two vectors of lengths $\ell$ and $s$ and obtain a vector of length $j$ outside this range.

Furthermore, if $s < \ell$ the number of $j$ multiplets is $(2s + 1)$ while the average $j$ of the multiplets is $\ell$, which means that the number of states is the $(2s + 1)(2\ell + 1)$ as mentioned before.

**Clebsch Gordan Coefficients**

Changing from the $m_\ell, m_s$ basis to the $j, m_j$ basis is described by the overlap of matrix elements,

$$\langle \ell, s, j, m_j | \ell, s, m_\ell, m_s \rangle. \tag{9}$$

Such matrix elements are known as Clebsch Gordan coefficients and are refered to through a variety of confusing notations, such as $C(\ell, s, m_\ell, m_s; j, m)$ and nearly every other possible permutation of the arguments. Sometimes the coeeficients are labeled by superscripts and subscripts and sometimes they look like matrix elements $\langle j, m_j | \ell, s, m_\ell, m_s$. The notation is remarkably confusing given that the only purpose of not advantage, compared to writing down the matrix element is that the labels $\ell$ and $s$ are not written down twice.

To emphasize that the coefficients are matrix elements and that the two indices $\ell$ and $s$ remain unchanged in the transformation, we will refer to the coefficients in terms of the matrix elements in this lecture.

Finding the matrix elements is straight-forward given the algebras for raising and lowering angular momentum. First, remember that the matrix elements are all proportional to $\delta_{m_j, m_\ell + m_s}$. Now, since there is only one multiplet with $m_j = \ell + s$ that matrix element is simple to write down.

$$\langle \ell, s, j = \ell + s, m_j = \ell + s | \ell, s, m_\ell = \ell, m_s = s \rangle = 1 \tag{10}$$

To generate the coefficients involving the asame $j = \ell + s$ but reduced $m_j$, one can use the lowering operators,

$$\begin{aligned} |\ell, s, j, m_j - 1\rangle &= \frac{1}{\sqrt{j(j+1) - m_j(m_j - 1)}} J_- |\ell, s, j, m_j\rangle && (11)\\ &= \frac{1}{\sqrt{j(j+1) - m_j(m_j - 1)}} \left(L_- + S_-\right) |\ell, s, j, m_j\rangle && (12) \end{aligned}$$

Applying this to the case where $m_j = j = \ell + s$ one generates an expression for the matrix elements with $m_j = \ell + s - 1$,

$$
\begin{aligned}
|\ell, s, j = \ell + s, m_j = \ell + s - 1\rangle &= \frac{1}{\sqrt{j(j+1) - m_j(m_j-1)}} (L_- + S_-)\, |\ell, s, m_\ell = \ell, m_s = s\rangle && (13)\\
&= \frac{1}{\sqrt{j(j+1) - m_j(m_j-1)}} && (14)\\
&\cdot \Big(\sqrt{\ell(\ell+1) - m_\ell(m_\ell-1)}|\ell, s, m_\ell = \ell - 1, m_s = s\rangle && (15)\\
&+ \sqrt{s(s+1) - m_s(m_s-1)}|\ell, s, m_\ell = \ell, m_s = s - 1\rangle\Big) && (16)
\end{aligned}
$$

One can now read off the Clebsch Gordan coefficients. For instance,

$$\langle \ell, s, j = \ell + s, m_j = \ell + s - 1 | \ell, s, m_\ell = \ell - 1, m_s = s\rangle = \frac{\sqrt{\ell(\ell+1) - m_\ell(m_\ell-1)}}{\sqrt{j(j+1) - m_j(m_j-1)}}. \quad (17)$$

Finding the Clebsch Gordan coefficient for $j \neq \ell + s$ is a bit trickier. By knowing that the $j = \ell + s - 1$ states are orthogonal to the $j = \ell + s$ states, allows one to write down the $j = \ell + s - 1$ states down by inspection. For instance,

$$
\begin{aligned}
|\ell, s, j = \ell + s - 1, m_j = \ell + s - 1\rangle &= && (18)\\
\frac{1}{\sqrt{j(j+1) - m_j(m_j-1)}} &\cdot \Big(\sqrt{\ell(\ell+1) - m_\ell(m_\ell-1)}|\ell, s, m_\ell = \ell, m_s = s - 1\rangle && (19)\\
&- \sqrt{s(s+1) - m_s(m_s-1)}|\ell, s, m_\ell = \ell - 1, m_s = s\rangle\Big) && (20)
\end{aligned}
$$

Of course, one could multiply the states by any arbitrary phase and the coefficients would work as well. The convention is that the coefficient $\langle j_1, j_2, j, j | j_1, j_2, m_1 = j_1, m_2 = j - j_1\rangle$ is real and positive.

**Example:**

Find $\langle j_1 = 3/2, j_2 = 1, j = 3/2, m = 3/2 | j_1 = 3/2, j_2 = 1, m_1 = 3/2, m_2 = 0\rangle$.

First, using $J_- = J_{1,-} + J_{2,-}$

$$
\begin{aligned}
|j = 5/2, m = 5/2\rangle &= |m_1 = 3/2, m_2 = 1\rangle\\
\sqrt{(5/2)(7/2) - (5/2)(3/2)}|j = 5/2, m = 3/2\rangle &= \sqrt{(3/2)(5/2) - (3/2)(1/2)}|m_1 = 1/2, m_2 = 1\rangle + \sqrt{(}\\
|j = 5/2, m = 3/2\rangle &= \sqrt{\frac{3}{5}}|m_1 = 1/2, m_2 = 1\rangle + \sqrt{\frac{2}{5}}|m_1 = 3/2, m_2 = 0\rangle
\end{aligned}
$$

Now, since the state $|j = 3/2, m = 3/2\rangle$ is orthogonal to the state above,

$$|j = 3/2, m = 3/2\rangle = \sqrt{\frac{3}{5}}|m_1 = 3/2, m_2 = 0\rangle - \sqrt{\frac{2}{5}}|m_1 = 1/2, m_2 = 1\rangle \quad (24)$$

**Another Example:**

A neutron and proton are each in an $s$ wave of a nuclear potential. The two particles feel a spin-spin interaction,

$$V_{ss} = \alpha \mathbf{S}_p \cdot \mathbf{S}_n, \tag{25}$$

and also feel a magnetic field of strength $B$,

$$V_b = -\mu_p \mathbf{B} \cdot \mathbf{S}_p - \mu_n \mathbf{B} \cdot \mathbf{S}_n. \tag{26}$$

In terms of $\alpha$, $\mu_p$, $\mu_n$ and $B$, find the four energy eigenvalues.

This problem is made difficult by the fact that $V_b$ is diagonal in the $m_p, m_n$ basis, while $V_{ss}$ is diagonal in the $j, m$ basis. (We will omit the $s_p = 1/2, s_n = 1/2$ labels in the bras and kets to save space.)

$$\begin{aligned} \langle j, m | V_{ss} | j', m' \rangle &= \delta_{j,j'} \delta_{m,m'} \frac{\alpha \hbar^2}{2} \left( j(j+1) - s_p(s_p+1) - s_n(s_n+1) \right) & (27) \\ \langle m_p, m_n | V_b | m_p', m_n' \rangle &= \delta_{m_p,m_p'} \delta_{m_n,m_n'} B\hbar \left( \mu_p m_p + \mu_n m_n \right) & (28) \end{aligned}$$

To proceed further, one must choose a basis. We choose the $j, m$ basis with the following eigenvalues,

$$|j=1, m=1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad |j=1, m=-1\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \quad |j=1, m=0\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad |j=0, m=0\rangle = \Bigg( \tag{29}$$

In this basis $V_{ss}$ is diagonal,

$$V_{ss} = \begin{pmatrix} \alpha\hbar^2/4 & 0 & 0 & 0 \\ 0 & \alpha\hbar^2/4 & 0 & 0 \\ 0 & 0 & \alpha\hbar^2/4 & 0 \\ 0 & 0 & 0 & -3\alpha\hbar^2/4 \end{pmatrix} \tag{30}$$

while writing $V_b$ requires first rewriting each of the states in the $m_n, m_p$ basis.

$$\begin{aligned} |j=1, m=1\rangle &= |m_p = 1/2, m_n = 1/2\rangle & (31) \\ |j=1, m=-1\rangle &= |m_p = -1/2, m_n = -1/2\rangle & (32) \\ |j=1, m=0\rangle &= \frac{1}{\sqrt{2}} \left( |m_p = 1/2, m_n = -1/2\rangle + |m_p = -1/2, m_n = 1/2\rangle \right) & (33) \\ |j=0, m=0\rangle &= \frac{1}{\sqrt{2}} \left( |m_p = 1/2, m_n = -1/2\rangle - |m_p = -1/2, m_n = 1/2\rangle \right) & (34) \end{aligned}$$

If the problem involved higher angular momentum, one would have to go through the procedure of the previous exercise, utilizing raising and lowering operators, to write the $j, m$ states in terms of the $m_1, m_1$ basis.

From the above form, we can see that $V_b$ will mix the two states with with $m =$ as they are not eigenstates in the $m_p, m_n$ basis.

$$V_b = \begin{pmatrix} (\mu_p + \mu_n)\hbar B/2 & 0 & 0 & 0 \\ 0 & -(\mu_p + \mu_n)\hbar B/2 & 0 & 0 \\ 0 & 0 & 0 & (\mu_p - \mu_n)\hbar B/2 \\ 0 & 0 & (\mu_p - \mu_n)\hbar B/2 & 0 \end{pmatrix} \tag{35}$$

Thus the first two eigenvalues are simple to write down

$$\begin{aligned} \epsilon_1 &= \alpha\hbar^2/4 + (\mu_p + \mu_n)\hbar B/2 & (36) \\ \epsilon_2 &= \alpha\hbar^2/4 - (\mu_p + \mu_n)\hbar B/2, & (37) \end{aligned}$$

while the last two eigenvalues are most easily found by writing the lower-right 2 × 2 submatrix in terms of $\sigma$ matrices,

$$V_{2\times 2} = -\alpha\hbar^2/4 + (\alpha\hbar^2/2)\sigma_z + [(\mu_p - \mu_n)\hbar B/2]\,\sigma_x \tag{38}$$

The eigenvalues of the submatrix are

$$\epsilon_\pm = -\alpha\hbar^2/4 \pm \sqrt{\alpha^2\hbar^4/4 + (\mu_p - \mu_n)^2\hbar^2 B^2/4} \tag{39}$$

## Symmetries and Conservation Laws

Two classes of symmetries are continuous symmetries and discrete symmetries. Examples of continuous symmetries are rotational and translation symmetries while parity and time reversal are examples of discrete symmetries. Rotational symmetries are continuous because of the continuum of rotations under which the system can be rotated. A third class of symmetries are finite translations or rotations by a finite angle. For instance, a lattice is invariant under translations of size $na$ where $n$ is an integer and $a$ is the lattice spacing. A circular chain can also have symmetry under rotations of $2\pi/n$.

In classical mechanics and in field theory, one studies Noether's theorem which associates a conserved charge with any continuous symmetry. There exists an analogous relation in quantum mechanics which is perhaps easier to see. A continuous symmetry can be expressed

$$U^\dagger(\theta)HU(\theta) = H, \tag{1}$$

where $H$ is the Hamiltonian and $U$ represents the unitary transformation by a continuous variable $\theta$. One can write such a transformation as

$$U = e^{-iG\theta/\hbar}, \tag{2}$$

where $G$ is an operator which generates the transformation. As $\theta \to 0$,

$$U = 1 - iG\theta/\hbar, \tag{3}$$

and

$$U^\dagger(\theta)HU(\theta) = H - i[H,G]\theta/\hbar, \tag{4}$$

which shows that $H$ must commute with $G$ if the Hamiltonian is to be left invariant. Also, such a commutation implies that $\langle G\rangle$ is a constant of the motion.

$$\frac{\partial}{\partial t}\langle G\rangle = i\langle [H,G]\rangle/\hbar = 0 \tag{5}$$

The degeneracies of levels is also intimately related to the symmetry. For instance, if one considers an electron orbiting a proton, even with spin-orbit splitting, the Hamiltonian commutes with $J^2$, and since one may rotate such states into one another, the $(2j+1)$ states must be degenerate. If one explicitly breaks the symmetry by adding an interaction with an external magnetic field, the degeneracy is no longer expected to exist.

## Parity

The parity operator $\pi$ reflects the system about some point, $x \to -x$, $y \to -y$, $z \to -z$. One can also have a system invariant under only a subset of the parity operator, e.g. $\pi_x$. Both the coordinate and momentum operators should flip sign under parity. However, the angular momentum operator,

$$\mathbf{L} \equiv \mathbf{r} \times \mathbf{p} \tag{6}$$

is invariant under parity. Since $\pi^2$ should return one to the original state, eigenstates of $\pi$ should have eigenvalues of $\pm 1$. Thus pseudo-vectors which are produced by taking the cross products of two vectors rotate like vectors but have the opposite behavior under parity. Examples of pseudo vectors are angular momenta and the magnetic field **B**.

Most Hamiltonians are even under parity. In that case, the solutions are either even or odd since they must be eigenstates of the parity operator. The eigenvalues are ±1 since $\pi^2$ must return one to the original state. If the Hamiltonian has any odd-parity terms, then the eigenstates have admixtures. For instance, the weak interaction of an electron with a nucleus mixes the $2s$ and $2p$ states in the Hydrogen atom.

Finally, we point out that parity allows one to label many matrix elements as being zero. For instance, if one looks at the matrix element,

$$\langle\phi|A|\psi\rangle, \tag{7}$$

where the parities of the two states and the operator are $(-1)^{p_\phi}$, $(-1)^{p_A}$ and $(-1)^{p_\psi}$, the matrix element will be zero if $p_\psi + p_\phi + p_A$ is an odd number. This can be understood by just considering what should happen when integrating over even or odd functions of $x$.

### Time Reversal

Time reversal is an odd kind of symmetry. It suggests that a motion picture of a physical event could be run in reverse without the viewer being able to tell something is wrong. Of course, this does not apply whenever dissipation (friction) is included. In classical mechanics the motion of a particle in a potential $V(r)$ should be equally valid when watched in reverse. In electrodynamics, the motion should be fine as long as the direction of the magnetic field is reversed. Summarizing the time reversal behavior of particles in classical electrodynamics,

$$\mathbf{E} \to \mathbf{E},\ \mathbf{B} \to -\mathbf{B},\ \mathbf{j} \to -\mathbf{j}, \rho \to \rho \tag{8}$$

should describe an equally valid evolution.

In quantum mechanics, we expect the following behavior under time reversal,

$$t \to -t,\ \mathbf{r} \to \mathbf{r},\ \mathbf{p} \to -\mathbf{p}. \tag{9}$$

If one refers to the time-reversal operator as $\Theta$, time-reversal invariance implies

$$(1 - iH\delta t/\hbar)\Theta|\alpha\rangle = \Theta(1 - iHt(-\delta t)/\hbar)|\alpha\rangle. \tag{10}$$

But this is clearly wrong by inspection. Thus, the time reversal must entail an additional property, that of taking the complex conjugate.

One may also see that time reversal entails taking the complex conjugate by considering Schrödinger's wave equation,

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t) + V(x)\Psi(x,t) = i\frac{\partial}{\partial t}\Psi(x,t). \tag{11}$$

If $\Psi(x,t) = \psi(x)e^{-iEt}$ is a solution, taking the complex conjugate and reversing the time also gives a solution to the Hamiltonian. In fact, since $H$ is real one may write $\psi(x)$ as a purely real function or purely imaginary function. A purely real function would be even under time-reversal symmetry while a purely imaginary function would be odd. For instance a plane wave solution is neither even nor odd as it has both real and imaginary parts. In that case taking the complex conjugate changes the direction of the momentum, thus signifying the motion reversal mentioned before.

An easy example is to consider plane waves

$$\Psi(x,t) = e^{ikx}e^{-iEt}. \tag{12}$$

By taking the complex conjugate and reversing the sign of $t$, one obtains a new solution where the momentum is reversed.

Of course, when one gets away from the Schrödinger equation, there are many Hamiltonians which are not real but are Hermitian, $e.g. \sigma_y$. Nonetheless there usually exists a time-reversal symmetry though it may be more complicated than merely taking the complex conjugate. In particle physics, the symmetry of switching times is clearly linked to the existence of solutions with opposite energy (anti-particles). In that case the operation which includes taking the complex conjugate is associated with finding negative-energy or antiparticle solutions, but that is material for another course.

The time reversal operator acts only to the right because it entails taking the complex conjugate. If one defines the time-reversal operator in terms of bras and kets,

$$\langle\tilde{\beta}|\tilde{\alpha}\rangle = \langle\alpha|\beta\rangle = \langle\beta|\alpha\rangle^* \tag{13}$$

where $|\tilde{\alpha}\rangle \equiv \Theta|\alpha\rangle$ and $|\tilde{\beta}\rangle \equiv \Theta|\beta\rangle$ are the time-reversed states. One can then easily show that expectation operators must satisfy the identity

$$\langle\tilde{\beta}|\Theta A\Theta^{-1}|\tilde{\alpha}\rangle = \langle\alpha|A^\dagger|\beta\rangle = \langle\beta|A|\alpha\rangle^*, \tag{14}$$

or is equivalent to saying that the time reversed operator $\Theta A\Theta^{-1}$ sandwiched between time-reversed states gives the complex conjugate of the same matrix element without the time reversals.

Most operators of interest are either even or odd under time reversal.

$$\Theta A\Theta^{-1} = \pm A \tag{15}$$

Clearly an operator that is a linear combination of an odd and an even operator would be neither. Examples of odd and even operators are:

$$\Theta\mathbf{P}\Theta^{-1} = -\mathbf{p},\ \Theta\mathbf{A}\Theta^{-1} = -\mathbf{A},\ \Theta\mathbf{r}\Theta^{-1} = \mathbf{r},\ \Theta\mathbf{L}\Theta^{-1} = -\mathbf{L}. \tag{16}$$

Note that the commutation relations,

$$[x,p] = i\hbar\ ,\quad [L_i, L_j] = i\hbar\epsilon_{ijk}L_k, \tag{17}$$

have apparently different behaviors under reversal on the left and right-hand sides of the equations, until one remembers to consider the $i\hbar$, which flips sign under the time-reversal operator. Notice that the raising and lowering operator for a harmonic oscillator, $x + ip$, is even under time reversal.

Hamiltonians are usually invariant under time reversal. Here we list a few terms which might appear in a Hamiltonian and discuss whether they violate time reversal or parity.

1. $\mathbf{p}^2/2m$ is invariant under both.
2. $\mathbf{p}\cdot\mathbf{r}$ is invariant under parity but not time reversal.
3. $\mathbf{L}\cdot\mathbf{p}$ is invariant under time reversal but not parity.
4. $\mathbf{S}\cdot\mathbf{B}$ and $\mathbf{p}\cdot\mathbf{A}$ are invariant under both.

### Time Reversal and Angular Momentum

The time reversal operator acts in a surprisingly complex manner when operating on eigenstates of angular momentum. For integer-spin particles, one can understand the behavior by considering properties of the $Y_{\ell,m}$s. By taking the complex conjugates, one sees

$$\Theta|j,m\rangle = (-1)^m|j,-m\rangle. \tag{18}$$

However, we should realize that the $(-1)^m$ is basically the result of a phase convention and should not be taken too seriously.

The case of spin 1/2 particles is more surprising. In this case the spins can not be represented by $Y_{\ell,m}$s and one must instead consider the two-component system where $|+\rangle$ and $|-\rangle$ refer to spin-up and spin-down with the direction being chosen along the $z$ axis. In this case an arbitrary state may be written,

$$|\alpha\rangle = e^{i\delta_1}\left(\begin{array}{c} \cos\theta/2 \\ e^{i\gamma_1}\sin\theta/2 \end{array}\right) \tag{19}$$

while the time-reversed state must be the opposite state, and must therefore be orthogonal with the opposite spin,

$$\Theta|\alpha\rangle = e^{i\delta_2}\left(\begin{array}{c} -e^{-i\gamma_1}\sin\theta/2 \\ \cos\theta/2 \end{array}\right) \tag{20}$$

The phases $\delta_1$ and $\delta_2$ are arbitrary, and labeling their difference as $\eta \equiv \delta_2 - \delta_1$ we see that $\Theta$ must equal

$$\Theta = e^{i\eta}\left(\begin{array}{cc} 0 & 1 \\ -1 & 0 \end{array}\right)K, \tag{21}$$

where $K$ is an operator which takes the complex conjugate. The surprising property of $\Theta$ is viewed by squaring the operator,

$$\Theta^2 = \left(\begin{array}{cc} 0 & 1 \\ -1 & 0 \end{array}\right)^2 = -1, \tag{22}$$

independent of the choice of $\eta$.

Making an arbitrary choice of $e^{i\eta} = -i$, one sees that

$$\Theta|+\rangle = i|-\rangle\ ,\quad \Theta|-\rangle = -i|+\rangle. \tag{23}$$

This allows one to summarize both the integral and half-integral results with

$$\Theta|j,m\rangle = i^{2m}|j,-m\rangle \tag{24}$$

To make the time-reversal operator in spin 1/2 systems seem a bit more peculiar it is often written as

$$\Theta = \sigma_y K, \tag{25}$$

which makes the operator look odd because the $y$ direction appears to be preferentially singled out. However, this has nothing to do with the $y$ direction, but only with the fact that the only the operator which flips spin must change the place of the two components and change one sign to make an orthogonal state. One could have associated any of the three sigma matrices with the $x$ , $y$ and $z$ directions, but the time reversal operator must be proportional to the anti-symmetric off-diagonal matrix.

### A particle in a periodic potential

A second class of discrete symmetries involves particles moving in a periodic lattice. In that case translational invariance gives

$$\tau_a H \tau_a^{-1} = H \quad \text{or} \quad V(x+a) = V(x). \tag{26}$$

One thus expects the solution to be an eigenstate of the translation operator,

$$\tau_a \psi(x) = \psi(x+a) = e^{ika}\psi(x), \tag{27}$$

where the eigenvalue is $e^{ika}$. We label the eigenvalue by $k$, which must be real if the wave function is to remain finite.

As an example, we consider the Kronig-Penney model, which is a 1-d model with delta-function potentials separated by $a$,

$$V(x) = \sum_n \beta\delta(x - na). \tag{28}$$

The solution between $x = 0$ and $x = a$ may be written as

$$\psi(x) = e^{iqx} + Be^{-iqx}, \tag{29}$$

with boundary conditions,

$$\psi(a) = e^{ika}\psi(0)\ , \quad \frac{d}{dx}\psi(x)|_{x=a-\epsilon} - e^{ika}\frac{d}{dx}\psi(x)|_{x=\epsilon} + \frac{2m\beta}{\hbar^2}\psi(a) = 0. \tag{30}$$

The boundary conditions can be written as

$$\begin{aligned} e^{iqa} + Be^{-iqa} &= e^{ika}(1+B) & (31)\\ iq\left(e^{iqa} - Be^{-iqa} - e^{ika} + e^{ika}B\right) &= -\frac{2m\beta}{\hbar^2}e^{ika}(1+B) & (32) \end{aligned}$$

Eliminating $B$, one can find a transcendental expression for $q$.

$$p\sin(qa) - 2q\cos(qa) + 2q\cos(ka) = 0, \tag{33}$$

where $p \equiv 2m\beta/\hbar^2$. Notice that the solution only depends on $\cos(ka)$ thus there are solutions for $-\pi < ka < \pi$ with the solutions symmetric about $k = 0$. However, for any $k$ there are a variety of solutions $q$ to the transcendental equation. Plotting the solutions as a function of $k$ yields bands. In the limit $p \to 0$, the solutions are given by $q = k$, otherwise they are shifted, especially near the points where $\cos(ka) = 0$.

### A periodic object

Another example of a discrete symmetry is the case where the object has a symmetry of its own, rather than the potential. An example is a circular chain with $n$ equally spaced identical particles fixed to the chain that can rotate together. In this case the position of the chain is specified by an angle

$$0 < \theta < 2\pi/n. \tag{34}$$

The boundary condition must be that the wave function is returned to the same state by a rotation by $2\pi/n$.

$$\psi(\theta) = e^{mi\theta} \ , \quad m = \cdots, -2n, -n, 0, n, 2n, \cdots \tag{35}$$

Thus the first rotational state is at a higher energy if the symmetry is higher. In fact if the chain was perfectly circular one could not rotate it. This has implications for nuclear and atomic physics. Many nuclei are elliptical and therefore behave similarly to chains with $n = 2$ meaning $\psi(\hat{n}) = \psi(-\hat{n})$. Thus only even values of $\ell$ are allowed.

## Approximation Methods I

In this lecture, we study 3 kinds of approximation methods:

1. WKB Method
2. Variational Method
3. Sudden and Adiabatic Approximations

In the next lectures we cover stationary-state and time-dependent perturbation theory.

### WKB Approximation

The WKB (Wentzel-Kramer-Brillouin) approximation is a useful method for estimating wave functions and tunneling probabilities for smooth potentials or for potentials with only a few discontinuities. The WKB approximation for a wave function can be written as:

$$\begin{aligned} \psi(x) &= A_+(x)e^{i\phi(x)} + A_-(x)e^{-i\phi(x)} && (1)\\ \phi(x) &= \int^x dx' p(x')/\hbar, && (2) \end{aligned}$$

where the lower limit of the integral is absorbed by the arbitrary phases in $A_+$ and $A_-$. The function $p(x)$ is defined by

$$p(x) \equiv \sqrt{2m(E - V(x))} \tag{3}$$

and can be thought of the momentum of a classical particle with energy $E$ at position $x$.

To see the accuracy of the approximation one must apply the Schrödinger equation to the assumed form for $\psi$. Here we use only the $A_+$ term.

$$\begin{aligned} (H-E)\psi(x) &= -\hbar^2 \frac{\partial^2}{\partial x^2}\psi(x) - (E-V)\psi(x) && (4)\\ &= \left\{ \frac{p(x)^2}{2m} - E - V(x) \right\} A_+(x)e^{i\phi(x)} + \frac{i\hbar}{2m}\left\{ 2p(x)\frac{\partial}{\partial x}A_+(x) + A_+(x)\frac{\partial}{\partial x}p(x) \right\} e^{i\phi(x)} && (5)\\ &\quad - \frac{\hbar^2}{2m}\left\{ \frac{\partial^2}{\partial x^2}A_+(x) \right\} e^{i\phi(x)} && (6) \end{aligned}$$

The first term disappears from our choice of $p(x)$ while the second term will vanish if we choose

$$A_+(x) \propto p(x)^{-1/2}. \tag{7}$$

The last term does not vanish, but is neglected in the limit that $\hbar$ is small as it is proportional to $\hbar^2$. One can understand the accuracy of the approximation by taking the second derivative of $A_+(x)$ in the last term and comparing it to the other terms. One then sees that what is important is whether characteristic lengths of the the potential $\ell$ are much longer than $\hbar/p(x)$.

Physically, one may understand the $p^{-1/2}$ dependence of $A_+$ by realizing that the WKB approximation has no reflection associated with it, thus conservation of flux requires $p|A|^2$ to be constant.

To estimate a bound state wave function, one sets the phase $\phi(x)$ to be zero at one turning point (a point where $p(x) = 0$), then solves for $\phi(x)$ at the other turning point. By finding an energy for which the phase changes by $\pi$ one then has a solution. For one may then combine such a solution with the $A_-$ solution to return to the original turning point incurring a net phase change of $2\pi$.

Perhaps the most common use of the WKB approximation is in estimating tunneling probabilities. In this case the wave functions have exponentially growing and decaying amplitudes. In fact, one usually ignores the $x$ dependence of the amplitude and merely states that the tunneling probability form going from turning point $a$ to turning point $b$ is

$$P_{a\to b} \approx \exp\left\{-\frac{2}{\hbar}\int_a^b dx\sqrt{2m(V(x)-E)}\right\}, \tag{8}$$

with the factor of two coming from squaring the amplitude.

As an example, we estimate the ground state energy of a particle of mass $m$ in the one-dimensional harmonic oscillator potential

$$V(x) = \frac{1}{2}m\omega^2x^2. \tag{9}$$

In this case one fourth of $2n\pi$ must result from integrating $\int k(x)dx$ from zero to the turning point.

$$\frac{n\pi}{2} = \frac{\sqrt{2m}}{\hbar}\int_0^a dx\sqrt{\frac{1}{2}m\omega^2a^2 - \frac{1}{2}m\omega^2x^2}, \tag{10}$$

where the turning point $a$ depends on the unknown ground state energy, $E = m\omega^2a^2/2$. Solving the equation above for $a$ gives

$$a^2 = \frac{2n\hbar}{m\omega} \tag{11}$$

$$E = n\hbar\omega, \tag{12}$$

which is correct aside from an extra $\hbar\omega/2$.

## Variational Theory

Variational calculations are used to calculate ground state wave functions by using the simple fact that all states must have energies greater or equal to that of the ground state. Thus, by writing a state in terms of some parameters $\alpha_i$, and minimizing $E = \langle\vec{\alpha}|H|\vec{\alpha}\rangle$ with respect to the parameters $\alpha_i$, one knows that the energy can never fall below the true ground state energy. The minimization procedure therefore can be used to estimate the ground state energy and ground state wave functions.

As an example, we consider the potential

$$V(r) = -\frac{e^2}{r}. \tag{13}$$

We suppose that we were lucky and guessed the hydrogen atom wave functions for the trial form,

$$\psi(r) = \frac{2}{\sqrt{4\pi a^3}}e^{-r/a}, \tag{14}$$

where $a$ is the variational parameter. One would then minimize the expectation of $\langle H\rangle$ with respect to $a$.

$$\langle H\rangle = \frac{\hbar^2}{2ma^2} - \frac{e^2}{a}. \tag{15}$$

The minimization, $(\partial/\partial a)\langle H\rangle = 0$, yields

$$a = \frac{\hbar^2}{me^2}, \tag{16}$$

which in this case gives the exact wave function and ground state energy, but only due to the fortunate choice for the form of the wave function. In general, one would obtain an approximate wave function with on overestimate of the ground state energy.

Variational calculations are popular in a variety of many-body applications where the interactions and many-body wave functions can be extremely complicated.

### Sudden Approximation

The sudden approximation can be used for calculating transition probabilities for cases where the Hamiltonian changes rapidly between two times $t_1$ and $t_2$ . In fact there is no real technique involved in the approximation, but merely an understanding that the reaction was so quick that one can approximate the transition amplitude by a simple overlap,

$$\langle\alpha|U(t_2,t_1)|\beta\rangle \approx \langle\alpha|\beta\rangle, \tag{17}$$

where $|\beta\rangle$ is usually an eigenstate of the Hamiltonian before $t_1$ and $|\alpha\rangle$ is usually an eigenstate of the Hamiltonian after $t_2$.

When a potential is changed slowly, the probability remains assigned to the same state. This is because for each differential change in the potential, a differential change $\epsilon$ is induced in the wave function. However, if the changes occur at much different times, the differential amplitudes contribute with uncorrelated phases and the net change in the probability goes as $\sum|\epsilon|^2 = 0$. Thus if a particle is in the ground state, and the well changes slowly, it remains in the ground state afterward. This also implies that entropy is not generated, hence the term adiabatic.

### Expanding Well Example:

The most common example used to illustrate the sudden approximation is the case of the expanding well. Here, we consider an inifinte square well confining particles to the region $0 < x < a$ which suddenly expands at time $t = 0$ to allow particles to occupy the region $0 < x < 2a$.

Assuming a particle was in the ground state of the old well,

- What is the probability of being in the ground state of the new well?
- What is the probability of being in the state $n$ of the new well? Here, $\psi_n(x) \propto \sin[n\pi x/(2a)]$
- What is the expectation of the energy $\langle H\rangle$ after the expansion of the well?

The sudden approximation can be used whenever the times $t_1$ and $t_2$ are so close that the relevant energies multiplied by $(t_2 - t_1)/\hbar$ are small. The sudden approximation is commonly used in nuclear reaction theory. For instance, one may consider a deuteron where an electric field from a relativistic particle flies by and accelerates the proton to a new velocity while leaving the neutron unchanged. One might then use the sudden approximation (or the Glauber approximation which is similar) to estimate the chance that the deuteron remains in its ground state.

## Approximation Methods II

In this lecture we present stationary-state perturbation theory which is also known as Rayleigh-Schrödinger perturbation theory. In such a theory one solves for states and their energies in an expansion of powers of $\lambda$ where the Hamiltonian is

$$H = H_0 + \lambda V. \tag{1}$$

The potential $V$ is known as the perturbation and is assumed to be small while $\lambda$ is assumed to be unity and is only used to keep tally of the expansion of $V$, i.e. and expansion in $\lambda$ is an expansion in $V$.

Before one embarks on perturbation theory, one assumes that one has already solved for the states $|n\rangle$ and the energies $\epsilon_n$ which are eigenstates of $H_0$. The goal is to express solutions for the new Hamiltonian as an expansion in terms of solutions of $H_0$.

We assume that both the eigenstates and eigenenergies of the new Hamiltonian can be written as an expansion if powers of $\lambda$,

$$\begin{aligned} |N\rangle &= |n\rangle + \lambda|N^{(1)}\rangle + \lambda^2|N^{(2)}\rangle + \cdots & (2) \\ E_n &= \epsilon_n + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \cdots & (3) \end{aligned}$$

Here, the terms $|n^{(j)}\rangle$ and $E_n^{(j)}$ denote the corrections to the eigenstates and energies of order $\lambda$.

We are also free to make an assumption about normalization of the state $|N\rangle$.

$$\langle n|N\rangle = 1, \tag{4}$$

which is equivalent to saying that the additional parts of the wave function have no $|n\rangle$ component,

$$\langle n|N^{(k)}\rangle = 0. \tag{5}$$

The Schrödinger equation

$$(H_0 + \lambda V)|N\rangle = E_n|N\rangle, \tag{6}$$

must be satisfied to every power of $\lambda$. by looking at the $j^{\text{th}}$ power of $\lambda$, this gives

$$H_0|N^{(j)}\rangle + V|N^{(j-1)}\rangle = \sum_{k=0,j} E_n^{(k)}|N^{(j-k)}\rangle. \tag{7}$$

Here, the sum over $k$ goes from zero to $j$ with the understanding that $|N^{(0)}\rangle = |n\rangle$ and $E^{(0)} = \epsilon_n$.

We solve for the expressions iteratively. That is, one first finds $E^{(k)}$ then finds $|N^{(k)}\rangle$, then given those states move onto $k+1$. To find $E_n^{(k))}$, one takes the overlap of Eq. (**??**) with $\langle n|$ and using the normalization definitions one obtains.

$$\langle n|V|N^{(j-1)}\rangle = E^{(j)} \tag{8}$$

For the case where $j = 1$, one gets the lowest-order perturbation theory answer for the energy.

$$E_n^{(1)} = \langle n|V|n\rangle. \tag{9}$$

The state $|N^{(j)}\rangle$ is defined by its overlap with the states $\langle m|$ where $m \neq n$. Given one knows $E_n^{(j)}$ one can find the $\langle m|N^{(j)}\rangle$ by taking the overlap of $\langle m|$ with Eq. (**??**).

$$\epsilon_m\langle m|N^{(j)}\rangle + \langle m|V|N^{(j-1)}\rangle = \sum_{k=0,j} E_n^{(k)}\langle m|N^{(j-k)}\rangle. \tag{10}$$

Solving for the $j^{\text{th}}$ part which is unknown,

$$\langle m|N^{(j)}\rangle = \frac{1}{\epsilon_m - \epsilon_n}\left(-\langle m|V|N^{(j-1)}\rangle + \sum_{k=1,j} E_n^{(k)}\langle m|N^{(j-k)}\rangle\right) \tag{11}$$

One can then solve for the first-order correction to the wave function,

$$|N^{(1)}\rangle = \sum_{m\neq n} |m\rangle\frac{1}{\epsilon_m - \epsilon_n}\langle m|V|n\rangle \tag{12}$$

Using the state $|N^{(1)}\rangle$, one can then find the expression for $E_n^{(2)}$,

$$E_n^{(2)} = -\sum_{m\neq n}\frac{|\langle m|V|n\rangle|^2}{\epsilon_m - \epsilon_n}. \tag{13}$$

Several important principles can be realized by observing the form of $E_n^{(2)}$. First, two states energies are pushed apart in 2nd-order perturbation theory. Secondly, if the levels are initially close, the energies are more affected. In fact, if they are degenerate perturbation, theory breaks down, and one must apply degenerate perturbation theory which is the topic of the next lecture. Of special significance is noticing that the ground state is always lowered in 2nd order perturbation theory.

**Example** We will work the problem of the Harmonic oscillator Hamiltonian with a perturbation,

$$V = \beta x, \tag{14}$$

and show that the correction to the ground state energy, $E^{(2)}$, surprisingly gives the exact answer for this case.

### Degenerate-State Perturbation Theory

Due to terms of the form

$$\frac{\langle m|V|n\rangle}{\epsilon_m - \epsilon_n},$$

perturbation theory falls apart when the perturbation mixes degenerate states. This can be corrected by first separting the part of the potential that mixes the degenerate states $V_d$ from the potential that mixes the degenerate states with the other states $V'$, then diagonalizing $V_d$ and use perturbation theory for $V'$.

Formally, this means breaking the potential as follows,

$$\begin{aligned} V &= V_d + V' && (15)\\ V_d &= P_d V P_d && (16)\\ V' &= (1-P_d)V(1-P_d) + P_d V(1-P_d) + (1-P_d)VP_d, && (17) \end{aligned}$$

where $P_d$ is the projection operator that projects the subset of states that are degenerate

$$P_d = \sum_{m\in d} |m\rangle\langle m| \tag{18}$$

Since $\langle m_1|V'|m_2\rangle = 0$ when $m_1$ and $m_2$ are in the degenerate set, there is no longer any problem. Note that by diagonalizing $V_d$, $V_d$ essentially becomes part of $H_0$.

The only example we will discuss is the Stark effect. Actually, in this example we will only consider the diagonalization of $V_d$ and forget about the perturbative part entirely. The Stark effect refers to the placement of a hydrogen atom in an electric field,

$$V = e\mathcal{E}z.$$

We are interested in calculating the splitting of the 2s and 2p levels. In this case the matrix elements of $V$ are zero along the diagonal of the 4×4 matrix that describes $V$. This arises because the three $p$ states and the $s$ states have good parity. However, the $s$ state can be mixed with the $p$ states by the interaction. Thus there is an off-diagonal matrix element

$$\langle n=2, \ell=1, m_\ell=0|V|n=1, \ell=0\rangle \neq 0.$$

All other matrix elements are zero. Using the forms for the wave functions given in a previous lecture, one can solve for the matrix element,

$$\langle 2s|V|2p, m=0\rangle = \int d\Omega r^2 dr R_{2,0}(r)R_{2,1}(r) r\cos\theta Y_{0,0}(\theta,\phi)Y_{1,0}(\theta,\phi) = 3ea_0|\mathbf{E}|$$

Thus the eigenstates of $V$ are $\pm 3ea_0|\mathbf{E}|$.

## Time-Dependent Interactions

Many problems in quantum problems involve time-dependent interactions. Obvious examples include spin magnetic resonance problems where the interaction explicitly varies in time. A less obvious example is a scattering problem where the incoming wave packet slowly enters the region where it feels the potential then leaves. This problem is treated by considering asymptotic momentum states with a potential that slowly turns off and on with time, rather than with a fixed potential with wave packets. Thus, nearly all perturbative scattering (e.g. Feynmann diagrams) treatments are application of time-dependent perturbatin theory even though the potential is not actually varying with time.

## The Two-State Problem, an Exactly Solvable Model

Consider two states $|1\rangle$ and $|2\rangle$ interacting through the potential,

$$\begin{aligned} H_0 &= \hbar\omega_1|1\rangle\langle 1| + \hbar\omega_2|2\rangle\langle 2| = \frac{\hbar}{2}(\omega_1+\omega_2) + \frac{\hbar}{2}(\omega_1-\omega_2)\sigma_z && (1)\\ V_t &= \gamma\cos(\omega t)\sigma_x + \gamma\sin(\omega t)\sigma_y && (2) \end{aligned}$$

or written as a matrix,

$$H = \left(\begin{array}{cc} E_1 & \gamma e^{i\omega t} \\ \gamma e^{-\omega t} & E_2 \end{array}\right). \qquad (3)$$

This is the form of an interaction with time-dependent magnetic field,

$$H = H_0 + \vec{\mu}\cdot\vec{B}(t), \quad B(t) = B_0\hat{z} + B_\perp\left[\hat{x}\cos(\omega t) + \hat{y}\sin(\omega t)\right]. \qquad (4)$$

One can make the substitution,

$$|\psi\rangle \rightarrow e^{-i\bar{\omega}t}|\psi\rangle,\ \bar{\omega} \equiv \frac{E_1+E_2}{2\hbar} \qquad (5)$$

to write the new Hamiltonian as

$$H = \left(\begin{array}{cc} \omega_{12}/2 & \gamma e^{i\omega t} \\ \gamma e^{-\omega t} & -\omega_{12}/2 \end{array}\right), \qquad (6)$$

where $\omega_{12} \equiv (E_1 - E_2)/2$.

Writing the evolution in the interaction picture for the components $\psi_1$ and $\psi_2$,

$$\begin{aligned} \frac{\partial}{\partial t}\psi_1(t) &= -i\frac{\omega_{12}}{2}\psi_1(t) - i\frac{\gamma}{\hbar}e^{-i\omega t}\psi_2(t) && (7)\\ \frac{\partial}{\partial t}\psi_2(t) &= -i\frac{\omega_{12}}{2}\psi_2(t) - i\frac{\gamma}{\hbar}e^{i\omega t}\psi_1(t) && (8)\\ & && (9) \end{aligned}$$

Now, by making the substituion,

$$\begin{aligned} \psi_1' &\equiv e^{-i\omega t/2}\psi_1 && (10)\\ \psi_2' &\equiv e^{i\omega t/2}\psi_2, && (11) \end{aligned}$$

one can derive the evolutions,

$$\begin{aligned}\frac{\partial}{\partial t}\psi_1'(t) &= -i\frac{(\omega_{12}-\omega)}{2}\psi_1'(t)+\frac{\gamma}{\hbar}\psi_2'(t) && (12)\\ \frac{\partial}{\partial t}\psi_2'(t) &= i\frac{(\omega_{12}-\omega)}{2}\psi_2'(t)+\frac{\gamma}{\hbar}\psi_1'(t). && (13)\end{aligned}$$

The problem now looks like a Hamiltonian without a time dependent interaction,

$$H' = \frac{\hbar(\omega_{12}-\omega)}{2}\sigma_z + \gamma\sigma_y. \tag{14}$$

This is the same problem as we worked out for neutrino oscillations. The evolution operator becomes

$$\begin{aligned}e^{-iH't} &= \cos(\Omega t)+\sigma_n\sin(\Omega t),\\ \Omega &= \sqrt{\frac{(\omega_{12}-\omega)^2}{4}+\frac{\gamma^2}{\hbar^2}}\\ \sigma_n &= \cos(\theta)\sigma_z+\sin(\theta)\sigma_y\\ \tan(\theta) &= \frac{2\gamma}{\hbar(\omega_{12}-\omega)}\end{aligned}$$

If the state begins polarized in the $z$ direction, the maximum probability of becoming a spin-down state is

$$\max|\langle\downarrow|e^{-iH't}|\uparrow\rangle|^2 = \frac{\gamma^2/\hbar^2}{\gamma^2/\hbar^2+(\omega-\omega_{12})^2/4} \tag{15}$$

Note the resonant condition, $\omega_{12}=\omega$. Also note that $\gamma$ plays the role of the half-width in the Lorentzian.

The Lorentzian is a common in time-dependent systems. The resonant form clearly displays that driving the system at the resonant frequency, $\omega=\omega_{12}$, results in the greatest chance for flipping the spin. NMR works on very similar principles, only in this case the time-dependent field usually oscillates only in one plane, i.e.

$$\vec{B}(t) = B_0\hat{z} + B_\perp\hat{x}\cos(\omega t). \tag{16}$$

This is a bit harder to work out as compared to our example but the resonant conditions remain the same.

### The Interaction Representation (Picture)

Before one can begin time-dependent perturbation theory, we need to consider the interaction representation, which is an alternative to the Schrödinger and Heisenberg representations. Summarizing the representations,

$$\begin{aligned}|\psi(t)\rangle_S &= e^{-iHt/\hbar}|\psi(t=0)\rangle_S && (17)\\ |\psi\rangle_H &= |\psi(t=0)\rangle_S \text{ (Heisenberg states are fixed in time.)} && (18)\\ |\psi(t)\rangle_I &= e^{iH_0t/\hbar}|\psi(t)\rangle_S, && (19)\end{aligned}$$

where the Hamiltonian is divided into an understood part, $H_0$ and a perturbation $V$. Note that if $V = 0$ that the interaction states become equal to the Heisenberg states.

Since matrix elements $\langle\phi|ABC|\psi\rangle$ must not depend on the representation, operators in the Heisenberg and Interaction representations are defined as:

$$\begin{aligned} A_H(t) &= e^{iHt/\hbar} A_S e^{-iHt/\hbar} && (20) \\ A_I(t) &= e^{iH_0t/\hbar} A_S e^{-iH_0t/\hbar}, && (21) \end{aligned}$$

where we have assumed that $H$ is not time dependents, otherwise $e^{-iHt/\hbar}$ would be replaced with an evolution operator.

Solving from the evolution of a state in the interaction representation,

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle_I &= -H_0|\psi(t)\rangle_I + e^{iH_0t/\hbar}(H_0+V)|\psi(t)\rangle_S && (22) \\ &= V_I(t)|\psi(t)\rangle_I. && (23) \end{aligned}$$

The subscript $I$ is omitted in most literature and the knowledge of which representation is being used is left to the astute reader. If the potential has an explicit time dependence, the explicit time dependence must be absorbed into $V_I(t)$.

$$V_S(t) = \sum_{m,n} \beta_{m,n}(t)|m\rangle\langle n|, \qquad (24)$$

then $V_I$ becomes,

$$V_I(t) = e^{i(\omega_m-\omega_n)t}\beta_{m,n}(t)|m\rangle\langle n|, \qquad (25)$$

where the eigenstates of $H_0$ are $\hbar\omega_n$.

**Time-Dependent Perturbation Theory**

Consider the evolution operator in the interaction picture defined by

$$|\psi(t)\rangle_I = U_I(t,t_0)|\psi(t_0)\rangle_I. \qquad (26)$$

Using the equations of motion,

$$i\hbar\frac{d}{dt}U(t,t_0) = V_I(t)U(t,t_0), \qquad (27)$$

with the boundary conditions,

$$U(t=t_0,t_0) = 1. \qquad (28)$$

One can rewrite the differential equation as a differential equation,

$$\begin{aligned} U(t,t_0) &= 1 - \frac{i}{\hbar}\int_{t_0}^{t} dt' V_I(t')U_I(t',t_0) && (29) \\ &= 1 - \frac{i}{\hbar}\int_{t_0}^{t} dt' V_I(t') + \left(\frac{-i}{\hbar}\right)^2 \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' V_I(t')V_I(t'') && (30) \\ & \cdots + \left(\frac{-i}{\hbar}\right)^n \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' \cdots \times \int_{t_0}^{t^{(n-1)}} dt^{(n)} V_I(t')V_I(t'')\cdots V_I(t^{(n)}) + \cdots && (31) \end{aligned}$$

This is known as the Dyson series, named after Freeman J. Dyson. Keeping only the first term in the expansion in $V$ amounts to first-order perturbation theory.

Also note the the operator $U_I$ is related to the Schrödinger evolution operator by

$$U_S = e^{-iH_0 t} U_I e^{iH_0 t}, \tag{32}$$

which means that transition probabilities (which go as the square of matrix elements, $|\langle n|U|i\rangle|^2$, are the same in both representations since the states are eigenstates of $H_0$.

To second order perturbation theory, the matrix element becomes

$$\begin{aligned} \langle n|U(t,t_0)|i\rangle &= -\frac{i}{\hbar}\int_{t_0}^{t} dt' \langle n|V_S(t')|i\rangle e^{i(E_n-E_i)t/\hbar} && (33) \\ &+ \left(\frac{-i}{\hbar}\right)^2 \sum_m \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' \langle n|V_S(t')|m\rangle\langle m|V_S(t'')|n\rangle e^{i(E_n-E_m)t'} e^{i(E_m-E_i)t''} && (34) \end{aligned}$$

Higher orders are simple to write down, it just takes space. Note that the this expression was accomplished by noting that

$$\langle n|V_I(t)|m\rangle = \langle n|V_S(t)|m\rangle e^{i(E_n-E_m)t/\hbar}. \tag{35}$$

## Fermi's Golden Rule

We will now derive one of the most important expressions derived in the class, Fermi's Golden Rule for the transion rate from the state $|i\rangle$ to the state $|n\rangle$. We will derive the same expression twice to demonstrate how robust the derivation is.

First we consider the case where we turn on the perturbation slowly,

$$\langle n|V_S(t)|n\rangle = e^{\eta t} V_{nm}, \quad \eta \to 0^+ \tag{36}$$

where the times being considered are less than or near zero, meaning the interaction was turned on slowly from $t = -\infty$. To first order,

$$\begin{aligned} \langle n|U_I(t,-\infty)|i\rangle &= -\frac{i}{\hbar} V_{ni} \int_{-\infty}^{t} dt' e^{i(E_n-E_i)t'/\hbar + \eta t'} && (37) \\ &= \frac{V_{ni}}{E_n - E_i - i\hbar\eta} e^{i(E_n-E_i)t/\hbar + \eta t} && (38) \end{aligned}$$

Thus the probability goes as,

$$P_{i\to n}(t) = \frac{|V_{ni}|^2}{(E_n-E_i)^2 + \hbar^2\eta^2} e^{2\eta t}, \tag{39}$$

In obtain Fermi's Golden Rule, one does not calculate $|\langle n|U|i\rangle|$, but instead calculates $(d/dt)|\langle n|U|i\rangle|^2$ to obtain transition rates rather than transition probabilities.

$$\frac{d}{dt} P_{i\to n}(t) = \frac{2\eta|V_{ni}|^2}{(E_n-E_i)^2 + \hbar^2\eta^2} \tag{40}$$

where we have finally made the approximation that $\eta t$ is small. From your homework problem, you can see that the $\eta$-dependent terms can be replaced with a $\delta$ function as $\eta \to 0^+$,

$$\frac{d}{dt}P_{i\to n}(t) = \frac{2\pi}{\hbar}|V_{ni}|^2\delta(E_n - E_i) \tag{41}$$

Thus, there is only a transition if the final state has the same energy as the initial state. This works for scattering or decays, where indeed there are many final states with a given energy. The $\delta$ function looks a bit peculiar, but makes sense when the states $n$ are in a continuum. For instance, one does not calculate the electromagnetic decay rate of a radioactive nucleus to a specific state where a photon has a momentum $k$, but instead to any state within a specific angle. By summing over all such states, using the density of states and integrating over $dE_\gamma$, the delta function simplifies the integration over final states.

### Harmonic Perturbations

Rather than having a potential that turned on slowly, one could envisage a a harmonic potential,

$$\langle n|V_S(t)|m\rangle = V_{nm}e^{\eta t}\cos(\omega t) = \frac{1}{2}V_{nm}e^{\eta t}\left(e^{i\omega t} + e^{-i\omega t}\right). \tag{42}$$

One can then follow the same derivation by noting that the only two differences are the factor of 1/2, which get squared to obtain a probability, and the extra phases in the two terms. If we consider each term separately $e^{i\omega t}$ and $e^{-i\omega t}$, one can write down the answer without much thought.

$$\frac{d}{dt}P_{i\to n}(t) = \frac{2\pi}{\hbar}\frac{|V_{ni}|^2}{4}\left[\delta(E_n - E_i + \hbar\omega) + \delta(E_n - E_i - \hbar\omega)\right] \tag{43}$$

Additionally there would be cross term from squaring the matrix elements, but that term behaves as $\cos(\omega t)$ and can be disregarded on the average.

### Example

Consider a particle of mass $m$ in the ground state of a $\delta$ function potential,

$$V_0(x) = -\beta\delta(x) \tag{44}$$

The particle feels a harmonic potential

$$V(t) = eEx\cos(\omega t), \quad \hbar\omega > |\text{G.S. energy}| \tag{45}$$

Estimate the ionization rate using first-order perturbaton theory. (This is a one-dimensional example).

To solve this problem,

1. Find the G.S. wave function and G.S energy of the delta function potential.
2. Calculate the matrix element $\langle k|V|0\rangle$ using a normalized state $\langle x|k\rangle = e^{ikx}/\sqrt{L}$ where $L$ is an arbitrarily large size to the box.
3. Sum the probability over states by writing it as a density of states. Notice how the size of the box falls out of the problem.

### Scattering in the Born approximation

Scattering cross sections can be thought of as giving the rate for scattering when multiplied by the particle flux.

$$R(\mathbf{k}_0 \to \mathbf{k}_f) = \sigma_{if}\frac{v}{V}, \tag{1}$$

where $V$ is the volume per individual projectile and $v$ is the velocity of the projectiles. Thus, one can write the cross section for scattering into any state,

$$\begin{aligned}\sigma &= \frac{V}{v}\sum_{\mathbf{k}_f} R(\mathbf{k}_0 \to \mathbf{k}_f) &(2)\\ &= \frac{2\pi V}{v\hbar}\sum_{\mathbf{k}_f} |\langle \mathbf{k}_f|V|\mathbf{k}_i\rangle|^2\delta(E_f - E_i) &(3)\end{aligned}$$

One may express the sum over states as an integral,

$$\sum_{\mathbf{k}_f} = \frac{V}{(2\pi)^3}\int d^3k_f, \tag{4}$$

and write the matrix element as,

$$\langle \mathbf{k}_f|V|\mathbf{k}_i\rangle = \int d^3r \frac{e^{-i\mathbf{k}_f\cdot\mathbf{r}}}{\sqrt{V}}V(\mathbf{r})\frac{e^{i\mathbf{k}_i\cdot\mathbf{r}}}{\sqrt{V}} \tag{5}$$

to obtain an expression for the cross section where the volume has canceled,

$$\begin{aligned}\sigma &= \frac{1}{4\pi^2\hbar v}\int d^3k_f\delta(E_f - E_i)|\int d^3rV(r)e^{i(\mathbf{k}_f-\mathbf{k}_i)\cdot\mathbf{r}}|^2 &(6)\\ &= \frac{m^2}{4\pi^2\hbar^4}\int d\Omega\left|\int d^3rV(r)e^{i(\mathbf{k}_f-\mathbf{k}_i)\cdot\mathbf{r}}\right|^2 &(7)\end{aligned}$$

One may express this as a differential cross section,

$$\frac{d\sigma}{d\Omega} = \frac{m^2}{4\pi^2\hbar^4}\left|\int d^3rV(r)e^{i(\mathbf{k}_f-\mathbf{k}_i)\cdot\mathbf{r}}\right|^2 \tag{8}$$

Thus the differential cross section is determined by the Fourier transform of the potential, where the momentum transfered to the target, $\mathbf{k}_i - \mathbf{k}_f$, enters the Fourier transform.

### Born Approximation Example

As a function of the scattering angle $\theta$ find the differential cross section for particles scattered off a spherically symmetric potential,

$$V(r) = V_0e^{-r^2/(2a^2)} \tag{9}$$

First calculate the Fourier transform of the potential which depends only on the magnitude of $\mathbf{k}_i - \mathbf{k}_f$.

$$\begin{aligned}V(q) &= V_0\int d^3re^{-r^2/(2a^2)}e^{i\mathbf{q}\cdot\mathbf{r}} &(10)\\ &= V_0a^3(2\pi)^{3/2}e^{-q^2a^2/2} &(11)\end{aligned}$$

where

$$\begin{aligned} q &= |\mathbf{k}_i - \mathbf{k}_f| && (12)\\ &= k\sqrt{(1-\cos\theta)^2 + \sin^2\theta} && (13)\\ &= k\sqrt{2(1-\cos\theta)} && (14)\\ &= 2k\sin(\theta/2) && (15) \end{aligned}$$

Thus the differential cross section is

$$\frac{d\sigma}{d\Omega} = \frac{2\pi m^2 a^6 V_0^2}{\hbar^4} e^{-4k^2\sin^2(\theta/2)} \tag{16}$$

Note that finding the total cross section would require performing a rather difficult integral over the solid angle, $d\Omega = 2\pi d\cos\theta$.

### Coulomb Scattering in the Born Approximation

In this case the potential is

$$V(\mathbf{r}) = \frac{e^2}{r}. \tag{17}$$

Note the cross sections will be the same whether the potential is attractive of repulsive in the Born approximation.

Performing the Fourier transform,

$$\begin{aligned} V(q) &= 2\pi \int r^2 dr \int_{-1}^{1} dx e^{iqrx} \frac{e^2}{r} && (18)\\ &= \frac{4\pi e^2}{q} \int dr \sin qr && (19)\\ &= -\frac{4\pi e^2}{q^2} \cos(qr)|_0^\infty && (20)\\ &= \frac{4\pi e^2}{q^2} && (21)\\ &= \frac{\pi e^2}{k^2\sin^2(\theta/2)}, && (22) \end{aligned}$$

The limit at $r \to \infty$ can be realized by adding an exponential damping term to the potential $e^{-\eta r}$, $\eta \to 0^+$, and repeating the integral to see that one gets the same answer with the evaluation at $\infty$ going to zero.

The expression for the differential cross section is then,

$$\frac{d\sigma}{d\Omega} = \frac{m^2 e^4}{4\hbar^4 k^4 \sin^4(\theta/2)}. \tag{23}$$

Coincidentally, this answer is identical to the Rutherford cross section in classical mechanics. Note that this cross section is ill-behaved at $\theta \to 0$, meaning that the total cross section is infinite.

## Diffraction

Often scattering is done within a material for the purpose of learning about the structure of the material rather than understanding the potential. In that case the Fourier transform of the potential can be written as,

$$\begin{aligned} V(\mathbf{q}) &= \sum_a \int d^3r e^{i\mathbf{q}\cdot\mathbf{r}} V(\mathbf{r}-\mathbf{a}) && (24) \\ &= \sum_a e^{i\mathbf{q}\cdot\mathbf{a}} \int d^3r e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{a})} V(\mathbf{r}-\mathbf{a}) && (25) \\ &= v(\mathbf{q})s(\mathbf{q}), && (26) \end{aligned}$$

where $s(\mathbf{q}) \equiv \sum_a e^{i\mathbf{q}\cdot\mathbf{a}}$.

This allows us to write the differential cross section ast

$$\frac{d\sigma}{d\Omega} = \frac{m^2}{4\pi^2\hbar^4}|v(\mathbf{q})^2|\ |s(\mathbf{q})|^2, \tag{27}$$

which means that if the potential is understood one may therefore determine $s(\mathbf{q})$.

The information from measuring the differential cross section is related to the probability that two scattering centers are separated by a distance $\mathbf{a}$.

$$\begin{aligned} |s(\mathbf{q}|^2 &= \sum_{a,a'} e^{i\mathbf{q}\cdot(\mathbf{a}-\mathbf{a}')} && (28) \\ &= N\sum_{\delta\mathbf{a}} e^{i\mathbf{q}\cdot\delta\mathbf{a}} && (29) \\ &= N\int d^3\delta a\ S(\delta\mathbf{a})e^{i\mathbf{q}\cdot\delta\mathbf{a}} && (30) \\ &= N\tilde{S}(\mathbf{q}), && (31) \end{aligned}$$

where $\mathbf{q}$ is the momentum transfer and $N$ is the number of scattering centers. Here $S$ is known as the structure function $S(\mathbf{x})$ and gives the probability of finding two scattering centers separated by $\mathbf{x}$. If the material is a lattice $\tilde{S}(\mathbf{q})$ has spikes for values of $\mathbf{q}$ which correspond to in-phase contributions from different sites. Whereas, if the material is a liquid, the spikes disappear since there is no long range order. The structure function $S(\mathbf{x})$ then has a hole near $\mathbf{x} = 0$ and perhaps a few wiggles before being flat for large $\mathbf{x}$.

Since the momentum transfer is very high in nuclear or particle experiments, one usually neglects the structure of the target in those experiments, whereas it comes into play for X-ray scattering or low-energy neutron scattering.

## Higher Order Expansions, The $T$-matrix

Decays, scattering cross sections and propagators (next topic) are all instances where one invokes Fermi's golden rule. In all these instances higher order calculations can be included by replacing the $V$ in Fermi's golden rule with the $T$ matrix.

Writing the transition matrix element to second order in time-dependent perturbation theory,

$$\langle n|U_I(t,-\infty)|i\rangle = -\frac{i}{\hbar}V_{ni}\int_{-\infty}^{t} dt' e^{i(E_n-E_i)t'/\hbar+\eta t'} \tag{32}$$

$$+\left(\frac{-i}{\hbar}\right)^2 V_{nm}V_{mi}\int_{-\infty}^{t} dt' \int_{-\infty}^{t'} dt'' e^{i(E_n-E_m)t'+\eta t'} e^{i(E_m-E_i)t''/\hbar+\eta t''} \tag{33}$$

$$= -\frac{i}{\hbar}\int_{-\infty}^{t} e^{i(E_n-E_i)/\hbar+\eta t'} \tag{34}$$

$$\cdot\left(V_{ni}+\frac{-i}{\hbar}e^{\eta t'}V_{nm}V_{mi}\int_{-\infty}^{t'} dt'' e^{i(E_i-E_m)(t'-t'')/\hbar+\eta(t''-t')}\right) \tag{35}$$

By inspection, one can see that by making the substitution,

$$T_{ni} \rightarrow V_{ni}-\frac{i}{\hbar}V_{nm}V_{mi}\int_{-\infty}^{t'} dt'' e^{i(E_i-E_m)(t''-t')/\hbar-\eta(t'-t'')} \tag{36}$$

$$= V_{ni}-\frac{V_{nm}V_{mi}}{E_i-E_m-i\hbar\eta} \tag{37}$$

one sees that the second order solution looks just like the first order solution with $T$ replacing $V$. (Note that this actually requires assuming $\eta \rightarrow 0$.)

One can thus perform higher order calculations in Fermi's Golden Rule by replacing $V$ with $T$, which is known as the T-matrix in the limit that all orders of perturbation theory are considered.

## Propagators (Time-ordered Evolution Operators)

A propagator, also known as a Green's function, is nothing more than the evolution operator with a theta function tacked on,

$$
\begin{aligned}
G(t) &\equiv e^{-iHt/\hbar}\Theta(t), \qquad (1)\\
g(t) &\equiv e^{-iH_0t/\hbar}\Theta(t). \qquad (2)
\end{aligned}
$$

The Theta function is tacked on because of the time-orderings involved in the expression for the evolution operator in the interaction representation. Rembering that the evolution operator in the interaction representation is

$$
\begin{aligned}
U_I(t-t_0) &= e^{iH_0(t-t_0)/\hbar}e^{-iH(t-t_0)} \qquad (3)\\
&= 1+\left(\frac{-i}{\hbar}\right)\int_{t_0}^{t} dt_1 e^{iH_0t_1}Ve^{-iH_0t_1} \qquad (4)\\
&+ \left(\frac{-i}{\hbar}\right)^2\int_0^t dt_1 e^{iH_0t_1}Ve^{-iH_0t_1}\int_0^{t_1} dt_2 iH_0t_2Ve^{-iH_0t_2}+\cdots \qquad (5)
\end{aligned}
$$

one can write the propagator as

$$
\begin{aligned}
G(t-t_0) &= e^{-iH_0(t-t_0)/\hbar}U_I(t)\Theta(t-t_0) \qquad (6)\\
&= e^{-iH_0(t-t_0)/\hbar}\Theta(t-t_0) \qquad (7)\\
&+ \left(\frac{-i}{\hbar}\right)\int_{-\infty}^{\infty} dt_1\; e^{-iH_0(t-t_1)/\hbar}\Theta(t-t_1)Ve^{iH_0(t_1-t_0)/\hbar}\Theta(t_1-t_0) \qquad (8)\\
&+ \left(\frac{-i}{\hbar}\right)^2\int_{-\infty}^{\infty} dt_1dt_2\; e^{-iH_0(t-t_1)/\hbar}\Theta(t-t_1)Ve^{iH_0(t_1-t_2)/\hbar}\Theta(t_1-t_2)Ve^{iH_0(t_2-t_0)/\hbar}\Theta(t_2-t_0)\\
&+ \cdots\\
&= g(t-t_0)+\left(\frac{-i}{\hbar}\right)\int_{-\infty}^{\infty} dt_1\; g(t-t_1)Vg(t-t_0) \qquad (9)\\
&+ \left(\frac{-i}{\hbar}\right)^2\int_{-\infty}^{\infty} dt_1dt_2\; g(t-t_1)Vg(t_1-t_2)Vg(t_2-t_0)\\
&\quad +\left(\frac{-i}{\hbar}\right)^3\int_{-\infty}^{\infty} dt_1dt_2dt_3\; g(t-t_1)Vg(t_1-t_2)Vg(t_2-t_3)Vg(t_3-t_0)+\cdots
\end{aligned}
$$

This expression has a nearly identical form to that for the evolution operator, the only apparent benefit being the incorporation of the $\Theta$ functions which allows one to more efficiently express the relations. The real benefits to this formalism comes when one considers the Fourier transform of $G$.

## The Fourier Transform of the Propagator, $\tilde{G}(\omega)$

Let us first consider the Fourier transform of $g$, the propagator without $V$. Assuming the states $|n\rangle$ and $|m\rangle$ are eigenstates of $H_0$,

$$
\begin{aligned}
\tilde{g}_{nm}(\omega) &= \int dte^{i\omega t}g_{nm}(t) \qquad (10)\\
&= \delta_{nm}\int dte^{i(\omega-iE_n)(t)/\hbar-\eta t}\Theta(t) \qquad (11)\\
&= \frac{i\delta_{nm}}{\omega-E_m/\hbar+i\eta},\ \eta\to 0. \qquad (12)
\end{aligned}
$$

The infinitesimal $\eta \to 0^+$ represents an extremely slow exponential decay at large time differences. By using Cauchy's theorem, one can integrate $\tilde{g}(\omega)e^{-i\omega t}/(2\pi)$ over all $\omega$ to see that the propagator $g(t)$ is recovered. In fact, if one flipped the sign of $\eta$ to $0^-$, the result would look the same except with $\Theta(-t)$.

The pole in $\tilde{g}(\omega)$ tells us at what energy the particle propagates. In this case one sees that the pole (where the propagator blows up) is at $\omega = E_n/\hbar - i\eta$. Note that if $\eta$ were replaced with a finite value $\Gamma/(2\hbar)$, that the square of the propagator would go as $e^{-\Gamma t/\hbar}$, thus $\Gamma/\hbar$ would be associated with the exponential decay constant.

**The simple case where $V$ is diagonal**

If $V$ and $\tilde{g}$ are both diagonal in the same basis, one can forego the matrix notation and consider the states one-at-a-time. One can then write the expression above for $\tilde{G}$ in a recursive form,

$$\begin{aligned}
\tilde{G}_{mm}(\omega) &= \tilde{g}_{mm}(\omega) + \frac{-i}{\hbar}\tilde{g}_{mm}(\omega)V_{mm}\tilde{G}_{mm}(\omega) && (13)\\
&= \frac{\tilde{g}_{mm}(\omega)}{1+(i/\hbar)\tilde{g}_{mm}(\omega)V_{mm}} && (14)\\
&= \frac{i}{\omega - E_m/\hbar - V_{mm}/\hbar + i\eta}. && (15)
\end{aligned}$$

Thus the only difference between the full propagator $\tilde{G}$ and the original propagator $\tilde{g}$ is that the energy of the pole is shifted by $V$, exactly as one would expect from knowing the eigenvalues of $H = H_0 + V$.

**The general case where $V$ has off-diagonal elements**

One can not do the same trick when $V$ has off-diagonal elements. However by inspection of the expansion of $\tilde{G}$, one sees that one could accomplish the same simplification by replacing $V$ with the diagonal matrix $\mathcal{T}$ defined by

$$\mathcal{T}_{km}(\omega) \equiv V_{km} + \frac{-i}{\hbar}V_{ki'}\tilde{g}_{i'i'}(\omega)V_{i'm} + \left(\frac{-i}{\hbar}\right)^2 V_{ki'}\tilde{g}_{i'i'}(\omega)V_{i'j'}\tilde{g}_{j'j'}V_{j'm} + \cdots \qquad (16)$$

Here, the primed sums refer to sums over all states except $m$. Thus $\mathcal{T}$ absorbs all the off-diagonal terms in the expansion of $G$,

$$\begin{aligned}
\tilde{G}_{mm}(\omega) &= \tilde{g}_{mm}(\omega) + \frac{-i}{\hbar}\tilde{g}_{mm}(\omega)\mathcal{T}_{mm}(\omega)\tilde{g}_{mm}(\omega) && (17)\\
&+ \left(\frac{-i}{\hbar}\right)^2 \tilde{g}_{mm}(\omega)\mathcal{T}_{mm}(\omega)\tilde{g}_{mm}(\omega)\mathcal{T}_{mm}(\omega)\tilde{g}_{mm} + \cdots && (18)\\
&= \frac{i}{\omega - E_m/\hbar - \mathcal{T}_{mm}/\hbar + i\eta}. && (19)
\end{aligned}$$

To second order in the potential $\mathcal{T}_{mm}$ can be separated into real and imaginary parts,

$$\begin{aligned}
\mathcal{T}_{mm}(\omega) &= V_{mi'}\frac{1}{\hbar\omega - E_m + i\hbar\eta}V_{i'm} && (20)\\
&= \sum_{i'}\left\{\frac{V_{mi'}V_{i'm}}{\hbar\omega - E_{i'}} + \pi i\delta(\hbar\omega - E_{i'})V_{mi'}V_{i'm}\right\} && (21)
\end{aligned}$$

One can now view the expression for $\tilde{G}_{mm}(\omega)$ for $\omega = E_m$ to see how the propagator is affected to second order,

$$\tilde{G}_{mm}(\omega) = \frac{i\hbar}{\hbar\omega - E_m - \Delta E + i\hbar\Gamma/2} \tag{22}$$

$$\Delta E_m = \sum_{i'} \frac{V_{mi'}V_{i'm}}{E_m - E_{i'}} \tag{23}$$

$$\Gamma = \frac{2\pi}{\hbar}\sum_{i'} V_{mi'}V_{i'm}\delta(E_m - E_{i'}) \tag{24}$$

Here we have used

$$\frac{1}{\omega - E/\hbar + i\eta} = \frac{\mathcal{P}}{\omega - E/\hbar} + \pi i\delta(\omega - E/\hbar) \text{ as } \eta \to 0, \tag{25}$$

Thus a pole of the propagator is adjusted by the interaction in such a way that the real part of the pole moves by an amount consistent with stationary state perturbation theory, while the imaginary part is consistent with Fermi's golden rule.

### Resonant Scattering

Here we consider the problem where an initial state $k$ scatters to a final state $k'$ through a resonant channel $R$. For simplicity, we consider the matrix element of the momentum state $k$ with the resonant state $R$ to be

$$\langle R|V|k\rangle = \frac{\alpha(k)}{\sqrt{V}}. \tag{26}$$

We will assume that one has performed all the necessary integrations to find the matrix element, and that we call it $\alpha$ aside from the $1/\sqrt{V}$ due to the normalization of the plane wave. To simplify our discussion we will assume that $\alpha$ has no dependence with respect to the direction of $k$.

One could calculate the rate of decay of the resonance using Fermi's golden rule and obtain

$$\Gamma_R = \frac{2\pi}{\hbar}\frac{|\alpha|^2}{V}\rho_k(E_R), \tag{27}$$

$$= \frac{k^2}{\pi v_k \hbar^2}|\alpha|^2 \tag{28}$$

where $\rho_k(E_R)$ is the density of states of the outgoing particle.

An example of resonant scattering could be a photon scattering off an atom. Here $k$ labels the momentum of the photon, while $R$ would refer to a specific excited state of the atom that could be attained due to the interaction with the photon. To simplify our derivation, we will assume that $\alpha$ has no dependence with respect to $k$.

It was shown in the previous lecture that the cross section for scattering could be written to second order as

$$\sigma = \frac{2\pi V}{v\hbar}\sum_{k'} |\mathcal{T}_{k'k}|^2\delta(E_{k'} - E_k) \tag{29}$$

$$\mathcal{T}_{k'k} = V_{k'k} + \frac{-i}{\hbar}\sum_m V_{k'm}\frac{i}{\omega - E_m/\hbar + i\eta}V_{mk}\bigg|_{\hbar\omega=E_k} \tag{30}$$

$$\tag{31}$$

One could have extended the treatment for scattering to find that by writing the propagator of the intermediate state in the form derived in the previous section, the answer could have been written as

$$\mathcal{T}_{k'k} = V_{k'k} + \frac{-i}{\hbar}\sum_{mm'} V_{k'm}G_{mm'}(\omega)V_{m'k}\bigg|_{\hbar\omega=E_k} \tag{32}$$

By resonant scattering we mean that the only interaction is between the resonant state $R$ and the momentum states. The matrix element then becomes

$$\mathcal{T}_{k'k} = \frac{-i}{\hbar}V_{k'R}\tilde{G}_{RR}(\omega)V_{Rk}\Big|_{\hbar\omega=E_k} \tag{33}$$

$$\tilde{G}_{RR}(\omega) = \frac{i}{\omega - E_R/\hbar + i\Gamma_R/2}, \tag{34}$$

where $\Gamma$ is the decay rate of the resonance.

The cross section is no longer infinite when $E_k = E_R$ due to the factor $\Gamma - R$ appearing in the denominator. Plugging the expression for $\mathcal{T}$ into the expression for the cross section one obtains

$$\begin{aligned}
\sigma &= \frac{2\pi V}{v\hbar}\sum_{k'}\frac{|\alpha|^4}{V^2}\frac{1}{(E_k - E_R)^2 + \hbar^2\Gamma_R^2/4}\delta(E_{k'} - E_k) && (35)\\
&= \frac{2\pi V}{v\hbar}\frac{|\alpha|^4}{V^2}\frac{1}{(E_k - E_R)^2 + \hbar^2\Gamma_R^2/4}\rho_k(E) && (36)\\
&= \frac{k^2}{\pi v^2\hbar^2}|\alpha|^4\frac{1}{(E_k - E_R)^2 + \hbar^2\Gamma_R^2/4} && (37)\\
&= \frac{4\pi}{k^2}\frac{(\hbar\Gamma_R/2)^2}{(E_k - E_r)^2 + (\hbar\Gamma_R/2)^2} && (38)
\end{aligned}$$

The last line is known as the Breit-Wigner form for scattering through a resonance. Note that the cross section is determined by two numbers, the width of the resonance and the Energy of the resonance.

If the resonance has spin $S_R$, then the effect is multiplied by the number of degenerate states through which one might scatter. If the incoming particles have spins $S_1$ and $S_2$, the effect is correspondingly reduced due to the fact that many of the states of the resonance would not be reached with particular combinations of $S_1$ and $S_2$.

The Breit-Wigner form for resonant scattering is then

$$\sigma = \frac{2S_R + 1}{(2S_1 + 1)(2S_2 + 1)}\frac{4\pi}{k^2}\frac{(\hbar\Gamma_R/2)^2}{(E_k - E_r)^2 + (\hbar\Gamma_R/2)^2} \tag{39}$$

**Example $\pi - \pi$ scattering through the $\rho$**

Consider a $\pi_+$ and a $\pi_0$ which are scalar mesons with masses 140 MeV/c$^2$ and 135 MeV/c$^2$. They scatter through the $\rho_+$ resonance which has spin 1, a mass of 770 MeV/c$^2$ and a width $\hbar\Gamma = 151 MeV$. Find the cross section at resonance.

**Solution:**

First, one must find the relative momentum **p** in the center of mass frame. In this frame the particles move with **p** and −**p**.

$$\begin{aligned} m_\rho &= \sqrt{m_+^2 + p^2} + \sqrt{m_0^2 + p^2} && (40) \\ p^2 &= \frac{m_\rho^4 + m_+^4 + m_-^4 - 2m_\rho^2 m_+^2 - 2m_\rho^2 m_-^2 - 2m_-^2 m_+^2}{4m_\rho^2} && (41) \end{aligned}$$

Here, we have neglected the factors of $c$. The value of $p$ at resonance is then 385 MeV/c.

The cross section at resonance is then

$$\sigma_R = \frac{12\pi}{(385/197.326)^2} = 9.9 \text{ fm}^2 = 99 \text{ mb} \qquad (42)$$

Here, I have used $\hbar c = 197.326$MeV·fm and used the fact that one squared femtometer equals 10 millibarns. Note that the maximum cross section depended only on the relative momentum at resonance and not on the width.

### Scattering, Central Potentials, Partial Waves and Phase Shifts

If potentials have spherial symmetry, one can solve the scattering problem through the consideration of spherical waves rather than plane waves. This effectively reduces the problem to the solution of one-dimensional Schrödinger equations, where each partial wave is characterized by a specific angular momentum $\ell$ and requires a different centrifugal potential.

First, we consider the kinetic part of the Hamiltonian. The Schrödinger equation can be written in either Cartesian coordinates or spherical coordinates,

$$\begin{aligned} -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right) &= -\frac{\hbar^2}{2m}\left(\frac{1}{r}\frac{\partial^2}{\partial r^2}r+\frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}\right) \quad (1)\\ &= -\frac{\hbar^2}{2m}\frac{1}{r}\frac{\partial^2}{\partial r^2}r+\frac{L^2}{2mr^2} \quad (2)\end{aligned}$$

If the potential spherically symmetric, angular momentum is a good quantum number and one can write solutions corresponding to a specific $\ell$ and $m$.

$$H\psi_{\ell,m}(\mathbf{r}) = E\psi_{\ell,m}(\mathbf{r}), \quad (3)$$

with the wave function being written as a product of a radial part and an angular part,

$$\psi_{\ell,m}(\mathbf{r}) = Y_{\ell,m}(\theta,\phi)R_\ell(r). \quad (4)$$

The radial wave function is a solution of the equation

$$-\frac{\hbar^2}{2m}\frac{1}{r}\frac{\partial^2}{\partial r^2}rR_\ell(r)+\frac{\hbar^2\ell(\ell+1)}{2mr^2}R_\ell(r)+V(r)R_\ell(r) = ER_\ell(r). \quad (5)$$

Remember that the radial wave function depends only on $\ell$ and not $m$ since the centrifugal potential is determined by $\ell$ only.

If the potential is zero, the solutions $R_\ell(r)$ are referred to as $j_\ell(r)$. Plane wave solutions can be expanded in terms of the spherical solutions through,

$$e^{i\mathbf{k}\cdot\mathbf{r}} = \sum_\ell (2\ell+1)i^\ell j_\ell(kr)P_\ell(\cos\theta), \quad (6)$$

where $\cos\theta \equiv \hat{k}\cdot\hat{r}$. This is known as the partial wave expansion. Note that the expansion are in terms of the Legendre polynomials,

$$P_\ell(\cos\theta) = \sqrt{\frac{4\pi}{2\ell+1}}Y_{\ell,m=0}(\theta,\phi).$$

All angular functions can be expanded in terms of $Y_{\ell,m}$s, and since $e^{i\mathbf{k}\cdot\mathbf{r}} = e^{ikr\cos\theta}$ does not depend on $\phi$ it is no surprise that the expansion contains only $Y_{\ell,m=0}$ terms. The partial wave expansion can be derived by combining orthogonality relations of the Legendre polynomials and spherical Bessel functions with the Rodriquez formula,

$$P_\ell(x) = \frac{1}{2^\ell\ell!}\frac{d^\ell(x^2-1)^\ell}{dx^\ell}.$$

The solutions $j_\ell$ are normalized as,

$$j_\ell(x)|_{x\rightarrow\infty} = \frac{(-i^\ell)e^{ix} - (i^\ell)e^{-ix}}{2ix}, \tag{7}$$

and are known as spherical Bessel functions. They are a linear combination of outgoing and incoming waves, each of which is a solution to the Schrödinger equation. The relative phase between the incoming and outging waves is chosen so that the solution goes to zero at $x = 0$. In fact,

$$j_\ell(x) \approx \frac{x^\ell}{(2\ell+1)!!}|_{x\approx 0} \tag{8}$$

As an exercise, one can verify the small $x$ expansion by applying Schrödinger's equation with the centrifugal potential. There also exist a class of solutions which are orthogonal to the spherical Bessel functions, but do not satisfy the boundary conditions at zero. These are known as spherical Neumann functions and have the opposite relative phase between the incoming and outgoing parts, while being quite divergent at the origin.

$$n_\ell(x) \approx \frac{(2\ell-1)!!}{x^{\ell+1}} \tag{9}$$

Examples of a few spherical functions for low $\ell$ are

$$j_0(x) = \frac{\sin x}{x}, \qquad n_0(x) = -\frac{\cos x}{x} \tag{10}$$

$$j_1(x) = \frac{\sin x}{x^2} - \frac{\cos x}{x}, \qquad n_1(x) = -\frac{\cos x}{x^2} - \frac{\sin x}{x} \tag{11}$$

$$j_2(x) = \left(\frac{3}{x^3} - \frac{1}{x}\right)\sin x - \frac{3}{x^2}\cos x, \qquad n_2(x) = -\left(\frac{3}{x^3} - \frac{1}{x}\right)\cos x - \frac{3}{x^2}\sin x \tag{12}$$

Both $j_\ell$ and $n_\ell$ are real.

The spherical Hankel functions are defined in terms of $j_\ell$ and $n_\ell$,

$$h_\ell(x) \equiv j_\ell(x) + in_\ell(x) \approx \frac{(-i)^{\ell+1}}{x}e^{ix}|_{x\rightarrow\infty} \tag{13}$$

$$h^*_\ell(x) \equiv j_\ell(x) - in_\ell(x) \approx \frac{i^{\ell+1}}{x}e^{-ix}|_{x\rightarrow\infty} \tag{14}$$

Here $h_\ell$ and $h^*_\ell$ behave as outgoing and incoming waves respectively.

### Scattering Phase Shifts

By making combinations, $j_\ell \pm in_\ell$, one finds solutions that correspond to incoming or outgoing waves. When adding a potential of finite range, there still exists solutions which look like $h_\ell(kr)$ or $h^*_\ell(kr)$ for $r$ beyond the range of the potential, but have modified forms at small $r$. Just as in the case with no potential, one can find a linear combination of the incoming and outgoing solutions which goes to zero at $r = 0$. However, the relative phase between the incoming and outgoing phase will be adjusted by a phase $e^{2i\delta_\ell}$ due to the existence of the potential. The large $x = kr$ behavior is then

$$R_\ell(x)|_{x>ka} = \frac{1}{2}\left(e^{2i\delta_\ell}h_\ell(x) + h^*_\ell(x)\right), \tag{15}$$

where $\delta$ is known as the phase shift. Here $a$ is any distance large enough such that the potential is zero. We define the overall phase of $R_\ell$ such that the incoming phase has the same phase as does the incoming part of $j_\ell$. .

If one scatters a plane wave off a potential, one can consider the solution to be the original plane wave, expanded in terms of partial waves, plus the correction due to the interaction,

$$\begin{aligned}\psi_{\mathbf{k}}(\mathbf{r}) &= \sum_\ell (2\ell+1) i^\ell R_\ell(kr) P_\ell(\cos\theta) &(16)\\ &= e^{i\mathbf{k}\cdot\mathbf{r}} + \sum_\ell (2\ell+1) i^\ell \left(R_\ell(kr) - j_\ell(kr)\right) P_\ell(\cos\theta), &(17)\end{aligned}$$

where the choice of phases in the definition of $R_\ell$ allows the incoming waves to be identical to those of the solution with no potential. Expanding the answer at large $r$, one obtains

$$\begin{aligned}\psi_{\mathbf{k}}(\mathbf{r})|_{r\to\infty} &= e^{i\mathbf{k}\cdot\mathbf{r}} + \sum_\ell (2\ell+1)\left(e^{2i\delta_\ell} - 1\right)\frac{e^{ikr}}{2ikr} P_\ell(\cos\theta) &(18)\\ &= e^{i\mathbf{k}\cdot\mathbf{r}} + \sum_\ell (2\ell+1) e^{i\delta_\ell}\sin\delta_\ell \frac{e^{ikr}}{kr} P_\ell(\cos\theta) &(19)\end{aligned}$$

Only the latter term contributes to scattering as the plane wave continues to travel forward after the wave packet leaves the region of the scatterer. One defines a quantity $f(\Omega)$ as the scattering amplitude and gives it dimension of length.

$$\begin{aligned}f(\Omega) &\equiv \sum_\ell (2\ell+1) e^{i\delta_\ell}\sin\delta_\ell \frac{1}{k} P_\ell(\cos\theta) &(20)\\ \psi_{\mathbf{k}}(\mathbf{r})|_{R\to\infty} &= e^{i\mathbf{k}\cdot\mathbf{r}} + \frac{e^{ikr}}{r} f(\Omega). &(21)\end{aligned}$$

Note that $f$ no longer depends on $r$. It can also be related to the differential cross section. To see this, we first relate the differential cross section to the flux of particles per solid angle,

$$\frac{v}{V}\frac{d\sigma}{d\Omega} = \frac{dN}{d\Omega dt} \tag{22}$$

The flux per unit area can be found by multiplying the square of the wave function in Eq. (**??**) by the velocity and dividing by the volume,

$$\frac{dN}{r^2 d\Omega dt} = \frac{v}{V}\frac{|f(\Omega)|^2}{r^2}, \tag{23}$$

Comparing the two equations above allows one to see that $f(\Omega)$ is directly related to the differential cross section.

$$\frac{d\sigma}{d\Omega} = |f(\Omega)|^2. \tag{24}$$

One can see that the differential cross section at a given energy is determined solely by the phase shifts $\delta_\ell(k)$.

Integrating over $d\Omega$ to obtain the whole cross section eliminates the cross terms involving different $\ell$s resulting from squaring $f(\Omega)$ due to the orthogonality of the Legendre Polynomials. In fact, one obtains

$$\sigma = \frac{4\pi}{k^2} \sum_{\ell} (2\ell+1) \sin^2 \delta_\ell. \tag{25}$$

**Example: Hard Sphere Scattering**:

Consider a hard sphere of radius $a$. Find the contribution to the cross section from $s$ and $p$ wave scattering as a function of the momentum.

The $\ell = 0$ case is simple as the solutions for ingoing and outgoing waves in the region $r > a$ are the Hankel functions which must go to zero at $r = a$.

$$R_0(a) = \frac{1}{2}\left(e^{2i\delta_0} h_0(ka) + h_0^*(ka)\right) = 0 \tag{26}$$

Plugging in the expressions for $h_0$, one obtains,

$$e^{2i\delta_0} (\sin(ka) - i\cos(ka)) + (\sin(ka) + i\cos(ka)) = 0 \tag{27}$$

which gives the $\ell = 0$ phase shifts,

$$\delta_0 = -ka \tag{28}$$

The contribution to the cross section from the $\ell = 0$ partial waves is then,

$$\sigma_0 = \frac{4\pi}{k^2} \sin^2(ka). \tag{29}$$

Note that as $k \to 0$, the cross section approaches $4\pi a^2$, four times the expected geometric cross section.

Calculating the contribution for the $\ell = 1$ partial waves is a bit difficult. In this case the incoming and outgoing waves are

$$R_1(a) = \frac{1}{2}\left(e^{2i\delta_1} h_1(ka) + h_1^*(ka)\right) = 0 \tag{30}$$

This yields the following expression for $\delta_1$ when requiring that $R_1(a) = 0$,

$$e^{2i\delta_1}\left(\frac{\sin(ka)}{ka} - \cos(ka) - i\frac{\cos(ka)}{ka} - i\sin(ka)\right) + \left(\frac{\sin(ka)}{ka} - \cos(ka) + i\frac{\cos(ka)}{ka} + i\sin(ka)\right) = 0. \tag{31}$$

Solving this for $\delta_1$,

$$\tan\delta_1 = \frac{\cos(ka) - \sin(ka)/(ka)}{\sin(ka) + \cos(ka)/(ka)} \tag{32}$$

The contribution to the cross section is

$$\sigma_1 = \frac{12\pi}{k^2} \sin^2 \delta_1. \tag{33}$$

### Solving for phase shifts for arbitrary potentials

Consider a potential that goes to zero for $r > b$. Rather than considering a solution for $R_\ell(r)$, it is easier to consider a solution for $u_\ell(r)$

$$\begin{aligned} u_\ell(r) &\equiv krR_\ell(r) && (34)\\ \frac{\hbar^2 k^2}{2m}u_\ell(r) &= -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r^2}u_\ell(r) + \frac{\hbar^2\ell(\ell+1)}{2mr^2}u_\ell(r) + V(r)u_\ell(r). && (35)\end{aligned}$$

Thus $u_\ell$ appears to be the solution to a one-dimensional Schrödinger equation with the effective potential,

$$V_{\text{eff}}(r) = V(r) + \frac{\hbar^2\ell(\ell+1)}{2mr^2}, \qquad (36)$$

and the extra condition that $u_\ell(r \to 0) = 0$.

The solution $u_\ell$ can be considered as the linear combination of an incoming and phase-shifted outgoing wave.

$$u_\ell(r) = u_\ell^{\text{in}}(r) + e^{2i\delta_\ell}u_\ell^{\text{out}}, \qquad (37)$$

where the incoming and outgoing waves are know solutions when $r > b$,

$$\begin{aligned} u_\ell^{\text{in}}(r) &= krh_\ell^*(r) && (38)\\ u_\ell^{\text{out}}(r) &= u_\ell^{\text{in},*}(r). && (39)\end{aligned}$$

To find the phase shift numerically, one can discretize space into steps of $\Delta$, then choose two points $r_{n+1}$ and $r_n$ which are chosen beyond $b$. One can calculate $u_\ell^{\text{in}}(r_{n+1})$ and $u_\ell^{\text{in}}(r_n)$. One can then numerically solve the discretized Schrödinger equation,

$$-\frac{\hbar^2}{2m\Delta^2}\left(u_\ell^{\text{in}}(r_{n+1}) - 2u_\ell^{\text{in}}(r_n) + u_\ell^{\text{in}}(r_{n-1})\right) = \left(\frac{\hbar^2k^2}{2m} - V_{\text{eff}}(r_n)\right)u_\ell^{\text{in}}(r_n), \qquad (40)$$

to find $u_\ell^{\text{in}}(r_{n-1})$. One can continue iteratively until one finds $u_\ell^{\text{in}}(r \to 0)$. The phase shift $\delta_\ell$ is then chosen to make $u_\ell(r \to 0) = 0$. Thus $\delta_\ell$ is determined by the phase of $u_\ell^{\text{in}}$ as $r \to 0$.

$$e^{2i\delta_\ell} = -\left.\frac{u_\ell^{\text{in},*}}{u_\ell^{\text{in}}}\right|_{r\to 0} \qquad (41)$$

An alternative method is to integrate from $r = 0$, then match logarithmic derivatives at $r = b$ to find the phase shifts. However, this method can be troublesome when it comes to larger $\ell$ since the wave functions grow as $r^{\ell+1}$ near $r = 0$.

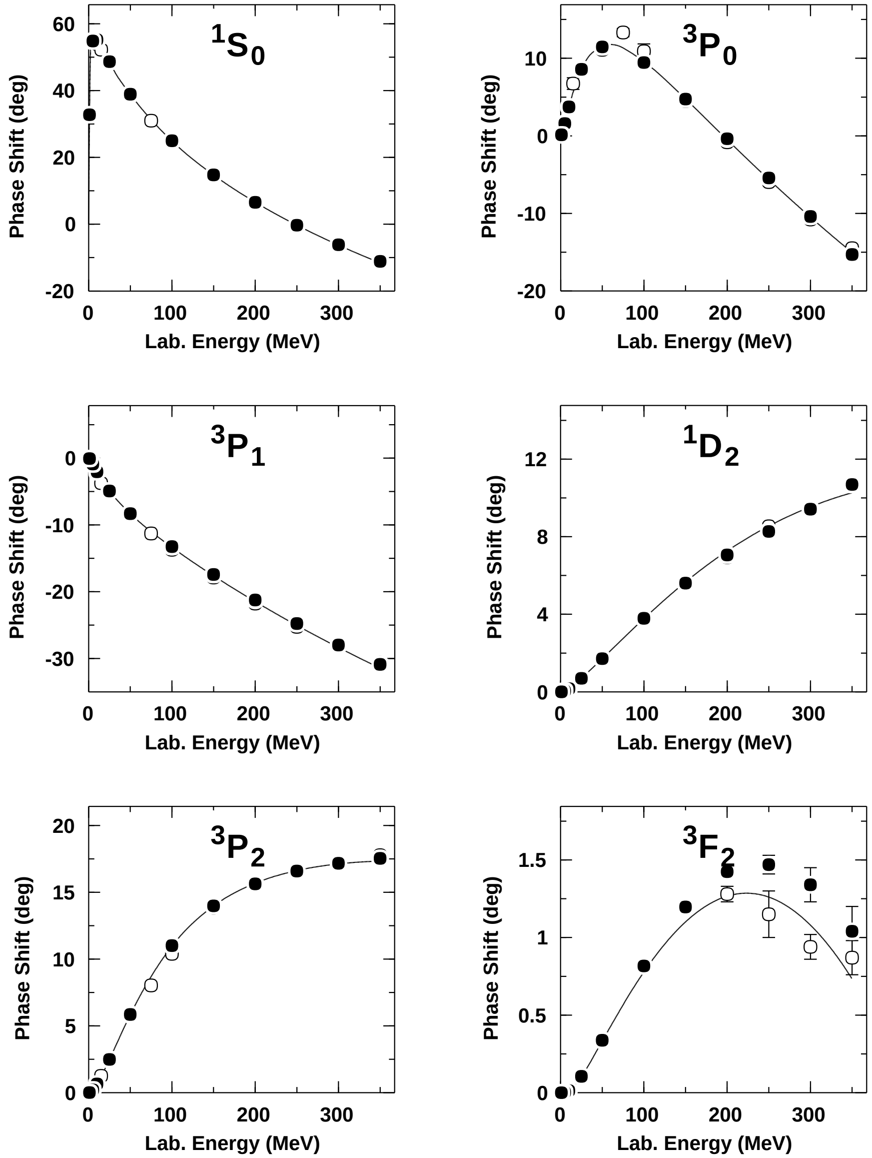
### Summary

Phase shifts offer a convenient means to express all the information required to describe scattering. In the presence of a spherically symmetric potential, each partial wave becomes a linear combination of the original incoming wave and a phase shifted outgoing wave. Since measurements are made outside the range of the potential the phase shifts, $\delta_\ell(E)$, completely describe all behavior.

One does not usually need to include higher values of $\ell$ in a phase shift analysis. This is because the partial waves tend to sample distances of order $r > \ell/k$. As $k \to 0$, $s$-wave scattering dominates the picture. Rarely does one see analyses for $\ell > 3$.

Phase shift analyses are common in low-energy nuclear scattering and in atomic physics. They become rather irrelevant at high energy due to the fact that inelastic channels ($A+B \to C+D+E$) tend to open at high energy, at which point the phase shift vocabulary is insufficient. Even when $\ell$ is not a good quantum number, e.g. spin-orbit scattering, but where $j$ is a good quantum number, one can still extract phase shifts using polarized beam, although in these cases the vocabulary includes mixing terms.

Finally, as an example I present a plot of proton-proton phase shifts to give an impression of the degree to which these quantities are analyzed. In this figure, the data (circles) are indistinguishable from two well-known models (Nijmegan and Bonn).



## Phase Shifts at Low Energy, Scattering Lengths

At low energy, one can solve the Schrödinger equation for a given partial wave between $r = 0$ and some point $r = b$ where $b$ is sufficiently large such that the potential is zero. Although the norm of $R_\ell$ is arbitrary, the logarithmic derivative is completely determined by the potential, the energy and the point $b$.

$$\alpha_\ell(k,b) \equiv \left.\frac{dR_\ell(k,r)/dr}{R_\ell(k,r)}\right|_{r=b} \tag{1}$$

We will consider $k \approx 0$, one can ignore the energy dependence of $\alpha_\ell$.

For $r > b$, $R_\ell(k,r)$ must have the form

$$R_\ell(k,r) \propto \left(h_\ell^*(kr) + e^{2i\delta}h_\ell(kr)\right), \tag{2}$$

which means that the logarithmic derivative at $r = b$ becomes

$$\alpha(k,b) = \frac{\partial/\partial r\left(h_\ell^*(kr) + e^{2i\delta}h_\ell(kr))\right)|_{r=b}}{h_\ell^*(kb) + e^{2i\delta}h_\ell(kb)}. \tag{3}$$

Using the definition of $h_\ell = j_\ell + in_\ell$ allows one (with some algebra) to write the phase shift in terms of $\alpha$, $j_\ell$ and $n_\ell$,

$$\cot(\delta_\ell) = \frac{\partial n_\ell/\partial r|_{r=b} - \alpha n_\ell(kb)}{\partial j_\ell(kr)/\partial r|_{r=b} - \alpha j_\ell(kb)}. \tag{4}$$

Thus, by finding the logarithmic derivative at $r = b$, one determines the phase shift. Note that if the potential is zero, $R_\ell$ would be proportional to $j_\ell$ and the denominator would diverge forcing the phase shift to zero.

We are now in a position to consider the behavior at low $k$ where $j_\ell$ and $n_\ell$ have the following behavior,

$$j_\ell(kr) \quad\rightarrow\quad \frac{(kr)^\ell}{(2\ell+1)!!} \tag{5}$$

$$n_\ell(kr) \quad\rightarrow\quad \frac{(\ell-1)!!}{(kr)^{\ell+1}}, \tag{6}$$

where $(2\ell+1)!! \equiv 1\cdot 3\cdot 5\cdots(2\ell+1)$. Inserting these into the expression for the phase shift above.

$$\cot\delta_\ell(k) \approx (kb)^{-(2\ell+1)}(2\ell-1)!!(2\ell+1)!!\frac{\ell+1+b\alpha_\ell(k,b)}{\ell-b\alpha_\ell(k,b)} \tag{7}$$

For low $k$, the kinetic term in Schrödinger's equation is negligible compared to the potential and $\alpha_\ell$ approaches a constant. Thus, the momentum dependence of the phase shifts at low relative momentum is

$$\sin\delta_\ell(k) \propto k^{2\ell+1}. \tag{8}$$

One can see that all phase shifts tend to an integral multiple of $\pi$ at $k = 0$, and that the cross section is dominated by the $s$-wave contribution at low energy. In fact the *scattering length*, $a$, is defined as the derivative of the $\ell = 0$ phase shift at $k = 0$,

$$a \equiv -\frac{\partial}{\partial k}\delta_0(k)|_{k=0}. \tag{9}$$

The cross section at very low energy is then,

$$\sigma \approx \frac{4\pi}{k^2}\sin^2(ka) = 4\pi a^2. \tag{10}$$

**Example: $s$-wave scattering off a square well**

Consider the repulsive potential

$$V(r) = \begin{cases} V_0, & r < b \\ 0, & r > b \end{cases} \tag{11}$$

Find the scattering length and the cross section at $k \approx 0$ for a particle of mass $m$.

We need only consider the $s$ wave in this case. Using the definition $u(k,r) \equiv rR_0(k,r)$, one knows that the Schrödinger equation for $u(k,r)$ looks exactly like a one-dimensional Schrödinger equation. Furthermore, the solution has the following form in the two regions,

$$u_I(k,r) = A\sinh\kappa r, \quad \kappa \equiv \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}, \tag{12}$$

$$u_{II}(k,r) = \sin(kr + \delta), \quad k \equiv \sqrt{\frac{2m(E)}{\hbar^2}} \tag{13}$$

Matching logarithmic derivatives at the boundary gives

$$\frac{1}{\kappa}\tanh\kappa b = \frac{1}{k}\tan(kb + \delta). \tag{14}$$

Solving for $\delta$ for small $k$,

$$\delta = -kb + \tan^{-1}\left(\frac{k}{\kappa}\tanh\kappa b\right) \tag{15}$$

$$\approx k\left(-b + \frac{1}{\kappa}\tanh\kappa b\right) \tag{16}$$

The scattering length and cross section are thus

$$a = b - \frac{1}{\kappa}\tanh\kappa b \tag{17}$$

$$\sigma(k=0) = 4\pi a^2. \tag{18}$$

Note that in the limit that $V_0 \to \infty$ that $\delta \to -kb$.

### Levinson's Theorem

As can be seen from the previous section all phase shifts begin life at multiples of $\pi$. If the phase shift at $k = 0$ were anything else an infinite cross section would result at small $k$. As $k \to \infty$, phase shifts all tend to zero. This asymptotic behavior at large $k$ can be understood by realizing that the in the high-energy limit the phase is changed by $V\Delta t/\hbar$, where $\Delta t$ is the time spent in the potential, which goes to zero as the particle moves very quickly.

Levinson's theorem relates the phase shift at zero energy, which is a multiple of $\pi$ to the number of bound states.

$$\delta_\ell(k = 0) = N_B \pi, \tag{19}$$

where $N_B$ is the number of bound states of angular momentum $\ell$.

In order to explain the physical motivation of Levinson's theorem we digress to consider the density of states of particles in a large sphere of radius $R$, which feels a short range potential $V(r)$, with the origin being located at the center of the sphere. The wave function at large $r$ is

$$\psi(r \to \infty) \propto \sin(kr + \delta_\ell), \tag{20}$$

so that the boundary conditions restrict the possible values of $k$ to

$$kR + \delta_\ell(k) = n\pi. \tag{21}$$

Thus the density of states in momentum is

$$\frac{dn}{dk} = \frac{R}{\pi} + \frac{1}{\pi}\frac{d\delta_\ell}{dk}. \tag{22}$$

The change of the density of states due to the non-zero potential is $(1/\pi)d\delta_\ell/dk$. Thus the number of extra states inserted between $k = 0$ and $k = \infty$ due to the potential is

$$\Delta N_{\text{cont.}} = \frac{\delta_\ell(k \to \infty) - \delta_\ell(k = 0)}{\pi}. \tag{23}$$

However, the net number of states under consideration is not affected by the potential. If $\Delta N_{\text{cont.}}$ states were pushed out of the continuum, then they must have become bound states.

$$N_B + \Delta N_{\text{cont.}} = 0. \tag{24}$$

Combining this constraint with the Eq. (**??**) and with the fact that $\delta_\ell(k \to \infty) = 0$ gives Levinson's theorem.

Levinson's theorem is important as it gives one an idea of the general behavior to expect from phase shifts. Attractive potentials tend to have positive phase shifts. If no bound state exists, the phase shifts rise near $k = 0$ indicating that the states in the continuum were pulled down to $k = 0$. Then at higher $k$, the phase shifts fall, indicating that the density of continuum states was depleted at higher $k$. If a bound state exists, the phase shift would generally start at $\pi$ and usually fall as a function of $k$. The falling phase shift denotes a negative correction to the density of states. These are the states from which the bound state was formed.

Phase shifts behave rather peculiarly when the potentials are at the threshold of creating a bound state. A small change in the potential causes the $\delta(k=0)$ to jump from zero to $\pi$. In these instances scattering lengths can be anomalously long. Such an example is neutron-neutron scattering. The scattering is length is nearly -20 fm. Thus the neutron-neutron cross section at low momentum is 100 times larger than $\pi R^2$, where $R$ is the range of the strong interaction.

### Coulomb waves

The Coulomb potential is not short-range, hence the incoming and outgoing spherical waves are not Hankel functions but are instead Coulomb waves. At large $r$ the spherical Coulomb waves behave as

$$R(r) \sim \frac{1}{r} e^{\pm i(kr - \gamma \log r)}, \tag{1}$$

where

$$\gamma \equiv \frac{\mu Z_1 Z_2 e^2}{\hbar^2 k} = -\frac{1}{a_0 k}. \tag{2}$$

When the potential is attractive, e.g. the Hydrogen atom, $\gamma$ is negative. The factor $\gamma$ is known as the Sommerfeld parameter.

The entire solutions for Coulomb waves are known as confluent hypergeometric functions which can be found in books of special functions such as Abramowitz and Stegun. They are also often simply called Coulomb wave functions.

When an extra potential is added to the problem, one can still classify the behavior in terms of phase shifts, but the problem becomes one of phase-shifted Coulomb waves rather than phase-shifted Hankel functions. Of course, all the relations for total cross sections are modified since the Coulomb force produces a scattering all it's own.

The expression for a plane wave plus it's scattered portion is written in terms of hypergeometric functions as

$$\psi_k(r) = \Gamma(1 + i\gamma) e^{-\pi\gamma/2} e^{ikz} {}_1F_1(-i\gamma; 1; ik(r - z)). \tag{3}$$

For small $r$ ($r << a_0$) the hypergeometric function ${}_1F_1$ goes to unity and the solution is approximately,

$$\begin{aligned} \psi_k(r << a_0) &= \Gamma(1 + i\gamma) e^{-\pi\gamma/2} e^{ikz} && (4) \\ |\psi_k(r << a_0)|^2 &= |\Gamma(1 + i\gamma)|^2 e^{-\pi\gamma} && (5) \\ &= \frac{2\pi\gamma}{e^{2\pi\gamma} - 1}. && (6) \end{aligned}$$

This last factor is referred to as the Gamow factor or penetrability.

Note that the Gamow factor is independent of $r$. For repulsive potentials. It can be thought of as the penetration probability of reaching the origin, relative to what it would have been if there were no Coulomb. Of course, in classical physics a charged particle never reaches the origin when there is a repulsive Coulomb barrier. If the potential is repulsive, gamma is positive. As $k \to 0$, $\gamma \to \infty$ and the Gamow factor goes to zero, meaning that low energy waves have great difficulty penetrating the barrier. As $k$ is increased and approaches $(2\pi a_0)^{-1}$ the penetrability rises.

For attractive potentials, the Gamow factor is greater than unity. In both the attractive and repulsive case, the factor approaches unity as $k \to \infty$.

The Gamow penetrability plays an important role in astrophysical rates. Fusion reactions would happen much more quickly if it were not for the Coulomb barrier. When the cross sections are measured the Gamow factor is divided out leaving what is known as the astrophysical S-factor.

## Quantum Fields and Second Quantization

Many transitions of interest involve not only a particle changing from one state to another, but the actual creation of a new particle. For instance the radiative decay of an atom or nucleus results in a system with a photon that did not exist before the decay. Most decays in particle physics also involve the creation of new particles. In fact, relativistic quantum field theory considers all interactions, e.g. the Coulomb force, as consisting of the creation and absorption of particles which are exchanged over a sufficiently short time so as not to contradict the energy-time uncertainty principle. For this class, we will constrain our goals to understanding simple decays.

Creation and destruction operators were introduced to describe the creation of energy quanta in a harmonic oscillator. The operators obeyed the relations,

$$[a_i, a_j^\dagger] = \delta_{ij}, \quad [a_i, a_j] = 0, \quad [a_i^\dagger, a_j^\dagger] = 0, \tag{1}$$

where $i$ specifies which oscillator is being affected. If one had $N$ harmonic oscillators, one would have $N$ creation operators and $N$ destruction operators. Note that the operators corresponding to different operators commute with one another as they are unrelated.

The essential feature of creation and destruction operators is that they increase/decrease the number of quanta, where the number of quanta of the oscillator $i$ is $N_i = a_i^\dagger a_i$. However, instead of counting only energy quanta, as in the case of the harmonic oscillator, the number operator could also refer to a number of particles in that level. Let us then consider a creation operator for each momentum eigenstate of a system, $a_k^\dagger$. The momentum state $|k\rangle$ is created by $a_k^\dagger$ operating on the vacuum.

$$|k\rangle = a_k^\dagger|0\rangle. \tag{2}$$

The state is normalized to unity, just as one would expect for creation operators.

$$\langle k'|k\rangle = \delta_{k'k}. \tag{3}$$

By operating twice with $a_k^\dagger$, one creates a state with two particles of momentum $k$.

### Example: Two oscillators with a mixing term

Consider two oscillator described by the creation operators $a_1^\dagger$ and $a_2^\dagger$. Let the Hamiltonian be

$$\begin{aligned} H &= H_0 + V \qquad (4)\\ H_0 &= \epsilon_1 a_1^\dagger a_1 + \epsilon_2 a_2^\dagger a_2 \qquad (5)\\ V &= \beta\left(a_2^\dagger a_1 + a_1^\dagger a_2\right) \qquad (6)\end{aligned}$$

Consider the operators $b_1^\dagger$ and $b_2^\dagger$ defined by

$$\begin{aligned} b_1^\dagger &\equiv \cos\theta a_1^\dagger + \sin\theta a_2^\dagger \qquad (7)\\ b_2^\dagger &\equiv \cos\theta a_2^\dagger - \sin\theta a_1^\dagger \qquad (8)\end{aligned}$$

First, show that $b_1$, $b_2$, $b_1^\dagger$ and $b_2^\dagger$ obey the commutation rules for destruction operators.

Find $E_1$, $E_2$ and $\theta$ such that

$$H = E_1 b_1^\dagger b_1 + E_2 b_2^\dagger b_2 \tag{9}$$

To find the answer substitute the expressions for $b_i^\dagger$ and $b_i$ and compare to the original expression for $H$.

$$\begin{aligned} H &= \frac{E_1+E_2}{2}\left(a_1^\dagger a_1 + a_2^\dagger a_2\right) + \frac{E_1-E_2}{2}\left(a_1^\dagger a_1 - a_2^\dagger a_2\right)\cos 2\theta + \frac{E_1-E_2}{2}\left(a_1^\dagger a_2 + a_2^\dagger a_1\right)\sin 2\theta \qquad (10) \\ &= \frac{\epsilon_1+\epsilon_2}{2}\left(a_1^\dagger a_1 + a_2^\dagger a_2\right) + \frac{\epsilon_1-\epsilon_2}{2}\left(a_1^\dagger a_1 - a_2^\dagger a_2\right) + \beta\left(a_1^\dagger a_2 + a_2^\dagger a_1\right) \qquad (11) \end{aligned}$$

By inspection, one sees that the Hamiltonians are equivalent when

$$\begin{aligned} \tan 2\theta &= \frac{2\beta}{\epsilon_1 - \epsilon_2} && (12) \\ E_1 + E_2 &= \epsilon_1 + \epsilon_2 && (13) \\ \left(\frac{E_1 - E_2}{2}\right)^2 &= \beta^2 + \left(\frac{\epsilon_1 - \epsilon_2}{2}\right)^2 . && (14) \end{aligned}$$

One can note the algebraic equivalence of this problem to the two-component problem with Hamiltonian

$$H = \frac{\epsilon_1+\epsilon_2}{2} + \frac{\epsilon_1-\epsilon_2}{2}\sigma_z + \beta\sigma_x \tag{15}$$

**Field operators: Creation and destruction in coordinate space**

Field operators are the coordinate-space analogs to $a_k^\dagger$. They are defined as

$$\Psi^\dagger(\mathbf{x}) = \sum_k a_k^\dagger \frac{e^{-i\mathbf{k}\cdot\mathbf{x}}}{\sqrt{V}}. \tag{16}$$

They obey the commutation rules,

$$\begin{aligned} [\Psi(\mathbf{x}), \Psi^\dagger(\mathbf{y})] &= \frac{1}{V}\sum_{k,k'} e^{-i(\mathbf{k}\cdot\mathbf{x} - \mathbf{k}'\cdot\mathbf{y})}[a_k, a_{k'}^\dagger] && (17) \\ &= \frac{1}{V}\sum_k e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})} && (18) \\ &= \frac{1}{(2\pi)^3}\int d^3k e^{-i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})} && (19) \\ &= \delta^3(\mathbf{x}-\mathbf{y}) && (20) \end{aligned}$$

These operators can create the state $|\mathbf{x}\rangle$,

$$|\mathbf{x}\rangle = \Psi^\dagger(\mathbf{x})|0\rangle, \tag{21}$$

which is a state with one particle at the position $\mathbf{x}$, and are normalized as

$$\langle\mathbf{x}|\mathbf{y}\rangle = \delta^3(\mathbf{x}-\mathbf{y}) \tag{22}$$

One can easily check that

$$\langle \mathbf{x}|\mathbf{k}\rangle = \frac{e^{-i\mathbf{k}\cdot\mathbf{x}}}{\sqrt{V}} \tag{23}$$

One should keep in mind the $\Psi(\mathbf{x})$ is an operator, not a wave function. If $\phi$ referes to a one-particle state, the relation to the wave function $\phi(x)$ is given by

$$\Psi(\mathbf{x})|\phi\rangle = \phi(x)|0\rangle,$$

where the wave function is defined by

$$\phi(\mathbf{x}) \equiv \langle \mathbf{x}|\phi\rangle$$

Charge densities and currents can also be considered as operators

$$\begin{aligned}\rho(\mathbf{x}) &= \Psi^\dagger(\mathbf{x})\Psi(\mathbf{x}) \\ \vec{j}(\mathbf{x}) &= \frac{\hbar}{2mi}\left((-\vec{\partial}\Psi^\dagger(\mathbf{x}))\Psi(\mathbf{x}) + \Psi^\dagger(\mathbf{x})\vec{\partial}\Psi(\mathbf{x})\right).\end{aligned}$$

If the state $|\phi\rangle$ and $|\chi\rangle$ are one-particle states, one sees that

$$\langle\chi|\vec{j}(\mathbf{x})|\phi\rangle = \frac{\hbar}{2mi}\left\{\chi^*(\mathbf{x})\vec{\partial}\phi(\mathbf{x}) - \left(\vec{\partial}\chi^*(\mathbf{x})\right)\phi(\mathbf{x})\right\} \tag{24}$$

**Free particle**

One can write the Hamiltonian for freely moving particles:

$$\begin{aligned}H_0 &= -\frac{\hbar^2}{2m}\int d^3x\Psi^\dagger(\mathbf{x})\nabla^2\Psi(\mathbf{x}). && (25)\\ &= \frac{\hbar^2}{2mV}\int d^3x\sum_{k,k'} k^2 e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}} a_k^\dagger a_{k'}. && (26)\end{aligned}$$

The integral over $\mathbf{x}$ gives zero due to the varying phase unless $\mathbf{k} = \mathbf{k}'$, at which point the phase is unity and the integral over $\mathbf{x}$ cancels the volume in the denominator.

$$H_0 = \sum_k \frac{\hbar^2 k^2}{2m} a_k^\dagger a_k. \tag{27}$$

Thus even though the Hamiltonian looks like the familiar expression for a wave function, it is far more powerfull as it correctly express the energy even when many particles are present in the system.

**Interaction with an external potential**

An interaction with a potential would be written as

$$H_{\text{int}} = \int d^3r\mathcal{V}(\mathbf{r})\Psi^\dagger(\mathbf{r})\Psi(\mathbf{r}). \tag{28}$$

This can be written in terms of momentum-space creation and destruction operators by substituting the expressions for $\Psi^\dagger$ above,

$$\begin{aligned} H_{\rm int} &= \frac{1}{V}\int d^3r \sum_{k,k'} a_k^\dagger a_{k'} e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}}\mathcal{V}(\mathbf{r}) && (29)\\ &= \frac{1}{V}\sum_{k,k'}\tilde{\mathcal{V}}(\mathbf{k}-\mathbf{k}')a_k^\dagger a_{k'}, && (30) \end{aligned}$$

where $\tilde{\mathcal{V}}$ is the Fourier transform of $\mathcal{V}$. Thus the form of the interaction is similar to that of the example above.

In fact, one can reduce the solution of the problem (finding the energy eigenvalues) to that of diagonalizing a matrix.

$$H = \sum_{k,k'} A_{k,k'}a_k^\dagger a_{k'}. \tag{31}$$

The simplified Hamiltonian results by rotating the states (perhaps in a high-dimensional space) such that $A$ is diagonalized. In this new basis,

$$H = \sum_{k} A'_{k,k}a_k^\dagger a_k. \tag{32}$$

One should keep in mind that if there are 10 single-particle levels that one still has an infinite number of states, as each level $k$ can hold an arbitrary number of particles. The ability of this formalism to include an arbitrary number of particles makes it the starting point for any study of many-body physics. It also represents the starting point for the study of relativistic physics due to the fact that even the vacuum might contain an arbitrary number of virtual particle-antiparticle pairs.

## Decays

The most common example where particles are destroyed and created is in the decays of particles or atoms. For instance a hydrogen atom in an excited state might decay to the ground state via the emission of a photon. The photon must be created in the process.

Creation of a photon is surprisingly complicated due to the fact that the photon is a massless spin-1 particle coupling to the current. Since the Lorentz structure of such a decay is potentially confusing, we will begin with a scalar form for a decay.

Consider hypothetical $\alpha$ and $\beta$ particles where the $\alpha$ particle has a mass $m_\alpha$ and the $\beta$ particle is massless. We assume both particles are spinless. The $\alpha$ particle is in the first excited state of a Harmonic oscillator characterized by frequency $\omega$. We wish to calculate the rate for decaying to the ground state via the emission of a $\beta$ particle which we will assume to be massless. We assume the interaction term is expressed

$$H_{\rm int} = g\int d^3r\Psi^\dagger_\alpha(\mathbf{r})\left(\Psi^\dagger_\beta(\mathbf{r}) + \Psi_\beta(\mathbf{r})\right)\Psi_\alpha(\mathbf{r}).$$

Using Fermi's golden rule the decay rate is

$$\Gamma = \frac{2\pi}{\hbar}\sum_{k_\beta}|\langle n_x = n_y = n_z = 0; k_\beta|H_{\rm int}|n_x = n_y = 0, n_z = 1\rangle|^2\,\delta(E_0 + E_1 - E_{k_\beta})$$

Before proceeding further, note that $H_{\rm int}$ has both a $\Psi_\beta$ and a $\Psi^\dagger_\beta$ piece in order to keep the Hamiltonian Hermittian. Since we are interested in the decay of the atom, which creates a particle, we can neglect the destruction term. Also, note that the initial state was assumed to be polarized along the $z$ axis. This choice is arbitrary since we are summing equally over all directions of $k$. If we were calculating a differential decay rate, $d\Gamma/d\Omega_k$, the answer would depend on the initial polarization.

One can now calculate the matrix element,

$$\langle n_x = n_y = n_z = 0; k|H_{\rm int}|n_x = n_y = 0, n_z = 1\rangle = g\int d^3r\phi^*_0(\mathbf{r})\frac{1}{\sqrt{V}}e^{i\mathbf{k}\cdot\mathbf{r}}\phi_{n_z=1}(\mathbf{r})$$

Writing the wave functions in terms of normalized 1-d harmonic oscillator wave functions $\psi_0(x)$,

$$\begin{aligned}
&\langle n_x = n_y = n_z = 0; k|H_{\rm int}|n_x = n_y = 0, n_z = 1\rangle \\
&= \frac{g}{\sqrt{V}}\int dx e^{ik_x x}\psi_0^2(x)\int dy e^{ik_y y}\psi_0^2(y)\int dz e^{ik_z z}z\sqrt{\frac{2m\omega}{\hbar}}\psi_0^2(z) \\
&= \frac{-igk_z a^2}{\sqrt{V}}\sqrt{\frac{m\omega}{2\hbar}}e^{-k^2a^2/4},
\end{aligned}$$

where $a$ is the characteristic size of the ground state.

$$a^2 \equiv \frac{\hbar}{m\omega}$$

Putting all this together

$$\begin{aligned}\Gamma &= \frac{4\pi g^2}{m\omega V}\sum_k k_z^2 e^{-k^2a^2/2}\delta(\hbar kc - \hbar\omega)\\ &= \frac{g^2}{2m\omega\pi}\int k^4 dk \cos^2\theta \; d\cos\theta e^{-k^2a^2/2}\delta(\hbar kc-\hbar\omega)\\ &= \frac{g^2k^4}{3\pi m\hbar\omega c}e^{-k^2a^2/2},\end{aligned}$$

where $k=\omega/c$, and $\omega$ is determined by energy conservation, $\hbar\omega = E_1 - E_0$.

### Electromagnetic decays

Electromagnetic decays are complicated due to the $\mathbf{j}\cdot\mathbf{A}$ nature of the coupling. Remember that minimal substitution, $\mathbf{p}\to(\mathbf{p}-e\mathbf{A}/c)$, results a term in the Hamiltonian which looks like

$$H_{\rm int} = \mathbf{j}\cdot\mathbf{A}/c + \frac{e^2}{2mc^2}\mathbf{A}^2 \tag{1}$$

representing the interaction with the vector potential. The last term will be neglected for now, but will play the defining role when we discuss the quantum Hall effect. Remember the current is given by

$$\mathbf{j}(\mathbf{x}) = \frac{ie}{2m}\left(\Psi^\dagger(\mathbf{x})\nabla\Psi - \nabla\Psi^\dagger(\mathbf{x})\Psi(\mathbf{x})\right).$$

First we must define the electromagnetic field operator in terms of creation and destruction operators that make real photons.

$$\vec{A}(\mathbf{r},t) = \sqrt{\frac{2\pi\hbar^2c^2}{V}}\sum_{k,s}\vec{\epsilon}_s\frac{1}{\sqrt{E_k}}\left(e^{i\mathbf{k}\cdot\mathbf{r}-iE_kt/\hbar}a_{k,s} + e^{-i\mathbf{k}\cdot\mathbf{r}+iE_kt/\hbar}a_{k,s}\right)$$

Here $s$ refers to the polarization (or spin) of the photon. For each $k$ there are two polarizations. Each must be perpendicular to the direction of $\mathbf{k}$. Aside from the polarization, the expression for $\mathbf{A}$ looks peculiar for all the prefactors and the $1/E_k$ term inside the sum. However all these terms are necessary to ensure that

$$\int d^3x\frac{\mathbf{E}^2+\mathbf{B}^2}{8\pi} = \sum_{k,s}E_k\left(a^\dagger_{k,s}a_{k,s}+\frac{1}{2}\right),$$

where the electromagnetic fields resulting from $\mathbf{A}$ are

$$\begin{aligned}\mathbf{E} &= -\frac{1}{c}\frac{\partial\mathbf{A}}{\partial t}\\ \mathbf{B} &= \nabla\times\mathbf{A}.\end{aligned}$$

We are now in position to consider the general problem of electromagnetic decay, where a particle of charge $e$ changes from state $i$ to state $f$ while emitting a photon of momentum $k$ and polarization $s$. Outlining the steps to solving the problem:

1. Write down Fermi's golden rule,

$$\Gamma = \frac{2\pi}{\hbar}\sum_{k,s}|\frac{1}{c}\langle f;k,s|\int d^3x\mathbf{j}(\mathbf{x})\cdot\mathbf{A}(\mathbf{x})|i\rangle|^2\delta(E_i - E_f - \hbar kc)$$

2. Write down the matrix element

$$\begin{aligned}\langle f;k,s|\frac{1}{c}\int d^3x\mathbf{j}(\mathbf{x})\cdot\mathbf{A}(\mathbf{x})|i\rangle &= \sqrt{\frac{2\pi\hbar^2}{E_kV}}\frac{e\hbar}{mi}\vec{\epsilon}_{k,s}\cdot\int d^3xe^{-i\mathbf{k}\cdot\mathbf{x}}\phi_f(\mathbf{x})\nabla\phi_i(\mathbf{x}) &(2)\\ &= \frac{e\hbar}{m}\sqrt{\frac{2\pi}{E_kV}}\vec{\epsilon}_{k,s}\cdot\vec{\mathcal{M}} &(3)\\ \vec{\mathcal{M}}(\mathbf{k},i,f) &\equiv \int d^3xe^{-i\mathbf{k}\cdot\mathbf{x}}\phi_f(\mathbf{x})\frac{\hbar}{i}\nabla\phi_i(\mathbf{x}) &(4)\end{aligned}$$

Note $\mathcal{M}$ does not depend on the polarization.

3. Change the sum over $k$ to an integral.

$$\sum_k \rightarrow \frac{V}{(2\pi\hbar)^3}\int d^3k = \frac{V}{(2\pi)^3}\int k^2dkd\Omega_k$$

Then eliminate the delta function in Fermi's golden rule.

$$\Gamma = \frac{e^2k}{2\pi\hbar m^2c^2}\sum_s\int d\Omega_k|\vec{\epsilon}_s\cdot\vec{\mathcal{M}}|^2$$

One can check the units of the above expression by noting that $e^2k$ has dimensions of energy (as it is the same as $e^2/r$) and that $\mathcal{M}$ has units of momentum which are the same as the units of $mc$, thus the overall expression has units of energy over $\hbar$ which is an inverse time. Remember that in many books and tables $\Gamma$ often refers to energies rather than rates, in which case one erases the $\hbar$ in the denominator.

4. Finally, perform the integral to find $\mathcal{M}$.

### The dipole approximation

For nuclear examples, typical $\gamma$ energies are on the order of one MeV, which gives wavelenths of a few hundred fm, approximately 100 times the size of a nucleus. For atomic examples, emitted photons usually have wavelengths of hundreds of nm, several thousand times the size of a typical atom. Thus, one might consider approximating the phase factor,

$$e^{-i\mathbf{k}\cdot\mathbf{x}} \approx 1.$$

This approximation is known as the dipole approximation. The term dipole can be explained by noting that in the dipole approximation,

$$\begin{aligned}\vec{\mathcal{M}} &\approx \langle f|\mathbf{P}|i\rangle\\ &= \frac{im}{\hbar}\langle f|[H_0,\mathbf{r}]|i\rangle\\ &= \frac{im(E_f-E_i)}{\hbar}\langle f|\mathbf{r}|i\rangle,\end{aligned}$$

thus giving it the dipole form.

The matrix element may be zero in the dipole approximation due to symmetry considerations, usually parity contraints. In that case, one should keep the next order term in the expansion of $e^{i\mathbf{k}\cdot\mathbf{x}}$. One then obtains terms in the matrix element that look like

$$\begin{aligned}(\vec{k}\cdot\vec{r})(\vec{P}\cdot\vec{\epsilon}) &= \frac{1}{2}\left\{(\vec{k}\cdot\vec{r})(\vec{P}\cdot\vec{\epsilon})-(\vec{\epsilon}\cdot\vec{r})(\vec{k}\cdot\vec{P})\right\}+\frac{1}{2}\left\{(\vec{k}\cdot\vec{r})(\vec{P}\cdot\vec{\epsilon})+(\vec{\epsilon}\cdot\vec{r})(\vec{k}\cdot\vec{P})\right\}\\ &= \frac{1}{2}\left\{(\vec{k}\cdot\vec{r})(\vec{P}\cdot\vec{\epsilon})-(\vec{\epsilon}\cdot\vec{r})(\vec{k}\cdot\vec{P})\right\}+\frac{1}{2}\left\{(\vec{P}\cdot\vec{\epsilon})(\vec{k}\cdot\vec{r})+(\vec{\epsilon}\cdot\vec{r})(\vec{k}\cdot\vec{P})\right\},\end{aligned}$$

where the last step was justified by the fact that $\vec{P}$ commuting with $\vec{k}\cdot\vec{r}$ yields a result proportional to $\vec{k}$ which is in turn orthogonal to $\vec{\epsilon}$.

Using a vector identity the first term can be written

$$\frac{1}{2}\left\{(\vec{k}\cdot\vec{r})(\vec{P}\cdot\vec{\epsilon})-(\vec{\epsilon}\cdot\vec{r})(\vec{k}\cdot\vec{P})\right\}=(\vec{r}\times\vec{P})\cdot(\vec{k}\times\vec{\epsilon})$$

This operator looks like $\mathbf{L}\cdot(\vec{\epsilon}\times\vec{k})/2$, thus it looks like the magnetic dipole operator multiplied into $\vec{\epsilon}\times\vec{k}$. Thus is is known as magnetic dipole radiation.

Using the identity

$$\vec{P}=\frac{m}{i\hbar}[\vec{r},H_0],$$

the second term can be written as

$$\frac{1}{2}\langle f|\left\{(\vec{k}\cdot\vec{r})(\vec{P}\cdot\vec{\epsilon})+(\vec{\epsilon}\cdot\vec{r})(\vec{k}\cdot\vec{P})\right\}|i\rangle=\frac{m}{i\hbar}(E_i-E_f)\langle f|(\vec{\epsilon}\cdot\vec{r})\cdot(\vec{k}\cdot\vec{r})|i\rangle.$$

Radiation through this term is know as electric quadrupole radiation. The term quadrupole comes from the fact that all such operators can be written in terms of $Y_{\ell=2,m}s$.

The symmetry constraints of the radiation pattern will be a major point of discussion later in the course when we discuss the Wigner-Eckart theorem.

## Isospin

The angular momentum algebra developed last semester has a broad range of applications, many of which have little or nothing to do with rotating systems but instead deal with symmetries in some other space. One such example is isospin. In nuclear and particle physics isospin represents a mirror of the spin mechanics used to discuss spin 1/2 particles. In quark language, the up quark is a $I = 1/2, I_z = 1/2$ particle while the down quark is a $I = -1/2, I_z = -1/2$ particle. In nuclear physics the proton and neutron form an isodoublet with the proton being the $I_z = 1/2$ particle.

The strong interaction is invariant to "rotations" in isospin space. This means that the symmetry is analagous to the rotational symmetries discussed with angular momentum. For instance, composite particles (those made of several quarks) have good isospin, which is determined by adding the isospin of several particles.

### Example: The $\rho$ meson

Consider the $\rho^{+,0,-}$ mesons which form an isotriplet ($I = 1$) and can decay into two pions. Pions, $\pi^{+,0,-}$, also form an isotriplet. Find the decay branches for each of the three $\rho \to 3\pi$ decays.

First, look at the $\rho^+$ or $\rho^-$. The only branchings for each decay are

$$\rho^+ \to \pi^+\pi^0 . \rho^- \to \pi^-\pi^0 .$$

However the $\rho^0$ might go into one of two branches

$$\rho^0 \to \pi^+, \pi^- \text{ or } \pi^0, \pi^0 .$$

To solve for the relative strengths of the two branches, find how to add two pion isospins to form a $I = 1, I_z = 0$ state. Start by writing the $I = 2, I_z = 2$ state

$$|I = 2, I_z = 2\rangle = |\pi^+, \pi^+\rangle$$

then use the lowering operator to find the $I = 2, I_z = 1$ state.

$$|I = 2, I_z = 1\rangle = \frac{1}{\sqrt{2}}|\pi^0, \pi^+\rangle + \frac{1}{\sqrt{2}}|\pi^+, \pi^0\rangle$$

By orthogonality,

$$|I = 1, I_z = 1\rangle = \frac{1}{\sqrt{2}}|\pi^0, \pi^+\rangle - \frac{1}{\sqrt{2}}|\pi^+, \pi^0\rangle$$

By applying the lowering operator,

$$\begin{aligned} \sqrt{1 \cdot (1+1) - 1 \cdot (1-1)}|I = 1, I_z = 0\rangle &= \frac{\sqrt{1 \cdot (1+1) + 0 \cdot (0-1)}}{2}|\pi^-\pi^+\rangle \\ &- \frac{\sqrt{1 \cdot (1+1) + 0 \cdot (0-1)}}{2}|\pi^+\pi^-\rangle \\ |I = 1, I_z = 0\rangle &= \frac{1}{\sqrt{2}}|\pi^-\pi^+\rangle - \frac{1}{\sqrt{2}}|\pi^+\pi^-\rangle \end{aligned}$$

Thus the two pions must both be charged if they are two couple to the $\rho^0$. Also, the fact that the two terms appear identical, except for the switching of the $\pi^+$ and $\pi^-$ tells us that the two final spatial (momentum) states of the pions must be antisymmetric to cancel the antisymmetry of the isospin wave function. This is accomplished by requiring the $\rho$ to decay into a $p$ wave. Note that the $\rho^+$ and $\rho^-$ isospin wave functions were also antisymmetric.

The angular momentum algebra applies to any system built out of two constituents where a rotation $e^{i\sigma_i\phi/2}$ leaves the Lagrangian unchanged. Isospin is not an "exact" symmetry. Although the strong interaction conserves isospin, the electromagnetic interaction manifestly violates isospin. Thus the $\rho^0$ does not decay with 100% probability into two charged pion, but has a very small probability to decay into $\pi_0\pi_0$ that is not even listed in the particle data book (http://pdg.lbl.gov).

Conservation of isospin plays a large role in nuclear physics. In this case the proton and neutron form the basis. Two nucleons can form both an isotriplet $pp$, $(pn+np)/\sqrt{2}$, $nn$ or an isosinglet $(pn-np)/\sqrt{2}$. The isosingle forms a bound state (the deuteron) while the isotriplet states are all unbound. A nucleus like $^{12}C$ which has $I_z = 0$ might have states of total isospin, $I = 0, 1, 2, \cdots 6$. The nucleus $^{12}N$ which has $I_z = 1$ can not have isospin zero. The ground state of $^{12}C$ has $I = 0$ and has no analog in Boron or Nitrogen, but there does exist an excited state of $^{12}C$ with $I = 1$ which has very similar properties to the ground states of $^{12}N$ and $^{12}B$.

Finally, we should mention that sometimes symmetries involve more than just the rotation of two states into one another. For instance, although the strange quark is much more massive than the up and down quarks, one can consider the three quarks to form a basis. This basis has a greater symmetry as it involves rotations among three constituents, SU(3), rather than the SU(2) symmetry discussed before. In SU(3) the mechanics are a bit more complicated compared to the SU(2) mechanics used to study angular momentum or isospin.

## Adding Three Angular Momenta

When we studied two angular momenta, we described the "addition" as a change of basis where the state with labels $|j_j, j_1, m_1, m_2\rangle$ was written as a linear combination of states with labels $|j_1, j_2, J, M\rangle$. When adding three angular momenta the change of basis is

$$|j_1, j_2, j_3, m_1, m_2, m_3\rangle \leftrightarrow |(j_1, j_2), j_3, J_{12}, J, M\rangle$$

Again, $M$ is the projection of the total angular momentum $J$ with values from $-J$ to $J$.

In order to couple the three angular momenta $j_1$ and $j_2$ were coupled to $J_{12}$ before $j_3$ and $J_{12}$ were coupled to $J$. Thus $J_{12}$ survives as a quantum number, which is necessary as the original state had six labels, which requires six labels for the final state.

The change of basis can be described in terms of Clebsch-Gordan coefficients. First we describe an intermediate state with $j_1$ and $j_2$ coupled to $J_{12}$.

$$\begin{aligned} |j_1, j_2, J_{12}, j_3, M_{12}, m_3\rangle &= \sum_{m_1, m_2} |j_1, j_2, j_3, m_1, m_2, m_3\rangle\langle j_1, j_2, j_3, m_1, m_2, m_3|j_1, j_2, J_{12}, j_3, M_{12}, m_3\rangle \\ &= \sum_{m_1, m_2} C^{j_1, j_2}_{m_2, m_2; J_{12}, M_{12}} |j_1, j_2, j_3, m_1, m_2, m_3\rangle \end{aligned}$$

One can now consider the states with total angular momentum $J$ created by coupling $J_{12}$ to $j_3$.

$$\begin{aligned} |(j_1, j_2), j_3, J_{12}, J, M\rangle &= \sum_{M_{12}, m_3} |j_1, j_2, j_3, J_{12}, M_{12}, m_3\rangle\langle j_1, j_2, j_3, J_{12}, M_{12}, m_3|(j_1, j_2), j_3, J_{12}, J, M\rangle \\ &= \sum_{m_1, m_2, m_3, M_{12}} C^{J_{12}, j_3}_{M_{12}, m_3; J, M} C^{j_1, j_2}_{m_1, m_2; J_{12}, M_{12}} |j_1, j_2, j_3, m_1, m_2, m_3\rangle \end{aligned}$$

The choice of coupling $j_1$ with $j_2$ to $J_{12}$ was arbitrary, as one might have instead chosen to couple $j_1$ to $j_3$ or $j_2$ to $j_3$. This choice represents a change of basis which can be represented by Racah coefficients $W$.

$$\begin{aligned} &\langle (j_1, j_2), j_3, J_{12}, J, M|j_1, (j_2, j_3), J_{23}, J, M\rangle \\ &\quad = \delta_{M,M'} \sqrt{(2J_{12}+1)(2J_{23}+1)} W(j_1, j_2, j_3, J; J_{12}, J_{23}) \\ &\quad = \delta_{M,M'} (-1)^{j_1+j_2+j_3+J} \sqrt{(2J_{12}+1)(2J_{23}+1)} \left\{ \begin{array}{ccc} j_1 & j_2 & J_{12} \\ j_3 & J & J_{23} \end{array} \right\}, \end{aligned}$$

where the quantity in brackets is known as the Wigner $6-j$ symbol, which is simply another incarnation of the Racah coefficient. As a homework problem you will be asked to express the Racah coefficient $W$ in terms of Clebsch-Gordan coefficients.

## Tensor Operators, rotation operators, and the Wigner-Eckart theorem

Often physics involves calculating transition elements of the form

$$\langle \ell', m' | T^k_q | \ell, m \rangle, \tag{1}$$

where the labels in the kets and bras denote the angular momentum of the initial and final states and $T^k_q$ is an operator that transforms like spherical harmonics $Y_{k,q}$ under rotation. Such operators are known as irreducible tensor operators. Example are

1. $L_z$ which transforms $Y_{1,0}$
2. $L_+$ which transforms as $Y_{1,1}$
3. $r^2$ which transforms as $Y_{0,0}$
4. $x$ or $p_x$ which transform as $-Y_{1,1} - Y_{1,-1}$

$\vdots$

Operators such as $x^2$ can be written as a sum over $Y^2_m$s, and the coefficients can be found by viewing the expressions for the $Y^\ell_m$s. Clearly, one could expand any analytic function of $x$, $y$ and $z$ in terms of irreducible tensor operators.

The term irreducible refers to the fact that under rotations the operators mix only amongst irreducible subsets,

$$R(\vec{\alpha}) T^k_q R^{-1}(\vec{\alpha}) = d^k_{q,q'} T^k_{q'}. \tag{2}$$

The rotations mix only the $2k+1$ operators with the same $k$ but different $q$. The term irreducible refers to the fact that rotations can mix in any of the different $q$ components.

The rotation matrices $d_{q,q'}(\vec{\alpha})$ can be expressed in terms of the overlaps

$$d^\ell_{m,m'}(\vec{\alpha}) = \langle \ell m' | R(\vec{\alpha}) | \ell, m \rangle = \langle \ell m' | e^{-i\vec{J}\cdot\vec{\alpha}/\hbar} | \ell, m \rangle \tag{3}$$

The $d$ matrices have a variety of properties, many of which are related to those of the spherical harmonics. For instance, the orthogonal property is

$$\int d\omega d^{(j_1)}_{m_1',m_1}(\vec{\omega})^* d^{(j_2)}_{m_2',m_2}(\vec{\omega}) = \frac{\delta_{j_1,j_2}\delta_{m_1,m_2}\delta_{m_1',m_2'}}{2j_1+1} \tag{4}$$

### Finding the $d$ matrix elements

Finding the $d$ matrices as a function of $\alpha$ can be painful, but luckily canned routines exist in standard computer languages. If one needs to calculate them, it is best to consider the rotation $\alpha$ in terms of Euler angles,

$$R(\phi, \theta\psi) = e^{-iJ_{z'}\psi/\hbar} e^{-iJ_{y'}\theta/\hbar} e^{-iJ_z\phi/\hbar}, \tag{5}$$

where the $y'$ axis is the $y$ axis after an initial rotation around the original $z$ axis by an angle $\phi$ and $z'$ is the new $z$ axis formed after the rotation of $\theta$ about the $y'$ axis. Thus,

$$\begin{aligned} e^{-iJ_{y'}\theta/\hbar} &= e^{-iJ_z\phi/\hbar}e^{-iJ_y\theta/\hbar}e^{iJ_z\phi/\hbar} && (6)\\ e^{-iJ_{z'}\psi/\hbar} &= e^{-iJ_{y'}\theta/\hbar}e^{-iJ_z\psi/\hbar}e^{iJ_{y'}\theta/\hbar} && (7)\end{aligned}$$

Substituting these into the expression for $R$ allows one to write the rotation matrices without mentioning primed axes.

$$R(\phi,\theta,\psi) = e^{-iJ_z\phi/\hbar}e^{-iJ_y\theta/\hbar}e^{-iJ_z\psi/\hbar} \tag{8}$$

One is now in a position to find the elements. Simple expressions follow for when either $m$ or $m'$ is zero or when some of the angles are zero, but otherwise it can be bit tedious to find the elements. The elements can be written in terms of the $Y_{\ell,m}$s.

### The Wigner Eckart theorem

Since $T_q^k$ rotates like an angular momentum state, one can define the state

$$|\tilde{\beta},k,j,j',m'\rangle \equiv \sum_{q,m}\langle k,j,q,m|k,j,j',m'\rangle T_q^k|\beta,j,m\rangle \tag{9}$$

which must rotate as an object with angular momentum $j'$ and projection $m'$. Here, we have written the Clebsch-Gordan coefficients with the convention $\langle \ell_1\ell_2,j,m|\ell_1,\ell_2,m_1,m_2\rangle$.

Furthermore, a matrix element formed with this state would be zero unless the angular momentum of the bra state are identical.

$$\langle\beta'',k,j,j'',m''|\tilde{\beta},k,j,j',m'\rangle = \delta_{m'',m'}\delta_{j'',j'}f(\beta'',\beta,k,j,j') \tag{10}$$

This conclusion follows from the fact that the matrix element should be invariant under equal rotations of both the bra and the ket, which requires both matrix elements to behave identically under rotation and therefore have the same angular momenta. Furthermore, the matrix element should be independent of $m$. Since rotations mix values of $m$, the function $f$ can not depend on $m$. This result can be proven rigorously using orthogonality relations of the rotation operators $d$ (See Baym or Messiah).

Expanding the state $|\tilde{\beta},j,m,j',m'\rangle$,

$$\sum_{q,m}\langle\beta''j'',m''|T_q^k|\beta,j,m\rangle\langle k,j,q,m|k,j,j',m'\rangle = \delta_{m'',m'}\delta_{j'',j'}f(\beta'',\beta,k,j,j'). \tag{11}$$

Multiplying both sides by Clebsch Gordan coefficients and using the orthogonality relations,

$$\begin{aligned} &\sum_{q,m,j',m'}\langle\beta''j'',m''|T_q^k|\beta,j,m\rangle\langle k,j,q,m|k,j,j',m'\rangle\langle k,j,j',m'|k,j,q',m'''\rangle && (12)\\ &= \langle\beta'',k,j,j'',m''|T_{q'}^k|\beta,j,m'''\rangle && (13)\\ &= \langle k,j,j'',m''|k,j,q',m'''\rangle f(\beta'',\beta,k,j,j''). && (14)\end{aligned}$$

This is the statement of the Wigner-Eckart theorem. It is usually expressed in the following form:

$$\langle\beta',k,j,j',m'|T_q^k|\beta,j,m\rangle = \langle k,j,j',m'|k,j,q,m\rangle\frac{\langle\tilde{\beta}',j'||T^{(k)}||\beta,j\rangle}{\sqrt{2j'+1}} \tag{15}$$

The funny looking matrix element with the double bars is refered to as the reduced matrix element and the $\sqrt{2j'+1}$ is arbitrary but conventional.

The Wigner Eckart theorem is profound for two reasons.

1. An irreducible tensor operator $T^k_q$ will not link two states of good angular momentum unless the Clebsch Gordan coefficient coupling the angular momentum of the ket with the angular momentum of $T$ to the angular momentum of the bra is not vanishing. Thus a vector operator can not connect a $j=2$ state to a $j=0$ state. Also, the projections must add up zero, $q+m=m'$.

2. If one needs to calculate $\langle \beta', k, j, j', m' | T^k_q | \beta, j, m\rangle$ for some given set of $m, m'$ and $q$, one can choose any values of $m, m'$ and $q$ that might make calculation of the matrix element most simple then use the fact that the desired matrix element is the calculated matrix element multiplied by the ratio of the Clebsch Gordan coefficients. For example if one needs to calculate a matrix element with $m'=1,\ m=-1$ and $q=2$, one could simple calculate the matrix element with all three projections equal to zero, then multiply by the ratio of Clebsch Gordan coefficients.

$$\begin{aligned} &\langle \beta', k, j, j', m'=1 | T^k_{q=2} | \beta, j, m=-1\rangle \\ &\qquad = \langle \beta', k, j, j', m'=0 | T^k_{q=0} | \beta, j, m=0\rangle \frac{\langle k, j, j', 1 | k, j, 2, -1\rangle}{\langle k, j, j', 0 | k, j, 0, 0\rangle}. \end{aligned} \tag{16}$$

   This is handy because the integrals required to find the matrix element may be much easier to perform with the projections all set to zero, and if one needs to find the elements for many values of the projections, the matrix element must be calculated only once, as Clebsch Gordan coefficients may be used to find all other matrix elements.

The reduced matrix element is confusing, as it implies that it is an object that one may calculate directly. This is not true. One must first find one of the matrix elements, then generate the reduced matrix element. Finally, from the reduced matrix element one can find all other matrix elements.

## Fermions

When a single particle is in a system, it does not matter that it is a Fermion or a boson. However, when multiple particles are present, the behavior is entirely different. The difference between fermions and bosons can be explained by a variety of perspectives.

1. When considering populations of single-particle levels, no more than one fermion of a given type and spin can be assigned to a particular level, while an arbitrary number of bosons can be placed in a given level. This constraint on fermions is known as the Pauli exclusion principle.
2. For identical fermions of the same spin, the wave function $\psi(x_1, x_2, x_3)$ must be completely antisymmetric, while the wave function for bosons must be symmetric.
3. Creation and destruction operators for fermions obey anticommutation relations while those for bosons obey commutation relations.

Examples of fermions are electrons, quarks and neutrinos. Examples of bosons are photons and gluons. Composite particles made of an odd number of fermions, e.g. a proton which is made of three quarks, are also fermions. Composite particles made of an even number of fermions are bosons, e.g. a $^{12}$C atom which is made of 6 protons, 6 neutrons and 6 electrons. All bosons have integral spin while all fermions have half integral spin. The relation of statistics to spin is a profound consequence of time reversal property in quantum field theories.

In this lecture we will consider some of the consequences of the Pauli exclusion principle, and leave the discussion of field operators and wave functions for the next chapters.

## Fermi gases

Consider a large number $N$ of fermions of spin $s$ and mass $m$ in a box of volume $V$. If the fermions are placed in the lowest levels consistent with the Pauli exclusion principle, the highest single-particle energy is known as the Fermi energy $\epsilon_f$ and the momentum of that state is known as the Fermi momentum $p_f$. The density is a function of the Fermi momentum,

$$\begin{aligned} N &= (2s+1)\frac{V}{(2\pi\hbar)^3}\int^{p<p_f} d^3p && (1)\\ n &= \frac{N}{V} = (2s+1)\frac{1}{6\pi^2\hbar^3}p_f^3 && (2) \end{aligned}$$

Note that the Fermi momentum is directly dependent on the density and does not depend on the particle's mass. Of course, the Fermi energy does depend on the mass, $\epsilon_f = p_f^2/(2m)$.

One example where the Fermi energy plays a pivotal role is in neutron stars. Due to beta decays neutrons can change into protons through the emission of an electron and neutrino.

$$n \rightarrow p + e + \bar{\nu}, \quad p + e \rightarrow n + \nu \tag{3}$$

Since neutrinos can exit the star due to their neglibible masses and small crossections, they need not be considered with respect to conservation laws. However, baryon number (neutrons plus protons) and electric charge must be conserved, In fact the electric charge density must be zero. Thus beta decays, and inverse beta decays, can proceed as long as the following constraints are met,

$$\begin{aligned} n_n + n_p &= n_B && (4) \\ n_e &= n_p && (5) \end{aligned}$$

Beta decays will proceed until the energy is minimized for the given value of the baryon density $n_B$. Neutrons are more massive than protons by an amount $(m_n - m_p)c^2 = 1.3$ MeV which more than accounts for the electron's mass of 0.511 MeV. When the energy is minimized, changing a neutron to a proton plus electron must leave the energy unchanged if the particles are added and removed from the top of the Fermi surfaces. Thus,

$$\epsilon_f^n + 1.3 \text{ MeV} = \epsilon_f^e + \epsilon_f^p + 0.511 MeV \tag{6}$$

Combining this equation with the two constraints allows one to find all three Fermi momenta in terms of $n_B$.

At low density, the extra 1.3 MeV favors protons over neutrons. Therefore in normal stars, protons are much more numerous than neutrons. At high density the electron Fermi momentum plays the pivotal role. Since electrons and protons have the same density, they have the same Fermi momentum, but the electron's Fermi energy is much higher due to it's lighter mass,

$$\epsilon_f = \sqrt{m^2 + p_f^2} - m \approx p_f^2/(2m). \tag{7}$$

Thus at high density the system must try to reduce the electron density which in turn requires a reduction in the proton density and results in a large excess of neutrons. This is certainly the case for the interior of neutron stars where densities are of the order 0.1 baryons per cubic fm. The resulting electron Fermi energy is on the order of 10 MeV as is the resulting neutron Fermi energy. Thus the electrons are extremely relativistic while the protons and neutrons remain nonrelativistic.

### Filling the harmonic oscillator with fermions

As a second example we consider the filling of harmonic oscillator energy levels. This simple picture provides a surprising amount of insight into the structure of light nuclei.

First, we must understand the degeneracy the single-particle levels in a 3-d harmonic oscillator with an energy of $(N + 3/2)\hbar\omega$. Considering the problem in a Cartesion basis, there are $N_\perp + 1$ ways to arrange $n_x + n_y = N_\perp$. Then the number of ways to arrange $n_x, n_y$ and $n_z$ to add up to $N$ is

$$d(N) = \sum_{N_\perp=0}^{N} N_\perp + 1 = \frac{(N+1)(N+2)}{2}. \tag{8}$$

Thus there is one combination of $n_x, n_y$ and $n_z$ to get $N = 0$, three combinations to get $N = 1$, six to get $N = 2$, etc.

Next, we wish to calculate the number of states of a specific $N$ with a given orbital angular momentum $\ell$. This will come in handy when we consider the spin-orbit coupling on top of the harmonic oscillator structure. The solution will be that the states with excitation $N$ are accounted for with one $\ell = N$ multiplet, one $\ell = N-2$ multiplet, one $\ell = N-4$ multiplet, etc. To prove that this is the case, we make an inductive proof assuming it is true for $N-2$. For every state with excitation $N-2$ there is a state with the same angular momentum with excitation $N$ which is reached by applying the operator $(a_x^\dagger a_x^\dagger + a_y^\dagger a_y^\dagger + a_z^\dagger a_z^\dagger)$ which is a rotational scalar. There are $(N-1)N/2$ such states. Furthermore, there must be at least one $\ell = N$ multiplet because the state $(a_x^\dagger + i a_y^\dagger)^N|0\rangle$ transforms like part of a $\ell = N$ multiplet. But one $\ell = N$ multiplet with degeneracy $(2N+1)$, and the $(N-1)N$ states accounted for by counting the states with excitation $N-2$ completely account for all the states with excitation $N$,

$$\frac{(N+1)(N+2)}{2} = \frac{(N-1)N}{2} + (2N+1). \tag{9}$$

Thus, increasing the excitation by $2\hbar\omega$ adds one more multiplet with $\ell = N$. As an example, for $N = 4$, there are multiplets with $\ell = 4, 2, 0$ with degeneracy $9 + 5 + 1 = 15 = 5 \cdot 6/2$.

If no spin orbit terms were present, adding neutrons to a harmonic oscillator would lead to shell closures with neutron numbers equal to 2, 8, 20, 40 and 70, meaning that 40 neutrons exactly fills the $N = 0, 1, 2, 3$ shells. Adding the spin orbit term adjusts the single-particle energies by an amount

$$E_{\text{s.o.}} = \beta\vec{\ell} \cdot \vec{s} = \frac{\beta}{2}\left\{j(j+1) - \ell(\ell+1) - s(s+1)\right\}. \tag{10}$$

For every value of $\ell$ there are two values of $j$, $j = \ell \pm 1/2$. Thus, one finds the energy levels by first labeling the states by $N$ and $\ell$. Then splitting each level into it's two values of $j$ and finding its energy,

$$E = (N + 3/2)\hbar\omega + \frac{\beta}{2}\left\{j(j+1) - \ell(\ell+1) - s(s+1)\right\}. \tag{11}$$

The shell structure changes due to the spin-orbit interaction, and the numbers of neutrons required to reach a condition where there is a large gap are called magic numbers. In nuclei, the magic numbers are 2, 8, 20, 28, 50, 82 and 126. Nuclei are considered doubly magic if both the neutron and proton numbers are magic numbers. Examples are $^{4}$He, $^{16}0$, $^{40}_{20}$Ca, $^{48}$Ca, $^{56}_{28}$Ni, $^{48}$Ni, $^{78}Ni$, $^{100}_{50}Sn$ and $^{208}_{82}Pb$. The magic numbers of nuclei were only explained by assuming an anomalously large spin-orbit coupling. The reason this large coupling surprising and will be explained later in the semester when we discuss the Dirac equation.

## Zero-point surface energy for Fermions

It costs energy to divide a piece of metal into two pieces. The associated surface energy, energy per surface area, has a component deriving from the penalty associated with the kinetic energies of the particles. To understand the source of this energy, we first consider the one-dimensional case. Consider a box of length $L$, which is divided into two boxes, each of length $L/2$. The initial energy levels are given by,

$$E_n = \frac{\hbar^2 k^2}{2m}, \quad kL = n\pi, \quad n = 1, 2, 3, \cdots \tag{12}$$

But after splitting the box the energy levels are given by

$$E_n = \frac{\hbar^2 k^2}{2m}, \quad kL = n\pi, \quad n = 2, 4, 6, \cdots, \tag{13}$$

with the new levels being able to hold twice as many particles because there are now two boxes.

Thus, in one dimension the energy penalty can be thought of as arising from forcing half the particles to move up by one rung on the energy diagram ladder. If all the particles had moved up one rung, the net penalty would be the Fermi energy, but since half the particles moved up, the penalty is

$$\Delta E = \epsilon_f/2. \tag{14}$$

In three dimensions, there are three quantum numbers, $n_x$, $n_y$ and $n_z$, corresponding to $k_x$, $k_y$ and $k_z$.

$$k_x L_x = n_x\pi, \quad k_y L_y = n_y\pi, \quad k_z L_z = n_z\pi. \tag{15}$$

If the box is divided in two along the $x$ axis, $L_x \to L_x/2$, the penalty for all levels with a fixed $n_y$ and $n_z$ is,

$$\delta E(n_y, n_z) = \frac{1}{2}\frac{\hbar^2(k_f^2 - k_y^2 - k_z^2)}{2m}. \tag{16}$$

This result follows from the fact that half the particles moved up a notch on the $n_x$ ladder, with the top energy being such that the overall energy (including the $y$ and $z$ components) adds up to the Fermi energy.

One can now find the entire energy cost by summing over $n_y$ and $n_z$.

$$\begin{aligned}
\Delta E &= \frac{L_y L_z}{(2\pi)^2}\int_{|k|<k_f} dk_y dk_z \delta E(n_y, n_z) && (17)\\
&= \frac{\hbar^2 L_y L_z}{8m\pi}\int_0^{k_f} kdk(k_f^2 - k^2) && (18)\\
&= L_y L_z \frac{\hbar^2 k_f^4}{32m\pi} && (19)\\
&= L_y L_z \frac{k_f^2}{16\pi}\epsilon_f. && (20)
\end{aligned}$$

Dividing by $2L_xL_z$ (as extra area is added to both sides of the split) gives the surface energy. Of course, one would also multiply the result by the spin degeneracy.

$$\frac{\Delta E}{A} = \frac{k_f^2}{32\pi}\epsilon_f. \tag{21}$$

In real systems the surface energy is of this order. It is lessened by the fact that the electron density is not sharply cut off at the surface, but dies out smoothly. An additional positive contribution can result from finite-range attractive interactions between the particles. In nuclear physics, the above expression overpredicts the surface energy by approximately a factor of two.

### Symmetrization and antisymmetrization for fermions

Consider a multi-particle state $|\alpha_1, \alpha_2 \cdots\rangle$, where the ordering $\alpha_1, \alpha_2, \cdots$ signifies that the first particle is measure to be in the state $\alpha_1$, the second in $\alpha_2$, etc. The permutation operator $\mathcal{P}_{ij}$ is defined by

$$\mathcal{P}(12)|\alpha_1, \alpha_2, \alpha_3, \cdots\rangle = |\alpha_2, \alpha_1, \alpha_3, \cdots\rangle = p|\alpha_1, \alpha_2, \alpha_3, \cdots\rangle \tag{1}$$

Any multiparticle state $|\phi\rangle$should have a good symmetry with respect to permutation since the particles are identical. This means that all states of the system should be eigenstates of the permutation operator $\mathcal{P}$.

$$\mathcal{P}(i,j)|\phi\rangle = (\pm 1)|\phi\rangle \tag{2}$$

Only ±1 are possible eigenvalues of the permutation operator since $\mathcal{P}^2 = 1$.

In order for the state to be an eigenstate of all permutations, the $N$-particle state must be either totally symmetric or totally antisymmetric.

$$\phi \;=\; \frac{1}{\sqrt{N!}} \sum_{\text{perm.s}} (\pm 1)^{n_p} \mathcal{P}|\alpha, \beta, \gamma \cdots\rangle, \tag{3}$$

where $n_p$ is the number of pairwise permutations required to make the desired permutation. For fermions, no two states, e.g. $\alpha$ and $\beta$ can be identical.

### Fermi creation and destruction operators

Writing states as a sum over various permutations is a rather clumsy way to consider the Fermi nature of the particles as it requires assuming there is a “first” particle, “second” particle, and so on. The algebra of anticommuting creation and destruction operators offers a more natural means to incorporate antisymmetrization. With this formalism, a state can be noted simply by their labels with no mention of permutations. Matrix elements are then calculated according to the algebra of the creation and destruction operators which account for the symmetrization.

The operators obey the algebra

$$\{a_\alpha, a_\beta^\dagger\} \;=\; \delta_{\alpha,\beta} \tag{4}$$

$$\{a_\alpha, a_\beta\} \;=\; \{a_\alpha^\dagger, a_\beta^\dagger\} = 0 \tag{5}$$

Any time two creation operators or two destruction operators with the same index are next to one another the result is zero, $a_\alpha a_\alpha = a_\alpha^\dagger a_\alpha^\dagger = 0$. This enforces the Pauli exclusion principle. Similar to the Bose example, the vacuum is annihilated by the destruction operator.

$$a_\alpha|0\rangle = 0. \tag{6}$$

The commutation rules written above assumed the states $\alpha, \beta, \cdots$ were orthogonal. If the indices refer to states which are from different different bases, the algebra becomes

$$\{a_\alpha, a_j^\dagger\} = \sum_k \{\langle\alpha|k\rangle a_k, a_j^\dagger\} = \langle\alpha|j\rangle. \tag{7}$$

We are now in a position to calculate arbitrary matrix elements for $N$ particle states,

$$\begin{aligned}\langle i,j,k,\cdots|\alpha,\beta,\gamma\rangle &= \langle 0|(a_i a_j a_k\cdots)(a^\dagger_\gamma a^\dagger_\beta a^\dagger_\alpha\cdots)|0\rangle &(8)\\ &= \sum_{\text{perm.s of } i,j,\cdots} (-1)^{n_p}\langle i|\alpha\rangle\langle j|\beta\rangle\langle k|\gamma\rangle\cdots &(9)\end{aligned}$$

As an example we consider two-particle matrix elements

$$\langle i,j|\alpha,\beta\rangle = \langle i|\alpha\rangle\langle j|\beta\rangle - \langle j|\alpha\rangle\langle i|\beta\rangle$$

If $i$ and $j$ refered to positions $x$ and $y$, the result would read

$$\langle x,y|\alpha,\beta\rangle = \phi_\alpha(x)\phi_\beta(y) - \phi_\alpha(y)\phi_\beta(x),$$

which signifies that the two particles can not be at the same position. Note that the overlap of an $N$ particle matrix element would yield $N!$ terms. Thus it seems little has been gained using field operators rather than writing symmetrized/antisymmetrized wave functions which also have $N!$ terms. However, when writing the bra and ket with all permutations, both the bra and ket have $N!$ terms, with the extra $N!$ being cancelled by the $1/\sqrt{N!}$s in the normalization of the wave functions.

It should also be noted that all the same results are valid for bosons, except that the $(-1)$s disappear.

**Fermionic field operators and the density operator**

The field operators $\Psi^\dagger(x)$ and $\Psi(x)$ create and destroy a particle in the state $x$. They obey the anticommutation relations,

$$\{\Psi(\mathbf{x}),\Psi^\dagger(\mathbf{y})\} = \delta^3(\mathbf{x}-\mathbf{y}) \tag{10}$$

The field operators commute with other operators as

$$\{\Psi(\mathbf{x}),a^\dagger_\alpha\} = \phi_\alpha(\mathbf{x}), \tag{11}$$

where $\phi(\mathbf{x}) = \langle\mathbf{x}|\alpha\rangle$ is the single particle wave function of a particle in the state $\alpha$. Thus the field operators are no different than other creation and destruction operators, except that their dimension is length$^{-3/2}$ and their anticommutation relations are expressed in terms of Dirac deltas instead of Kronecker deltas.

The density operator is

$$\rho(\mathbf{x}) = \Psi^\dagger(\mathbf{x})\Psi(\mathbf{x}). \tag{12}$$

The expectation of the density operator in the state $|\alpha,\beta,\cdots...\rangle$ is

$$\begin{aligned}\langle\alpha,\beta,\gamma,\cdots|\Psi^\dagger(\mathbf{x})\Psi(\mathbf{x})|\alpha,\beta,\gamma,\cdots\rangle &= \langle 0|(a_\alpha a_\beta a_\gamma\cdots)\Psi^\dagger(\mathbf{x})\Psi(\mathbf{x})(\cdots a^\dagger_\gamma a^\dagger_\beta a^\dagger_\alpha)|0\rangle &(13)\\ &= \sum_{\kappa\in\alpha,\beta\cdots}\phi^*_\kappa(\mathbf{x})\phi_\kappa(\mathbf{x}) &(14)\end{aligned}$$

Then density operator can also appear in a transition element. Consider the bra and ket to differ in one label, $\gamma \to \gamma'$,

$$\begin{aligned} \langle \alpha, \beta, \gamma', \cdots | \Psi^\dagger(\mathbf{x}) \Psi(\mathbf{x}) | \alpha, \beta, \gamma, \cdots \rangle &= \langle 0 | (a_\alpha a_\beta a_{\gamma'} \cdots) \Psi^\dagger(\mathbf{x}) \Psi(\mathbf{x}) (\cdots a_\gamma^\dagger a_\beta^\dagger a_\alpha^\dagger) | 0 \rangle \quad (15) \\ &= \phi_{\gamma'}^*(\mathbf{x}) \phi_\gamma(\mathbf{x}) \quad (16) \end{aligned}$$

This simple result followed because it was assumed that the final state was described by the same single particle states, except for a single particle. In more realistic models, the transition might be between states where many of the wave functions were altered. For instance, in a many electron atom, the other levels are affected by whether an electron in the state $\gamma$ is excited to the state $\gamma'$. A second inherent assumption was that the initial state could be written as a "product" state. A product state is produced by operating with a single string of orthogonal creation operators on the vacuum. The most general state could be expressed as a linear combination of product states. Going beyond simple product states requires sophisticated many-body treatments which are outside the scope of this class.

## Interacting Fermi systems – the Hartree Fock approximation

### Two-point interactions

The simplest sort of interaction is a two-point interaction.

$$H_2 = \sum_{\alpha,\beta} V_{\alpha,\beta} a_\alpha^\dagger a_\beta. \tag{1}$$

Such an interaction allows particles to behave independently. To demonstrate what is meant by "independent", consider the evolution of the product state

$$\begin{aligned} |\phi(t)\rangle &= e^{-iHt/\hbar} a_\delta^\dagger \cdots a_\beta^\dagger a_\alpha^\dagger |0\rangle & (2)\\ &= \left(e^{-iHt/\hbar} a_\delta^\dagger e^{iHt/\hbar}\right) \cdots \left(e^{-iHt/\hbar} a_\beta^\dagger e^{iHt/\hbar}\right) \left(e^{-iHt/\hbar} a_\alpha^\dagger e^{iHt/\hbar}\right) |0\rangle. & (3) \end{aligned}$$

Thus, the evolution in time simply adjusts the creation operators to time-dependent quantities

$$\begin{aligned} a_\alpha^\dagger(t) &= \left(e^{-iHt/\hbar} a_\alpha^\dagger e^{iHt/\hbar}\right) & (4)\\ i\hbar \frac{\partial}{\partial t} a_\alpha^\dagger(t) &= \left[H, a_\alpha^\dagger(t)\right] & (5)\\ &= e^{-iHt/\hbar} \left[H, a_\alpha^\dagger\right] e^{-iHt/\hbar} & (6)\\ &= \sum_\beta V_{\beta,\alpha} a_\beta^\dagger(t). & (7) \end{aligned}$$

Therefore, a two-point interaction leaves a product state as a product state, and the evolution can be reduced to the evolution of independent creation operators.

Unfortunately, physics is not usually so simple. If all interactions were of the two-point type all problems could be solved by considering the independent motion of independent operators and there would be no need for many-body theory. Interactions of the type

$$H = \int dx \left( -\frac{\hbar^2}{2m} \Psi^\dagger(x) \frac{\partial^2}{\partial x^2} \Psi(x) + V(x) \Psi^\dagger(x) \Psi(x) \right), \tag{8}$$

are of the two-point form and can be solved by considering a single particle in the system, then creating the many-particle system as a product of many single-particle solutions.

### Four-point interactions

An interaction between particles separated by $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ is written classically as

$$H_{\text{int}} = \frac{1}{2} \int d^3r_1 d^3r_2 \rho(\mathbf{r}_1) \rho(\mathbf{r}_2) V(\mathbf{r}_1 - \mathbf{r}_2). \tag{9}$$

The factor of 1/2 corrects for double counting since the integral is without a $r_1 < r_2$ qualifier.

Written in terms of field operators, this interaction becomes

$$H_{\text{int}} = \frac{1}{2} \int d^3r_1 d^3r_2 V(\mathbf{r}_1 - \mathbf{r}_2) \psi^\dagger(\mathbf{r}_1) \psi^\dagger(\mathbf{r}_2) \psi(\mathbf{r}_2) \psi(\mathbf{r}_1). \tag{10}$$

For the moment, we will omit spin indices and assume only particles of a specific spin are involved.

One peculiar aspect of the Hamiltonian is that the two $\Psi^\dagger$s are on the left while the two $\Psi$s are on the right, whereas the product of densities would suggest a product of $\Psi^\dagger\Psi$s. However, such a product would result in an energy for a one-particle state, as the particle would interact with itself.

Four-point interactions (or three-point interactions, e.g. the electromagnetic interaction $\mathbf{J}\cdot\mathbf{A}$) are infinitely more complicated than two-point interactions. For one, if one wishes to calculate the evolution of $a_\alpha^\dagger(t)$, one needs to commute the Hamiltonian with $a_\alpha^\dagger$. However, commuting a four-point function which is a product of four creation/destruction operators with a single creation operator results in a product of three creation/destruction operators. This destroys the independent-particle nature of the evolution. In fact, the eigenstates of a Hamiltonian with four-point terms is not a product state, but is instead a complicated linear combinations of product states. In fact, such problems are in general not solvable, forcing one to resort to approximations. One such approximation is the Hartree-Fock approximation.

**Example: correlations in a Fermi gas**

Consider a one-dimensional gas of fermions moving in a large region of length $L$.

1. Find the correlation function, relating the ratio of the probability of finding two particles separated by $r$ to the probability of finding the two particles at arbitrary locations.

   To do this problem, we first write down the two-particle probability,

$$\begin{aligned} P_2(x_1,x_2) &= \langle\phi|\Psi^\dagger(x_1)\Psi^\dagger(x_2)\Psi(x_2)\Psi(x_1)|\phi\rangle. && (11)\\ |\phi\rangle &= \prod_{k<k_f} a_k^\dagger|0\rangle. && (12)\end{aligned}$$

   Commuting the field operators $\Psi(x_2)$ and $\Psi(x_1)$ towards the ket yields

$$\begin{aligned} \Psi(x_2)\Psi(x_1)\prod_{k<k_f} a_k^\dagger|0\rangle &= \sum_{k_1,k_2<k_f}\frac{e^{ik_1x_1}}{\sqrt{L}}\frac{e^{ik_2x_2}}{\sqrt{L}}a_{k_1}a_{k_2}\left(\prod_{k<k_f}a_k^\dagger\right)|0\rangle && (13)\\ &= \sum_{k_1,k_2<k_f}(\pm)(-)^{n_1+n_2}\frac{e^{ik_1x_1}}{\sqrt{L}}\frac{e^{ik_2x_2}}{\sqrt{L}}\left(\prod_{k<k_f,k\neq k_1,k\neq k_2}a_k^\dagger\right)|0\rangle && (14)\end{aligned}$$

   Here, the sign $(\pm)$ depends on whether $a(k_1)a(k_2)$ appear in the same/opposite order as $a^\dagger(k_1)a^\dagger(k_2)$ in the product of creation operators.

   One can find a similar expression for $\langle\phi|\Psi^\dagger(x_1)\Psi^\dagger(x_2)|\phi\rangle$. The overlap of the two states is zero unless $k_1$ and $k_2$ are the same in the expressions for the bra and ket. This yields

$$\langle\phi|\Psi^\dagger(x_1)\Psi^\dagger(x_2)\Psi(x_2)\Psi(x_1)|\phi\rangle = \sum_{k_1,k_2<k_f}\frac{1}{L^2}\left(1-\cos\left(k_2-k_1\right)(x_2-x_1)\right) \qquad (15)$$

   Taking the ratio of the two-particle density to the square of the one particle density gives the correlation function.

$$g(r\equiv x_2-x_1) = \frac{\sum_{k_1,k_2<k_f}\left(1-\cos\left(k_2-k_1\right)(x_2-x_1)\right)}{\sum_{k_1,k_2<k_f}} \qquad (16)$$

The sums can be changed into integrals,

$$\begin{aligned} g(r) &= 1 - |I|^2 && (17) \\ I &= \frac{\int_{-k_f<k<k_f} dk e^{ikr}}{\int_{-k_f<k<k_f} dk} && (18) \\ &= \frac{\sin(k_f r)}{k_f r} && (19) \end{aligned}$$

2. The particles now feel a mutual interaction,

$$V(x) = \alpha x^2 \Theta(a - |x|) \tag{20}$$

Find the exchange contribution to the energy per unit length due to the interaction in first-order perturbation theory.

In first-order perturbation theory the correction to the energy is

$$\begin{aligned} \langle H \rangle &= \frac{1}{2} \int dx_1 dx_2 \langle \phi | \Psi^\dagger(x_1) \Psi^\dagger(x_2) \Psi(x_2) \Psi(x_1) | \phi \rangle V(x_1 - x_2) && (21) \\ &= L \frac{1}{2} \int dr \langle \phi | \Psi^\dagger(0) \Psi^\dagger(r) \Psi(r) \Psi(0) | \phi \rangle V(r), && (22) \end{aligned}$$

where we have used the fact that the two particle density depends only on $x_1 - x_2$. By using the results of #1 one can find the energy per length,

$$\begin{aligned} \frac{\langle H \rangle}{L} &= \frac{1}{2} n^2 \int_{-\infty}^{\infty} dr \; g(r) V(r) && (23) \\ &= \frac{n^2}{k_f^2} \alpha \int_0^a dr \left( k_f^2 r^2 - \sin^2(k_f r) \right) && (24) \\ &= \alpha \frac{n^2}{k_f^3} \left\{ \frac{1}{3}(k_f a)^3 - \frac{1}{2} k_f a + \frac{1}{4} \sin(2 k_f a) \right\} && (25) \end{aligned}$$

where $n$ is the number of particles per unit length. Note that the first term describes the potential energy one would expect from particles with a uniform density interacting through the potential $V(x_1 - x_2)$. This is called the direct term, while the remainder is referred to as the exchange term.

### Hartree Fock

The Hartree-Fock approximation yields an expression for the ground state of a many-particle system. It is basically a manifestation of the variational approximation. One assumes a form of the wavefunction, then solves for the parameters that minimize the energy. The assumed form of the wave function is

$$|\phi\rangle = a_\delta^\dagger \cdots a_\beta^\dagger a_\alpha^\dagger |0\rangle, \tag{26}$$

that is one confines the search to product states.

Next, one writes down the expectation of the Hamiltonian,

$$\begin{aligned}\langle\phi|H|\phi\rangle &= \langle\phi|\int d^3r\Psi^\dagger(\mathbf{r})\left(-\frac{\hbar^2}{2m}\nabla^2\right)\Psi(\mathbf{r})+\int d^3rU(r)\Psi^\dagger(\mathbf{r})\Psi(\mathbf{r})|\phi\rangle &(27)\\ &+\langle\phi|\frac{1}{2}\int d^3r_1d^3r_2V(\mathbf{r_2}-\mathbf{r}_1)\Psi^\dagger(\mathbf{r}_1)\Psi^\dagger(\mathbf{r}_2)\Psi(\mathbf{r}_2)\Psi(\mathbf{r}_1)|\phi\rangle, &(28)\end{aligned}$$

where the spin indices have been omitted temporarily.

One can now write down the energy in terms of the wave functions of the occupied states $\alpha$.

$$\begin{aligned}\langle\phi|H|\phi\rangle &= \sum_\alpha\int d^3r\phi^*_\alpha(\mathbf{r})\left(-\frac{\hbar^2}{2m}\nabla^2+U(\mathbf{r})\right) &(29)\\ &+ \frac{1}{2}\sum_{\alpha,\alpha'}\int d^3rd^3r'\left(\phi^*_\alpha(\mathbf{r})\phi^*_{\alpha'}(\mathbf{r}')\phi_{\alpha'}(\mathbf{r}')\phi_\alpha(\mathbf{r})\pm\phi^*_\alpha(\mathbf{r})\phi^*_{\alpha'}(\mathbf{r}')\phi_\alpha(\mathbf{r}')\phi_{\alpha'}(\mathbf{r})\right)\end{aligned}$$

The second term in the two-body interaction, where the ± refers to bosons/fermions, is known as the exchange term, with the name coming from the exchange of the $\alpha$ and $\alpha'$ indices.

The next step in the variational procedure is to minimize $\langle\phi|H|\phi\rangle$ with respect to changes in the wave functions subject to the constraint that each wave function is properly normalized. One accounts for the constraint by multiplying the constraint by a Lagrange multiplier $\lambda$ then adding it to the function one wishes to minimize,

$$\frac{\delta}{\delta\phi_\gamma(\mathbf{r})}\left\{\langle\phi|H|\phi\rangle-\lambda_\gamma\int d^3r\phi^*_\gamma(\mathbf{r})\phi_\gamma(\mathbf{r})\right\}=0. \tag{30}$$

More correctly, one would vary both the real and imaginary parts of $\phi_\gamma$ which is equivalent to varying either $\phi_\gamma$ or $\phi^*_\gamma$. The resulting expression is

$$\begin{aligned}\lambda_\gamma\phi_\gamma(\mathbf{r}) &= \left(-\frac{\hbar^2}{2m}\nabla^2+U(\mathbf{r})\right)\phi_\gamma(\mathbf{r}) &(31)\\ &+ \sum_{\alpha'}\int d^3r'V(\mathbf{r}-\mathbf{r}')\left\{\phi^*_{\alpha'}(\mathbf{r}')\phi_{\alpha'}(\mathbf{r}')\phi_\gamma(\mathbf{r})\pm\phi^*_{\alpha'}(\mathbf{r}')\phi_\gamma(\mathbf{r}')\phi_{\alpha'}(\mathbf{r})\right\}\end{aligned}$$

The two terms involving $V(\mathbf{r}-\mathbf{r}')$ are known as the Hartree and Fock terms respectively. The Hartree term looks like a potential felt by the particles due to the presence of the other particles. Thus the Hartree equation can be solved by self-consistently finding the solutions to the effective potential

$$V_{\mathrm{Hartree}}(\mathbf{r})=\sum_{\alpha'}\int d^3r'V(\mathbf{r}-\mathbf{r}')\phi^*_{\alpha'}(\mathbf{r}')\phi_{\alpha'}(\mathbf{r}') \tag{32}$$

The Hartree equations are often solved iteratively. One guesses at the wave functions, finds the Hartree-potential, solves the Schrödinger equation for the single-particle wave functions, then iterates the procedure until the wavefunctions converge.

The Fock term presents a different challenge since $\phi_\gamma(\mathbf{r})$ can not be factored out of the differential equation. The Fock term is non-local in that $\phi_\gamma(\mathbf{r}')$ appears in its place.

The Lagrange multiplier $\lambda_\gamma$ plays the role of a single-particle energy. However, one should remember that since the interaction energy between two states is contained in the single-particle energy for both states, that the total energy is not the sum of the $\lambda_\gamma$s. The Hartree Fock approximation is especially useful for finding density distributions or even changes in energies (e.g. separation energies), but is not particularly accurate at calculating total binding energies.

Finally, we return to the problem of including the spin indices. When spin indices are included the Fock term disappears unless the two states are the same species and the same spin. Hence a factor $\delta_{s,s'}$ accompanies the Fock term.

## Multi-electron atoms

### The Thomas-Fermi approximation

A very crude way to find the density of fermions in an external well is the Thomas-Fermi approximation. This approximation is semiclassical and assumes that the local density is a function of the local potential only,

$$n = \frac{2s+1}{6\pi^2}k_f^3, \quad \frac{\hbar^2 k_f(\mathbf{r})^2}{2m} + V(\mathbf{r}) = \epsilon_f \tag{1}$$

The density would extend only in the region where $V(\mathbf{r}) < \epsilon_f$. Given the potential and $\epsilon_f$ it is straight forward to find the density. For a finite system with a fixed particle number, one would have to adjust $\epsilon_f$ to get the correct total number of particles.

The Thomas-Fermi approximation is crude, and gives rather non-sensical results for atoms, but is more reasonable for estimating the electron density near surfaces. As a general rule it is valid for large systems where the potential changes slowly.

### Hartree Fock

The principle difficulty in handling multi-electron atoms comes from the fact that the electrons interact with one another. If it were not for the mutual interactions of the electrons, one could treat the electrons independently. Of course, this would yield horribly unphysical results. For instance, one could place an infinite number of electrons into the the hydrogen atom, where in reality no more than two electrons can be bound to hydrogen.

The Hartree approximation is the first method one might consider for treating such atoms. One then solves the Schrödinger equation with the potential,

$$V_i(\mathbf{r}) = -\frac{Ze^2}{r} + \sum_{j\neq i}\int d^3r' |\phi_j(\mathbf{r}')|^2 \frac{e^2}{|\mathbf{r}-\mathbf{r}'|} \tag{2}$$

If there are $n$ electrons, one must solve $n$ coupled equations.

One can go one step further and solve the Hartree Fock equations,

$$\left(-\frac{\hbar^2\nabla^2}{2m} - \frac{Ze^2}{r}\right)\phi_i(\mathbf{r}) + \sum_j \int d^3r' \frac{e^2}{|\mathbf{r}-\mathbf{r}'|}\phi_j^*(\mathbf{r}')\left[\phi_j(\mathbf{r}')\phi_i(\mathbf{r}) - \delta_{s,s'}\phi_j(\mathbf{r})\phi_i(\mathbf{r}')\right] = \lambda_i\phi_i(\mathbf{r}) \tag{3}$$

to find the wavefunctions. One can then find the energy by calculating $\langle\phi|H|\phi\rangle$. Again, this requires solving coupled differential equations, but the Fock term also makes the equations non-local which brings along an added computational difficulty.

The difference of the energy found by solving the Hartree Fock equations and the Hartree equations is the exchange energy. Since the Hartree Fock wave functions force the electrons to stay away from one another due to antisymmetrization, the repulsive Coulomb interacton between electrons is weakened which means that the exchange energy is negative.

The Hartree Fock equations were derived with the assumption that the solution is a product state. As that is a variational assumption, the true ground state energies are about 1 eV lower than Hartree Fock solutions. This difference is refered to as "correlation" energy. It can be calculated perturbatively by considering the mixing of one-particle-one-hole and two-particle-two-hole states into the wave functions. This is done perturbatively by considering the $n$-electron Hartree Fock ground state as the ground state. Then one considers excited states as being those $n$-particle $n$-hole states formed by considering $n$ of the single-particle solutions of the Hartree Fock ground state to be replaced by $n$ single-particle solutions from the set of single-particle states left unfilled in the Hartree Fock ground state.

### The periodic table

Single-electron wave functions are labeled by $n$, $\ell$, $s$, $j$ and $m_j$. In an atom with only one electron, the energy depends principally on $n$ as states with same $n$ but different $\ell = 0, 1, \cdots n-1$ are degenerate aside from the spin-orbit interaction. Of course, $s$ always equals $1/2$ and $j$ can be either $\ell + 1/2$ or $\ell - 1/2$.

The existence of the other electrons destroys the "accidental" degeneracy of the hydrogen atom and allows states with different $\ell$ and the same $n$ to have significantly different energy. This is due to the screening of the positive charge. The "accidental" degeneracy allowed states with fewer nodes in the radial wave function but larger angular momentum to have the same energy as states with smaller angular momentum but more nodes in the radial wave function. By screening the charge an advantage is created for states that have a relatively greater probability of being near the origin. Since radial wave functions behave as $r^\ell$ near the origin, a state with a lower $\ell$ but the same $n$ will have lower energy due to screening. This difference can be large enough at times to allow a state to move lower than states of higher $n$ but higher angular momentum. For instance, in some cases the $4s$ states can move below the $3d$ states, and similarly the $4d$ and $5s$ shells compete as well. The $5s$ shell is always well below the $4f$ shell. When shells compete, e.g. the $4s$ and $3d$ electrons, the choice of orbitals is non-trivial. In these cases the configuration can vary from one element to the next, and in fact, solutions might contain a mixture of configurations. Chemical properties are determined largely by the outermost electrons. When shells are filled, the elements are less reactive. The rare gases (also know as inert gases) all have filled $p$ shells with the exception of Helium.

The set of orbitals with a specific $n$ and $\ell$ is known as a "shell". The degeneracy of a shell is $4\ell + 2$. Electronic "configurations" are labeled by the shells and the filling, e.g.,

$$(1s)^2(2s)^2(2p)^3,$$

with the superscript labeling the number of electrons in the shell.

### Configuration splitting

Different configurations are generally split by a few electron volts. Within a configuration, the splitting is complicated. Although there are $4\ell + 2$ single-particle orbitals, the number of ways to arrange several electrons among these levels can be rather large.

Ignoring the spin-orbit interaction, the total angular momentum $\mathbf{L}$ and total spin $\mathbf{S}$ of the electrons commute with the Hamiltonian. The $(2L+1)(2S+1)$ states of an $LS$ multiplet are then further split by the spin-orbit interaction. Thus the spin-orbit interaction invalidates $M_L$ and $M_S$ as good quantum numbers, and replaces them with $J$ and $M_J$.

Hund's rules determine which $LSJ$ combination has the lowest energy:

1. The largest $S$ is most favorable as it has the most symmetric spin wave functions, therefore totally antisymmetric spatial wave functions, which minimizes the probability that electrons are close to one another, and therefore minimizing their repulsive interaction.
2. For a given $S$, the $LS$ multiplet with the largest $L$ has the lowest energy. This can be understood by considering two electrons rotating about a nucleus. If $L$ is large, both electrons are moving about with essentially the same orbit as $m_1$ and $m_2$ can be large and of the same sign. As such electrons spend less time crossing one another's path they miminize their repulsive interaction.
3. Different $LS$ multiplets are typically split by tenths of electron volts. A given $LS$ multiplet is again split by the spin-orbit interaction but only by a few hundredths or a few thousandths of an electron volt. The spin-orbit interaction gives preference to states with the minimum $J$ when the shells are less than half filled and behaves in the opposite way when the shells are more than half filled.

Configurations are labeled by $S$, $L$ and $J$, which should not be confused with the $\ell$ of the single-particle orbitals. The notation is

$$^{2S+1}L_J.$$

For instance, the state $^3D_3$ would have the spins coupled to $S = 1$, $L = 2$ and $J = 3$. Note the upper-case angular momentum labels $S, P, D, F \cdots$.

## Slater Determinants

One way to write antisymmetric wave functions is through a determinant. Imagine three identical particles with states described by the wave functions $\phi_a(x)$, $\phi_b(x)$ and $\phi_c(x)$. The total wave function $\Phi(x_1, x_2, x_3)$ can be written as:

$$\Phi(x_1, x_1, x_3) = \frac{1}{\sqrt{3!}} \begin{vmatrix} \phi_a(x_1) & \phi_b(x_1) & \phi_c(x_1) \\ \phi_a(x_2) & \phi_b(x_2) & \phi_c(x_2) \\ \phi_a(x_3) & \phi_b(x_3) & \phi_c(x_3) \end{vmatrix} \tag{1}$$

By expanding the determinant, one can see that the overall wave function is antisymmetric.

$$\begin{aligned} \Phi(x_1, x_1, x_3) &= \frac{1}{\sqrt{3!}} \{\phi_a(x_1)\phi_b(x_2)\phi_c(x_3) - \phi_a(x_1)\phi_c(x_2)\phi_b(x_3) - \phi_b(x_1)\phi_a(x_2)\phi_c(x_3) \\ &\quad + \phi_b(x_1)\phi_c(x_2)\phi_a(x_3) + \phi_c(x_1)\phi_a(x_2)\phi_b(x_3) - \phi_c(x_1)\phi_b(x_2)\phi_a(x_3)\} \qquad (2) \end{aligned}$$

## Angular and spin wave functions

The overall wave function for a many-electron state described by $L$, $S$ and $J$ can be written as the sum over products of angular and spin wave functions.

$$|L, S, J, M_J\rangle = \sum_{M_L, M_S} \langle L, S, J, M_L | M_L, M_S\rangle |L, M_L\rangle |S, M_S\rangle \tag{3}$$

The angular/spin wave functions $|L, M_L\rangle|S, M_S\rangle$ must first be written in terms of products of singular particle wave functions summed over with the help of Clebsch-Gordan technology.

As an example we consider a two-electron state with orbital/spin wave functions in a shell of angular momentum $\ell$.

$$\begin{aligned} \Psi_{L,S,J,M_J}(\Omega, \Omega'; m_s, m_s') &= \langle \Omega, \Omega'; m_s, m_s' | L, S, J, M_J\rangle & (4) \\ &= \sum_{M_L, M_S} \langle L, S, J, M_J | M_L, M_S\rangle \langle \Omega, \Omega' | L, M_L\rangle \langle m_s, m_s' | S, M_S\rangle & (5) \\ &= \sum_{M_L, M_S} \langle L, S, J, M_J | M_L, M_S\rangle & (6) \\ &\quad \cdot \left( \sum_{m_\ell, m_\ell'} \langle \ell, \ell, L, M_L | m_\ell, m_\ell'\rangle Y_{\ell, m_\ell}(\Omega) Y_{\ell, m_\ell'}(\Omega') \right) \\ &\quad \cdot \left( \sum_{m_s'', m_s'''} \langle 1/2, 1/2, S, M_S | m_s'', m_s'''\rangle \langle m_s | m_s''\rangle \langle m_s' | m_s'''\rangle \right) \\ &= \sum_{M_L, M_s, m_\ell, m_\ell'} \langle L, S, J, M_J | M_L, M_S\rangle \langle \ell, \ell, L, M_L | m_\ell, m_\ell'\rangle & (7) \\ &\qquad \langle 1/2, 1/2, S, M_S | m_s, m_s'\rangle Y_{\ell, m_\ell}(\Omega) Y_{\ell, m_\ell'}(\Omega'). \end{aligned}$$

The expression would be even more complicated if there were three electrons in the shell.

## Example: Constructing the $^1S_0$ state in Carbon

The two electrons in the $p$ shell of Carbon can be in any number of configurations. Using the expression above,

$$\begin{aligned}
&\Psi_{L=0,S=0,J=0,M_J=0}(\Omega,\Omega',m_s,m_s') \qquad (8)\\
&\quad= \sum_{m_\ell,m_\ell'} \langle L,S,J,M_J|M_L,M_S\rangle\langle \ell=1,\ell=1,L=0,M_L=0|m_\ell,m_\ell'\rangle\\
&\qquad\qquad \cdot\langle 1/2,1/2,S=0,M_S=0|m_s,m_s'\rangle Y_{\ell=1,m_\ell}(\Omega)Y_{\ell=1,m_\ell'}(\Omega')\\
&\quad= \sum_{m_\ell,m_\ell'} \langle \ell=1,\ell=1,L=0,M_L=0|m_\ell,m_\ell'\rangle Y_{\ell=1,m_\ell}(\Omega)Y_{\ell=1,m_\ell'}(\Omega') \qquad (9)\\
&\qquad\qquad \cdot\frac{1}{\sqrt{2}}\left(\delta_{m_s,1/2}\delta_{m_s',-1/2}-\delta_{m_s,-1/2}\delta_{m_s',1/2}\right)\\
&\quad= \frac{1}{\sqrt{6}}\left\{Y_{1,1}(\Omega)Y_{1,-1}(\Omega')+Y_{1,-1}(\Omega)Y_{1,1}(\Omega')-Y_{1,0}(\Omega)Y_{1,0}(\Omega')\right\} \qquad (10)\\
&\qquad\qquad \cdot\left(\delta_{m_s,1/2}\delta_{m_s',-1/2}-\delta_{m_s,-1/2}\delta_{m_s',1/2}\right)
\end{aligned}$$

Note that the wave function is symmetric with respect to interchange of $\Omega$ with $\Omega'$ and antisymmetric with respect to interchange of $m_s$ and $m_s'$, making the overall wave function antisymmetric.

### Permutation symmetry

When coupling two particles together the permutation symmetry goes as $(-1)^L$ for the spatial part, while the interchange of spins is symmetric/antisymmetric for $S=1/0$. For this reason one can notice that for two electrons in the (2p) shell (carbon) the orbital states must be $L=0$ or $L=2$ if the the spin state is $S=0$ and must be $L=1$ if $S=1$. Thus the possible states in carbon are ${}^1S_0$, ${}^1D_2$, ${}^3P_0$, ${}^3P_1$ and ${}^3P_2$.

Coupling a higher number of particles together can lead to "mixed" symmetries. In this case the angular wave functions may be neither symmetric or antisymmetric, while the spin wave functions might be mixed as well. However, the overall wave function needs to be antisymmetric. For example, the flavor and spin wave functions of the three quarks that constitute a proton or neutron are in states of mixed symmetry. This will be discussed in detail later.

### Zeeman Effect

A particle in a magnetic field feels the interaction,

$$H_{\text{mag}} = -\frac{eB}{2mc}(L_z+2S_z), \qquad (11)$$

where the magnetic field is assumed to point in the $z$ direction. We wish to calculate the change in energy for an atom in a state of good $J, M_J$ due to the interaction.

$$\begin{aligned}
\Delta E_{LSJM_J} &= -\frac{eB}{2mc}\langle L,S,J,M_J|L_z+2S_z|L,S,J,M_J\rangle \qquad (12)\\
&= -\frac{eB}{2mc}\left(M_J+\langle L,S,J,M_J|S_z|L,S,J,M_J\rangle\right). \qquad (13)
\end{aligned}$$

The challenge in calculating the splitting comes from finding $\langle S_z \rangle$. We expect this to be proportional to $M_J$ as it is the only label available. The Wigner Eckart theorem and Clebsch-Gordan technology come to the rescue.

$$\frac{\langle L, S, J, M_J | S_z | L, S, J, M_J \rangle}{\langle L, S, J, M_J | J_z | L, S, J, M_J \rangle} = \frac{\langle L, S, J || S || L, S, J \rangle}{\langle L, S, J || J || L, S, J \rangle}. \tag{14}$$

This follows by applying the Wigner Eckart theorem to both $\langle S_z \rangle$ and $\langle J_z \rangle$ and noticing that the same Clebsch Gordan coefficients appear in both terms.

Thus if we can find the ratio of the reduced matrix elements we will have fulfilled our mission. To do this, we first step aside to perform a proof. Consider a vector operator $\mathbf{A}$.

$$\begin{aligned} \langle JM | \mathbf{A} \cdot \mathbf{J} | JM \rangle &= \sum_{-1 \le m' \le 1} \langle JM | A_{m'} J_{-m'} | JM \rangle & (15) \\ &= \sum_{-1 \le m' \le 1, -J \le M'' \le J} \langle JM | A_{m'} | JM'' \rangle \langle JM'' | J_{-m'} | JM \rangle, & (16) \end{aligned}$$

Note that the inserted states were only those within the same $JM$ multiplet. This is valid since $J_m$ does not mix different multplets. Now, by applying the Wigner Eckart theorem, one can write the matrix element $\langle \mathbf{A} \cdot \mathbf{J} \rangle$ as

$$\begin{aligned} \langle JM | \mathbf{A} \cdot \mathbf{J} | JM \rangle &= f(J, M) \langle J || A || J \rangle \langle J || J || J \rangle & (17) \\ f(J, M) &= \sum_{-1 \le m' \le 1, -J \le M'' \le J} & (18) \\ & \cdot \langle 1, J, J, M | m', M'' \rangle \langle 1, J, J, M | -m', M'' \rangle \frac{1}{2J+1} & (19) \end{aligned}$$

Since $f$ is determined solely by Clebsch-Gordan coefficients, one can see that

$$\frac{\langle JM | \mathbf{A} \cdot \mathbf{J} | JM \rangle}{\langle JM | \mathbf{J} \cdot \mathbf{J} | JM \rangle} = \frac{\langle J || A || J \rangle}{\langle J || J || J \rangle} \tag{20}$$

Now that our proof is finished we can see that

$$\begin{aligned} \frac{\langle L, S, J || S || L, S, J \rangle}{\langle L, S, J || J || L, S, J \rangle} &= \frac{\langle L, S, J, M_J | \mathbf{J} \cdot \mathbf{S} | L, S, J, M_J \rangle}{\langle L, S, J, M_J | \mathbf{J} \cdot \mathbf{J} | L, S, J, M_J \rangle} & (21) \\ &= \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)}, & (22) \end{aligned}$$

where we have taken advantage of the fact that

$$\mathbf{J} \cdot \mathbf{S} = \frac{1}{2} \left( J(J+1) - S(S+1) - L(L+1) \right) \tag{23}$$

Finally, we are able to insert our result for the ratio of the reduced matrix elements into our expression for the splitting to get

$$\begin{aligned} \Delta E &= -g \frac{e\hbar B}{2mc} M_J & (24) \\ g &= 1 + \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)}. & (25) \end{aligned}$$

The factor $g$ is known as the Landé $g$ factor.

In some undergraduate modern physics books the Landé $g$ factor is derived from simple geometric arguments. If one considers the vector $J$ precessing about the $z$ axis and the vector $S$ precessing about $\mathbf{J}$, one would expect that the expectation of $\mathbf{S}$ for a given orientation of $\mathbf{J}$ would be

$$\langle \mathbf{S} \rangle = \mathbf{J} \frac{\mathbf{S} \cdot \mathbf{J}}{|J|^2}, \tag{26}$$

since as $\mathbf{S}$ precesses about $\mathbf{J}$ the component of $\mathbf{S}$ perpendicular to $\mathbf{J}$ averages to zero. Finally, averaging over the direction of $\mathbf{J}$ gives the result we expected.

### Molecules and the adiabatic approximation

The force felt between atoms largely derives from the distortion of the electronic wave functions due to the proximity of a second potential. Since atoms move slowly with respect to the electronic motion, electronic wave functions largely adjust in such a way as to remain in the ground state for a given atomic separation. This was refered to as the adiabatic or Born-Oppenheimer approximation. Examples where the adiabatic approximation were applied included a particle in a slowly expanding box. If a box were slowly expanded or contracted, a particle would remain in the ground state of the box. Of course, this implies that the energy of the particle is not kept constant. For the example of an expanding box, the ground state energy falls as the volume expands, and the lost energy appears in the kinetic energy of the piston. In fact, that energy is equal to the work, $PdV$, done by the expansion.

In the case of atoms, the gain or loss of the electronic energy appears as a loss or gain of the heavy ion's kinetic energy. The electronic energy, calculated as a function of the ion's separation $r$, serves as a potential for the atoms. In a previous problem set, we worked out the energy felt by two electrons in harmonic oscillator potentials situated far apart, such that they felt a dipole-dipole interaction. Calculating the correction to the energy, it was found that the energy went as $1/r^6$.

### Example: A neutral atom and an ion separated far apart

For this example we consider an electron and a positive ion, where we assume the states available to the electron are described as those of a harmonic oscillator with frequency $\omega$. An ion of charge $Ze$ is placed a distance $R$ from the atom. The perturbative potential between the ion and the atom is

$$\begin{aligned} V &= Ze^2\left\{\frac{1}{R}-\int d^3r\rho(\mathbf{r})\frac{1}{|\mathbf{R}-\mathbf{r}|}\right\} && (1)\\ &\approx -Ze^2\int d^3r\rho(\mathbf{r})\frac{z}{R^2} && (2)\\ &= -\frac{Ze^2}{R^2}z_{\rm op}. && (3)\end{aligned}$$

One can then calculate the energy to second order perturbation theory,

$$\begin{aligned} \Delta E &= -\frac{Z^2e^4}{R^4}\frac{|\langle n_z=1|z_{\rm op}|0\rangle|^2}{\hbar\omega} && (4)\\ &= -\frac{Z^2e^4}{2R^4m\omega^2}. && (5)\end{aligned}$$

This energy serves as the potential between the atom and the ion. Note that if one were to consider an induced dipole moment proportion to the electric field, multiplied by the electric field which falls off as $1/R^2$, one would have expected the $1/R^4$ behavior.

### Example: $^+H_2$ ion

Consider two protons separated by a distance $R$, with the addition of a single electron. In the adiabatic approximation the binding energy of the electron, $\epsilon(R)$ serves as the potential between the protons when combined with the proton-proton interaction. At large distances the binding energy is one Rydberg, while one would expect an increase in the magnitude of the binding energy as $R$ is shortened. At very short distances, one expects the interaction to become repulsive when one penetrates the electronic cloud and the interaction is dominated by the Coulomb interaction between the protons.

Calculating the binding energy as a function of $R$ can be crudely accomplished with a variational calculation assuming a trivial form of the wave function,

$$\psi(\mathbf{r}) = C_\pm \left[\psi_A(\mathbf{r}) \pm \psi_B(\mathbf{r})\right], \tag{6}$$

where $\psi_A$ and $\psi_B$ are the bound state wave functions of an electron to each of the protons,

$$\psi_A(\mathbf{r}) = (\pi a_0^3)^{-1/2} e^{-|\mathbf{r}-\mathbf{R}_A|/a_0}. \tag{7}$$

The factor $C_\pm$ is merely a normalization constant,

$$\begin{aligned} C_\pm &= \frac{1}{\sqrt{2 \pm 2S(R)}} && (8)\\ S(R) &= \int d^3r \psi_A(\mathbf{r})\psi_B\mathbf{r}) && (9)\\ &= \left(1 + \frac{R}{a_0} + \frac{R^2}{3a_0^2}\right) e^{-R/a_0} && (10) \end{aligned}$$

This can be considered as a variatonal calculation with zero variational parameters.

This integral $S(R)$ is most easily calculated in elliptic coordinates, where the three components of $\mathbf{r}$ are replaced by

$$\begin{aligned} u &\equiv \frac{|\mathbf{r}-\mathbf{R}_A| + |\mathbf{r}-\mathbf{R}_B|}{R}, && (11)\\ v &\equiv \frac{|\mathbf{r}-\mathbf{R}_A| - |\mathbf{r}-\mathbf{R}_B|}{R}, && (12)\\ \phi &\equiv \arctan y/x. && (13) \end{aligned}$$

Thus $u$ is the scaled sum of the distances to the two protons, $v$ is the scaled difference of the two distances and $\phi$ is the usual azimuthal angle with respect to the axis defined by the two protons. Some Jacobian manipulations would reveal,

$$\int d^3r f(\mathbf{r}) = \int_1^\infty du \int_{-1}^1 dv \int_0^{2\pi} d\phi \frac{R^3}{8}(u^2 - v^2) f(\mathbf{r}). \tag{14}$$

Once one has made a transformation into these coordinates the integral becomes rather trivial since

$$\psi_A(\mathbf{r})\psi_B(\mathbf{r}) = (\pi a_0^3)^{-1} e^{-uR/a_0} \tag{15}$$

If you have not worked with elliptic coordinates before, you can understand the name "elliptical" since the set of points with a fixed sum of distances, $|\mathbf{r}-\mathbf{R}_A| + |\mathbf{r}-\mathbf{R}_B|$, defines an ellipse.

One is now in the position to calculate the expectation of the energy,

$$\begin{aligned} \langle H \rangle_\pm = \epsilon_\pm(R) &= \frac{\langle A|H|A\rangle + \langle B|H|B\rangle \pm 2\langle A|H|B\rangle}{2 \pm 2S} && (16) \\ &= \frac{\langle A|H|A\rangle \pm \langle A|H|B\rangle}{1 \pm S}, && (17) \end{aligned}$$

where

$$\begin{aligned} \langle A|H|A\rangle &= \epsilon_1 + \frac{e^2}{R} - \int \psi_A^2(\mathbf{r}) \frac{e^2}{|\mathbf{r} - \mathbf{R}_B|} d^3r && (18) \\ &= \epsilon_1 + \frac{e^2}{R}\left(1 + \frac{R}{a_0}\right) e^{-2R/a_0}, && (19) \end{aligned}$$

and

$$\langle A|H|B\rangle = \left(\epsilon_1 + \frac{e^2}{R}\right) S - \int d^3r \psi_A(\mathbf{r}) \psi_B(\mathbf{r}) \frac{e^2}{|\mathbf{r} - \mathbf{R}_B|} \qquad (20)$$

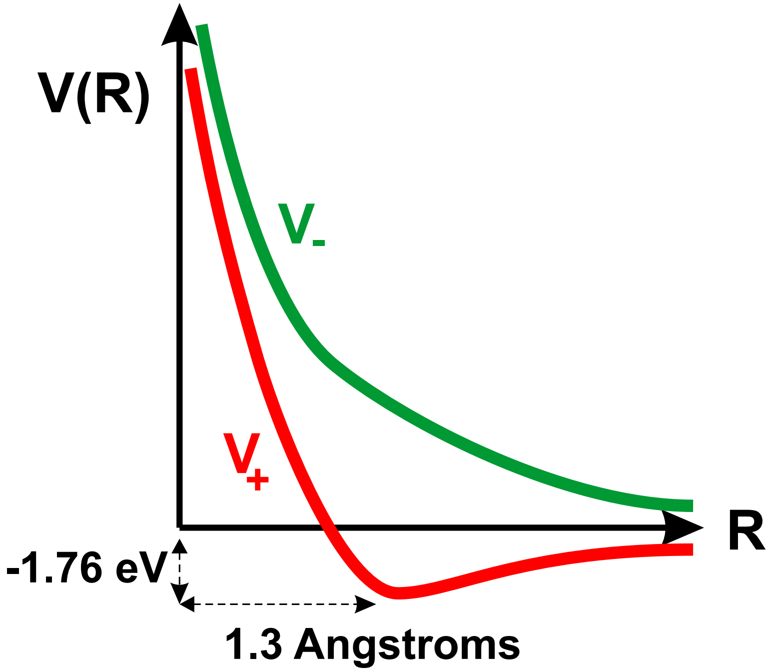
$$= \left(\epsilon_1 + \frac{e^2}{R}\right) S - \frac{e^2}{a_0}\left(1 + \frac{R}{a_0}\right) e^{-R/a_0} \qquad (21)$$

The term $\epsilon_1$ is merely the electronic binding energy of one electron with a proton, -1.0 Rydbergs. The integrals were calculated with the help of the tranformation into elliptic coordinates.

The potential between the atoms is effectively

$$V_\pm(R) = \langle H \rangle_\pm - \epsilon_1. \qquad (22)$$

When plotted against $R$ the resulting curves looks like,



In the adiabatic approximation, where the mass of the proton is considered to be very large, the binding energy should simply be the minimum of the potential. In reality the binding energy is deeper by an entire eV. However, one could improve the calculation by considering a variational calculation with more than zero variational parameters.

The difference between $V_+$ and $V_-$ comes from the fact that the parities of the two wave functions were positive and negative respectfully. The positive-parity solution has lower energy because the probability density is larger in the region between the protons where the interaction with the protons is maximized, and because the negative-parity solution has an extra node, which increases the kinetic energy.

### The Hydrogen Molecule and pairing

The neutral Hydrogen molecule has two electrons. One can pursue a variational calculation as performed in the previous problem; only in this instance the variational wave function is a two-electron wave function. When we discussed multi-electron atoms, Hund's first rule stated that the prime criteria for multielecton states to minimize the energy is to form states of largest $S$ so that the spatial wave function will be maximally antisymmetrized thus minimizing the electron-electron repulsive interaction. However, in the case of the $H_2$ molecule, the driving determination is that both electrons should be in the even-parity $\psi_+$ state, which through the Pauli exclusion principle requires that the electrons be in a spin singlet with $S = 0$.

When two electrons form a spin-singlet they are called a pair. Much of the systematics of molecular binding can be understood by considering pairing. Pairing that involves $p$ states is somewhat more complicated. Of the three $p$ states, the $m_\ell = 0$ state extends along the $z$ axis and thus more strongly samples the attractive interaction with the other proton. Pairing between the $m_\ell = \pm 1$ states can also take place but is usually weaker. The two pairings are refered to as $\sigma$ and $\pi$ bondings. The $\pi$ label refers to the fact that the transverse pairing allows an angular momentum about the molecular axis.

For atoms where $p$ and $s$ states are nearly degenerate, pairing with neighboring atoms can be especially strong. In these cases the wave function can be a linear combination of an $s$ state and a $p$ state with $m_\ell = 0$. Separately, both states have equal weight on the $z$-positive and $z$-negative sides of the atom. However, linear combination of an even-parity and an odd-parity state will result in a wave function with higher probability on one side. Given the presence of a neighboring atom, this can lead to an energetically favorable situation. By taking a linear combination of such a "hybrid" state with a hybrid state using the opposing atom as it's center, one can make states with overall good reflection symmetry about the half-way point between the atoms.

## Cooper Pairs

Pairing of electrons is responsible for the phenomena known as superconductivity. The connection between forming pairs and reducing the conductivity to zero is actually rather tenuous. The formed pairs, which have net negligible momentum, can coalesce and move as a coherent unit through the material.

One could imagine resistance coming from several sources:

1. As we will see, a gap energy will be associated with the pairs. In order for the moving pairs to de-excite one must excite the pairs by at least the gap energy. If one imagines a current moving through a circular loop at a temperature near zero, there is not enough thermal energy available to break a pair.
2. One could imagine a drag force acting on the condensate due to moving the condensate through the liquid of non-condensate particles. The drag force would then behave as

   $$F_{\rm drag} \propto u^2, \quad P \propto u^3 \tag{1}$$

   where $u$ is the condensate velocity. Since the power goes as $u^3$ and the resistance is defined as

   $$P = I^2 R, \ I^2 \propto u^2, \tag{2}$$

   one sees that since the power from drag contributes at a higher power of $u$, drag can be neglected with respect to it's contribution to the resistance if $u$ is small. Since the coalesced pairs move as a unit, they can carry a large current with a very small velocity.

Our goal in this section will not be to understand the correlated structure of the pairs, but only to show that pairs exist as a lower-energy solution than a Fermi gas.

In order for electrons to pair there must exist an attractive interaction between two electrons with momenta near the Fermi surface. The idea of two electrons interacting attractively is most peculiar since electrons have the same charge. The excuse for assuming an attractive interaction is that the electrons interact with one another via the lattice. An electron might interact with an ion, which might then interact with the other electron. Intuitively, one might expect such an interaction to provide an effective polarizability that reduces the electric repulsion, but does not reverse it. However, electrons are not static in a medium and the movement of the electrons, seemingly miraculously, results in an effectively attractive interaction.

For our purposes, we will follow the work of Bardeen, Cooper and Schraefer (BCS) and assume a simplified interaction between electrons,

$$\langle \mathbf{k}_1 \mathbf{k}_2 | \mathcal{V} | \mathbf{k}_1' \mathbf{k}_2' \rangle = \left\{ \begin{array}{cl} -\frac{v_0}{V}\delta_{k_1+k_2,k_1'+k_2'}, & k_f < k_1, k_2, k_1', k_2' < k_a \\ 0, & \text{otherwise} \end{array} \right. \tag{3}$$

where $v_0$ sets the scale of the interaction, $V$ is the volume, and $k_a$ is close to $k_f$. Thus the model assumes the attractive interaction is confined to particles within the neighborhood of the Fermi surface.

Since total momentum is a good quantum number, eigenstates can have the form,

$$|\mathbf{K}\text{ paired}\rangle = \sum_{\mathbf{k}'}{}' a_{\mathbf{k}'}(\mathbf{K})|\mathbf{k}_1' = \mathbf{K}/2+\mathbf{k}', \mathbf{k}_2' = \mathbf{K}/2-\mathbf{k}'\rangle, \tag{4}$$

where the primed sum is over all relative momenta $\mathbf{k}' \equiv (\mathbf{k}_1' - \mathbf{k}_2')/2$ such that both $\mathbf{k}_1'$ and $\mathbf{k}_2'$ are inside the region between $k_f$ and $k_a$.

Solving for the eigenstates,

$$\begin{aligned} \langle \mathbf{k}_1, \mathbf{k}_2|H|\mathbf{K}\text{ paired}\rangle &= \langle \mathbf{k}_1, \mathbf{k}_2|E|\mathbf{K}\text{ paired}\rangle, & (5)\\ -\frac{v_0}{V}\sum_{\mathbf{k}'}{}' a_{\mathbf{k}'}(\mathbf{K}) &= (E - \epsilon_{\mathbf{k}_1} - \epsilon_{\mathbf{k}_2})a_{\mathbf{k}}(\mathbf{K}) & (6)\end{aligned}$$

Summing both sides over $\mathbf{k}$,

$$\sum_{\mathbf{k}}{}' a_{\mathbf{k}}(\mathbf{K}) - \frac{v_0}{V}\sum_{\mathbf{k}}{}' \frac{1}{E - \epsilon_{\mathbf{k}_1} - \epsilon_{\mathbf{k_2}}}\sum_{\mathbf{k}'}{}' a_{\mathbf{k}'}(\mathbf{K}) = 0. \tag{7}$$

Now, one can see how the simplifying assumption that the matrix element $v_{k,i'}$ was independent of $k$ and $k'$ in the subspace simplifies the problem. It allows the sum over amplitudes to be canceled from both sides of the equation above and result in,

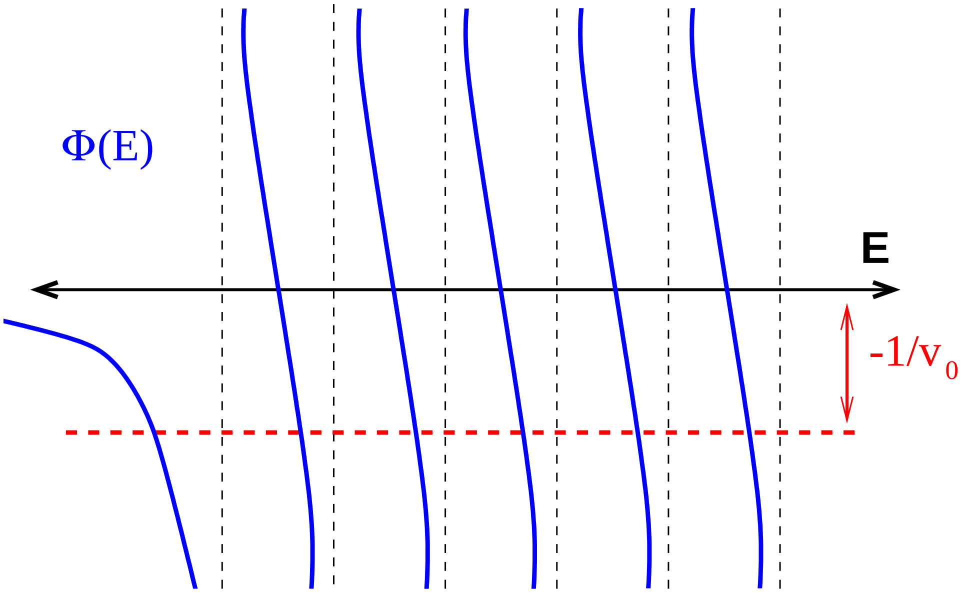
$$\begin{aligned} -\frac{1}{v_0} &= \frac{1}{V}\sum_{\mathbf{k}}{}' \frac{1}{E - \epsilon_{\mathbf{k}_1} - \epsilon_{\mathbf{k}_2}} & (8)\\ &= \frac{1}{V}\sum_{\mathbf{k}}{}' \frac{1}{E - \epsilon_{\mathbf{K}+\mathbf{k}} - \epsilon_{\mathbf{K}-\mathbf{k}}} & (9)\\ &= \frac{1}{V}\sum_{\mathbf{k}}{}' \frac{1}{E - \hbar^2K^2/(4m) - \hbar^2k^2/m}, & (10)\end{aligned}$$

where the last step involved writing the energy as a center-of-mass energy plus an energy-of-relative-motion.

The solutions to the above equation can be found graphically. To illustrate the solutions, we consider the function

$$\Phi_K(E) \equiv \frac{1}{V}\sum_{\mathbf{k}}{}' \frac{1}{E - \hbar^2K^2/m - \hbar^2k^2/(4m)}, \tag{11}$$

and graph the function to see for what energies, $E$, the function $\Phi(E)$ equals $-1/v_0$.



Every time $E$ passes an energy, $\hbar^2K^2/(4m)+\hbar^2k^2/m$, $\Phi$ changes from $-\infty$ to $+\infty$. Thus for every value of $\mathbf{k}$ there exists a solution with $E < \hbar^2K^2/(4m) + \hbar^2k^2/m$ where $\Phi = -1/v_0$. The vertical dashed lines in the figure represent the energies $\hbar^2K^2/(4m) + \hbar^2k^2/m$, which would be the eigen-energies if $v_0$ were to be zero. The intersections of the blue curves with the horizontal dashed line represent the solutions.

If $\mathbf{K} = 0$, the first value of $\mathbf{k}$ that enters the primed sum is $|\mathbf{k}| = k_f$. Thus there exists a solution with energy $E < 2\epsilon_f$, even though the solution was formed from momentum states above $k_f$. Thus the paired is energetically favorable compared to being a momentum state at the Fermi surface. Note that as $v_0$ is increased the solution for the energy becomes lower.

### The Gap

The expression for $\Phi$ in Eq. (11) can be integrated analytically for the case with $K = 0$ if one approximates the sum over states as

$$\sum_{\mathbf{k}}{}' \rightarrow \rho(\epsilon_f) \int_{\epsilon_f}^{\epsilon_a} d\epsilon_k. \tag{12}$$

This amounts to assuming the density of states, $\rho(\epsilon_k)$, is constant in the region of integration. The expression for $\Phi$ then becomes

$$\begin{aligned} \Phi(E) &= \rho(\epsilon_f) \int_{\epsilon_f}^{\epsilon_a} dE_k \frac{1}{E - 2\epsilon_k} && (13) \\ &= -\frac{\rho(2\epsilon_f)}{2} \log\left|\frac{2\epsilon_a - E}{2\epsilon_f - E}\right|, && (14) \end{aligned}$$

where

$$\rho(\epsilon_f) = \frac{mk_f}{2\pi^2\hbar^3}. \tag{15}$$

Solving for $E$,

$$E = \frac{-2\epsilon_a + 2\epsilon_f e^{2/(\rho v_0)}}{e^{2/(\rho v_0)} - 1}. \tag{16}$$

The difference between this energy and $2\epsilon_f$ is known as the gap energy, $\Delta$.

$$\begin{aligned} \Delta &\equiv \frac{2\epsilon_f - E}{2} && (17) \\ &= \frac{\epsilon_a - \epsilon_f}{e^{2/[\rho(\epsilon_f)v_0]} - 1}. && (18) \end{aligned}$$

One can do a similar calculation for $K \neq 0$, but the binding energy would be smaller since the interaction links fewer pairs as both electrons in the pair, with momenta $k_\pm = K/2 \pm k$, must lie within the shell in momentum space.

One can see that the energy required to break the pair is $2\Delta$, because in order to break the pair one must move the electrons outside the Fermi sea, that is, increase their energy beyond $2\epsilon_f$.

**Wave Functions**

The relative wave function can be found by Fourier transforming the wave function in coordinate space. For $\mathbf{K} = 0$, the relative wave functions, as seen from Eq. (6) in momentum and coordinate space are:

$$\begin{aligned} \langle \mathbf{K} = \mathbf{0}, \mathbf{k} | \phi \rangle &= a_{\mathbf{k}}(\mathbf{K} = \mathbf{0}) \sim \frac{1}{E - 2\epsilon_k} && (19) \\ \langle \mathbf{r} | \phi \rangle &\sim \int' d^3k \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{E - 2\epsilon_k} && (20) \\ &= \frac{4\pi}{r} \int_{k_f}^{k_a} kdk \frac{\sin(kr)}{E - 2\epsilon_k} && (21) \end{aligned}$$

This integral results in rather obtuse combinations of cosine-integral and sine-integral functions. One can expand the result and see that for large $r$,

$$\langle \mathbf{r} | \phi \rangle |_{r\to\infty} \sim \frac{\cos k_f r - \cos k_a r}{r^2}. \qquad (22)$$

As a homework problem, you are to show that this is square-integrable, but that $\langle r^2 \rangle = \infty$.

Since $\langle r^2 \rangle = \infty$, one should use a different criteria for finding the effective size. One such criteria is to find the square of the wave function at zero.

$$|\Psi(r = 0)|^2 = \frac{\left| \int' d^3k \frac{1}{E - 2\epsilon_k} \right|^2}{\int d^3r \left| \int' d^3k \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{E - 2\epsilon_k} \right|^2} \qquad (23)$$

One can define an effective radius that corresponds to a sphere that would give the equivalent density at $r = 0$.

$$\frac{1}{4\pi R_{\text{eff.}}^3/3} \equiv |\Psi(r = 0)|^2. \qquad (24)$$

The resulting effective radius is a complicated function of the reduced mass, the Fermi energy, $\epsilon_a$ and the gap $\Delta$. For larger gaps, one finds smaller radii.

### Superconductivity

As mentioned at the beginning of this lecture, the pairs move as a coherent unit through the material. Acting as a unit derives from the fact that once they are paired they act as bosons. Thus many pairs can occupy the same state as long as the density of pairs does not exceed $1/R^3$ where $R$ is the size of a pair. Since the density of pairs is saturated, the pairs interact strongly with one another and thus move as a unit.

Current can dissipate through two mechanisms. First, the entire coherent unit could slow due to drag forces. However, the drag is negligible due to the small velocity of the charge. Secondly, pairs could be broken off from the larger coherent unit where they would then scatter and no longer contribute to the current. This is small because the pairs have saturated and there is no phase space into which to scatter the pair. In fact the best way to remove a pair from the coherent unit is to break a pair which requires an energy of $2\Delta$. The resistance then behaves proportional to $e^{-2\Delta/T}$. Since the temperatures are much lower than $\Delta$, currents can remain moving for long periods of time even after the driving voltage is turned off.

## Landau Levels and the Integral Quantum Hall Effect

Consider particles of mass $m$ and charge $e$ moving in a two-dimensional world, the x-y plane. A magnetic field is present, $\mathbf{B} = B\hat{z}$. The Hamiltonian for such particles is

$$H = (\mathbf{p} - e\mathbf{A}/c)^2 /(2m). \tag{1}$$

If one chooses as a vector potential,

$$\mathbf{A} = Bx\hat{y}, \tag{2}$$

one obtains the desired magnetic field. Since there is no $y$ dependence in the Hamiltonian, solutions can be chosen as eigenstates of the operator $P_y$ with eigenvalue $p_y$. One can then rewrite the Hamiltonian,

$$H = \frac{P_x^2}{2m} + \frac{(p_y - eBx/c)^2}{2m}, \tag{3}$$

where $p_y$ is simply a number and $P_x$ is an operator. Since $p_y$ is a number, one can consider the second term an offset harmonic oscillator potential,

$$\begin{aligned} H &= \frac{P_x^2}{2m} + \frac{1}{2}m\omega^2\left(x - \frac{p_y c}{eB}\right)^2, & (4)\\ \omega &\equiv \frac{eB}{mc}. & (5) \end{aligned}$$

Thus, the Hamiltonian looks like a one-dimensional Harmonic oscillator with a frequency equal to the Larmor frequency. The harmonic oscillator is centered at $x = p_y c/(eB)$.

Note that the eigen-energies, $(n + 1/2)\hbar\omega$, do not depend on $p_y$. Thus, there are many solutions with different $p_y$ that have identical energies. The energy levels are referred to as Landau levels.

Each level has a degeneracy equal to the number of values of $p_y$ for which there exist solutions. The density of such states is

$$\frac{dN}{dp_y} = \frac{L_y}{2\pi\hbar}, \tag{6}$$

where $L_y$ is the size of the sample in the $y$ direction. The limits on $p_y$ are determined by the $x$ dimension. Since $p_y$ is related to the offset of the center of the Harmonic oscillator in the $x$ direction,

$$0 < \frac{p_y c}{eB} < L_x. \tag{7}$$

Thus the number of such states is

$$N = \frac{eBL_yL_x}{2\pi\hbar c}. \tag{8}$$

Assume the sample has a number of free electrons per unit area $n$. If the number of free electrons exactly fits an integer number of Landau levels, the levels will be exactly filled and the conductance will be relatively small. Thus varying the magnetic field one sees conductance minima for

$$m = \frac{2\pi\hbar c n}{eB} = \text{integers}. \tag{9}$$

This is known as the integer quantum Hall effect. It corresponds to an integral number of levels being exactly filled.

The fractional quantum Hall effect refers to conductance minima for fractional, e.g. one third, values of $m$. This is much more difficult to explain, but is related to the sharing of electrons between adjacent orbitals, similar to the sharing of electrons in the covalent bonds in solids.

### Adding an Electric Field

Consider the same problem as above, only with an electric field $E$ pointing along the $y$-axis. The electric and magnetic fields can then be generated with the vector potential,

$$\mathbf{A} = Bx\hat{y} + Et \tag{10}$$

One can then rewrite the Schrödinger equation

$$\begin{aligned} H &= \frac{P_x^2}{2m} + \frac{(p_y - eBx/c - eEt)^2}{2m} \\ &= \frac{P_x^2}{2m} + \frac{1}{2}m\omega^2\left(x - x_0 - v_0 t\right)^2 \\ x_0 &= p_y c/eB \\ v_0 &= -cE/B \end{aligned}$$

The solution to this equation, $H\phi(x,t) = i\hbar\partial/\partial t\phi(x,t)$, can be written as a product of the the solution for a static harmonic oscillator with a phase factor responsible for the momentum,

$$\phi(x,t) \propto e^{-(x-x_0-v_0t)^2/(2a^2)} e^{imv_0x/\hbar} e^{-iEt/\hbar}. \tag{11}$$

Here $a^2 = \hbar/(m\omega)$, and $E = \hbar\omega/2 + mv_0^2/2$. This solution can be simply interpreted as a static solution moving with velocity $v = cE/B$. Note that the electric field was in the $y$ direction, but the velocity is along the $x$ direction.

This peculiar result can be understood in terms of the Lorentz transformation properties of tehe $\mathbf{E}$ and $\mathbf{B}$ field. Under the transformation,

$$E_y \to \gamma\left(E_y - \frac{v_x}{c}B_z\right). \tag{12}$$

Thus by moving to a frame with velocity $v_x = cE_y/B_z$ one would not observe electric fields and the solutions would be stationary, in agreement with the above result – which had no relativistic assumptions!

Lecture 36, February 7, 2001

---

## The Klein-Gordon Equation

In relativistic kinematics energy and momentum appear on an equal footing, as do postion and time. For instance,

$$E^2 - p^2c^2 = m^2c^4. \tag{1}$$

Rewriting energy and momentum as operators, one obtains the Klein-Gordon equation,

$$\left(-\hbar^2 \frac{\partial^2}{\partial t^2} + \hbar^2 c^2 \nabla^2 - m^2 c^4\right) \psi(\mathbf{r}, t) = 0 \tag{2}$$

It differs from the Schrödinger equation in that the time appears as the second derivative.

The Klein-Gordon equation has plane wave solutions,

$$\begin{aligned} \psi_{\mathbf{p}}(\mathbf{r}) &\sim e^{i\mathbf{p}\cdot\mathbf{r}/\hbar - iE_\pm(p)t/\hbar}, & (3) \\ E_\pm(p) &= \pm\sqrt{p^2c^2 + m^2c^4} & (4) \end{aligned}$$

If one expands the energy for small $p$,

$$E_+(p) \approx mc^2 + p^2/2m. \tag{5}$$

Thus, in the non-relatistic limit, the energy appears identical to the that of the Schrödinger equation aside from the inclusion of the rest mass energy. If mass were conserved this would merely add a constant to the energy along with an unobservable phase, $e^{iMc^2t/\hbar}$. However, for cases where particles are generated, the phase can play an important role.

Perhaps the most unusual feature in the solutions is the appearance of negative-energy solutions. The negative-energy solutions can only be understood when one writes field operators in second quantization. The field operators (remember the case for photons) will then be written as

$$\begin{aligned} \Phi(\mathbf{r}, t) &= \sqrt{\frac{\hbar c}{V}} \sum_p \frac{1}{\sqrt{E_p}} \left(e^{ip\cdot r/\hbar} b_{\mathbf{p}}^\dagger + e^{-ip\cdot r/\hbar} a_{\mathbf{p}}\right) & (6) \\ &= \sqrt{\frac{\hbar c}{V}} \sum_p \frac{1}{\sqrt{E_p}} e^{-i\mathbf{p}\cdot\mathbf{r}/\hbar} \left(e^{iEt/\hbar} b_{\mathbf{p}}^\dagger + e^{-iEt/\hbar} a_{-\mathbf{p}}\right). & (7) \end{aligned}$$

where $p \cdot r \equiv E_p t - \mathbf{p} \cdot \mathbf{r}$. Thus, in the language of field operators, the negative-energy solution is associated with the destruction of antiparticles moving with opposite momentum. We note that if the field were a real field, rather than a complex field, $b^\dagger$ would be replaced by $a^\dagger$. It only seems natural that a relativistic theory should require the consideration of field operators to make sense, since the creation and destruction of particles is an intimate element of relativistic treatments.

Remembering the expression for non-relativistic field operators,

$$\begin{aligned} \Psi(\mathbf{r}, t) &= \frac{1}{\sqrt{V}} \sum_k e^{-iE_k t + i\mathbf{k}\cdot\mathbf{r}} a_{\mathbf{k}} & (8) \\ \Psi^\dagger(\mathbf{r}, t) &= \frac{1}{\sqrt{V}} \sum_k e^{iE_k t - i\mathbf{k}\cdot\mathbf{r}} a_{\mathbf{k}}^\dagger & (9) \end{aligned}$$

If the field operators referred to electrons, one can think of $\Psi^\dagger(\mathbf{r})$ as creating a negative particle at $\mathbf{r}$, while $\Psi(\mathbf{r})$ would destroy a negative particle. With relativistic fields, the operator that creates a negative particle also has a piece that destroys the positive antiparticle. This can be considered a particle-antiparticle symmetry that derives from the existence of negative-energy solutions. The same symmetry will result from the Dirac equation, which is the topic of the next lecture.

### Current conservation

The current density should have the form of a relativistic four-vector. Furthermore, the current density should be conserved,

$$\partial_\mu j^\mu(\mathbf{r},t) = 0. \tag{10}$$

Non-relativistically, the charge density $j^0$ appeared in the form

$$\rho = \psi^*(\mathbf{r},t)\psi(\mathbf{r},t), \tag{11}$$

while the current density had the form

$$\vec{j}(\mathbf{r},t) = \frac{-i\hbar}{2m}\left(\psi^*(\mathbf{r},t)\vec{\partial}\psi(\mathbf{r},t) - \vec{\partial}\psi^*(\mathbf{r},t)\psi(\mathbf{r},t)\right). \tag{12}$$

This clearly violates the relativistic spirit where the time and space components of a four vector should appear with similar forms.

As an ansatz, we guess a form for the current density,

$$\begin{aligned} j^0(\mathbf{r},t) &= \frac{-i}{2c}\left(\phi^*(\mathbf{r},t)\frac{\partial}{\partial t}\phi(\mathbf{r},t) - \frac{\partial}{\partial t}\phi^*(\mathbf{r},t)\phi(\mathbf{r},t)\right) && (13)\\ \vec{j}(\mathbf{r},t) &= \frac{-ic}{2}\left(\phi^*(\mathbf{r},t)\vec{\partial}\phi(\mathbf{r},t) - \vec{\partial}\phi^*(\mathbf{r},t)\phi(\mathbf{r},t)\right). && (14)\end{aligned}$$

It is now straight-forward to see that

$$\partial_\mu j^\mu(\mathbf{r},t) = 0, \tag{15}$$

by taking the four divergence of $j^\mu$ and then applying the Klein-Gordon equation.

Furthermore, one can see that the look at the form of $j^\mu$ in terms of field operators. One then obtains, after integrating over space,

$$\begin{aligned} \int d^3r\; j^0(\mathbf{r},t) &= \sum_p \left(a^\dagger_{\mathbf{p}} a_{\mathbf{p}} - b_{\mathbf{p}} b^\dagger_{\mathbf{p}}\right) && (16)\\ \int d^3r\; \vec{j}(\mathbf{r},t) &= \sum_p \frac{c^2\mathbf{p}}{E_p}\left(a^\dagger_{\mathbf{p}} a_{\mathbf{p}} - b_{\mathbf{p}} b^\dagger_{\mathbf{p}}\right) && (17)\end{aligned}$$

Of course, one would also multiply by the charge $e$ to get a charge density or current density, but the velocity does come in with the correct factor $c^2\mathbf{p}/E_p$, and the particles and antiparticles do come in with opposite signs.

A peculiar aspect of the expression is that the contribution from the antiparticles comes in with the creation and destruction operators reversed. This implies that an extra charge of -1 is associated with each momentum mode after making the substitution,

$$a^\dagger a - bb^\dagger = a^\dagger a - b^\dagger b - 1. \tag{18}$$

This suggests that the vacuum has a charge of -1 associated with each mode, which translates into an infinite negative charge since there are an infinite number of modes. If one wrote down an expression for the Hamiltonian in terms of field operators one would find,

$$\begin{aligned} H &= \sum_p E_p \left( a^\dagger_{\mathbf{p}} a_{\mathbf{p}} + b_{\mathbf{p}} b^\dagger_{\mathbf{p}} \right) & (19)\\ &= \sum_p E_p \left( a^\dagger_{\mathbf{p}} a_{\mathbf{p}} + b^\dagger_{\mathbf{p}} b_{\mathbf{p}} + 1 \right). & (20) \end{aligned}$$

Thus the vacuum also has an infinite positve energy associated with it. When we consider the Dirac equation, which is applicable for Fermions, the same problem will appear, but with opposite signs. That is, the energy of the vaccum will be $-E_p$ for each mode. This result serves as one of the motivations for super symmetry, where every bosonic mode has a corresponding Fermionic mode.

### Coupling to the electromagnetic field

In the Schrödinger equation, incorporating the electromagnetic field could be accomplished by minimal substition,

$$\begin{aligned} -i\hbar\vec{\partial} &\rightarrow -i\hbar\vec{\partial} + e\vec{A}/c & (21)\\ i\hbar\frac{\partial}{\partial t} &\rightarrow i\hbar\frac{\partial}{\partial t} - e\Phi, & (22) \end{aligned}$$

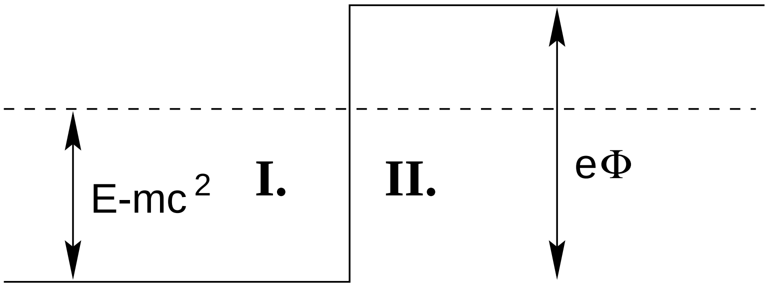
where $\Phi$ is the "scalar" field. However, in relativistic electromagnetism, $\Phi$ is the zeroth component of the four vector $A^\mu$.

In relativistic treatments, coupling to the electromagnetic field is also incorporated with the same minimal substitution. One result of coupling to an electromagnetic field is that the charge and current densities are modified,

$$\begin{aligned} j^0(\mathbf{r},t) &= \frac{-i}{2c}\left(\phi^*(\mathbf{r},t)\frac{\partial}{\partial t}\phi(\mathbf{r},t) - \frac{\partial}{\partial t}\phi^*(\mathbf{r},t)\phi(\mathbf{r},t)\right) - \frac{e\Phi(\mathbf{r},t)}{\hbar c}\phi^*(\mathbf{r},t)\phi(\mathbf{r},t) & (23)\\ \vec{j}(\mathbf{r},t) &= \frac{-ic}{2}\left(\phi^*(\mathbf{r},t)\vec{\partial}\phi(\mathbf{r},t) - \vec{\partial}\phi^*(\mathbf{r},t)\phi(\mathbf{r},t)\right) + \frac{e\vec{A}}{\hbar}\phi^*(\mathbf{r},t)\phi(\mathbf{r},t). & (24) \end{aligned}$$

### Reflection off a potential step

A seemingly simple example that becomes surprisingly difficult is the reflection off a potential step, where the potential step is due to jump in $A_0$. Consider the one-dimensional problem,



$$\Phi(x) = \begin{matrix} 0, & x < 0 \\ \Phi, & x > 0 \end{matrix} \tag{25}$$

Consider a wave incident from the left, with a reflected and transmitted wave,

$$\psi_I(x) = e^{ikx} - Be^{-ikx} \tag{26}$$

$$\psi_{II}(x) = Ce^{ik'x}, \tag{27}$$

where the energy of the particle is

$$E = \sqrt{\hbar^2 k^2 c^2 + m^2 c^4}. \tag{28}$$

Before solving for $B$ and $C$, one must find $k'$. Applying the Klein-Gordon equation,

$$(E - e\Phi)^2 = \hbar^2 k'^2 c^2 + m^2 c^4, \tag{29}$$

one may find the limits for $k'^2$ being positive or negative.

$$k'^2 > 0 \quad \text{when } 0 < \Phi < E - mc^2, \tag{30}$$

$$k'^2 < 0 \quad \text{when } E - m < \Phi < E + mc^2, \tag{31}$$

$$k'^2 > 0 \quad \text{when } \Phi > E + mc^2. \tag{32}$$

The first two regions for $\Phi$ correspond to the usual case for non-relativistic physics. That is, when the barrier is small the particle penetrates with a reduced velocity. For larger barriers, the particle is confined to region I and the wave function exponentially dies in region II.

However, the surprise here is that for very large $\Phi$, there again appears to be a solution with the particle moving through the barrier. This surprising result can be understood by calculating the charge and current densities in region II. One finds that the charge density in region II is opposite to that of region I. The solution describes an incoming wave that splits into two outgoing waves, one of particles moving to the left and one of antiparticles moving to the right. This behavior owes itself to the large field. When the voltage difference exceeds twice the mass, it becomes possible to create pairs of particles. Since the antiparticle feels a potential of $-e\Phi$, it is perfectly willing to go to into region II, and many do so spontaneously if the step has enough energy to overcome the mass penalty, $2mc^2$. This behavior does not exist should one consider a problem where the regions have different masses rather than different $A^0$s.

## The Dirac Equation

The Dirac is another example of a relativistic wave equation. However, the Dirac equation differs in that it describes spin 1/2 particles whereas the Klein-Gordon equation works for spinless particles.

Dirac was motivated by finding a linear equation that was consistend with the relativistic constraint $H^2 = P^2c^2 + m^2c^4$. By linear, Dirac was looking for and equation that was linear in the derivatives. In order to accomplish this Dirac needed to use a matrix equation,

$$H = \alpha_x cP_x + \alpha_y cP_y + \alpha_z cP_z + \beta mc^2, \tag{1}$$

where $\alpha_i$ and $\beta$ are matrices. Given that one needs to satisfy our knowledge of relativity,

$$H^2 = p^2c^2 + m^2c^4, \tag{2}$$

there are constraints on the matrices,

$$\{\alpha_i, \alpha_j\} = 2\delta_{ij}, \beta^2 = 1, \{\alpha_i, \beta\} = 0. \tag{3}$$

Two-by-two matrices are insufficient, as one can only come up with three anticommuting matrices (the Pauli matrices), but one needs four. Three-by-three matrices are also insufficient, but four-by-four matrices are sufficient. The following four-by-four matrices satisfy the equations.

$$\vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \tag{4}$$

Actually, there exist an infinite number of choices as one can transform the matrices by a unitary tranformation,

$$U\vec{\alpha}U^\dagger, \tag{5}$$

and find a new choice of matrices. The choice above is known as the Dirac representation, which is convenient for massive particles. For highly relativistic particles, it is sometimes convenient to employ the chiral representation,

$$\vec{\alpha} = \begin{pmatrix} \vec{\sigma} & 0 \\ 0 & -\vec{\sigma} \end{pmatrix}, \quad \beta = -\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \tag{6}$$

We will confine our discussions to the Dirac representation.

It should be stressed that the four components of the wave function are not a relativistic four vector. They correspond to spin-up, spin-down, and the two corresponding anti-particle solutions. Like any wave function, the components of the wave functions mean nothing physically. Only expectations have a physical meaning. By changing the arbitrarily chosen representation, the solutions are changed.

## Conserved Quantities

The particle current,

$$j_0(\mathbf{r},t) \equiv \psi^\dagger(\mathbf{r},t)\psi(\mathbf{r},t), \quad \vec{j}(\mathbf{r},t) \equiv c\psi^\dagger(\mathbf{r},t)\vec{\alpha}\psi(\mathbf{r},t), \tag{7}$$

is conserved. One can demonstrate the conservation of the current by taking the four divergence, $\partial_\mu j^\mu$, and by applying the Dirac equation,

$$\begin{aligned} \frac{\partial}{\partial t}\psi + c\vec{\alpha}\cdot\vec{\nabla}\psi &= i\frac{mc^2}{\hbar}\psi, & (8)\\ \frac{\partial}{\partial t}\psi^\dagger + c\vec{\alpha}\cdot\vec{\nabla}\psi^\dagger &= -i\frac{mc^2}{\hbar}\psi^\dagger, & (9)\end{aligned}$$

to see that

$$\frac{\partial}{\partial t}j_0 + \nabla\cdot\mathbf{j} = 0. \tag{10}$$

Now, we consider conservation of angular momentum. Unlike the Schrödinger equation, the Dirac Hamiltonian does not commute with the orbital angular momentum.

$$[H, \vec{r}\times\vec{p}] = -i\hbar\vec{\alpha}\times\vec{p}. \tag{11}$$

One can also define a spin operator, $S = \hbar\vec{\Sigma}/2$, where

$$\begin{aligned} \Sigma_i &= -\frac{i}{2}\epsilon_{ijk}\alpha_i\alpha_j & (12)\\ \vec{\Sigma} &= \begin{pmatrix} \vec{\sigma} & 0 \\ 0 & \vec{\sigma} \end{pmatrix}, & (13)\end{aligned}$$

The spin is also not conserved.

$$\begin{aligned} [H, S_i] &= \sum_j \frac{\hbar p_j}{2}[\alpha_j, \Sigma_i] & (14)\\ &= \sum_{jkl} \frac{-i\hbar p_j}{4}\epsilon_{ikl}[\alpha_i, \alpha_k\alpha_l] & (15)\\ &= \sum_{jk} \frac{-i\hbar p_j}{2}\left(\epsilon_{ijk}\alpha_k - \epsilon_{ikj}\alpha_k\right) & (16)\\ &= i\hbar\sum_{jk}\epsilon_{ijk}\alpha_j p_k. & (17)\end{aligned}$$

Thus, the combination $\vec{J} = \vec{r}\times\vec{p} + \vec{S}$ is conserved.

$$[H, \vec{J}] = 0. \tag{18}$$

### Solutions for free particles

Analogously to the Klein-Gordon equation, the Dirac equation will have both positive-energy and negative-energy solutions. The positive-energy solutions with a given momentum, $\vec{p}$, are referred to as $u_s(\vec{p})$ while the negative-energy solutions are referred to as $v_s(\vec{p})$. The label $s$ refers to the spin.

$$\begin{aligned} E_p u(\vec{p}) &= \vec{\alpha}\cdot\vec{p}cu(\vec{p}) + \beta mc^2 u(\vec{p}) && (19) \\ -E_p v(\vec{p}) &= \vec{\alpha}\cdot\vec{p}cv(-\vec{p}) + \beta mc^2 v(-\vec{p}). && (20) \end{aligned}$$

The momentum labels on the negative-energy solutions were labeled with the opposite momenta since they would correspond to the destruction of anti-particles with momentum $-\vec{p}$ rather than the creation of particles of momentum $\vec{p}$.

To find the solutions, first find the solutions for $p = 0$. The solutions are then

$$u_\uparrow(p=0) = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \tag{21}$$

$$u_\downarrow(p=0) = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \tag{22}$$

$$v_\downarrow(p=0) = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \tag{23}$$

$$v_\uparrow(p=0) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \tag{24}$$

Note that the solutions $v$ are labeled with a spin index opposite to the eigenvalue of $\vec{\Sigma}$. Again, this is because the solution will correspond to the destruction of an antiparticle.

It is easy to check that these solutions are eigenstates of the Dirac equation with eigenvalues $\pm mc^2$.

Finding solutions for non-zero momentum can be accomplished by multiplying the zero-momentum solutions by the operator $mc^2\beta + \vec{\alpha}\cdot\vec{p}c \pm E_p$. This results in a solution to the Dirac equation because

$$(E - \vec{\alpha}\cdot\vec{p}c - \beta mc^2)(E + \vec{\alpha}\cdot\vec{p}c - \beta mc^2) = 0. \tag{25}$$

Thus we define the solution $u_s(\vec{p})$ to be

$$u_s(\vec{p}) = \frac{E_p + \vec{\alpha}\cdot\vec{p}c + \beta mc^2}{\sqrt{2mc^2(mc^2 + E_p)}} u_s(p=0), \tag{26}$$

which will also be a solution to the Dirac equation.

$$(E - \vec{\alpha}\cdot\vec{p}c - \beta mc^2)u(\vec{p}) = 0. \tag{27}$$

The square root in the denominator was chosen to result in the normalization

$$u_s^\dagger(p)u_s(p) = E_p/m. \tag{28}$$

The choice of normalization is motivated by the fact that $u^\dagger u$ turns out to be related to the zeroth component of the current, which must transform like the zeroth part of a four vector $(E, \vec{p}c)/m$.

As an example, we find $u_\uparrow(\vec{p})$ where $\vec{p}$ is along the $z$ axis. For instance,

$$\begin{aligned} u_\uparrow(p_z) &= \frac{1}{\sqrt{2mc^2(E_p+mc^2)}} \begin{pmatrix} E_p+mc^2 & 0 & p_zc & 0 \\ 0 & E_p+mc^2 & 0 & -p_zc \\ p_zc & 0 & E_p-mc^2 & 0 \\ 0 & -p_zc & 0 & E_p-mc^2 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} & (29) \\ &= \frac{1}{\sqrt{2mc^2(E_p+mc^2)}} \begin{pmatrix} E_p+mc^2 \\ 0 \\ p_zc \\ 0 \end{pmatrix} & (30) \end{aligned}$$

Thus, one can see that at non-zero momentum, the positive-energy solutions have a mixture of upper (top two) and lower (bottom two) components.

### Non-relativistic limit and the $g$ factor

Interaction with the electromagnetic field can be accommodated by replacing $\vec{p}$ with $\vec{p}-e\vec{A}/c$ and $i\hbar\partial/\partial t$ with $i\hbar\partial/\partial t - e\Phi$, where $\Phi$ is the electric potential.

Using the Dirac representation, one can write the four components in terms of two two-component vectors $\phi$ and $\chi$, where $\phi$ and $\chi$ refer to the upper/lower components.

$$\psi = \begin{pmatrix} \phi \\ \chi \end{pmatrix}. \tag{31}$$

One can now write the Dirac equation as two equations for $\phi$ and $\chi$.

$$\begin{aligned} i\hbar\frac{\partial\phi}{\partial t} &= c\left(\frac{\hbar}{i}\nabla - \frac{e}{c}\mathbf{A}\right)\cdot\vec{\sigma}\chi + (e\Phi + mc^2)\phi & (32) \\ i\hbar\frac{\partial\chi}{\partial t} &= c\left(\frac{\hbar}{i}\nabla - \frac{e}{c}\mathbf{A}\right)\cdot\vec{\sigma}\phi + (e\Phi - mc^2)\chi & (33) \end{aligned}$$

In the non-relativistic limit the lower components will be small, and one can make the replacement

$$i\hbar\frac{\partial}{\partial t}\chi = mc^2\chi + \cdots, \tag{34}$$

which results in a simple substition for $\chi$ using Eq. (33).

$$2mc^2\chi \approx c\left(\frac{\hbar}{i}\nabla - \frac{e}{c}\mathbf{A}\right)\cdot\vec{\sigma}\phi. \tag{35}$$

Substituting this expression into Eq. (32),

$$i\hbar\frac{\partial}{\partial t}\phi = \frac{1}{2m}\left[\left(\frac{\hbar}{i}\nabla - \frac{e}{c}\mathbf{A}\right)\cdot\vec{\sigma}\right]^2 \phi + (e\Phi + mc^2)\phi. \tag{36}$$

If the gradient and vector potential operator commuted with one another, one would use the anticommutation relations to obtain the usual kinetic energy piece in the Schrödinger equation from squaring the $\mathbf{p} - e\mathbf{A}/c$ term and employing the anticommutation relation. However, taking account of such terms yields an extra piece.

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\phi &= \frac{1}{2m}\left[\left(\frac{\hbar}{i}\nabla - \frac{e}{c}\mathbf{A}\right)\right]^2 \phi + (e\Phi + mc^2)\phi + \frac{\hbar}{2mi}\sum_{i\neq j}\sigma_i\sigma_j(\partial_i A_j + A_i\partial_j)\phi & (37)\\ &= \frac{1}{2m}\left[\left(\frac{\hbar}{i}\nabla - \frac{e}{c}\mathbf{A}\right)\right]^2 \phi + (e\Phi + mc^2)\phi - \frac{e\hbar}{2mc}\vec{\Sigma}\cdot\vec{B}\phi. & (38)\end{aligned}$$

Since $\hbar\vec{\Sigma} = 2\vec{S}$, the last term explains why the $g$ factor of the electron is 2. Previously, this had been inserted by hand. However, the Dirac equation requires that the $g$ factor be exactly two. Note that the $g$ factor of the proton and neutron are not equal to two, because they are composite particles.

The only difference between the expression above and the usual Schrödinger equation is in the additional term $mc^2$. However, this merely adds a constant to the energy as long as mass is conserved, and does not affect any observable in the non-relativistic limit.

### The spin-orbit interaction

One can make a rigorous expansion of Eq.s (32) and (33) by iterating Eq. (33),

$$\begin{aligned} \chi &= \frac{1}{2mc}\left(\frac{\hbar}{i}\nabla - \frac{e}{c}\mathbf{A}\right)\cdot\vec{\sigma}\phi - \frac{1}{2mc^2}\left(i\hbar\frac{\partial}{\partial t} - mc^2 - e\Phi\right)\chi & (39)\\ &= \frac{1}{2mc}\left(\frac{\hbar}{i}\nabla - \frac{e}{c}\mathbf{A}\right)\cdot\vec{\sigma}\phi - \frac{1}{2mc^2}\left(i\hbar\frac{\partial}{\partial t} - mc^2 - e\Phi\right) & (40)\\ &\qquad \left\{\frac{1}{2mc}\left(\frac{\hbar}{i}\nabla - \frac{e}{c}\mathbf{A}\right)\cdot\vec{\sigma}\phi \quad - \frac{1}{2mc^2}\left(i\hbar\frac{\partial}{\partial t} - mc^2 - e\Phi\right)\chi\right\}. & (41)\end{aligned}$$

One can repeat the iterative substitution and find an expression for $\chi$ to arbitrary power in $1/m$. Once a satisfactory level for $\chi$ has been found, it may be substituted into Eq. (32) to obtain a wave equation for $\phi$.

If one pursues the expansion one step beyond what was done previously with the magnetic field to find the $g$ factor of the electron, one finds (with a substantial amount of work) that the approximate Hamiltonian for the upper components $\phi$ has the extra terms,

$$\delta H = -\left[\frac{p^4}{8m^3c^2} + \frac{e\hbar}{4m^2c^2}\vec{\sigma}\cdot(\vec{E}\times\vec{p})\right]. \tag{42}$$

The first term is merely the next-order expansion of $E = \sqrt{p^2c^2 + m^2c^4}$, while the second term is the spin-orbit term. To show that the second term is the spin-orbit term, we note that

$$\vec{E} \times \vec{p} = \frac{E(r)}{r} \vec{r} \times \vec{p}, \tag{43}$$

for a radial electric field $\vec{E}$.

Finally, it is noted that one may go through the same exercise without any electromagnetic field, but instead with a position dependent mass $m(r)$. One then finds that the spin-orbit term looks identical except that

$$\vec{E} \to \frac{\partial m(r)}{\partial r}. \tag{44}$$

This has the opposite contribution for an attractive interaction. This is important for understanding nuclear physics where the spin-orbit interaction is surprisingly large. It can be explained by an attractive scalar interaction (like a position dependent mass) and a repulsive vector interaction (similar to a Hydrogen atom, but with opposite sign). The interactions cancel each other out to a large degree as far as the binding energies are concerned but the contributions from the spin-orbit terms add together.

The Dirac equation is one of the great triumphs of twentieth century physics. Motivated by aeshtetic considerations, several previously ad-hoc assumptions fall out naturally: the $g$ factor, particle-antiparticle symmetry, the spin-orbit coupling, etc. When combined with the relativistic coupling to the quantum electromagnetic field, incredibly accurate calculations can be made of $g-2$ using perturbation theory. But, this is the material for another course.

### More notation – $\gamma$ matrices

To more clearly demonstrate the covariant nature of the equations, it is common to define the Dirac $\gamma$ matrices.

$$\gamma^0 \equiv \beta, \quad \vec{\gamma} \equiv \beta\vec{\alpha}. \tag{45}$$

The three space-like $\gamma$ matrices are anti-Hermitian, while $\gamma^0$ is Hermitian. The convenient covariant behavior of the $\gamma$ matrices comes from the property,

$$\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu}, \tag{46}$$

where $g^{\mu\nu}$ is the metric tensor

$$g^{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}. \tag{47}$$

This property means that the $\gamma$ matrices transform like four vectors.

A very common notation is

$$\not{p} \equiv p^\mu \gamma_\mu, \tag{48}$$

which means that the Dirac equation (multiplied by $\gamma_0$) can be expressed as

$$(\not{p} + m)\psi = m\psi. \tag{49}$$

This has the attraction that $\not{p}$ is a scalar.

One can write the current as

$$j^\mu = \bar{\psi}\gamma^\mu\psi, \tag{50}$$

where

$$\bar{\psi} \equiv \psi^*\gamma_0. \tag{51}$$

This seems a bit peculiar, but $\bar{\psi}\psi$ is a scalar rather than $\psi^*\psi$ which transforms like the zeroth component of the four current.

To more rigorously see the Lorentz structure of all the terms and more consistently derive the expressions for the currents, it is best to start with the Lagrangian density,

$$\mathcal{L} = \bar{\psi}(\not{p} + m)\psi, \tag{52}$$

then use Noether's theorem to derive the equations of motion and conserved currents. Note that the use of $\bar{\psi}$ rather than $\psi^*$ is necessary to obtain a Hermitian Hamiltonian.

Lecture 38, April 13, 2001

---

## States without fixed particle number

Usually, we concern ourselves with states with fixed particle number,

$$|n\rangle = \frac{1}{\sqrt{n!}}(a^\dagger)^n|0\rangle. \tag{1}$$

However, sometimes there are motivations for considering states which are not eigenstates of particle number. We consider three such examples here. First, we revisit the mass term in the Dirac equation and show how it represents a mixing of particle-creation and antiparticle-destruction operators. Secondly, we revisit the pairing problem in superconductivity and discuss approximate solutions where particle number is not conserved. Finally, we consider "coherent" state formalism which is commonly used to describe laser pulses, and is also used in the calculation of path integrals.

## The Dirac equation and the mass term

The Hamiltonian for the Dirac equation for massless particles can be written in terms of creation and destruction operators,

$$H_0 = \sum_{\mathbf{k}} \hbar k c(b^\dagger_{\mathbf{k}} b_{\mathbf{k}} + d^\dagger_{-\mathbf{k}} d_{-\mathbf{k}}), \tag{2}$$

where $b^\dagger$ and $d^\dagger$ correspond to creation and destruction operators for particles and antiparticles respectively.

If the mass term is treated like a perturbation, it can also be written in terms of the same creation/destruction operators,

$$V = \sum_{\mathbf{k}} mc^2(b^\dagger_{\mathbf{k}} d^\dagger_{-\mathbf{k}} + d_{-\mathbf{k}} b_{\mathbf{k}}). \tag{3}$$

For each momentum mode we can define two new operators,

$$\begin{aligned} \alpha^\dagger_k &\equiv \cos\theta_k b^\dagger_{\mathbf{k}} + \sin\theta_k d_{-\mathbf{k}}, &(4)\\ \beta^\dagger_k &\equiv \cos\theta_k d^\dagger_{-\mathbf{k}} - \sin\theta_k b_{\mathbf{k}}. &(5)\end{aligned}$$

These operators satisfy the commutation relations,

$$\{\alpha_k, \alpha^\dagger_q\} = \{\beta_k, \beta^\dagger_q\} = \delta_{k,q}, \tag{6}$$

$$\{\alpha_k, \beta_q\} = \{\beta_k, \alpha^\dagger_q\} = \{\alpha_k, \beta^\dagger_q\} = \{\alpha^\dagger_k, \beta^\dagger_q\} = 0 \tag{7}$$

If one considers the Hamiltonian,

$$\begin{aligned} H &= \sum_k E_k(\alpha^\dagger_k \alpha_k + \beta^\dagger_k \beta_k) &(8)\\ &= E\cos 2\theta_k \left[b^\dagger_{\mathbf{k}} b_{\mathbf{k}} + d^\dagger_{-\mathbf{k}} d_{-\mathbf{k}}\right] + 2E\sin^2\theta + E\sin 2\theta \left[b^\dagger_{\mathbf{k}} d^\dagger_{-\mathbf{k}} + d_{-\mathbf{k}} b_{\mathbf{k}}\right], &(9)\end{aligned}$$

one may see that the definitions

$$\begin{aligned} E_k &= \sqrt{\hbar^2 k^2 c^2 + m^2 c^4} &(10)\\ \tan 2\theta_k &= \frac{mc}{\hbar k} &(11)\end{aligned}$$

allow one to reproduce the Hamiltonian within a constant.

$$H = H_0 + V + 2\sum_k E_k \sin^2\theta_k. \tag{12}$$

The last term is a correction to the vacuum energy but does not incorporate the creation and destruction operators. Thus, one can see that eigenstates of the new Hamiltonian are not eigenstates of the number operators of the unperturbed Hamiltonian.

Finally, one can calculate the energy of the new ground state,

$$\langle H\rangle = \sum_k 2E_k \sin^2\theta_k = \sum_k \left(\sqrt{\hbar^2k^2c^2 + m^2c^4} - \hbar kc\right)$$

The change in the vacuum energy is thus the difference of the energies with and without a mass added to the problem. This can be thought of as an alteration to the energy of the Dirac sea.

**Exercise**

Show that

$$b^\dagger_{\mathbf{k}} b_{\mathbf{k}} - d^\dagger_{-\mathbf{k}} d_{-\mathbf{k}} = \alpha^\dagger\alpha - \beta^\dagger\beta. \tag{13}$$

This demonstrates that the eigenstates of the new Hamiltonian are still eigenstates of the charge operator written in the old basis.

**Another Exercise**

Show that the state

$$|\tilde{0}\rangle \equiv \cos\theta|0\rangle + \sin\theta d^\dagger_{-\mathbf{k}} b^\dagger_{\mathbf{k}}|0\rangle$$

is destroyed by both $\alpha_k$ and $\beta_k$. This is the vacuum in the new basis.

**Bogoliubov operators and Cooper pairs**

The pairing term in BCS theory can be written in terms of creation and destruction operators as

$$V = -\frac{v_0}{V}\sum_{k,k'}{}' b^\dagger_{\mathbf{k}} d^\dagger_{-\mathbf{k}} d_{-\mathbf{k}'} b_{\mathbf{k}'}. \tag{14}$$

Here, we have only considered pairs that sum to total momentum zero. The $b^\dagger$ and $d^\dagger$ operators refer to electron spin-up and spin-down creation operators. We do this rather than fouling the formalism with more subscripts. The interaction represents the scattering of particles of opposite momenta $\mathbf{k}'$ and $-\mathbf{k}'$ into states $\mathbf{k}$ and $-\mathbf{k}$. The primed sum limits the sum to a region near the Fermi surface.

Now, we consider as a variational wave function a state where each momentum mode is defined as

$$|\Psi\rangle = \prod_k{}' \left(\cos\theta_k + \sin\theta_k b^\dagger_{-\mathbf{k}} d^\dagger_{\mathbf{k}}\right)|0\rangle \tag{15}$$

For $\theta_k$ becomes non-zero, this state is no longer an eigenstate of the number operator, or electric charge. The expectations of the relevant creation/destruction operator combinations are

$$\langle b^\dagger_{\mathbf{k}} b_{\mathbf{k}} + d^\dagger_{-\mathbf{k}} d_{-\mathbf{k}}\rangle = 2\sin^2\theta_k, \quad \langle b_{\mathbf{k}} d_{-\mathbf{k}}\rangle = \frac{1}{2}\sin 2\theta_k. \tag{16}$$

Next, we consider the energy of particles in the primed region,

$$\begin{aligned}\langle H_0+V\rangle &= \sum_k{}' \epsilon_k \langle b^\dagger_{\mathbf{k}} b_{\mathbf{k}} + d^\dagger_{-\mathbf{k}} d_{-\mathbf{k}}\rangle - \frac{v_0}{V}\sum_k{}' \langle b^\dagger_{\mathbf{k}} d^\dagger_{-\mathbf{k}}\rangle \sum_{k'}{}' \langle b_{\mathbf{k}'} d_{-\mathbf{k}'}\rangle &(17)\\ &= \sum_k{}' \left(2\epsilon_k \sin^2\theta_k - \frac{\Delta}{2}\sin 2\theta_k\right), \quad \text{where } \Delta \equiv \frac{v_0}{2V}\sum_{k'}{}' \sin 2\theta_{k'} &(18)\end{aligned}$$

The important step here is in writing $\langle b^\dagger_{\mathbf{k}} d^\dagger_{-\mathbf{k}} d_{-\mathbf{k}'} b_{\mathbf{k}'}\rangle = \langle b^\dagger_{\mathbf{k}} d^\dagger_{-\mathbf{k}}\rangle \langle b_{\mathbf{k}'} d_{-\mathbf{k}'}\rangle$. This follow from the ansatz for the product form of the state, Eq. (15), and from ignoring terms where $\mathbf{k} = \mathbf{k}'$. These terms are ignored because they are an infinitesimal fraction of the terms in the continuum limit where many states are included in the sum.

Now, one must choose the angles $\theta_k$ such that the energy is minimized compared to the extra particles coming from a reservoir with chemical potential $\mu$. (Usually $\mu$ is the Fermi energy).

$$\frac{\partial}{\partial\theta_k}\sum_k{}' \left((\epsilon_k-\mu)2\sin^2\theta_k - \frac{v_0}{4V}\sin 2\theta_k \sum_{\mathbf{k}'}{}' \sin 2\theta_{\mathbf{k}'}\right) = 0. \tag{19}$$

This leads to the solution

$$\tan 2\theta_k = \frac{\Delta}{\epsilon_k - \mu}. \tag{20}$$

Of course after finding the angles $\theta_k$, one must find the new $\Delta$, then iterate until a consistent solution is found.

One can find the probability that a state $\mathbf{k}$ is occupied by a particle,

$$\langle b^\dagger_{\mathbf{k}} b_{\mathbf{k}}\rangle = \sin^2\theta_{\mathbf{k}} = \frac{1}{2} - \frac{1}{2}\frac{(\epsilon_k-\mu)}{\sqrt{(\epsilon_k-\mu)^2+\Delta^2}}.$$

The occupation is 1/2 when $\epsilon_k = \mu$, is zero for $\epsilon_k >> \mu$ and is unity for $\epsilon_k << \mu$. Pairing smooths the step function one expects for non-interacting particles with a scale $\Delta$.

We also note the difference of this solution with the relativistic Dirac problem above. In that case the ground state was a mixture of the old vacuum and a particle/anti-particle pair, $|0\rangle$ and $b^\dagger_k d^\dagger_{-k}|0\rangle$. However, in this example the solution is a mixture of zero-electron and two-electron states, thus not even electric charge is fixed. The analogy between superconductivity and particle/nuclear physics is reflected in the jargon, as the generation of masses due to spontaneous symmetry breaking is referred to as the creation of a gap.

**Exercise: Show that same-spin particles don't pair**

If we had considered particles of the same spin,

$$|\Psi\rangle = \prod_k{}' \left(\cos\theta_k + \sin\theta_k b^\dagger_{\mathbf{k}} b^\dagger_{-\mathbf{k}}\right)|0_k\rangle,$$

the resulting expectation for the pairing would be zero. This follows because

$$(b_{\mathbf{k}} b_{-\mathbf{k}} + b_{-\mathbf{k}} b_{\mathbf{k}})\left(\cos\theta_k + \sin\theta_k b^\dagger_{\mathbf{k}'} b^\dagger_{-\mathbf{k}'}\right)|0\rangle = 0.$$

The cancellation results from the fact that $\mathbf{k}$ could equal either $\mathbf{k}'$ or $-\mathbf{k}'$. There is only one possible connection for the case where the product of $b_{\mathbf{k}}b_{-\mathbf{k}}$ is replaced by $b_{\mathbf{k}}d_{-\mathbf{k}}$. One way of stating this result is that an $s$-wave coupling must combine with an antisymmetric spin combination since the overall pair wave function must be antisymmetric. If the original potential had had odd-parity, e.g. it was proportional to $k$, then one could form a $p$ wave like state with symmetric spin. The wave function might have a form

$$|\Psi\rangle = \prod_k{}' \left(\cos\theta_k + f(\mathbf{k})\sin\theta_k b_{\mathbf{k}}^\dagger b_{-\mathbf{k}}^\dagger\right)|0_k\rangle,$$

where $f$ is an odd-parity function of $\mathbf{k}$.

### Coherent states

The last example of a state with non-conserved particle number is refered to as a "coherent" state.

$$\begin{aligned} |\eta\rangle &= e^{-\eta^*\eta/2}e^{\eta a^\dagger}|0\rangle && (21)\\ &= e^{-\eta^*\eta/2}\sum_n \frac{(\eta a^\dagger)^n}{n!}|0\rangle, && (22)\end{aligned}$$

where $\eta$ is a complex number. One can check to see that this state is properly normalized by calculating the overlap,

$$\begin{aligned} \langle 0|e^{\eta^* a}e^{\eta a^\dagger}|0\rangle &= \langle 0|\sum_m \frac{(\eta^* a)^m}{m!}\sum_n \frac{(\eta a^\dagger)^n}{n!}|0\rangle && (23)\\ &= \sum_n \langle 0|\frac{(\eta^*\eta)^n}{(n!)^2}a^n(a^\dagger)^n|0\rangle && (24)\\ &= \sum_n \frac{(\eta^*\eta)^n}{n!} = e^{\eta^*\eta}. && (25)\end{aligned}$$

A coherent state is an eigenstate of the destruction operator.

$$\begin{aligned} a|\eta\rangle &= e^{-\eta^*\eta/2}a\sum_n \frac{(\eta a^\dagger)^n}{n!}|0\rangle && (26)\\ &= \sum_n \frac{n\eta^n(a^\dagger)^{n-1}}{n!}|0\rangle && (27)\\ &= \eta|\eta\rangle. && (28)\end{aligned}$$

Thus, it is simple to calculate matrix elements of coherent states. For example,

$$\langle\gamma|(a^\dagger)^3a^2|\eta\rangle = (\gamma^*)^3\eta^2\langle\gamma|\eta\rangle. \qquad (29)$$

### Coherent states as a solution to emission via coupling through a classical current

The physical importance of coherent states comes from the fact that they are the solution to the following Hamiltonian.

$$\begin{aligned} H(t) &= H_0 + V(t). && (30)\\ H_0 &= \epsilon a^\dagger a, \quad V(t) = j(t)[a^\dagger + a]. && (31)\end{aligned}$$

Here $j$ plays the role of an external classical current that couples to a quantum field, e.g. $j \cdot A$.

To see that this is a solution of the Hamiltonian, consider the state $|\eta(t)\rangle_I$ to be a solution in the interaction representation,

$$\begin{aligned} |\eta(t)\rangle_I &= e^{i\phi(t)} e^{-\eta^*(t)\eta(t)/2} e^{\eta(t)a^\dagger}|0\rangle, && (32)\\ & \quad \text{where } \eta(t) \equiv -i\int_{-\infty}^{t} dt' e^{-i\epsilon t'/\hbar} j(t'). && (33)\end{aligned}$$

Viewing the evolution of $|\eta\rangle_I$ with time,

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}|\eta(t)\rangle_I &= \left\{-\hbar\frac{d\phi}{dt} + \frac{1}{2}j(t)e^{-i\epsilon t/\hbar}\eta(t) - \frac{1}{2}j(t)e^{i\epsilon t/\hbar}\eta^*(t) + j(t)e^{i\epsilon t/\hbar}a^\dagger\right\}|\eta(t)\rangle_I && (34)\\ &= \left\{-\hbar\frac{d\phi}{dt} - \frac{1}{2}j(t)e^{i\epsilon t/\hbar}\eta(t) - \frac{1}{2}j(t)e^{-i\epsilon t/\hbar}\eta^*(t)\right. && (35)\\ &\qquad \left. + j(t)e^{-i\epsilon t/\hbar}a + j(t)e^{i\epsilon t/\hbar}a^\dagger\right\}|\eta(t)\rangle_I, && (36)\end{aligned}$$

where we have used that fact that $a|\eta(t)\rangle = \eta(t)|\eta(t)\rangle$. The last two terms can be recognized as $V_I(t)$. Thus, if one defines the phase $\phi(t)$ by

$$\phi(t) \equiv -\frac{1}{2}\int_{-\infty}^{t} dt' \left(e^{i\epsilon t'}\eta(t') + e^{-i\epsilon t'}\eta^*(t')\right) j(t')/\hbar, \tag{37}$$

one can find that the time evolution for $|\eta(t)\rangle_I$ in a simple form.

$$i\hbar\frac{\partial}{\partial t}|\eta(t)\rangle_I = V_I(t)|\eta(t)\rangle_I. \tag{38}$$

This demonstrates that our guess at $|\eta(t)\rangle_I$ was correct.

Coupling to an external current is a common consideration in a wide variety of physical problems. Even when spatial degrees of freedom are considered, e.g. $j \cdot A$, one finds simple analytic solutions. They then often have the form

$$|\eta\rangle \sim \exp\left\{-i\int d^3p\ j(\mathbf{p})a^\dagger_{\mathbf{p}}\right\}|0\rangle, \quad j(\mathbf{p}) \sim \int d^4x\ e^{ip\cdot x}j(x). \tag{39}$$

Any large current will radiate particles in a coherent state. Some types of lasers are associated with coherent states.

### Completeness relations for coherent states

A useful property of any basis is completeness,

$$\sum_\alpha \langle m|\alpha\rangle\langle\alpha|n\rangle = \delta_{mn}. \tag{40}$$

Coherent states provide a complete basis when all values of $\eta$ in the complex plane are considered.

$$\frac{1}{\pi}\int d\eta_R d\eta_I \langle m|\eta\rangle\langle\eta|n\rangle = \delta_{mn} \tag{41}$$

To prove this, we expand the matrix elements.

$$\langle m|\eta\rangle\langle\eta|n\rangle = e^{-|\eta|^2}\frac{\eta^m(\eta^*)^n}{\sqrt{n!m!}}. \tag{42}$$

Writing the integral over the real and imaginary parts of $\eta$ as

$$\int d\eta_R d\eta_I \to \int d\phi|\eta|d|\eta|, \tag{43}$$

where $\phi$ is the complex phase of $\eta$, allows one to see that the integral over $\phi$ will eliminate all terms with $m \neq n$ since

$$\langle m|\eta\rangle\langle\eta|n\rangle = e^{-|\eta|^2}e^{i(m-n)\phi}\frac{|\eta|^{m+n}}{\sqrt{n!m!}}. \tag{44}$$

One may now rewrite the expression using the fact that integrating over $\phi$ constrains the result to be proportional to $\delta_{mn}$.

$$\frac{1}{\pi}\int d\eta_R d\eta_I\langle m|\eta\rangle\langle\eta|n\rangle = 2\delta_{mn}\int |\eta|d|\eta|\ e^{-|\eta|^2}\frac{|\eta|^{2n}}{n!}. \tag{45}$$

By making the substitution $u \equiv |\eta|^2$, one can perform the integral and see that

$$\frac{1}{\pi}\int d\eta_R d\eta_I\langle m|\eta\rangle\langle\eta|n\rangle = \delta_{mn}. \tag{46}$$

Completeness, combined with the fact that the coherent states are eigenstates of the destruction operator, allows one to calculate all matrix elements

$$\langle\alpha_f|e^{-iHt}|\alpha_i\rangle = \sum_{\alpha_i}\langle\alpha_f|e^{-iH(t-t_1)}|\alpha_1\rangle\langle\alpha_1|e^{-iH(t_1-t_2)}|\alpha_2\rangle\langle\alpha_2|e^{-iH(t_2-t_3)}|\alpha_3\rangle\cdots\langle\alpha_n|e^{-iH(t_n-t_i)}|\alpha_i\rangle \tag{47}$$

as an integral over complex fields $\eta_i$ rather than a sum over discrete states $\alpha_i$. Furthermore, if the Hamiltonian is normal ordered, that is each term has all creation operators pushed to the left,

$$\langle\eta_n|e^{-iH(a^\dagger,a)\delta t}|\eta_{n+1}\rangle = \{1 - iH(\eta_n^*, \eta_{n+1})\delta t\}\langle\eta_n|\eta_{n+1}\rangle. \tag{48}$$

The process of breaking up the evolution operator into the product of many individual pieces $e^{-iH\delta t}$, inserting a complete set of states between each piece, and integrating over all states is known as a path integral. In addition to being useful for calculating evolution operators, they also can be applied to thermodynamics partition functions which require calculating the trace of $e^{-\beta H}$. Lattice gauge theory is the numeric enterprise of calculating such path integrals for QCD.