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1 September 9th, 2004

1.1 Basic rules of QM

Any physical state of a system is described by a state vector $|\psi\rangle$ in a linear Hilbert space:

$$\langle \psi_1 | \psi_2 \rangle = \langle \psi_2 | \psi_1 \rangle^*, \quad |\psi\rangle = |\psi_1\rangle + |\psi_2\rangle$$  \hspace{1cm} (1)

Note that in classical mechanics, it does not make sense to superpose, say, position states of a system.

Any physical observable $A$ is represented by a Hermitean operator $\hat{A}$, on that space. $\hat{A}$ has real eigenvalues $\lambda_n$, which are the possible outcomes of a measurement:

$$\hat{A} |\psi\rangle \in \text{Hilbert space}$$

$$\hat{A} |\psi_1\rangle + \hat{A} |\psi_2\rangle = \hat{A} (|\psi_1\rangle + |\psi_2\rangle)$$  \hspace{1cm} (2)

$$\hat{A} |\psi_n\rangle = \lambda_n |\psi_n\rangle$$  \hspace{1cm} (3)

Example, position:

$$\hat{x} |\vec{x}\rangle = \vec{x} |\vec{x}\rangle,$$  \hspace{1cm} (4)

where $\hat{x}$ is a Hermitean operator, $|\vec{x}\rangle$ an eigenstate with eigenvalue $\vec{x}$. The eigenstates $|\vec{x}\rangle$ (and those of any Hermitean operator) are a complete orthonormal basis of states:

$$\langle \vec{x}_1 | \vec{x}_2 \rangle = \delta(\vec{x}_1 - \vec{x}_2)$$  \hspace{1cm} (5)

Any state, $|\psi\rangle$ can therefore be written as a linear combination (in this case, a continuous sum) of these eigenstates:

$$|\psi\rangle = \int |\vec{x}\rangle \langle \vec{x}| \psi \rangle d^3\vec{x}$$  \hspace{1cm} (6)

$\psi(\vec{x}) \equiv \langle \vec{x}| \psi \rangle$ is the wave function of the state $|\psi\rangle$ in position. Note from Eq. 6 the closure relation

$$1 = \int |\vec{x}\rangle \langle \vec{x}| d^3\vec{x}$$  \hspace{1cm} (7)

The outcome of a measurement of a general operator $\hat{A}$ will be one of its eigenvalues, $\lambda_n$. For a state $|\psi\rangle = \sum_n c_n |\psi_n\rangle, c_n \equiv \langle \psi_n | \psi \rangle$, the probability that the result of the measurement is $\lambda_n$ is $P_n = |\langle \psi_n | \psi \rangle|^2$. The closure relation here (with a discrete spectrum) is

$$1 = \sum_n |\psi_n\rangle \langle \psi_n|$$  \hspace{1cm} (8)

Recall the Time-Dependent Schrödinger Equation (TDSE)

$$i\hbar \frac{\partial}{\partial t} |\psi\rangle = \hat{H} |\psi\rangle,$$  \hspace{1cm} (9)
where \( \hat{H}(\vec{p}, \vec{x}) \) is the Hamiltonian. In some cases, exact solutions are known: free particle, harmonic oscillator, two-state systems (e.g. spin 1/2), hydrogen atom, etc. We solve the TDSE by first solving the Time-Independent Schrödinger Equation (TISE)

\[
i \hbar \frac{\partial}{\partial t} |\psi_n\rangle = \hat{H} |\psi\rangle = E_n |\psi_n\rangle \]

\[
|\psi_n\rangle (t) = e^{-\frac{i}{\hbar} E_n t} |\psi_n\rangle , \quad |\psi_n\rangle (0) \equiv |\psi_n\rangle
\]

\[
|\psi\rangle (t) = \sum_n c_n e^{-\frac{i}{\hbar} E_n t} |\psi_n\rangle
\]

But this does not explain why a hydrogen atom in an excited 'energy eigenstate' emits a photon to get to a lower eigenstate, rather than staying in the initial state forever.

Postulate in QM (ex. momentum and position relations):

\[
[\hat{p}_k, \hat{x}_l] = \hbar i \delta_{kl}, \quad \hat{p} = \hbar \frac{\partial}{\partial \vec{x}}
\]

2 September 14th, 2004

2.1 Maxwell Equations

For a particle with charge \(-e\) and mass \(m\),

\[
m \frac{d^2 \vec{x}}{dt^2} = F_{\text{Lorentz}} = -e \vec{E} - \frac{e}{c} \vec{v} \times \vec{B}
\]

In terms of vector and scalar potentials, \(\vec{A}(\vec{x}, t)\) and \(\phi(\vec{x}, t)\)

\[
\vec{B} = \nabla \times \vec{A}, \quad \vec{E} = -\nabla \phi - \frac{1}{c} \frac{d \vec{A}}{dt},
\]

since

\[
\nabla \cdot \vec{B} = 0 \quad \text{(no magnetic monopoles)}, \quad \nabla \times \vec{E} + \frac{1}{c} \frac{\partial \vec{B}}{\partial t} = 0.
\]

These potentials are not unique, i.e. invariant under gauge transformation: if \(A \rightarrow A - \nabla f\), \(\vec{B}\) is unchanged (\(\nabla \times \nabla f = 0\)); if \(\phi \rightarrow \phi + \frac{1}{c} \frac{\partial f}{\partial t}\), \(\vec{E}\) is unchanged.

2.2 Hamiltonian of a particle in an EM field

We start from the Hamiltonian

\[
H(\vec{p}, \vec{x}, t) = \frac{1}{2m} \left( \vec{p} - \frac{e}{c} \vec{A}(\vec{x}, t) \right)^2 + e\phi(\vec{x}, t).
\]

In classical mechanics, Hamilton’s equations are

\[
\frac{d\vec{x}}{dt} = \frac{\partial H}{\partial \vec{p}}, \quad \frac{d\vec{p}}{dt} = -\frac{\partial H}{\partial \vec{x}}
\]
whereas in quantum mechanics,

\[ i\hbar \frac{\partial}{\partial t} |\psi\rangle = H |\psi\rangle, \quad [p_k, x_l] = \frac{\hbar}{i} \delta_{kl}. \]  

(17)

Hamilton’s equations are satisfied at the level of expectation values:

\[ \frac{d}{dt} \langle \vec{x} \rangle = \langle \frac{\partial H}{\partial \vec{p}} \rangle, \quad \frac{d}{dt} \langle \vec{p} \rangle = -\langle \frac{\partial H}{\partial \vec{x}} \rangle. \]  

(18)

Proof:

\[ \frac{d}{dt} \langle \psi|\vec{p}|\psi \rangle = \left( \frac{d}{dt} \langle \psi| \right) \vec{p} \langle \psi \rangle + \langle \psi| \vec{p} \left( \frac{d}{dt} \langle \psi \rangle \right) = \]

\[ = \frac{i}{\hbar} \langle \psi| [H, \vec{p}] |\psi \rangle = \langle \psi \rangle - \frac{\partial H}{\partial \vec{x}} \langle \psi \rangle \]  

(19)

In the above, we have used the following:

\[ i\hbar |\psi\rangle = H |\psi\rangle, \quad -i\hbar \langle \psi| = \langle \psi| H, \quad \vec{p} = \frac{\hbar}{i} \frac{\partial}{\partial \vec{x}}. \]  

(20)

Aside: For any operator \( A \) that is time-independent,

\[ \frac{d}{dt} \langle A \rangle = \frac{i}{\hbar} \langle [H, A] \rangle \]  

(21)

so any time-independent operator that commutes with the Hamiltonian is conserved (e.g. \( \vec{p} \) conserved if \( H \) does not explicitly depend on \( \vec{x} \)). Note that if \( A \) had explicit time-dependence, then

\[ \frac{d}{dt} \langle A \rangle = \frac{i}{\hbar} \langle [H, A] \rangle + \langle \frac{\partial A}{\partial t} \rangle. \]  

(22)

It can be shown that \( H = \frac{1}{2m} (\vec{p} + \frac{e}{c} \vec{A})^2 + e\phi \) is the correct Hamiltonian from which the Lorentz force can be obtained. Moreover, this Hamiltonian indicates that momentum and velocity are not proportional in an EM field, but instead have the following relation:

\[ \frac{d\vec{x}}{dt} = \frac{1}{m} \left( \vec{p} + \frac{e}{c} \vec{A} \right) \]  

(23)

\[ \frac{dp_l}{dt} = -\frac{e}{mc} \left( p_k + \frac{e}{c} A_k \right) \frac{\partial A_k}{\partial x_l} + e \frac{\partial \phi}{\partial x_l}, \]  

(24)

where \( l = 1, 2, 3 \) for \( x, y, z \).

Conclusion: Hamiltonian has the form

\[ H (\vec{p}, \vec{x}) = \frac{1}{2m} \left( \vec{p} + \frac{e}{c} \vec{A} (\vec{x}, t) \right)^2 + e\phi (x, t) \]  

(25)
Remark:
\[ L = \frac{1}{2} m \dot{x}^2 - \frac{e}{c} \vec{A}(\vec{x}, t) \cdot \dot{\vec{x}} + e \phi(\vec{x}, t) \]
\[ H = \dot{\vec{x}} \cdot \frac{\partial L}{\partial \dot{\vec{x}}} - L \]
\[ \vec{p} = \frac{\partial L}{\partial \dot{\vec{x}}} \]  
(26)

Consider the case where \( \vec{E} = 0 \), and \( \vec{B} = \vec{B}(\vec{x}) \) (no time dependence). Stokes theorem gives the magnetic flux, \( \Phi \), as
\[ \Phi = \int_S \vec{B} \cdot d\vec{a} = \int_C \vec{A} \cdot d\vec{x} \]  
(27)
where \( \vec{B}(\vec{x}) = \nabla \times \vec{A}(\vec{x}) \).

2.3 Aharonov-Bohm Effect

Consider the two slit experiment, with a (confined) region of magnetic field. In regions where \( \vec{B} = 0 \), \( \vec{A} = \nabla f \). (Note that \( \vec{B} = 0 \) does not imply \( \vec{A} = 0 \), unless the space for which \( \vec{B} = 0 \) is simply connected, in which case a gauge transformation can be applied to set \( \vec{A} = 0 \)). Let’s look at the Schrödinger equation (SE) for \( \phi = 0 \) and \( \vec{A} = \vec{A}(x) \):
\[ i \hbar \frac{\partial}{\partial t} \psi(\vec{x}, t) = \frac{1}{2m} \left[ \frac{\hbar}{i} \frac{\partial}{\partial \vec{x}} + \frac{e}{c} \vec{A}(\vec{x}) \right]^2 \psi(\vec{x}, t). \]  
(28)
The SE is invariant under the following transformation:
\[ \psi(\vec{x}, t) \rightarrow e^{\frac{i}{\hbar} \frac{e}{c} f(\vec{x})} \psi(\vec{x}, t), \]  
\[ \vec{A}(\vec{x}) \rightarrow \vec{A}(\vec{x}) - \frac{\partial f(\vec{x})}{\partial \vec{x}}. \]  
(29)
(30)

Note that the quantity \( |\psi|^2 \), as well as the expectation value of any operator, is invariant under the above transformation as well. In the region where \( \vec{B} = 0 \), \( \nabla \times \vec{A} = 0 \), so \( \vec{A} = \nabla f(\vec{x}) \), where
\[ f(\vec{x}) = \int_p \vec{A}(\vec{x}) \cdot d\vec{x}, \]  
(31)
where \( p \) is some arbitrary position in the space where \( \vec{B} = 0 \); we can set \( f(p) = 0 \).

Consider two different paths, \( C_1 \) and \( C_2 \), connecting \( p \) and \( \vec{x} \), and let \( f_1(\vec{x}) \) and \( f_2(\vec{x}) \) be the functions obtained by integration along these separate paths. Then, \( f_1(\vec{x}) - f_2(\vec{x}) \) is the integral of \( \vec{A}(\vec{x}) \cdot d\vec{x} \) along the closed curve, \( C = C_1 - C_2 \). By Stokes theorem, this is equivalent to the magnetic flux through the surface bounded by \( C \). In the region where \( \vec{B} = 0 \), \( \vec{A} = \nabla f \), and we can set \( \vec{A} = 0 \) by transforming both \( \vec{A} \) and \( \psi \) according to Eq. 29. Then, \( \psi \) is shifted by a phase factor, in a such a way that the interference pattern depends on \( \vec{B} \). See handout: Gasiorowicz pp. 230-232.
3 September 16th, 2004

3.1 Two ways of doing QM

\[ |\psi_S\rangle = \frac{1}{\sqrt{2}} \left( |\psi_S\rangle + e^{-iHt} |\psi_H\rangle \right) \]

\[ |\psi_H\rangle = \frac{1}{\sqrt{2}} \left( |\psi_S\rangle + e^{iHt} |\psi_H\rangle \right) \]

Note that

\[ (\langle \psi_S | A_S | \psi_S \rangle) = (\langle \psi_H | A_H | \psi_H \rangle) \]

Consider the Hamiltonian

\[ H = \frac{1}{2m} \left( \vec{p} + \frac{e}{c} \vec{A} \right)^2 + e\phi. \]

In the Heisenberg picture,

\[ \frac{d\vec{x}}{dt} = \frac{i}{\hbar} [H, \vec{x}] = \frac{1}{m} \left( \vec{p} + \frac{e}{c} \vec{A} \right), \]

\[ \vec{p} = m\vec{x} - \frac{e}{c} \vec{A}. \]

As an exercise, derive the Lorentz for law:

\[ m\ddot{\vec{x}} = -e \left[ \vec{E} + \frac{1}{c} \vec{\times} \vec{B} \right] \]

3.2 The constant B-field problem

For a constant B-field, \( \vec{B} = B\hat{z} = (0, 0, B) \), we can choose the following vector potential:

\[ \vec{A}(x, y) = \left( -\frac{B}{2} y, \frac{B}{2} x, 0 \right). \]

The corresponding Hamiltonian is

\[ H = \frac{1}{2m} \left[ \left( p_x - \frac{eB}{2c} y \right)^2 + \left( p_y + \frac{eB}{2c} \right)^2 + p_z^2 \right], \]

which can be rewritten as

\[ H = \frac{1}{2m} \left( p_x^2 + p_y^2 + p_z^2 \right) + \frac{1}{2} m\omega^2 \left( x^2 + y^2 \right) + \omega (x p_y - y p_x), \]
with \( \omega = \frac{eB}{2mc} = \frac{1}{2} \omega_L \), where \( \omega_L \) is the Larmor frequency. Note that \( (xp_y - yp_x) = L_z \), the angular momentum in the z-direction. Recall that \( \frac{d}{dt} \mathcal{A}_H = \frac{i}{\hbar} [H, \mathcal{A}_H] \).

Here, \( \frac{dp_z}{dt} = \frac{i}{\hbar} \mathcal{A}_H \), so we can ignore the motion in z and consider the Hamiltonian as that of two harmonic oscillators:

\[
H = \frac{1}{2m} (p_x^2 + p_y^2 + p_z^2) + \frac{1}{2} m\omega^2 (x^2 + y^2).
\]

### 3.2.1 Reminder: the harmonic oscillator

A one-dimensional harmonic oscillator has the following Hamiltonian:

\[
H_o = \frac{1}{2m} p^2 + \frac{1}{2} m\omega^2 x^2.
\]

The equations of motion are

\[
\dot{x} = \frac{i}{\hbar} [H, x] = \frac{p}{m}, \quad \dot{p} = \frac{i}{\hbar} H_p = -m\omega^2 x.
\]

We can define the following creation and annihilation operators, respectively:

\[
a^\dagger = \sqrt{\frac{m\omega}{2\hbar}} x - i\sqrt{\frac{1}{2m\hbar\omega}} p, \\
a = \sqrt{\frac{m\omega}{2\hbar}} x + i\sqrt{\frac{1}{2m\hbar\omega}} p.
\]

As a homework exercise, show that

\[
\dot{a} = -i\omega a, \quad \dot{a}^\dagger = i\omega a^\dagger, \quad [a, a^\dagger] = 1.
\]

The Hamiltonian can be written as:

\[
H_o = \hbar\omega \left( a^\dagger a + \frac{1}{2} \right),
\]

which has eigenstates

\[
|n\rangle = \frac{1}{\sqrt{n!}} (a^\dagger)^n |0\rangle, \quad \text{where } a |0\rangle = 0;
\]

i.e., \( H_o |0\rangle = \frac{1}{2} \hbar\omega |0\rangle \), and \( H_o |n\rangle = \frac{1}{2} \hbar\omega |n\rangle \). Note also that, in the Heisenberg picture

\[
a(t) = e^{-i\omega t} a(0), \quad a^\dagger(t) = e^{i\omega t} a^\dagger(0).
\]
3.2.2 Diagonalizing the equations of motion

We would like to find creation and annihilation operators for the Hamiltonian

\[ H = \frac{1}{2} \left( p^2 + \frac{1}{2} m \omega^2 (x^2 + y^2) + \omega L_z \right). \] (52)

First, as a aside, consider the last term alone: \( H_1 = \omega L_z \). Note that

\[ \dot{x} = \frac{i}{\hbar} [H, x] = -\omega y, \quad \dot{y} = \frac{i}{\hbar} [H, y] = -\omega x. \] (53)

We can define these operators

\[ x^+ = x + iy, \quad x^- = x - iy, \] (54)

which have the following properties:

\[ \dot{x}^+ = -i\omega x^+, \quad \dot{x}^- = i\omega x^-; \] (55)

\[ x^+ (t) = e^{-i\omega t} x^+ (0), \quad x^- (t) = e^{i\omega t} x^- (0), \] (56)

much like \( a \) and \( a^\dagger \) for the simple harmonic oscillator. Now, back to the Hamiltonian in 52. Recall that we have ignored the motion in the z-direction. We first note the following equations of motion:

\[ \dot{x} = \frac{p_x}{m} - \omega y, \quad \dot{y} = \frac{p_y}{y} + \omega x; \]

\[ \dot{p}_x = m \omega^2 x - \omega p_y, \quad \dot{p}_y = m \omega^2 y - \omega p_x. \] (57)

Introducing operators \( a_k \) and \( a_k^\dagger \), where \( k=1,2 \) for the x- and y- directions, defined as:

\[ x_k = \sqrt{\frac{\hbar}{2m \omega}} (a_k + a_k^\dagger) , \quad p_k = \sqrt{\frac{\hbar m \omega}{2}} (a_k - a_k^\dagger) , \] (58)

where \( x_{1,2} = x, y \) and \( p_{1,2} = p_x, p_y \). These operators behave as:

\[ \dot{a}_x = -i\omega a_x - \omega a_y, \quad \dot{a}_x^\dagger = i\omega a_x^\dagger - \omega a_y^\dagger, \]

\[ \dot{a}_y = -i\omega a_y + \omega a_x, \quad \dot{a}_y^\dagger = i\omega a_y^\dagger - \omega a_x^\dagger. \] (59)

Note also the following properties:

\[ [a_{x,y}^\dagger, a_{x,y}] = -1, \quad [a_x, a_y] = 0, \text{ etc.} \] (61)

We can further rearrange these operators to form yet a new set of operators as follows:

\[ a_\pm = (a_x \pm ia_y) / \sqrt{2}, \quad a_{\pm}^\dagger = (a_x^\dagger \pm ia_y^\dagger) / \sqrt{2}. \] (62)

These operators behave as:

\[ \dot{a}_+ = -i\omega a_+ , \quad \dot{a}_- = i\omega a_-, \]

\[ \dot{a} = 0 , \quad \dot{a}_{-} = 0. \] (64)
with the following commutation properties:
\[
[a_\pm, a_\mp^\dagger] = 1, \quad [a_+, a_-] = 0 \quad \text{etc.} \quad (65)
\]
Hence, for the Hamiltonian in Eq. 52, \(a_\pm\) and \(a_\mp^\dagger\) look like good “ladder operators” (analogous to those used to solve the harmonic oscillator). In particular, \(a_+\) and \(a_-^\dagger\) do not change in time (as though they correspond to a harmonic oscillator with \(\omega = 0\)). As a homework exercise, show that
\[
L_z = \hbar \omega \left( a_+^\dagger a_+ - a_-^\dagger a_- \right). \quad (66)
\]
In terms of the newly defined operators, the Hamiltonian for a charged particle in a constant B-field Eq. 52 is:
\[
H = \hbar \omega \left( a_+^\dagger a_+ + a_-^\dagger a_- + 1 \right) + \hbar \omega \left( a_+^\dagger a_+ - a_-^\dagger a_- \right) =
\]
\[
= 2\hbar \omega \left( a_+^\dagger a_+ + \frac{1}{2} \right) =
\]
\[
= \hbar \omega L \left( a_+^\dagger a_+ + \frac{1}{2} \right), \quad (67)
\]
where \(\omega_L = \frac{eB}{m}\) is the Larmor frequency, as before.

**Summary of method:** We write the equations of motion, as in Eq. 57, and realize that they are linear in all the variables. We then try to find clever linear combinations of these to diagonalize these equations of motion, as in Eq. 63. Now we are left to solve the Hamiltonian: \(H = \hbar \omega_L \left( a_+^\dagger a_+ + \frac{1}{2} \right)\), which has the exact same form as that of a simple, one-dimensional harmonic oscillator. Having found the operators \(a_\pm\) and \(a_\mp^\dagger\), we can “build” the Hilbert space spectrum with the following basis:
\[
|n_+, n_-\rangle = \frac{\left( a_+^\dagger \right)^n_+ \left( a_-^\dagger \right)^n_-}{\sqrt{n_+!} \sqrt{n_-!}} |0\rangle, \quad (68)
\]
where \(a_+ |0\rangle = a_- |0\rangle = 0\). The eigenenergies are
\[
H |n_+, n_-\rangle = \hbar \omega_L \left( n_+ + \frac{1}{2} \right) |n_+, n_-\rangle, \quad (69)
\]
which are independent of \(n_-\) (since \(a_-\) does no appear in \(H\)). Thus, all states are infinitely degenerate, including the ground state:
\[
H |0, n_-\rangle = \frac{1}{2} \hbar \omega_L |0, n_-\rangle, \quad \text{for all} \ n_- . \quad (70)
\]
This degeneracy reflects the fact that the Hamiltonian is invariant under translation on the x-y plane; in other words, the particle’s energy is independent of it’s position on the x−y plane.
4 September 21st, 2004

4.1 The constant B-field problem continued: coherent states and Landau levels

Consider a state, $|\alpha\rangle$, defined as $|\alpha\rangle = e^{\alpha a^\dagger} |0,0\rangle$, (71)

where $\alpha$ is a complex number. This state has the following useful properties: first,

$$a_- |\alpha\rangle = a_- e^{\alpha a^\dagger} |0,0\rangle = \alpha e^{\alpha a^\dagger} |0,0\rangle = \alpha |\alpha\rangle,$$ (72)

and second,

$$H |\alpha\rangle = He^{\alpha a^\dagger} |0,0\rangle = \left( [H,e^{\alpha a^\dagger}] + e^{\alpha a^\dagger} H \right) |0,0\rangle = \frac{1}{2} \hbar \omega_L \alpha;$$ (73)

so all states $|\alpha\rangle$, for any complex $\alpha$, are ground states. As a homework exercise, prove that:

$$\langle x_1 \rangle = \frac{\langle \alpha | x_1 | \alpha \rangle}{\langle \alpha | \alpha \rangle} = \sqrt{\frac{\hbar}{2m\omega}} \text{Re} (\alpha),$$

$$\langle x_2 \rangle = \frac{\langle \alpha | x_2 | \alpha \rangle}{\langle \alpha | \alpha \rangle} = \sqrt{\frac{\hbar}{2m\omega}} \text{Im} (\alpha),$$ (74)

namely, that $\alpha$ tells us the position of the particle: $\text{Re}(\alpha)$ the $x$-coordinate and $\text{Im}(\alpha)$ the $y$ coordinate. Let us denote the fact that $|\alpha\rangle$ is an energy ground state by writing $|0;\alpha\rangle \equiv |\alpha\rangle$. In this notation, the energy spectrum is obtained by letting $a^\dagger_+$ and $a_+$ act on an energy eigenstate, $|n;\alpha\rangle$:

$$a^\dagger_+ |n;\alpha\rangle = \sqrt{n+1} |n+1;\alpha\rangle, \quad a_+ |n;\alpha\rangle = \sqrt{n} |n-1;\alpha\rangle.$$ (75)

Energy levels of a particle in a constant magnetic field, also known as Landau levels:

$$H |n;\alpha\rangle = \hbar \omega_L \left( n + \frac{1}{2} \right) |n,\alpha\rangle,$$ (76)

and $|0,\alpha\rangle$ is called the “lowest Landau level.”
4.2 Reminder: The Zeeman effect

Recall the Hamiltonian for an electron in a hydrogen atom,

\[ H = \frac{\vec{p}^2}{2m} - \frac{e^2}{r}, \]  

(77)

has the spectrum:

\[ H |n, l, m\rangle = E_{n,l} |n, l, m\rangle, \]  

(78)

where the quantum numbers \( n, l, m \) correspond, respectively, to the energy, the orbital angular momentum, and the orbital angular momentum in the (arbitrary) \( z \)-direction, \( L_z \). If an external magnetic field is present, the system is no longer rotationally invariant, thus breaking the \((2l + 1)\)-fold degeneracy that would otherwise exist for every \( l \), for a given \( n \). This is known as the Zeeman effect.

The Hamiltonian for an electron in a hydrogen atom, in a constant magnetic field in the \( z \)-direction, is

\[ H = \frac{1}{2m} (p_x^2 + p_y^2 + p_z^2) + \frac{eB}{2mc} L_z + \frac{e^2B^2}{8mc^2} (x^2 + y^2) - \frac{e^2}{r}. \]  

(79)

For a sufficiently weak magnetic field, we can ignore the term quadratic in \( B \) (Also, \( x^2 \) and \( y^2 \) are small if the electron is to remain inside the atom). Thus, the Hamiltonian simplifies to

\[ H = H_0 + H_1, \]

where \( H_0 = \frac{1}{2m} (p_x^2 + p_y^2 + p_z^2) - \frac{e^2}{r}, \]

and \( H_1 = \frac{eB}{2mc} L_z, \)

(80)

for which the spectrum is

\[ (H_0 + H_1) |n, l, m\rangle = (E_{n,l} + E_{m}^{(1)}) |n, l, m\rangle, \]

(81)

\[ H_1 |n, l, m\rangle = \frac{\hbar eB}{2mc} m |n, l, m\rangle, \]

(82)

where \( E_{m}^{(1)} \) is the correction to the spectrum for the \( B = 0 \), unperturbed, system in Eq. 77; we shall solve this using perturbation theory.

4.3 Reminder: Time Independent Perturbation Theory

Consider, in general, a Hamiltonian consisting of two parts:

\[ H = H_0 + H_1, \]

(83)

where \( H_0 \) is the unperturbed Hamiltonian (the “large part”, for which exact solutions to eigenstates are known), and \( H_1 \) is the perturbation (the “small part”). As a book-keeping trick, we rewrite this as

\[ H = H_0 + \lambda H_1, \]

(84)
where \( \lambda \), a small parameter, is introduced to keep track of “size” (of contribution to the total energy) in our computations. Let \( \{ \psi_n^{(0)} \} \) be the set of (orthonormal) unperturbed eigenstates: namely, \( H_0 = \psi_n^{(0)} \rangle \langle \psi_n^{(0)} \), and \( \langle \psi_n^{(0)} | \psi_m^{(0)} \rangle = \delta_{nm} \). We can write the eigenstates and eigenenergies of \( H \) in Eq. 84 as:

\[
\psi_n^{(1)} = \psi_n^{(0)} + \lambda \psi_n^{(1)} + \lambda^2 \psi_n^{(2)} + \ldots ,
\]

\[
E_n^{(1)} = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \ldots .
\]

First order time-independent perturbation theory:

\[
(H = H_0 + \lambda H_1) \left( \psi_n^{(0)} + \lambda \psi_n^{(1)} + \ldots \right) = \left( E_n^{(0)} + \lambda E_n^{(1)} + \ldots \right) \left( \psi_n^{(0)} + \lambda \psi_n^{(1)} + \ldots \right) .
\]

From the above, the zeroth-order (\( \lambda^0 \)) equation is simply \( H_0 = \psi_n^{(0)} \rangle \langle \psi_n^{(0)} \). The first-order (\( \lambda^1 \)) equation is:

\[
H_0 \psi_n^{(1)} + H_1 \psi_n^{(0)} = E_n^{(1)} \psi_n^{(0)} + E_n^{(0)} \psi_n^{(1)} .
\]

Taking the inner product of \( \langle \psi_n^{(0)} | \) with Eq. 88, we obtain

\[
E_n^{(1)} = \langle \psi_n^{(0)} | H_1 \psi_n^{(0)} \rangle .
\]

Thus we have found the first order correction to the energy, \( E_n^{(1)} \).

5 September 23rd, 2004

5.1 Multiparticle systems

Consider a system of \( N \) particles in \( d \)-dimensions. Such a configuration can be described in \( (N \times d) \)-dimensional space. We can define \( |\vec{x}_1, \vec{x}_2, ..., \vec{x}_N \rangle \) as an eigenstate of the position for each and all the particles. The wavefunction,

\[
\psi(\vec{x}_1, \vec{x}_2, ..., \vec{x}_N) = \langle \vec{x}_1, \vec{x}_2, ..., \vec{x}_N | \psi \rangle ,
\]

is, in general, not a product of functions of individual particles.

5.2 Indistinguishable particles

One electron is indistinguishable from another electron; the same goes for protons, photon, quarks etc. However, internal quantum numbers (spin, color, excitation) can distinguish one of these particles from another of the same ‘species.’
Consider a system with two indistinguishable particles. A position eigenstate of this system is \(|\vec{x}_1, \vec{x}_2\rangle\). The operation of exchanging the two particles,
\[
P_{12} |\vec{x}_1, \vec{x}_2\rangle = |\vec{x}_2, \vec{x}_1\rangle,
\]
commutes with the Hamiltonian ([\(P_{12}, H]\) = 0), and is a symmetry of the system. Evidently, \(P_{12}^2 = 1\), so the eigenvalues of \(P_{12}\) are \(\pm 1\). The eigenstates of \(P_{12}\):
\[
\frac{1}{\sqrt{2}} (|\vec{x}_1, \vec{x}_2\rangle \pm |\vec{x}_2, \vec{x}_1\rangle)
\]
with eigenvalues \(\pm 1\), are suitable (“good”) states for describing bosons and fermions. In other words, states that describe bosons and fermions must be symmetric and antisymmetric, respectively.

The Pauli Exclusion Principle states that no two indistinguishable fermions can be in the same state. Two identical fermions can be described by the general wavefunction, \(\psi (\vec{x}_1, \vec{x}_2) = (\psi_a (\vec{x}_1) \psi_b (\vec{x}_2) - \psi_b (\vec{x}_1) \psi_a (\vec{x}_2))\); thus, \(\psi (\vec{x}_1, \vec{x}_2) = 0\) if \(\psi_a = \psi_b\).

The consequences of these rules for indistinguishable particles include the exchange forces, the Periodic Table, and, in solids, the Fermi energy, white dwarfs, neuron stars, superconductivity, and the quantum Hall effect. We will be discussing some of these soon.

### 5.3 Spin and statistics

Particles with 1/2 integer spin are fermions (examples: electrons, proton, quarks, neutrons); these are “matter particles.” Particles with integer spin are bosons (examples: photon, gluons, phonons, Higgs); these are “force carriers.” For two indistinguishable (spin \(\frac{1}{2}\)) electrons, the possible (allowable) spin-states are:

- \(|\uparrow\rangle_1 |\uparrow\rangle_2\),
- \(\frac{1}{\sqrt{2}} (|\uparrow\rangle_1 |\downarrow\rangle_2 + |\downarrow\rangle_1 |\uparrow\rangle_2)\),
- \(|\downarrow\rangle_1 |\downarrow\rangle_2\),
- \(\frac{1}{\sqrt{2}} (|\uparrow\rangle_1 |\downarrow\rangle_2 - |\downarrow\rangle_1 |\uparrow\rangle_2)\).

The first three of the above are symmetric under interchange of 1,2: this group is called a spin triplet. The last state is antisymmetric, and is called a spin singlet state. The complete wavefunction of these two electrons must be antisymmetric, therefore we have these possibilities:

- \(\psi_- (\vec{x}_1, \vec{x}_2) \times [\text{triplet state}]\),
- \(\psi_+ (\vec{x}_1, \vec{x}_2) \times [\text{singlet state}]\),

where \(\psi_-\) must be antisymmetric, and \(\psi_+\) symmetric.
As another example, consider quarks: spin $\frac{1}{2}$, with 3 ‘colors’ (green, blue, and red). It turns out that quarks must ‘exist’ in combinations that are ‘color neutral.’ Hence, the following is an example of an allowable state of 3 quarks:

$$\psi_{\text{symm}}(\vec{x}_1, \vec{x}_2, \vec{x}_3) \times (|\downarrow\rangle_1, |\downarrow\rangle_2, |\downarrow\rangle_3)$$

$$\times (|rgb\rangle - |grb\rangle + |gbr\rangle - |rbg\rangle + |brg\rangle - |bgr\rangle); \quad (93)$$

the spatial and spin parts are symmetric, which imply that the color part must be antisymmetric (there, it is a color singlet that is antisymmetric under interchange of any two quarks) such that the wavefunction as a whole is antisymmetric. The above combination corresponds to a color neutral particle with charge $2e$ and spin $\frac{3}{2}$.

### 5.4 Exchange forces (Griffiths 5.1.2)

Suppose there are two possible position states an electron can be in: $\psi_a(\vec{x})$ and $\psi_b(\vec{x})$. A system with two indistinguishable electrons can either be in a symmetric or antisymmetric position state:

$$\psi_{\pm} = (\psi_a(\vec{x}_1) \psi_b(\vec{x}_2) \pm \psi_b(\vec{x}_1) \psi_a(\vec{x}_2)).$$

We can calculate the mean square distance between the two electrons to be:

$$\langle (\vec{x}_1 - \vec{x}_2)^2 \rangle = \langle \psi_\pm | (\vec{x}_1 - \vec{x}_2)^2 | \psi_\pm \rangle = \langle \vec{x}^2 \rangle_a + \langle \vec{x}^2 \rangle_b - 2\langle \vec{x} \rangle_a \cdot \langle \vec{x} \rangle_b \mp 2|\langle \vec{x} \rangle_{ab}|^2,$$

where $\langle \vec{x}^2 \rangle_{a,b} = \langle \psi_{a,b} | \vec{x}^2 | \psi_{a,b} \rangle$, $\langle \vec{x} \rangle_{ab} = \langle \psi_a | \vec{x} | \psi_b \rangle$. Evidently, $\langle (\vec{x}_1 - \vec{x}_2)^2 \rangle$ is smaller if the spatial wavefunction is symmetric.

### 5.5 Solids: Fermi energy

Consider a free Fermi gas of $N$ noninteracting electrons in a cubic box with side length $L$. The Hamiltonian for this system is:

$$H = \sum_j \frac{p_j^2}{2m}, \quad \text{where } j = 1, 2, 3 \text{ for } x, y, z. \quad (94)$$

Recall that the energy eigenstate for one electron ($N = 1$) can be solved by separation of variables:

$$\psi_{x,y,z} = \left(\frac{2}{L}\right)^{3/2} \sin(k_x x) \sin(k_y y) \sin(k_z z), \quad (95)$$

where $k_{x,y,z} = \frac{n_{x,y,z}\pi}{L}$, $n_{x,y,z} = 1, 2, 3, \ldots$. The eigenenergies are

$$E_{1\text{-particle}} = \frac{\pi^2 \hbar^2}{2mL^2}\left(n_x^2 + n_y^2 + n_z^2\right). \quad (96)$$

Now, consider the states in $k$-space (momentum space). In this space, the eigenstates are situated on a lattice, occupying the sites: $(k_x, k_y, k_z) = \frac{2\pi}{L}(n_x, n_y, n_z)$. 15
The distance between each site is uniformly \( \frac{\pi}{L} \), so each ‘cube’ of the lattice has volume \( \frac{\pi^3}{L^3} \). We see from the form of the eigenstates in Eq. 95, that a complete, linearly independent basis of the Hilbert space that represents all the physical states of this system is obtained by including only states with \( n_{x,y,z} > 0 \). Therefore, we consider only states occupying the positive octant of \( k \)-space.

For a system with \( N \) \textit{noninteracting} electrons in the same box, the wavefunction is separable with respect to each electron, and the states in \( k \)-space accessible for each electron are identical to those accessible to an electron that occupies this box alone. Each of these momentum states can be occupied by no more than \textit{two} electrons (spin degree of freedom) according to the Pauli Exclusion Principle. So, these \( N \) electrons must ‘fill’ the cubic lattice in the positive octant of \( k \)-space. Usually, we are concerned with the case where \( N \) and \( L \) are both very large (many, say \( 10^{23} \) electrons, occupying a box much greater than their typical wavelengths). In such a case, we can approximate a continuum of states in \( k \)-space.

The lowest energy configuration, or ground state, of this Fermi gas is one where the electrons fill the \( \frac{N}{2} \) lowest energy states: in other words, they fill an octant of a sphere (centered at \( \vec{k} = 0 \)) with a radius defined as \( k_F = \frac{\pi}{L} n_F \), with the corresponding energy, \( E_F = \frac{\hbar^2 k_F^2}{2m} \), known as the \textbf{Fermi energy}. Given \( N \) and \( L \), we can compute \( E_F \):

\[
N = 2 \left( \frac{1}{8} \right) \left( \frac{4}{3} \pi n_F^3 \right) = \frac{\pi n_F^3}{3}; \tag{97}
\]

(the factor of 2 is for the two spin states; \( \frac{1}{8} \), for considering only one octant in \( k \)-space), so

\[
E_F = \frac{\hbar^2 \pi^2}{2m} \left( 3\pi^2 \rho \right)^{\frac{3}{2}}, \tag{98}
\]

where \( \rho \equiv \frac{N}{V} \).

We see that the Fermi energy depends on the density, not the volume, of the gas. The total energy of the gas is:

\[
E_{\text{tot}} = 2 \left( \frac{\hbar^2 \pi^2}{2mL^2} \right) \sum_{|\vec{n}| \leq n_F} \vec{n}^2, \tag{99}
\]

where \( \vec{n} = (n_x, n_y, n_z) \). This can be approximated as (assuming \( N \) and \( L \) very large):

\[
E_{\text{tot}} = 2 \left( \frac{\hbar^2 \pi^2}{2mL^2} \right) \int_{\text{octant}} \vec{n}^2 \, d\vec{n}. \tag{100}
\]

The integral in \( \vec{n} \) equals \( \int_0^{n_F} \frac{4\pi n^2}{3} \, dn = \frac{\pi}{3} n_F^3 \), where \( 4\pi n^2 \, dn \) is the volume of a spherical shell at radius \( n \). Thus,

\[
E_{\text{tot}} = \frac{\hbar^2 \pi^3}{10mL^2} n_F^5 = \frac{\hbar^2}{10\pi^2 m} \left( \frac{3\pi^2 N}{V} \right)^{\frac{3}{2}}. \tag{101}
\]

We note that \( E_{\text{tot}} \) scales with volume, i.e. it is an \textit{extensive property}.
5.5.1 Degeneracy pressure

A Fermi gas has a pressure even at zero temperature, because particles “don’t want to be on top of each other.” This is known as degeneracy pressure. Suppose $N$ is fixed; if we try to compress the box, we will need to put energy into the system: all wave numbers have to increase ($k_n x / L$), so the electrons become more energetic. The pressure is defined as the partial derivative of the energy with respect to volume, keeping total number of states and $N$ constant:

$$ P = - \left( \frac{\partial E}{\partial V} \right)_{S,N}. $$

So for the Fermi gas,

$$ P_{\text{degeneracy}} = \left( \frac{3}{2} \pi \right)^{\frac{3}{2}} \frac{\hbar^2}{\rho^2} \frac{2}{5} m. $$

As expected, the degeneracy pressure is an intensive property. If both the volume and the shape of the box were changed, then there will be small correction terms that get smaller as $V$ gets bigger.

5.6 Bose gas (i.e. Photon gas)

The energy of a photon is

$$ E_k = \hbar c | \vec{k} | = \hbar \omega. $$

Only two spin states, corresponding to two polarizations perpendicular to the direction of motion, occur for the photon (despite the fact that it is a spin 1 particle). The number of photons is not a conserved quantity, but instead depends on the temperature.

Consider a state with $N$ photons in a box with side lengths $L$. Let the number of photons with wavenumber $\vec{k} = \frac{\pi}{L} \vec{n}$ be $N(\vec{n}) = N(\vec{k})$. Then,

$$ N = \sum_{\vec{n}} N(\vec{n}), $$

and the total energy of the photon gas is:

$$ E_{\text{tot}} = \sum_{|\vec{n}|} \hbar \omega (\vec{n}) N(\vec{n}) = \sum_{|\vec{n}|} \frac{\hbar c \pi}{L} |\vec{n}| N(\vec{n}). $$

Now, let us digress for a moment to consider a string of length $L$, held fixed at both ends. The shape of the string as a function of time is described by $u(x, t)$:

$$ u(x, t) = \sum_{n=1}^{\infty} q_n(t) \sin \left( \frac{\pi}{L} nx \right), $$
where \( \sin \left( \frac{\pi}{L} nx \right) \) are the normal modes of the string. The equation of motion for \( q_n(t) \) is

\[
\frac{d^2}{dt^2} q_n(t) = -\omega_n^2 q_n(t),
\]

where \( \omega_n = \frac{n\pi}{L} c \), where \( c \) is the velocity of sound in the string. 

(As a homework exercise, show that

\[
\frac{1}{c^2} \frac{\partial^2}{\partial t^2} u(x, t) = \frac{\partial^2}{\partial x^2} u(x, t)
\]

has solutions of the form:

\[
u(x, t) = f_+ (x - ct) + f_- (x + ct).
\]

The Hamiltonian of the string is

\[
H = \sum_{n=1}^{\infty} \left( \frac{p_n^2}{L} + \frac{L}{4} \omega_n^2 q_n^2 \right),
\]

where \( p_n \) = momentum of \( q_n = \frac{L}{2} \dot{q}_n \), from Hamilton’s equations. The quantization postulate is, of course, \([p_n, q_n] = i \hbar \delta_{nm}\). The string is like a set of infinite harmonic oscillators, with frequencies \( \omega_n = \frac{n\pi}{L} c \), where \( n = 0, 1, 2, \ldots \).

Let \( N(n) \) be the excitation level of the harmonic oscillator with frequency \( \omega_n \). As an operator, \( N(n) = a_n^\dagger a_n \). Recall the usual commutation relations between the creation and annihilation operators:

\[
[a_n^\dagger, a_m] = \delta_{nm}.
\]

In terms of these operators, the Hamiltonian is

\[
H = \sum_n \hbar \omega_n \left( N(n) + \frac{1}{2} \right).
\]

In other words, \( a_n^\dagger \) creates a phonon of frequency \( \omega_n \), and \( N(n) \) counts the number of phonons of frequency \( \omega_n \). We can call this system of the excited string a phonon gas in 1 + 1 dimensions (space+time). We can apply what we have done so far to a photon gas, by defining \( c \) to be the speed of light. In that case, the formula gives the total energy for the photon gas, if we ignore a factor of 1/2. Photons can be considered excitation of harmonic oscillators: the excitation level \( N(n) \) is equivalent to the number of photons with frequency \( \omega_n \).

6 September 30th, 2004

6.1 Quantization of the electromagnetic field (Griffiths 5.4.4)

Emission of photons:

\[
\vec{A}(\vec{x}, t) \sim \sqrt{n} \vec{E} e^{i(k \cdot \vec{x} - \omega t)},
\]

18
where $\epsilon$ is the polarization.

**Spontaneous emission** ($n = 0$): although $n = 0$, fields still present, just as there is energy in the ground state of a harmonic oscillator.

**Stimulated emission** ($n > 0$): atom interacts with photons (i.e. EM fields) to emit photons.

Absorption of photons:

$$\vec{A}(\vec{x},t) \sim \sqrt{n}\epsilon e^{i(\vec{k} \cdot \vec{x} - \omega t)}$$

### 6.2 Planck blackbody spectrum

In an empty box, the temperature determines the number of photons, $N$, present inside it. The expected number of photons of a given mode with frequency $\omega$ at temperature $T$ is

$$\langle N(\omega) \rangle = \frac{1}{e^{\frac{\omega}{k_B T}} - 1} \times 2,$$

where the factor of 2 accounts for the two polarizations. Note that there may many modes (or states) with the same frequency (or energy). The thermal expectation value of a quantity $A$ is

$$\langle A \rangle = \sum_n \langle n | A | n \rangle e^{\frac{E_n}{k_B T}},$$

where the sums are over all energy eigenstates. Recall, from the harmonic oscillator, that $N = a^\dagger a$; as an exercise, show that

$$\langle N(\omega) \rangle = \frac{1}{e^{\frac{\omega}{k_B T}} - 1}.$$

### 6.3 Planck Spectrum

The average number of photons per unit volume with frequency between $\omega$ and $\omega + d\omega$

$$\rho(\omega) d\omega$$

equals $\langle N(\omega) \rangle$, from above, times the number of photon states at that frequency (i.e. density of states for non-interacting particles in a box). Thus,

$$\rho(\omega) d\omega = \frac{1}{e^{\frac{\omega}{k_B T}} - 1} \left( \frac{L^3}{c^3 \pi^3} \right) \pi \omega^2 \left( \frac{1}{L^3} \right) =$$

$$= \frac{\omega^2}{\pi^2 c^3} \left( \frac{1}{e^{\frac{\omega}{k_B T}} - 1} \right).$$

The energy density is $h\omega \rho(\omega)$:

$$\frac{h\omega^3}{\pi^2 c^3} \left( \frac{1}{e^{\frac{\omega}{k_B T}} - 1} \right).$$

19
6.4 Thermal distributions

There are three thermal distributions according to the statistical properties of different particles:

\[
n(\varepsilon) = \begin{cases} 
  e^{-(\varepsilon-\mu)/k_B T}, & \text{Maxwell-Boltzmann (distinguishable particles),} \\
  \frac{1}{e^{(\varepsilon-\mu)/k_B T}-1}, & \text{Bose-Einstein (bosons),} \\
  \frac{1}{1-e^{-(\varepsilon-\mu)/k_B T}}, & \text{Fermi-Dirac (fermions),}
\end{cases}
\]  

(122)

where \(n(\varepsilon)\) is the thermal expectation of the number of particles with energy \(\varepsilon\) in each case, and \(\mu\) is the chemical potential. Note that for fermions, \(n(\varepsilon) \leq 1\) always, which is consistent with the exclusion principle. The Fermi-Dirac distribution at \(T = 0\) is a step function that drops abruptly to zero at \(\varepsilon = \mu\):

\[
n_{FD}(\varepsilon) = \begin{cases} 
  1, & \varepsilon < \mu, \\
  0, & \varepsilon > \mu.
\end{cases}
\]  

(123)

Here, the chemical potential is called the Fermi energy. In the ground state of a Fermi gas, particles fill the lowest energy states (obeying the exclusion principle) up to the Fermi energy. For finite temperatures, fermions have thermal energy and some will have total energy about that of the Fermi level.

Using the Maxwell-Boltzmann distribution, we can find the energy of \(N\) distinguishable particles in a box, at temperature \(T\). The number of particles in a box of volume \(V\) is:

\[
N = \int_0^\infty dk \frac{4\pi k^2}{8} \frac{V}{\pi^3} e^{-\left(\frac{\varepsilon^2}{2m} - \mu\right)/k_B T} = V e^{\mu/k_B T} \left(\frac{mk_B T}{2\pi \hbar^2}\right)^{\frac{3}{2}}.
\]  

(124)

The total energy of the gas is:

\[
E = \int_0^\infty dk \frac{4\pi k^2}{8} \frac{V}{\pi^3} e^{-\left(\frac{\varepsilon^2}{2m} - \mu\right)/k_B T} \frac{\hbar^2 k^2}{2m} = \frac{3}{2} NkT.
\]  

(125)

which is the familiar result for a low density, monatomic ideal gas.

6.5 White dwarf (Griffiths: Problem 5.3.1)

This problem asks us to compute the total energy (energy of electrons + gravitational energy) of a white dwarf star. Let \(N=\) number of nucleons, \(q=\) number of electrons per nucleon, \(m=\) electron mass, \(M=\) nucleon mass, and \(R=\) radius of star. The Fermi energy of the electrons is:

\[
E_F = \frac{\hbar^2 \pi^2}{2mV^{2/3}} n_F^2.
\]  

(126)
where \( k_F = \frac{\pi}{n_F} \). The total energy of the electrons can be found by integrating up to the Fermi energy:

\[
E_{\text{electrons}} = \frac{\hbar^2 \pi^2}{10mV^{2/3}n_F^5}.
\]

(127)

where \( n_F \) is related to the total number of electrons as follows:

\[
Nq = \frac{24\pi}{3} n_F^3.
\]

(128)

Thus, the energy of the electrons can be written as:

\[
E_{\text{electrons}} = \frac{\hbar^2 (3\pi Nq)^{5/3}}{10\pi^2 m^{2/3}R^2}.
\]

(129)

Notice that this energy scales as \( \frac{1}{R^2} \). This is reasonable: as the star gets larger, wavelengths that "fit" in the "box" get longer so that more levels at lower energies become available. This energy also scales with the electron density, \( \rho = Nq/V \):

\[
E_{\text{electrons}} = \frac{\hbar^2 (3\pi \rho)^{5/3}V}{10\pi^2 m^2},
\]

(130)

which means that, even in a very big start, electrons locally notices a change in the size of the star (which changes \( \rho \)).

We now want to calculate the gravitation energy assuming uniform mass distribution, \( \rho_{\text{mass}} \):

\[
E_{\text{grav}} = -G\rho_{\text{mass}}^2 \int_0^R dr \frac{4\pi r^2 \left( \frac{4}{3} \pi r^3 \right)}{r} = -\frac{16}{15} G\rho_{\text{mass}}^2 \pi^2 R^5.
\]

(131)

This can be written in terms of the total (nucleon) mass of the star, \( \frac{4\pi}{3} \rho_{\text{mass}} R^3 = NM \):

\[
E_{\text{grav}} = -\frac{3}{5} GN^2 M^2 R.
\]

(132)

The total energy of the white dwarf is the sum of the electron energy and the gravitational energy; it has the following dependence on \( R \):

\[
E_{\text{tot}}(R) = \frac{A}{R^2} - \frac{B}{R}
\]

(133)

where \( A \) and \( B \) are constants of \( R \). From this \( E_{\text{tot}}(R) \), we can find the size of the star that minimizes the energy.
7 October 5th, 2004

7.1 Band Structure

Consider an electron interacting with nuclei in a solid (crystal lattice). The hamitonian for the electron is:

\[ H = \frac{\vec{p}^2}{2m} + V(\vec{x}), \] (134)

where \( V(\vec{x}) \) is a periodic potential. Consider a 1-D case, \( V(\vec{x}) = V(x) \). The potential has a discrete translational symmetry:

\[ V(x) = V(x + a), \] (135)

unlike the free electron hamiltonian, which has a continuous translational symmetry. The operator \( T_a : x \rightarrow x + a \) commutes with the hamiltonian; it is therefore possible to simultaneously diagonalize \( T_a \) and \( H \). Consider an eigenfunction, \( \psi(x) \), of \( T_a \):

\[ T_a \psi(x) = \psi(x + a) = \lambda_a \psi(x). \] (136)

In general,

\[ T_{a+b} = T_a T_b \Rightarrow \lambda_{a+b} = \lambda_a \lambda_b, \] (137)

similarly,

\[ \psi(x + Na) = \lambda^N \psi(x), \] (138)

which implies that

\[ |\lambda_a| = 1, \] (139)

because the wavefuncton cannot grow exponentially when translated. We can write the eigenvalue as

\[ \lambda_a = e^{ika}. \] (140)

Recall that the momentum operator, \( p \), generates infinitesimal translation in \( x \); for a free particle, \( [H, p] = 0 \), and so \( H \) is symmetric with respect to such a translation. For a particle in a potential with periodicity \( a \), the hamiltonian is symmetric with respect to a discrete translation by \( a \), generated by \( T_a \).

**Bloch’s Theorem**: In a periodic potential, we can take \( \psi(x + a) = e^{ika} \psi(x) \).

The crystal momentum here takes values from \(-\frac{\pi}{a}\) to \(\frac{\pi}{a}\). Since \( V(x) \) is periodic, we can write it as a Fourier Series:

\[ V(x) = \sum_{m=-\infty}^{\infty} V_m e^{i\frac{2\pi m}{a} x}. \] (141)

So we can consider the crystal momentum as contributing to the potential: when acted on \( \psi(x) \), \( T_a \) changes the momentum by an amount proportional to \( \frac{2\pi m}{a} \).

Example: "Dirac’s Comb" Consider the following periodic potential,

\[ V(x) = -\sum_{n=-\infty}^{\infty} V_0 \delta(x - na), \quad V_0 > 0. \] (142)
We would like to solve for the eigenfunctions, $\psi(x)$, given:

\[
H\psi(x) = E\psi(x), \quad \psi(x + a) = e^{ika}\psi(x).
\]  

Before solving this, we can take a look at the Fourier transform of the potential $\tilde{V}(q)$ to give some insight into the problem.

\[
\tilde{V}(q) = \int_{-\infty}^{\infty} dx e^{iqx} V(x) = \sum_{n=-\infty}^{\infty} V_0 e^{inaq} = \sum_{m=-\infty}^{\infty} V_0 \delta(q - \frac{2\pi m}{a}).
\]

We see that in momentum space, the potential is quantized in $2\pi/a$ due to the periodicity; we thus expect this momentum quantization in the wavefunctions as well. Let’s start with considering the function in the interval $0 < x < a$, where $H = \frac{p^2}{2m} = -\hbar^2 2m \frac{\partial^2}{\partial x^2}$. The eigenenergy is:

\[
E = \frac{\hbar^2 q^2}{2m}.
\]

The wavefunction and its derivative for $0 < x < a$ are

\[
\psi(x) = A \cos qx + B \sin qx, \\
\psi'(x) = -Aq \sin qx + Bq \cos qx.
\]

For $-a < x < 0$, we use Bloch’s Theorem to write the wavefunction:

\[
\psi(x) = e^{-ika}\psi(x + a) = e^{-ika}(A \cos q(x + a) + B \sin q(x + a)) = e^{-ika}(-Aq \sin q(x + a) + Bq \cos q(x + a)).
\]

Now we shall make use of the boundary conditions at $x = 0$:

1) continuity : $\psi_+(0) = \psi_-(0)$,

2) near $x=0$ : the first derivative of $\psi(x)$ is discontinuous

\[
\frac{d^2}{dx^2} \delta(x) (\psi'_+(0) - \psi'_-(0)) ;
\]

so that from the SE,

\[
\left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} - V_0 \delta(x) \right] \psi(x) = E\psi(x),
\]
we obtain

\[ \frac{\hbar^2}{2m} (\psi'_+(0) - \psi'_-(0)). \] (150)

So we have these equations:

\[ e^{-ika} (A \cos qa + B \sin qa) = A \]
\[ \Rightarrow A (e^{ika} - \cos qa) = B \sin qa; \] (151)
\[ \frac{\hbar^2 q}{2m} (e^{-ika} (-A \sin qa + B \cos qa) - B) = V_0 A \]
\[ \Rightarrow B (e^{-ika} \cos qa^{-1}) = A \left( \frac{2mV_0}{\hbar^2 q} + e^{-ika} \sin qa \right) \] (152)

Multiplying Eq. 151 and Eq. 152, we get:

\[ \cos qa - \frac{mV_0}{\hbar^2 q} \sin qa = \cos ka. \] (153)

If we choose a momentum \( q \), then 3) gives us \( k(q) \), the corresponding crystal momentum. Now, there exists values for \( q \) for which no \( k \) exists, since

\[ \cos qa - \frac{mV_0}{\hbar^2 q} \sin qa > 1. \] (154)

The result are "bands", or allowed regions in the energy spectrum for the particle to exist in.

8 October 7th, 2004

Midterm announcement: Oct. 21st, will cover Griffiths Ch. 1-4, 5(all except 5.2), 9.1(next week)

8.1 Remark on the Variational Principle

We shall not discuss this topic in detail. The main idea: sometimes we can’t solve \( H \), so we guess a ground state, and take the \( \langle H \rangle \) of that function, which we know must be greater than the actual ground state energy.

8.2 Band Structure continued

From last lecture, we arrived at the following results for the “Dirac Comb” problem:

\[ \cos qa - \frac{mV_0}{\hbar^2 q} \sin qa = \cos ka, \]
\[ E = \frac{\hbar^2 q^2}{2m}. \] (155)
where $k$ is the ‘crystal momentum’, and $E$ is the energy of the state. Recall that in the interval $0 < x < a$, the wave function takes the form:

$$\psi(x) = A \cos qx + B \sin qx, \quad 0 < x < a;$$  \hfill (156)

if $q$ is purely real, then the function as written above represents a *scattering state*. Alternatively, we can write:

$$\psi(x) = A' \cosh \kappa x + B' \sinh \kappa x, \quad 0 < x < a,$$

where $q = ik$; this represents a *bound state*, with energy $E = -\frac{\hbar^2 \kappa^2}{2m} < 0$. In this case, the boundary conditions yield the following relation:

$$\cosh \kappa a - \frac{mV_0}{\hbar^2 \kappa} = \cos \kappa a.$$  \hfill (158)

Consider now $N$ points in a lattice (with periodic boundary conditions), where there is attractive delta-function at each lattice site. The crystal momentum $k$ in this case takes values $\frac{2\pi m}{Na}$, where $m$ is an integer from $-N/2$ to $N/2$ (to see this, consider the eigenvalues of the operator $T_a : x \rightarrow x + a$). In this case, there will be $N$ energy levels in the 1st band (i.e. $2N$ electrons can occupy this band, taking into considering spin degree of freedom). If the lattice has two conducting electrons per ‘atom,’ then the first band will be filled, and the system behaves as an *insulator* because it will cost energy to excite electrons to overcome the gap of forbidden energy states. If the lattice has only one electron per lattice site, the first band will be half-filled so that electrons require little energy to excite and become ‘mobile’ – hence the system behaves as a conductor.

### 8.3 Quantum Hall Effect (reference: Gasiorowicz)

Consider the electrons confined in a slab of material extended in the $x-y$ plane, subject to the following electric and magnetic fields (we will ignore interactions with atoms):

$$\vec{E} = E\hat{y}, \quad \vec{B} = B\hat{z}. $$  \hfill (159)

The current density, $\vec{J}$, caused by the fields is:

$$\vec{J} = \sigma_0 \left( \vec{E} + \frac{\vec{v}}{c} \times \vec{B} \right) =$$

$$= -n_e e \vec{v},$$  \hfill (160)

where $n_e = \sigma_0/e$ is the electron density. From these, we get:

$$\vec{J} = \sigma_0 \left( \vec{E} - \frac{\vec{J} \times \vec{B}}{en_ee} \right) \Rightarrow$$

$$J_x = -\frac{\sigma_0 B}{en_ee} J_y, \quad J_y = \sigma_0 E_y + \frac{\sigma_0 B}{n_e ec} J_x.$$  \hfill (161)
Recall that solving the SE for an electron in \( \vec{B} = B\hat{z} \) gave us Landau levels with energies
\[
E_n = \hbar \omega_L (n + \frac{1}{2}), \quad \omega_L = \frac{eB}{mc} \text{ (Larmor frequency)}. \quad (162)
\]
From our homework, we found that the number of states, \( N \), in the lowest Landau Level \( n = 0 \) for a slab with length \( l \) and width \( w \) is:
\[
N = lw \frac{eB}{2\pi \hbar c}. \quad (163)
\]
We can define a “filling factor”, \( f \):
\[
n_e = fn_{\text{max}}, \quad n_{\text{max}} = \frac{N}{lw} = \frac{eB}{2\pi \hbar c}, \quad (164)
\]
which gives the number of filled bands, so that, if \( f > 1 \), the levels above the lowest Landau level begin to fill. The energy spectrum is composed of levels separated by \( \hbar \omega_L \), each of which has degeneracy \( N \). Experimentally, \( f \) is varied by changing \( n_{\text{max}} \) (i.e. changing \( B \)). In this experiments, we observe that for \( f = 1, 2, 3, \ldots \), i.e. as the Landau levels are filled,
\[
\frac{j_x}{E_y} \rightarrow 0, \quad \frac{j_x}{E_y} = -\frac{fe^2}{\hbar}. \quad (165)
\]
If \( j_x \) is finite, this means that \( j_y = 0 \). Also, since \( j_x = -\frac{eB}{n_e c} j_y \), the conductivity \( \sigma_0 \) is infinite. On the other hand, since \( n_e = \frac{E_y}{\hbar c} \) and \( j_y = \sigma_0 (E_y + \frac{\hbar}{fe} j_x) \), with \( j_x = -\frac{fe^2}{\hbar} E_y \), this implies that the conductivity \( \sigma \) vanishes.

In other words, it costs energy to kick electrons from one Landau level to the next when an integer number of bands are filled. On the other hand, the electric field causes all the electrons to move in the same \((x)\) direction. The vanishing of the resistance occurs because the atoms want to change the electron’s energy, but they cannot, because they’d have to kick electrons into the next higher Landau levels.

### 8.4 Symmetries in QM

**Symmetry transformation \( \Rightarrow \) conserved quantity \( \Rightarrow \) generator of the symmetry**

Examples of possible symmetries: Time-translations \( \Rightarrow H \) is time-independent), translations, rotations. We know that for any operator \( A \) which does not explicitly depend on time, \( \frac{\partial A}{\partial t} = i \hbar [H, A] \). This a statement that the Hamiltonian is a “generator” of time translations.

On the other hand, if \( A \) depends on time, \( \frac{\partial A}{\partial t} = i \frac{\hbar}{\tau} [H, A] + \frac{\partial A}{\partial \tau} \). Thus, if \( H \) depends on time, energy is not conserved, while if \( H \) is time-independent, energy (eigenvalues of \( H \)) are conserved.

If \( H \) does not depend on \( x \), this means translation symmetry in the \( x \) direction, so that \([p_x, H] = 0 \) and \( p_x \) is conserved. Noting that
\[
e^{i\vec{p}\cdot\vec{r}} f(x) = f + a \frac{\partial f}{\partial x} + \frac{a^2}{2} \frac{\partial f}{\partial x}^2 + \frac{a^3}{6} \frac{\partial f}{\partial x}^3 + \ldots = f(x + a), \quad (166)
\]
we see that the operator $T_a = e^{i \hbar p_x a}$, acts as $T_a f(x) = f(x + a)$. We also have that $T_a^\dagger = e^{-i \hbar p_x a}$ and $T_a^\dagger f(x) = f(x - a)$. In this sense, $p_x$ is the “generator” of translations in $x$.

The situation is similar with rotations. Consider the rotation matrix

$$R_z(\theta) = \begin{pmatrix} \cos \theta & -\sin \theta & 0 \\ \sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{pmatrix};$$  \hspace{1cm} (167)

its action on a vector is given by

$$R_z \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} \cos \theta x - \sin \theta y \\ \sin \theta x + \cos \theta y \\ z \end{pmatrix},$$  \hspace{1cm} (168)

and it can be represented as $R_z(\theta) = e^{i \theta L_z}$, if $H$ is rotation invariant around the $z$-axis, where

$$L_z = \hbar i \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix};$$  \hspace{1cm} (169)

in the spin-1 representation of the rotation group. The previous relation between $R_z$ and $L_z$ can be seen by starting at the definition of $\hat{L}_z := x\hat{p}_y - y\hat{p}_x$. This implies the following commutation relation

$$[\hat{L}_z, \begin{pmatrix} \hat{x} \\ \hat{y} \\ \hat{z} \end{pmatrix}] = \hbar i \begin{pmatrix} -\hat{y} \\ \hat{x} \\ 0 \end{pmatrix} = \hbar i \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \hat{x} \\ \hat{y} \\ \hat{z} \end{pmatrix}. \hspace{1cm} (170)$$

In other words, $L_z$ is the infinitesimal “generator” of rotations about the $z$-axis. In terms of operators, if we define the rotation operator as $\hat{R}_z(\theta) = e^{i \theta \hat{L}_z}$, then the action of this operator is equivalent to rotation:

$$\hat{R}_z^\dagger(\theta) \begin{pmatrix} \hat{x} \\ \hat{y} \\ \hat{z} \end{pmatrix} \hat{R}_z(\theta) = R_z(\theta) \begin{pmatrix} x \\ y \\ z \end{pmatrix}. \hspace{1cm} (171)$$

9 October 12th, 2004

What is a quantum jump? First, as an aside, if we were all in energy eigenstates, we would all just be sitting here looking at each other changing our phases — it would not be very interesting.

Consider, the process of a neutron undergoing beta decay, producing a proton, an electron and a neutrino. This is possible because the neutron is not an eigenstate of the full Hamiltonian of nature. This Hamiltonian can be seen as $H = H_0 + H_1(t)$, where the first term is the “free/unperturbed” part, and the second term is the “interaction”. Thus, we have to work with time dependent perturbation theory.
Consider a 2-state system, e.g. an atom that can be in either an excited or the ground state. These states and their eigenstates are

\[ \psi_a, \psi_b, \quad H_0 \psi_a = E_a \psi_a, \quad H_0 \psi_b = E_b \psi_b, \]

the states are chosen to be orthonormal, while an arbitrary state at the initial time can be decomposed as

\[ \psi(t = 0) = c_a \psi_a + c_b \psi_b, \quad |c_a|^2 + |c_b|^2 = 1. \]

(173)

Solving the Schrödinger Equation with \( H_0 \) is easy

\[ \psi(t) = c_a \psi_a e^{-i \omega_a t} + c_b \psi_b e^{-i \omega_b t}, \quad \omega_a = \frac{E_a}{\hbar}, \omega_b = \frac{E_b}{\hbar}. \]

(174)

However, we want to solve the full Schrödinger Equation:

\[ i \hbar \frac{\partial}{\partial t} \psi = (H_0 + H_1(t)) \psi \]

(175)

We start with the following “Ansatz”:

\[ \psi(t) = c_a(t) \psi_a e^{-i \omega_a t} + c_b(t) \psi_b e^{-i \omega_b t}, \]

(176)

since we can always write \( \psi(t) \) as a linear combination of \( \psi_a \) and \( \psi_b \). We extract the factor \( e^{i \omega t} \), because we want the coefficients \( c_a, c_b \) to be time-independent, if we turn off the perturbation.

Substituting this Ansatz to the Schrödinger Equation, we find

\[ (i \hbar \frac{\partial}{\partial t} - H_0) \psi = H_1 \psi \]

(177)

\[ i \hbar \left[ \frac{\partial c_a(t)}{\partial t} \psi_a e^{-i \omega_a t} + \frac{\partial c_b(t)}{\partial t} \psi_b e^{-i \omega_b t} \right] = H_1 (c_a(t) \psi_a e^{-i \omega_a t} + c_b(t) \psi_b e^{-i \omega_b t}). \]

(178)

Introducing the notation

\[ \langle \psi_a | H_1 | \psi_b \rangle = H'_{ab}(t), \]

(179)

we take the inner product of the Schrödinger Equation with \( \bar{\psi}_a \) and \( \bar{\psi}_b \) to get

\[ i \hbar \frac{\partial}{\partial t} c_a = c_a H'_{aa} + c_b H'_{ab} e^{-i (\omega_b - \omega_a) t}, \]

(180)

together with a similar equation for \( c_b \). Now, we make the simplifying assumptions that \( H'_{aa} = H'_{bb} = 0 \), and define \( \omega_0 = \omega_b - \omega_a \); for radiation of photons this is not really an assumption, since there \( H' \) corresponds to emission/absorption, which by definition change the state of the atom. If we are interested in another physical system, such that the assumption is non-trivial, we can avoid making it, with the main change being in the definition of \( \omega_0 \).
Using the above assumption, the evolution equations take the form:

\[
\dot{c}_a = -i \frac{\hbar}{\hbar} H'_{ab} e^{-i\omega_0 t} c_b, \quad (181)
\]

\[
\dot{c}_b = -i \frac{\hbar}{\hbar} H'_{ba} e^{i\omega_0 t} c_a. \quad (182)
\]

We see immediately, that if the system starts in \( \psi_a \), at a later time there’s a finite probability that it could be in \( \psi_b \). \( H'_{ba} \) is “responsible for a quantum jump”, \( H' \) can act on \( \psi_a \) and produce \( \psi_b \).

Example: If \( H' \) is time independent, these equations still say that a system that starts in \( \psi_a \), it can end up in \( \psi_b \). Assume that at time \( t = 0 \), \( c_a = 1 \) and \( c_0 = 0 \), and that \( H'_{ba} = \epsilon = \text{constant} \). Then

\[
c_b = -\frac{\epsilon}{\hbar \omega_0} (e^{i\omega_0 t} - 1), \quad (183)
\]

to 1st order, because \( c_a = 1 \). Note that \( |c_b|^2 \) is non-zero because \( \psi_a, \psi_b \) are not eigenstates of total \( H \), so we are describing time evolution in the wrong basis (couldn’t have gotten the right matrix by diagonalizing the perturbation).

Example: Neutrino oscillations. There are 3 neutrinos: \( |\nu_e\rangle, |\nu_{\mu}\rangle, |\nu_{\tau}\rangle \), but for simplicity we will consider only 2 of them. Thus, a neutrino can start as \( \nu_e \) and later become \( \nu_{\mu} \); this can be detected because they interact differently with matter (protons and neutrons). To study neutrinos in free space, the form

\[
\frac{i\hbar}{\hbar} \frac{\partial \psi}{\partial t} = \frac{p^2}{2m} \psi, \quad (184)
\]

of the Schroedinger Equation is not useful, because neutrinos are highly relativistic. A more correct version of the SE is

\[
\frac{i\hbar}{\hbar} \frac{\partial \psi}{\partial t} = \sqrt{p^2 c^2 + m^2 c^4} \psi; \quad (185)
\]

in the ultra-relativistic regime \( (p^2 \gg m^2) \) with \( c = 1 \), we expand the kinetic energy as

\[
\sqrt{p^2 c^2 + m^2 c^4} = |p| + \frac{m^2}{2|p|} + \ldots . \quad (186)
\]

Thus, the SE takes the form

\[
\frac{i\hbar}{\hbar} \frac{\partial \psi}{\partial t} = (|p| + \frac{m^2}{2|p|}) \psi. \quad (187)
\]

Here the \( m^2 \) is a 2 \( \times \) 2 matrix acting on the Hilbert space spanned by \( |\nu_e\rangle, |\nu_{\mu}\rangle \); thus the \( m^2 \) matrix mixes the states (it is not diagonal).

Let \( |\nu_1\rangle, |\nu_2\rangle \) be eigenstates of \( m^2 \). In general, we will have

\[
|\nu_e\rangle = \cos \theta |\nu_1\rangle + \sin \theta |\nu_2\rangle, \quad (188)
\]

\[
|\nu_{\mu}\rangle = -\sin \theta |\nu_1\rangle + \cos \theta |\nu_2\rangle; \quad (189)
\]
if $\theta = 0$, then $\nu_e$ stays $\nu_e$, and $\nu_\mu$ stays $\nu_\mu$ — $\theta$ is called the mixing angle. It belongs to the particle properties of the neutrinos: it affects how the particle interacts with matter, as well as how it propagates (through its appearance in the solution of the SE). Our definition of $|\nu_e\rangle, |\nu_\mu\rangle$ depend on how they interact with matter. We can change the basis to states that are eigenstates of Hamiltonian (which determines how they propagate). Quarks are the same way, but we have named them the other way: we gave the name “charm” to a particular mass, but sometimes the charm quark interacts like a strange quark.

Question: what is the probability that a neutrino that starts as $|\nu_e\rangle$ will later turn into $|\nu_\mu\rangle$? We start at $t = 0$ with $\psi(t) = |\nu_e\rangle$; then the probability that at time $t$ the particle is $\nu_\mu$ is given by computing

$$\psi(t) = e^{-i|\mathbf{p}|t/\hbar}(\cos \theta e^{-i\frac{\mathbf{m}_1^2t}{2\hbar}|\nu_1\rangle + \sin \theta e^{-i\frac{\mathbf{m}_2^2t}{2\hbar}|\nu_2\rangle}),$$

and taking the square of the transition amplitude:

$$\text{Prob.} = |\langle \nu_\mu | \psi(t) \rangle|^2 = \sin^2(2\theta) \sin^2 \left(\frac{\delta M t}{2}\right),$$

where

$$\delta M = \frac{m_1^2 - m_2^2}{2\hbar |\mathbf{p}|}.$$ 

In the sun, neutrinos are slowed down by their interactions, so that they effectively have an index of refraction. The electron neutrino has a larger index of refraction, because it interacts more with matter. As it oscillates, though, the index of refraction changes. This is shown in the figure below: because the energy levels can’t cross, they change (MSW effect).

The time dependence of the muon neutrino is given by

$$\nu_\mu = e^{-i|\mathbf{p}|t/\hbar}(-\sin \theta e^{-im_1^2t/2\hbar}|\nu_1\rangle + \cos \theta e^{-im_2^2t/2\hbar}|\nu_2\rangle),$$

while the transition amplitude equals

$$\langle \nu_\mu | \psi(t) \rangle = -\sin \theta \cos \theta + \sin \theta \cos \theta = 0.$$ 

Returning to the general case, we attempt to solve the linear system

$$\dot{c}_a = -\frac{i}{\hbar} H'_{ab} e^{-i\omega_0 t} c_b,$$

$$\dot{c}_b = -\frac{i}{\hbar} H'_{ba} e^{i\omega_0 t} c_a,$$

to the first order in perturbation theory. We start by expanding the coefficients as

$$c_a(t) = c_a^{(0)}(t) + c_a^{(1)}(t) + \ldots,$$

$$c_b(t) = c_b^{(0)}(t) + c_b^{(1)}(t) + \ldots.$$
Assume that the 0th order solution implies that \( c_a^{(0)} = 1, c_b^{(0)} = 0 \); then to 1st order

\[
\dot{c}_a^{(1)} = 0, \quad \dot{c}_b^{(1)} = -\frac{i}{\hbar} H'_{ba}(t) e^{i\omega_0 t} \cdot 1,
\]

so that

\[
c_b^{(1)}(t) = -\frac{i}{\hbar} \int_0^t H'_{ba}(t') e^{i\omega_0 t'} dt'.
\]

Comment: recall the Schroedinger and Heisenberg pictures. Another useful picture is the Dirac (or interaction) picture, where the Hamiltonian is decomposed as \( H = H_0 + H_1 \), and the vectors and operators in the Hilbert space transform as

\[
|\psi_D\rangle = e^{\frac{i}{\hbar} H_0 t} |\psi_S\rangle, \quad A_D = e^{\frac{i}{\hbar} H_0 t} A_S e^{-\frac{i}{\hbar} H_0 t}.
\]

The above transformations are unitary, meaning that

\[
\langle \psi_D | A_D | \psi_D\rangle = \langle \psi_S | A_S | \psi_S\rangle.
\]

Both operators and states evolve in time:

\[
\frac{\partial}{\partial t} A_D(t) = \frac{i}{\hbar} [H_D, A_D], \quad \frac{\partial}{\partial t} |\psi_D\rangle = H'_D |\psi_D\rangle.
\]

Note if the interaction vanishes, the Dirac wavefunction is identical to the Heisenberg wavefunction. These equations imply that the time evolution equation for the wavefunction in the Dirac picture can be written as

\[
\psi_D(t) = c_a(t) |\psi_a\rangle_S + c_b(t) |\psi_b\rangle_S.
\]

10 October 14th, 2004

Let’s summarize the definitions for the Dirac picture:

\[
H = H_0 + H_1(t), \quad |\psi\rangle_0 = e^{\frac{i}{\hbar} H_0 t} |\psi_S\rangle, \quad \frac{\partial}{\partial t} |\psi\rangle_S = H |\psi\rangle_S.
\]

The last relation implies that

\[
\frac{\partial}{\partial t} |\psi_D\rangle = \frac{\partial}{\partial t}(e^{iH_1 t/\hbar} |\psi\rangle_S) =
\]

\[
= -H^0 |\psi\rangle_0 + e^{iH_1 t/\hbar} H |\psi\rangle_S =
\]

\[
= e^{iH_1 t/\hbar} H \frac{1}{S} e^{-iH_1 t/\hbar} |\psi\rangle_D, \quad \text{(since } [H_1, H^0] \neq 0\).
\]
which can be written as
\[ i\hbar \frac{\partial}{\partial t} |\psi\rangle_D = H'_D |\psi\rangle_D, \] (213)
with
\[ H'_D = e^{iH^0 t/\hbar} \frac{1}{2} e^{-iH^0 t/\hbar}. \] (214)
Similarly, we find that
\[ i\hbar \frac{\partial}{\partial t} H'_D = i\hbar \frac{\partial}{\partial t} H'_D + [H'_D, H^0]; \] (215)
in general,
\[ i\hbar \frac{\partial}{\partial t} A_D = i\hbar \frac{\partial}{\partial t} A_D + [A_D, H^0]. \] (216)
The latter equation is easily seen to preserve the unitarity of the transformation
\[ \langle \psi_S | A_S | \psi_S \rangle = \langle \psi_D | A_D | \psi_D \rangle. \] (217)
more generally, if a quantity is independent on time and can be written as
\( f(x_D, p_D) \), then it also equals \( e^{iH^0 t/\hbar} f(x, p) e^{-iH^0 t/\hbar} \), as can be seen by substituting the definitions for \( x_D, p_D \) in the series expansion of the function \( f \). Thus, if an operator in the Schroedinger picture does not depend on time \textit{explicitly}, then it will not depend on time in the Dirac picture either. In other words, any conserved quantity relative to \( H^0 \) is the same in either picture.

Time-dependent perturbation theory: we start from the SE in the Dirac picture:
\[ i\hbar \frac{\partial}{\partial t} |\psi\rangle_D = H'_D |\psi\rangle_D, \] (218)
and write the state vector as
\[ |\psi_D\rangle = U(t) |\psi_D\rangle (0) = U(t) |\psi\rangle_H, \] (219)
where \( U \) is a unitary evolution operator called the evolution operator. This operator satisfies the evolution equation
\[ i\hbar \frac{\partial U(t)}{\partial t} = H'_D U(t). \] (220)
As an aside, we note that if \( H'_D(t) \) were actually time-independent, then \( U(t) = e^{-iH_D t}. \) Also, \([H'_D, H^0] = 0\).

When \( H'_D(t) \) does depend on time, the 0th order solution of the evolution equation for \( U \) is simply
\[ i\hbar \frac{d}{dt} U(t) = 0 \Rightarrow U(t) = 1, \] (221)
since at the initial time \( U(0) = 1 \). The 1st order solution of the evolution equation for \( U \) equals
\[ -\frac{i}{\hbar} \int_0^t H'_D(t') dt', \] (222)
and the second order equals

\[
\left( \frac{i}{\hbar} \right)^2 \int_0^t \int_0^{t'} H_D'(t')H_D''(t'')dt''dt';
\]

(223)

note that \( H_D'(t'') \) acts earlier than \( H_D'(t') \) since \( t'' < t' \). The above process can be carried to all orders, so that the whole series can be written formally as

\[
U(t) = Te^{-\frac{i}{\hbar} \int_0^t H_D'(t')dt'},
\]

(224)

where the symbol \( T \) stands for “time ordering”. The exponential should be expanded as a power series, where each operator has a time at which it acts. \( T \) means then that we should put the operator that acts earliest on the right.

Question: why do the factors \( \frac{1}{2}, \frac{1}{3} \) etc drop out of the series in the last expression. In order to see why, consider the 2nd order approximation, where the integration region equals a square \((t', t'') \in [0, t]^2\). The constraint \( t'' < t' \) describes the upper triangle in the square, so that we are including \( \frac{1}{2} \) of the square rather than integrating \( \int_0^t \int_0^t dt''dt' \).

If we differentiate the expression

\[
U(t) = Te^{-\frac{i}{\hbar} \int_0^t H_D'(t')dt'},
\]

(225)

we need to evaluate the integral at \( t \), under the constraint that “late” must be on the left. If the equation were

\[
i\hbar \frac{d}{dt} U = U(t)H_D'
\]

(226)

then we would have to invert the definition of time ordering.

10.1 1st order perturbation theory

To the 1st order we have

\[
U(t) = 1 - \frac{i}{\hbar} \int_0^t H_D'(t')dt',
\]

(227)

and

\[
|\psi\rangle_D = c_a(t)|\psi\rangle_a + c_b(t)|\psi\rangle_b.
\]

(228)

where

\[
H^0|\psi\rangle_{a,b} = E_{a,b}|\psi\rangle_{a,b}.
\]

(229)

The coefficients satisfy the evolution equations

\[
\dot{c}_a = -\frac{i}{\hbar} H_{ab}^* e^{-i\omega_0 t} c_b, \quad \dot{c}_b = -\frac{i}{\hbar} H_{ba} e^{i\omega_0 t} c_a,
\]

(230)

where

\[
\omega_0 = \frac{E_b - E_a}{\hbar},
\]

(231)
\[ H'_{ab} = \langle \psi_{a,D} | H'_S | \psi_{b,D} \rangle, \]  
(232)
so that
\[ H'_{ab} e^{-i\omega_0 t} = \langle \psi_{a,D} | H'_D | \psi_{b,D} \rangle^*. \]  
(233)

Note that the Dirac states equal the Heisenberg states to 0th order in perturbation theory.

Example: Let \( H'_{ab} = V'_{ab} \cos(\omega t) \), \( H'_{ba} = V_{ba} \cos(\omega t) \) describe a photon (E-field), and assume that \( \omega_0 > 0 \). To the 1st order in perturbation theory, \( c_a = 1 \) and \( c_b = 0 \) at \( t = 0 \). At later times,
\[
c_b(t) = -\frac{i}{\hbar} \int_0^t V_{ba} \cos(\omega t') e^{i\omega_0 t'} dt' = -\frac{i}{2\hbar} V_{ba} \int_0^t (e^{i(\omega_0 + \omega) t'} + e^{i(\omega_0 - \omega) t'}) dt' = -\frac{V_{ba}}{2\hbar} \left( \frac{e^{i(\omega_0 + \omega) t'} - 1}{\omega_0 + \omega} + \frac{e^{i(\omega_0 - \omega) t'} - 1}{\omega_0 - \omega} \right), \]  
(234)

The second term is important, because it implies a resonance. The physical system described by the above Hamiltonian has 2 energy levels, so it can be realized by for instance a 2-level atom. The last relation implies that the greatest probability of transition occurs for \( \omega \approx \omega_0 \):
\[
P_{a \rightarrow b}(t) = |c_b|^2 = \frac{|V_{ba}|^2 \sin^2 \frac{[\omega_0 - \omega] t}{2}}{\hbar^2 (\omega_0 - \omega)^2}. \]  
(235)

As \( t \to \infty \), the transition amplitude becomes more and more strongly peaked at \( \omega = \omega_0 \), and it is significant for a region of width \( 4\pi/\omega \) around that point.

The above discussion implies that because of the interaction, \( E_b \) is not stable, strictly speaking, but rather has a finite lifetime. Thus, the energy of the 2nd energy level is not quite well-defined: this is known generally as energy-time uncertainty.

Recall that for any physical quantity \( Q \) that does not depend explicitly on time, the time evolution equation becomes
\[
\frac{d}{dt} \langle Q \rangle = \frac{i}{\hbar} [H, Q] + \left( \frac{d}{dt} Q \right) = \frac{i}{\hbar} [H, Q]. \]  
(236)

Heisenberg uncertainty relation can be then written as
\[
\sigma_H^2 \sigma_Q^2 \geq \left( \frac{1}{2t} \langle [H, Q] \rangle \right)^2 = \left( \frac{\hbar}{2} \right)^2 \left( \frac{d}{dt} Q \right)^2, \]  
(237)
or
\[
\sigma_H \sigma_Q \geq \frac{\hbar}{2} \left| \frac{d}{dt} Q \right|. \]  
(238)
Denoting by $\delta t$ the amount of time for the expectation of $Q$ to change by one standard deviation,

$$\delta t \equiv \frac{\sigma_Q}{|\frac{d}{dt} \langle Q \rangle|},$$

we find that

$$\delta E \delta t \geq \frac{\hbar}{2}.$$  \hspace{1cm} (240)

In this case, $\delta t$ refers to the lifetime of the excited state. Since $\delta t \neq \infty$, $\delta E \neq 0$.

As a last note, the coefficients giving the expansion of the evolution functions,

$$c_a = c_a^{(0)} + c_a^{(1)} + c_a^{(2)} + \ldots,$$  \hspace{1cm} (241)

can be written as

$$c_a^{(0)} = 1, \quad c_a^{(1)} = 0, \quad |c_a(t)|^2 = 1 + O(\epsilon^2),$$

$$c_b^{(0)} = 0, \quad c_b^{(1)} = O(\epsilon), \quad |c_b(t)|^2 = O(\epsilon^2).$$  \hspace{1cm} (243)

11 October 19th, 2004

Consider an EM wave:

$$\vec{E}(z, t) = E_0 \cos(kz) \cos(\omega t) \vec{x},$$

$$\vec{B}(z, t) = B_0 \cos(kz) \cos(\omega t) \hat{y},$$

where $\omega = kc$ and $E_0 = B_0 c$.

The $\vec{B}$ field is not very important to the electrons in an atom, because the Lorentz force coming from $B$ is small compared to the force from $\vec{E}$.

Consider a standing wave, and put an atom at $z = 0$ so that it feels the maximum amplitude of the waves. Suppose that the wavelength $\lambda = \frac{2\pi}{k}$ is much larger than the size of the atom, so that the fact that EM wave depends on the position is not very important. Thus, expanding around $z \sim 0$, we have that the electric field approximately equals

$$\vec{E}(t) = E_0 \cos(\omega t) \vec{x} = -\nabla(E_0 \cos(\omega t)x),$$

since $\nabla x = \vec{x}$. Then the Hamiltonian of the electron can be written as

$$H = \left(\frac{\vec{p} - \frac{e}{c} \vec{A}}{2m}\right)^2 + e\phi,$$

which holds for weak enough $\vec{A}$, and where

$$e\phi = -\frac{Ze^2}{r} + eE_0 \cos(\omega t)x.$$  \hspace{1cm} (248)

We consider the second term as the perturbation Hamiltonian $H'(t)$; recall that the original Hamiltonian has the eigenfunctions $\psi_{n_l m}$,

$$H^0 \psi_{n_l m} = E_{n_l m}^0 |\psi_{n_l m}\rangle.$$  \hspace{1cm} (249)
To study absorption, suppose that at time \( t = 0 \), the electron is in the ground state, \( |\psi_0\rangle \). Then, at a later time \( t \), the state can be written as a linear combination

\[
|\psi_D\rangle = c_0(t) |0\rangle + \sum_{(n,l,m)\neq(1,0,0)} c_{nlm}(t) |\psi_{nlm}\rangle,
\]

where \( c_0(t) = 1 \) to 1st order and the rest of the coefficients are given by

\[
c_{nlm}(t) = -i \hbar \int_0^t e^{i(E_{nlm} - E_0)t'} e E_0 \cos(\omega t') \langle \psi_{nlm} | x | \psi_0 \rangle \, dt'.
\]

We see that the computation involves the matrix element of the electric dipole moment

\[
P = e \langle \psi_{nlm} | x | \psi_0 \rangle = \langle nlm | x | 0 \rangle,
\]

where the ket corresponds of course to \( n = 1, l = m = 0 \).

Let \( \omega = \frac{E_{nlm} - E_0}{\hbar} \) and assume that \( \omega \sim \omega_0 \). Then the transition amplitude equals

\[
P_{0\rightarrow nlm} = |c_{nlm}(t)|^2 = \left| \frac{E_0 P}{\hbar} \right|^2 \frac{\sin^2 \frac{(\omega_0 - \omega)t}{2}}{(\omega_0 - \omega)^2}.
\]

Note that even if \( \omega \neq \omega_0 \), it is still possible to get transition. However, for \( \omega - \omega_0 \) larger than about \( 2\pi/t \), the transition amplitude tends to 0, for large \( t \).

Recall the uncertainty principle: \( \delta E \delta t \sim \hbar/2 \). Suppose that we start with an atom at the ground state. Then, a little later, we measure the state, and we find that the atom is in the excited state, if the energy of the photons is less than \( \omega_0 \). Since we perform the measurement over a time \( t \), there is some energy uncertainty in your measuring apparatus.

Now, let us return to the case of a standing EM wave in volume \( V \),

\[
\vec{E} = E_0 \cos(kz) \cos(\omega t) \hat{x},
\]

and let us compute the total energy in the EM wave:

\[
E_{EM} = \int_V \frac{\varepsilon_0}{2} \left( \vec{E}_0^2 + \vec{B}_0^2 \right) d^3x = \frac{\varepsilon_0}{2} V E_0^2 \sim N \hbar \omega,
\]

where the last equality follows by considering the additivity of the photon energy. We see in this way that the amplitude of the field is proportional to the square root of the number of photons:

\[
E_0 = \sqrt{\frac{\hbar \omega N}{\varepsilon_0 V}}.
\]

What is really happening? The proper formula for the electric field is

\[
\vec{E} = \cos(kz) \cos(\omega t) \hat{x} \sqrt{\frac{\hbar \omega N}{\varepsilon_0 V}} (a^\dagger - a),
\]

where \( a, a^\dagger \) are the photon annihilation and creator operator, and

\[
E_0 = \sqrt{\frac{\hbar \omega N}{\varepsilon_0 V}} \langle N - 1 | (a^\dagger - a) | N \rangle.
\]
So at the moment that the electron goes from $\psi_0$ to $\psi_{nlm}$, there is one photon less in the final state. Clearly, if we consider simultaneously both the radiation field and the atom, energy is conserved.

$E_0$ is an operator, but it acts on the Hilbert space of all photons, and not on the Hilbert space of the atom.

### 11.1 Emission

Start with an excited state, and consider

$$P \equiv \langle 0 | x | nlm \rangle ;$$

what is this quantity equal to? From 1st order perturbation theory, we find as before that

$$c_{nlm}^{(0)} = 1, \quad c_{0}^{(0)} = 0, \quad |c_0(t)|^2 = \left( \frac{\epsilon_0 P}{\hbar} \right)^2 \frac{\sin^2 \frac{\omega_0 - \omega t}{2}}{\omega_0 - \omega} ,$$

where

$$E_0 = \sqrt{\frac{\hbar \omega}{2e_0 V}} [N + 1] (a^\dagger - a) |N\rangle \sim \sqrt{\frac{\hbar \omega (N + 1)}{e_0 V}} .$$

In short, we find that

$$|E_0|^2 \sim \frac{\hbar \omega}{eV} N$$

during absorption, and

$$|E_0|^2 \sim \frac{\hbar \omega}{eV} (N + 1)$$

during emission. The factor $N$ corresponds to stimulated emission, while the unit factor comes from spontaneous emission. Note that, even for $N = 0$, there is non-zero probability for emission; also, $P_{\text{stim}} = NP_{\text{spont}}$.

### 12 November 2nd, 2004 - Griffith 9.3

Consider an atom with two energy levels $E_1, E_2$ which is illuminated with a photon of energy $\omega_0$. Let

$$\omega_0 = \frac{E_1 - E_0}{\hbar} ;$$

the Hamiltonian for the system can be separated to the part describing the atom and the part describing the effect of the electromagnetic field:

$$H = H_0 + H_1 ,$$

where

$$H_0 = -eE_0 z \cos(\omega t) ;$$

here we assume that the radiation is polarized in the $z$ direction and we consider the electric field as approximately constant in the space occupied by the atom.
Under these assumptions, the probability for the transition from the ground to the excited state is given by

\[ P_{0\to 1} = |c_1|^2 = \frac{|\mathcal{P}|^2 E_0^2 \sin^2 \left( \frac{\omega_0 - \omega)t}{2} \right)}{\hbar^2 (\omega_0 - \omega)^2}, \tag{266} \]

where

\[ \mathcal{P} = e \langle \psi_1 | z | \psi_0 \rangle \tag{267} \]

is the dipole operator matrix element.

### 12.1 Incoherent perturbations

Suppose that the radiation is incident from many different directions and has different polarizations. The energy density of the electric field equals

\[ u = \frac{\varepsilon_0 E_0^2}{2}, \tag{268} \]

in terms of which the transition probability takes the form

\[ P_{0\to 1} = \frac{2u |\mathcal{P}|^2 \sin^2 \left( \frac{\omega_0 - \omega)t}{2} \right)}{\varepsilon_0 \hbar^2 (\omega_0 - \omega)^2}. \tag{269} \]

If we assume that the photons are in thermal equilibrium with a heat reservoir of temperature \(T\), then their energy density with respect to the angular frequency equals

\[ u(\omega) d\omega = \frac{\hbar \omega^3}{(e^{\hbar \omega/kT} - 1)\pi^2 c^3}, \tag{270} \]

and the transition probability is given by an integral over all possible frequencies:

\[ P_{0\to 1} = \frac{2}{\epsilon_0 \hbar^2} |\mathcal{P}|^2 \int_0^\infty \frac{\hbar \omega^3}{(e^{\hbar \omega/kT} - 1)\pi^2 c^3} \sin^2 \left( \frac{\omega_0 - \omega)t}{2} \right) d\omega \approx \frac{2}{\epsilon_0 \hbar^2} |\mathcal{P}|^2 u(\omega_0) \int_0^\infty \frac{\sin^2 \left( \frac{\omega_0 - \omega)t}{2} \right)}{(\omega_0 - \omega)^2} d\omega \approx \frac{2}{\epsilon_0 \hbar^2} |\mathcal{P}|^2 u(\omega_0) \int_{-\infty}^{\infty} \frac{\sin^2 \left( \frac{\omega_0 - \omega)t}{2} \right)}{(\omega_0 - \omega)^2} d\omega = \frac{2}{\epsilon_0 \hbar^2} |\mathcal{P}|^2 u(\omega)? \tag{271} \]

where the second equality follows because the factor \( \frac{\sin^2 \left( \frac{\omega_0 - \omega)t}{2} \right)}{(\omega_0 - \omega)^2} \) is large only at \( \omega \approx \omega_0 \) — this approximation becomes better for larger \( t \).

This can be seen as a special case of Fermi’s Golden Rule, since the rate of transition is given

\[ \rho = \frac{\pi}{\epsilon_0 \hbar^2} |\mathcal{P}|^2 u(\omega_0), \tag{272} \]
(if we also integrate over all polarization directions, we must multiply this expression by 1/3).

In conclusion, the probability for an atom to absorb a photon is given by

$$P_{0 \rightarrow 1} = \frac{\pi^2}{\epsilon_0 \hbar^2} |P|^2 u(\omega_0). \quad (273)$$

This probability increases, of course, if more photons are present.

The converse probability can be separated into two parts:

$$P_{1 \rightarrow 0} = P_{1 \rightarrow 0}^{\text{spont}} + P_{1 \rightarrow 0}^{\text{stim}}. \quad (274)$$

From the problem set, we have seen that

$$P_{1 \rightarrow 0}^{\text{stim}} = P_{0 \rightarrow 1}^{\text{abs}} = \langle n \rangle_{\text{thermal}} P_{1 \rightarrow 0}^{\text{spont}}, \quad (275)$$

where

$$\langle n \rangle_{\text{thermal}} = \frac{1}{e^{\hbar \omega/kT} - 1}. \quad (276)$$

12.2 Dipole

The dipole matrix element $\mathcal{P} = e \langle \psi_1 | z | \psi_0 \rangle$ is zero unless certain “selection rules” are met. For the hydrogen atom, the wavefunction for a given eigenstate can be separated as

$$\psi(r, \theta, \phi) = \Psi_{nlm}(r) Y_{lm}(\theta, \phi), \quad (277)$$

where the states $Y_{lm}$ (also denoted by $|lm\rangle$) are eigenstates of the angular momentum operator:

$$L^2 |lm\rangle = \hbar^2 l(l+1) |lm\rangle, \quad (278)$$

$$L_z |lm\rangle = \hbar m |lm\rangle. \quad (279)$$

The ground state is given by $n = 1, l = m = 0$, while the 1st excited state can be either an s-wave, $n = 2, l = m = 0$, or a p-wave, $n = 2, l = 1, m = \pm 1, 0$. In general, recall that the quantum numbers $l, m$ satisfy

$$0 \leq l \leq n, \quad -l \leq m \leq l, \quad (280)$$

so that there are $2l + 1$ $Y$’s for a given $l$.

12.3 Selection rules

The general matrix element $\mathcal{F} = -e \langle nlm | \vec{x} | n'lm' \rangle$ can be non-zero, i.e. a radiative transition is possible, if and only if

$$\delta l \equiv |l' - l| = 1, \quad \delta m \equiv |m' - m| = 0, 1. \quad (281)$$

This can be understood if we take into account that the photon has intrinsic angular momentum, i.e. spin, equal to 1.
13 November 4th, 2004

13.1 Fermi’s Golden Rule

This rule only applies for a perturbation which is constant in time, i.e. we are considering standing waves in a box. Examples of processes described by this rule are absorption, spontaneous emission and stimulated emission of a photon by an atom. The formula describing all these processes is

\[ R_{a \rightarrow b} = \frac{\pi}{3\epsilon_0 \hbar^2} |P|^2 \rho_{\text{Planck}}(\omega_0), \]  

where

\[ \omega_0 = \frac{E_1 - E_0}{\hbar}. \]

More generally, we have that

\[ R_{a \rightarrow b} = \frac{2\pi}{\hbar} |V_{fl}|^2 \rho(\omega), \]

where \( V_{fl} \) is the matrix element of the interaction Hamiltonian between the initial and final state, \( \rho(\omega) \) is the density of the photon states of energy \( \omega \), and

\[ \rho_{\text{Planck}} = \frac{\hbar}{\pi^2 c^3} \omega^3 e^{\omega/kT} - 1 \]

is the energy density per unit volume and unit frequency. Note that

\[ \rho_{\text{Planck}} = \hbar \omega \rho(\omega) V \langle n(\omega) \rangle, \]

where \( \rho(\omega) \) is the number of photon states per unit frequency, so that

\[ \rho(\omega) = \frac{V}{\pi^3} \frac{\omega^2}{c^3} = \frac{V}{\pi^2} \frac{\omega^2}{c^3}. \]

13.2 Einstein relations

Consider a number of atoms that can exist in either the ground or an excited state, and interacting with a gas of photons. If the two states have energies \( E_a < E_b \) and the number of atoms in each state is \( N_a, N_b \), we have the following differential equation that describes the evolution of the system with time

\[ \frac{\partial N_b}{\partial t} = -AN_b - B_{ba} \rho_{\text{Planck}}(\omega) N_b + B_{ab} \rho_{\text{Planck}}(\omega) N_a, \]

where the first term describes the spontaneous emission, the second term the stimulated emission, and the last term absorption of photons.

When the system reaches thermal equilibrium,

\[ \frac{\partial N_b}{\partial t} = 0, \]

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while the Gibbs distribution implies that

$$N_b \frac{N_a}{N_b} = e^{-(E_b - E_a)/kT}. \quad (290)$$

These equation imply that

$$A = \frac{\hbar \omega^3}{\pi e^4} B_{ba} = \hbar \omega \rho(\omega) B_{ba}, \quad (291)$$

so that the evolution equation takes the form

$$\partial N_b/\partial t = -B_{ba} \hbar \omega \rho(\omega) \frac{V}{3\epsilon_0 \hbar^2} (1 - (n(\omega))_b + (n(\omega))_a); \quad (292)$$

note that at zero temperature, we have $(n(\omega)) = 0$.

The previous relation can be understood by using Fermi’s Golden Rule:

$$A = R_{b \rightarrow a} = \frac{2\pi}{\hbar} |V_{fl}|^2 \rho(\omega) = \hbar \omega \rho(\omega) B_{ba} = \hbar \omega \frac{\rho(\omega)}{V} \frac{\pi}{3\epsilon_0 \hbar^2} |\mathcal{P}|^2 \quad (293)$$

where we used the fact that

$$R_{a \rightarrow b} = \frac{\pi}{3\epsilon_0 \hbar^2} |\mathcal{P}|^2 \rho(\omega) = B_{ab} \rho(\omega). \quad (294)$$

Recall that the dipole moment matrix element $\mathcal{P} = e \langle \psi_{nlm} | x | n_0 l_0 m_0 \rangle$ is only non-zero if $\delta m = 0, 1$. To prove this, we start with the commutation relations

$$[L_z, z] = 0, \quad i\hbar [L_z, x] = -y, \quad i\hbar [L_z, y] = x; \quad (295)$$

we then take the matrix element of this relations:

$$0 = \langle nlm | [L_z, z] | n_0 l_0 m_0 \rangle = \hbar (m_1 - m_0) \langle nlm | z | n_0 l_0 m_0 \rangle, \quad (296)$$

which implies that $\langle nlm | z | n_0 l_0 m_0 \rangle \neq 0$ only if $m_1 = m_0$. Similarly,

$$-\frac{\hbar}{i} \langle nlm | y | n_0 l_0 m_0 \rangle = \langle nlm | [L_z, x] | n_0 l_0 m_0 \rangle = \hbar (m_1 - m_0) \langle nlm | x | n_0 l_0 m_0 \rangle, \quad (297)$$

and

$$\frac{\hbar}{i} \langle nlm | x | n_0 l_0 m_0 \rangle = \langle nlm | [L_z, y] | n_0 l_0 m_0 \rangle = \hbar (m_1 - m_0) \langle nlm | y | n_0 l_0 m_0 \rangle = \frac{\hbar}{i} (m_1 - m_0)^2 \langle nlm | x | n_0 l_0 m_0 \rangle, \quad (298)$$

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so that either \((m_1 - m_0)^2 = 1\) or \(\langle nlm | x | n_0l_0m_0 \rangle = 0\).

Note that these selection rules are only valid to 1st order, meaning that higher order transitions are still allowed. However, they happen with much reduced rate, and are effectively suppressed.

As mentioned above, an “explanation” of the selection rules comes from the fact that the photon has spin 1. Thus, if the original atom had angular momentum \(l_1\) and absorbs a photon with angular momentum \(l_0 = 1\), the final state can have angular momentum \(l_2\) which according to the rules for the addition of angular momenta is constrained to take values in \(|l_0 - l_1|, \ldots, l_0 + l_1\).

As mentioned above the selection rules are accurate only to the 1st order.

The approximation that we used above, that \(e^{i\mathbf{k} \cdot \mathbf{r}} = 1\) holds only in the dipole approximation. The magnetic part only affects the electron because it is moving. In order for the resulting force to be comparable to that due to the electric field, the velocity of the electron has to be of the order of the speed of light. Thus, in general, the magnetic effect is much smaller than the electric effect. The transition caused by the corresponding term in the Hamiltonian is called the magnetic dipole transition. If we don’t assume that the electric field is constant in space, we get the quadrupole approximation.

### 13.3 WKB approximation

Consider a one-dimensional system described by the wavefunction \(\psi(x)\); as we know, this function obeys the Schroedinger equation

\[
\left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) \psi(x) = E\psi(x).
\]  

(299)

However, for many potentials, this equation is not exactly solvable. Suppose instead that the potential is constant; then the equation is solvable and the solutions are a linear combination of the factors \(e^{\pm ikx}\), where

\[
\frac{\hbar^2 k^2}{2m} + V = E \Rightarrow k = \frac{1}{\hbar} \sqrt{2m(E - V)}.
\]  

(300)

Returning to the general case, define a position dependent wavevector

\[
k(x) = \frac{1}{\hbar} \sqrt{2m(E - V(x))},
\]  

(301)

in terms of which the SE becomes

\[
\frac{2}{x^2} \psi(x) = k(x)^2 \psi(x).
\]  

(302)

We try to find solutions to this equation of the form

\[
\psi(x) = A(x)e^{i\phi(x)},
\]  

(303)

which implies that

\[
\frac{\partial \phi}{\partial x} = \pm k(x) \Rightarrow \phi(x) = \pm \int_0^x k(x')dx'.
\]  

(304)

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Note that this reduces to the right answer for constant \( k \).

The WKB approximation is valid when

\[
\frac{A''(x)}{A(x)} \ll k(x)^2.
\]  

(305)

In this case, we can write the solution as

\[
\psi(x) = \frac{C}{\sqrt{k(x)}} e^{\pm \int k(x') dx'} = \frac{C'}{\sqrt{p(x)}} e^{\pm \int p(x') dx'}.
\]  

(306)

The interpretation of this relation is that \( p(x) = mv(x) \) stands for the momentum of the particle at position \( x \) (like the classical case). Moreover,

\[
|\psi(x)| = \frac{|C'|^2}{p(x)},
\]  

(307)

which means that the particle has the largest probability of being at the place where it is moving slowly.

14 November 9th, 2004

We continue discussing the WKB approximation, also called the “semi-classical” approximation. This approximation is intermediate between the full SE and the Bohr-Sommerfeld interpretation, also known as the “old quantum mechanics”. The latter was first introduced in 1910, when Bohr postulated that angular momentum comes in units of \( \hbar \). He used this to justify the introduction of the Bohr-Sommerfeld quantization condition:

\[
\oint \vec{p} \cdot d\vec{r} = 2\pi n\hbar,
\]  

(308)

where the integral is to be computed over one electron orbit. This rule can be recovered from WKB. We start again from the time-independent SE:

\[
\left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) \psi(x) = E\psi(x),
\]  

(309)

which is satisfied approximately by the WKB wavefunction

\[
\psi(x) = \frac{C}{\sqrt{p(x)}} e^{\pm \int p(x') dx'}. \tag{310}
\]

Following Griffiths 8.2, we write \( \psi(x) = e^{i\phi(x)/\hbar} \), where \( \phi(x) \) can be complex. We expand this function formally,

\[
\phi(x) = \phi_0(x) + \hbar\phi_1(x) + \hbar^2\phi_2(x) + \ldots, \tag{311}
\]
and plug this into the SE to find
\[ i\hbar \phi''(x) - (\phi'(x))^2 + p^2(x) = 0, \tag{312} \]
where \( p^2(x) = 2m(E - V(x)) \). To order \( \hbar^0 \), this can be written as
\[ -(\phi_0')^2 + p^2(x) = 0 \Rightarrow \phi_0(x) = \pm p(x) \Rightarrow \phi_0(x) = \pm \int_x^p p(x')dx', \tag{313} \]
while to order \( \hbar \), we have
\[ i\hbar \phi''_0(x) - 2\hbar \phi_0'(x)\phi_0'(x) = 0 \Rightarrow \phi_1 = \frac{i}{2} \frac{\phi_0'}{\phi_0} = \frac{i}{2} \partial \log \phi_0 \partial x = \]
\[ \frac{i}{2} d \log \sqrt{\phi_0'} dx \Rightarrow \phi_1(x) = i \log \sqrt{\phi_0'}(x) + \text{const.}, \tag{314} \]
so that the wavefunction takes the form
\[ \psi(x) = e^{i\phi_0(x)}e^{i\phi_1(x)} = \frac{C}{\sqrt{\phi_0(x)}} e^{i\phi_0(x)} = \]
\[ \frac{C}{\sqrt{\pm p(x)}} e^{i \int p(x')dx'} = \frac{C}{\sqrt{|p(x)|}} e^{i \int p(x')dx'}. \tag{315} \]
This approximation is accurate if \( p(x) \) varies relatively slowly, i.e. there are many oscillations before \( p \) changes much (because \( \hbar \) is small).

For example, we consider the bumpy square well. The boundary conditions imply that \( \psi(0) = \psi(a) = 0 \). Note that the more kinetic energy the particle has, the more frequently it oscillates, and the better the WKB approximation becomes. Using this method, we can write
\[ \psi(x) = \frac{1}{\sqrt{p(x)}} \left( c_1 \sin \frac{\phi_0(x)}{\hbar} + c_2 \cos \frac{\phi_0(x)}{\hbar} \right); \tag{316} \]
the boundary condition \( \psi(0) = 0 \) implies that \( c_2 = 0 \), while the boundary condition \( \psi(a) = 0 \) implies that
\[ \frac{\phi_0(x)}{\hbar} = n\pi, \quad n = 1, 2, \ldots. \tag{317} \]
This equation can be written as
\[ \int_0^a p(x)dx = n\pi \hbar, \tag{318} \]
which is actually an equation for the energy, because of the definition of \( p \). Rewriting the above equation as
\[ \oint p(x)dx = 2n\pi \hbar, \tag{319} \]
it takes the form that Bohr used to extract the energy levels of an atom.
14.1 Tunneling

In 1928 Gamow used the WKB approximation to explain the alpha decay through the following model. An alpha particle is supposed to be trapped in the nucleus of electric charge $Z\epsilon$ by some potential that approximates the Coulomb interaction,

$$\frac{2Ze^2}{4\pi\epsilon_0 r^2}$$

for large distances, while being approximately constant and very negative for small distances less than $r_1$. The $\alpha$ particle has some non-zero probability of tunneling through the potential barrier and escaping the nucleus, which can be computed as follows. For $E < V(x)$, i.e. in the tunneling region, the momentum equals

$$p(x) = \sqrt{2m(E - V(x))} \Rightarrow |p(x)| = \sqrt{2m(V(x) - E)},$$

while the wavefunction becomes exponentially decaying

$$\psi(x) = \frac{C}{\sqrt{|p(x)|}} e^{\pm \frac{1}{\hbar} \int_{x'}^x p(x') dx'} = \frac{C}{\sqrt{|p(x)|}} e^{-\frac{1}{\hbar} \int_{x'}^x \sqrt{2m(V(x') - E)} dx'}.$$  

Normalizing the incoming wave that hits the barrier from the inside at $x = r_1$, we have that the transmission probability is given by

$$|T|^2 = \text{const.} e^{-2\gamma},$$

with

$$\gamma = \frac{1}{\hbar} \int_{r_1}^{r_2} \sqrt{2m(V(x) - E)} dx,$$

so that the transmission probability is exponentially small.

In the above computation, we dropped the positive sign in the exponential, because of the boundary condition that $\psi = 0$ at infinity. Continuing the evaluation of the transmission probability,

$$\gamma = \frac{1}{\hbar} \int_{r_1}^{r_2} \sqrt{2mE - \frac{2Ze^2}{4\pi\epsilon_0 r^2}} dx = \frac{\sqrt{2mE}}{\hbar} \int_{r_1}^{r_2} \sqrt{\frac{r_2}{r} - 1} dr \approx \frac{\sqrt{2mE}}{\hbar} \left( \frac{\pi}{2} r_2 - 2\sqrt{r_1 r_2} \right) \equiv K_1 \frac{Z}{\sqrt{E}} - K_2 \sqrt{Zr_1}.$$  

This relation is confirmed in experiments that find that the logarithm of the lifetime of a radiative nucleus is approximately inversely proportional to the square root of the energy of the emitted alpha particle.
14.2 Feynman path integral

Consider a particle moving between a position $x_0$ at time $t_0$ to a position $x_1$ at time $t_1$; what is the probability for this happening? We want to prove that the answer can be loosely written as

$$\psi = \sum_{x(t)} e^{i\frac{\hbar}{\lambda} S(x)}, \quad (326)$$

where

$$S(x) = \int_{t_0}^{t_1} L(x, \dot{x})dt \quad (327)$$

is the action for each path.

The classical path, which turns out to be the most probable path, is the one for which $S(x)$ is the minimum:

$$\delta S(x) = 0; \quad (328)$$

this leads to the Euler-Lagrange equations. The semiclassical approximation shows why the extremal path contributes the most to the path integral:

$$\psi(x) = \text{coeff.} e^{i\frac{\hbar}{\lambda} S(x_{\text{class}})} = e^{-\frac{i}{\hbar} E(t_1 - t_0) + \frac{i}{\hbar} \int_{x_0}^{x_1} \sqrt{2m(E - V(x))}dx}, \quad (329)$$

where

$$E = \frac{1}{2} m \dot{x}^2 + V(x), \quad \dot{x} = \sqrt{\frac{2}{m}(E - V(x))}. \quad (330)$$

The definition of the Lagrangian,

$$L(x, \dot{x}) = \frac{1}{2} m \dot{x}^2 - V(x), \quad (331)$$

implies that

$$L(x, \dot{x}) = 2(E - V(x)) - E, \quad (332)$$

so that the action can be written as

$$i\frac{\hbar}{\lambda} S(x) = i\frac{\hbar}{\lambda} \int_{t_0}^{t_1} L(x, \dot{x})dt =$$

$$= i\frac{\hbar}{\lambda} \int_{x_0}^{x_1} \frac{2[E - V(x)]}{dx/dt}dx - i\frac{\hbar}{\lambda} \int_{t_0}^{t_1} E dt =$$

$$= i\frac{\hbar}{\lambda} \int_{x_0}^{x_1} \sqrt{2m(E - V(x))}dx - c \frac{\hbar}{\lambda} E(t_0 - t_1). \quad (333)$$

We treat the first term in the WKB approximation, which is why it is also known as the semiclassical approximation.

In the case of tunneling, there is no classical path. If we allow, though, for the particle to move in imaginary time, then $dt$ gets a factor of $i$, which puts a negative exponential into the path integral.

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So far, we have seen how to use the WKB approximation in cases like the bumpy square well. To make more precise the use of the WKB approximation in the general case, consider a potential with a bump between the points \(x_1\) and \(x_2\). The condition in that case can be written as

\[
\int_{x_1}^{x_2} p(x) dx = \left( n - \frac{1}{2} \right) \pi \hbar,
\]

where the correction comes from a factor of \(-\frac{1}{4}\) from each side of the wall.

15.1 Scattering - Griffiths Ch. 11

If an atom absorbs, and then emits a photon, the photon is effectively scattered. For a rotationally symmetric potential, the scattered intensity leaving the target/scattering region depends on the solid angle \(\Omega\) only through the angle \(\theta\) and not through \(\phi\).

For a beam of incoming particles, the scattered particles come out in all directions. For the incoming particle, the Hamiltonian is simply

\[
H_0 = \frac{p^2}{2m},
\]

so that their wavefunction is a free particle with momentum \(\vec{\rho} = \hbar \vec{k}\),

\[
\psi_0(\vec{r}) = e^{i\vec{k} \cdot \vec{r}}.
\]

Note that in the case we are discussing, a infinite number of particles will eventually pass through the scattering region at a constant rate, so we can work with time-independent perturbation theory.

The differential cross section \(\frac{\partial \sigma}{\partial \Omega}\) is defined as the ratio of the number of particles seen by a detector at a solid angle element with the number of the particles incident per unit area on the target. Recall the definition of the probability current \(\vec{j}\):

\[
P(x) \equiv |\psi(x)|^2, \quad \frac{\partial P(x)}{\partial t} = \nabla \cdot \vec{j};
\]

for instance, if \(S\) is the surface of a sphere of volume \(V\), the rate of change of the probability to find the particle in the sphere equals the probability flowing out of the sphere

\[
\frac{d}{dt} \int_V P(x) d^3 x = \int_S \vec{j} \cdot d\vec{a}.
\]

Moreover, the probability current can be written as

\[
\vec{j} = \frac{\hbar}{2mi} (\psi^* \nabla \psi - \nabla \psi^* \psi).
\]
Example: for a free particle, $\psi_0 = e^{i\vec{k}\cdot\vec{r}}$, the probability current equals

$$\vec{j} = \frac{\hbar \vec{k}}{m},$$

(340)
which is constant, i.e. $\nabla \cdot \vec{j} = 0$. For every volume, an equal number of particles goes in and out. The probability currents tells us how many particles go through a particular volume element per unit time.

Outside the scattering region, the wavefunction has the form

$$\psi(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} + f(\theta) \frac{e^{ikr}}{r},$$

(341)

where $k = |\vec{k}|$; note that the second term is spherically symmetric — the situation is similar to that of surface waves in water.

This wavefunction solves the SE in the “vacuum” region outside the scattering domain:

$$(\nabla^2 + k^2) \psi(r) = 0.$$  (342)

In computing the probability current, if the detector is placed far from the direction of the incoming beam, we do not need to worry about cross terms between the terms $e^{i\vec{k}\cdot\vec{r}}$ and $\frac{e^{ikr}}{r}$ when finding $\vec{j}$. Thus, we have that the probability current of the scattered particles equals

$$\vec{j} = \frac{\hbar k}{m} \hat{r} \left| f(\theta) \right|^2 \frac{1}{r^2},$$

(343)
which means that the differential scattering cross section equals

$$\frac{\partial \sigma}{\partial \Omega} = \left| f(\theta) \right|^2.$$  (344)

In the scattering region, there is a localized potential $V(\vec{r})$. We look at scattering as a stationary process because there exists a continuous beam of incoming particles, so we only have to solve the time-independent SE:

$$\left( \frac{-\hbar^2 \nabla^2}{2m} + V(\vec{x}) \right) \psi(\vec{x}) = E \psi(\vec{x}),$$

(345)

where

$$E = \frac{\hbar^2 \vec{k}^2}{2m}.$$  (346)

This can be re-written as

$$\left( \nabla^2 + \vec{k}^2 \right) \psi(\vec{x}) = \frac{2mV(\vec{x})}{\hbar^2} \psi(\vec{x}),$$  (347)

where the potential term is treated as a perturbation. We can complete this calculation by using the Born approximation, which is usually good at low energies.
We start by separating the scattered term from the wavefunction,

\[ \psi(x) = \psi_0(x) + \psi_1(x), \]  

(348)

where the second term is treated as a small correction, because \( V \) is small, and the first term is the the free wave solution to the vacuum SE. Then we have that

\[ \left( \nabla^2 + k^2 \right) \psi_1(\vec{x}) = \frac{2mV(\vec{x})}{\hbar^2} (\psi_0(\vec{x}) + \psi_1(\vec{x})) \approx \frac{2mV(\vec{x})}{\hbar^2} \psi_0(\vec{x}). \]  

(349)

This equation can be solved by using the Green function, which are defined as the solution to the equation

\[ \left( \nabla^2 + k^2 \right) G(\vec{x} - \vec{y}) = \delta^3(\vec{x} - \vec{y}), \]  

(350)

where the 3-dimensional delta function is defined by the property that for all well-behaved functions \( F \),

\[ \int \delta^3(\vec{x} - \vec{y}) F(\vec{y}) d^3y = F(\vec{x}). \]  

(351)

The solution of the latter equation is given by

\[ G(\vec{x} - \vec{y}) = -\frac{e^{\pm ik|\vec{x} - \vec{y}|}}{4\pi |\vec{x} - \vec{y}|}, \]  

(352)

which for \( k = 0 \) corresponds to the Coulomb potential at \( \vec{x} \) due to a point charge at \( \vec{y} \),

\[ G(r) = -\frac{e^{ik|\vec{x} - \vec{y}|}}{4\pi |\vec{x} - \vec{y}|}. \]  

(353)

To check that the above solution is indeed the Green function, we define \( \vec{r} = \vec{x} - \vec{y} \), and compute

\[
\nabla^2 G(\vec{r}) = \nabla \cdot (\nabla G(\vec{r})) =
\]

\[
= -\frac{1}{4\pi} \nabla \cdot \left( e^{ikr} \nabla \left( \frac{1}{r} \right) + \frac{1}{r} \nabla e^{ikr} \right) =
\]

\[
= -\frac{1}{4\pi} \left( e^{ikr} \nabla^2 \left( \frac{1}{r} \right) + 2\nabla \left( \frac{1}{r} \right) \cdot \nabla e^{ikr} + \frac{1}{r} \nabla^2 e^{ikr} \right) =
\]

\[
= \delta^3(\vec{r}) + \frac{1}{4\pi} \frac{2ik}{r^2} e^{ikr} + \frac{k^2}{4\pi r} e^{ikr} - \frac{2ik}{4\pi r^2} e^{ikr} =
\]

\[
= \delta^3(\vec{r}) + \frac{k^2}{4\pi r} e^{ikr},
\]

(354)

where we used that

\[
\nabla e^{ikr} = i\vec{r} \cdot \vec{k} e^{ikr}, \quad \nabla \left( \frac{1}{r} \right) = \frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r},
\]

(355)
The solution to the equation for the wavefunction can be expressed in terms of the Green function as

\[ \psi(\vec{r}) = e^{i\vec{k} \cdot \vec{r}} + \frac{2m}{\hbar^2} \int G(\vec{r} - \vec{r}') V(\vec{r}') e^{i\vec{k} \cdot \vec{r}'} d^3r', \]  

(356)

which can be verified easily:

\[
(\nabla^2 + k^2) \psi_1(\vec{r}) = \frac{2m}{\hbar^2} \int \delta^3(\vec{r} - \vec{r}') V(\vec{r}') e^{i\vec{k} \cdot \vec{r}'} d^3r' = \frac{2m}{\hbar^2} V(\vec{r}) e^{i\vec{k} \cdot \vec{r}}.
\]

(357)

Looking back at the expression for the Green function,

\[ G(\vec{r} - \vec{r}') = \frac{e^{ik|\vec{r} - \vec{r}'|}}{4\pi|\vec{r} - \vec{r}'|}, \]

(358)

note that the variable \( \vec{r} \) refers to the position where the wavefunction is actually measured, i.e. at the detector, while \( \vec{r}' \) plays the role of the integration variable in the target region, because that is the only place where the potential does not vanish. In general, the size of the target region is much smaller than the distance of the detector from it, so that we have \( |\vec{r}| \gg |\vec{r}'| \). This implies that

\[
|\vec{r} - \vec{r}'|^2 = |\vec{r}|^2 + |\vec{r}'|^2 - 2\vec{r} \cdot \vec{r}' \approx r^2 - 2\vec{r} \cdot \vec{r}' = r^2 \left(1 - 2\frac{\vec{r} \cdot \vec{r}'}{r^2}\right) \Rightarrow |\vec{r} - \vec{r}'| \approx r \left(1 - \frac{\vec{r} \cdot \vec{r}'}{r^2}\right),
\]

(359)

so that the Green function takes the form

\[ G(\vec{r} - r\vec{r}') \approx \frac{e^{ikr} e^{-ik\cdot\vec{r}'}}{4\pi r}, \]

(360)

and the scattering amplitude takes the form of the Born approximation

\[ f(\theta) \approx -\frac{m}{2\pi \hbar^2} \int V(\vec{r}') e^{i(\vec{k} - k\hat{r}) \cdot \vec{r}'} d^3r'. \]

(361)

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In the above formula, \( \vec{k_i} = \vec{k} \) is the direction of the incoming beam, while \( \vec{k_f} = k\hat{r} \) is in the direction of the detector. The quantity

\[ \vec{k} = \hbar(\vec{k_i} - \vec{k_f}) \]

(362)
equals the change in the momentum due to the scattering of a single particle, and is also called the “momentum transfer”. Also, note that the correction to the original wavefunction looks like a matrix element from 1st order time-dependent perturbation theory:

\[ U(t) = 1 - i \frac{\hbar}{\hbar} \int_0^t e^{iH_0t'} V(t') e^{-iH_0t'} dt'. \]  

(363)

The limit of this expression as \( t \to \infty \) can be seen as the Born approximation, since

\[ U(\infty) = 1 - i \frac{\hbar}{\hbar} \int_0^\infty e^{iH_0t'} V(t') e^{-iH_0t'} dt'. \]  

(364)

and

\[ \int_0^\infty e^{\pm A} = -i \frac{\hbar}{A}. \]  

(365)

Returning to the geometry of the scattering problem, note that the initial and final momenta form a triangle bisected by the momentum transfer vector, so that its magnitude is given by

\[ |\vec{k}| = 2 |\vec{k}| \sin \frac{\theta}{2}. \]  

(366)

Now assume that the potential is rotationally invariant,

\[ V(\vec{r}) = V(|\vec{r}|), \]  

(367)

and choose the integration variable \( z' \) to be in the direction of \( \vec{k} \), so that

\[ \vec{k} \cdot \vec{r}' = kr' \cos \theta', \quad \int d^3\vec{r}' = 2\pi \int_0^\infty \int_0^{\pi} r'^2 \sin \theta' d\theta' dr'. \]  

(368)

Then the formula for the Born approximation simplifies to

\[ f(\theta) = -\frac{2m}{\hbar^2 \vec{k}} \int_0^\infty V(r') r' \sin(\vec{k}r') dr', \]  

(369)

with \( \vec{k} = 2k \sin \frac{\theta}{2} \).

As the first example of applying this formula, consider the Yukawa potential,

\[ V(r) = \beta e^{-\mu r}. \]  

(370)

The scattering amplitude is then given by

\[ f(\theta) = -\frac{2m\beta}{\hbar^2 \vec{k}} \int_0^\infty e^{-\mu r'} \sin(\vec{k}r') dr' = \]  

\[ = -\frac{m\beta}{i\hbar^2 \vec{k}} \int_0^\infty \left( e^{i(k-\mu)r'} - e^{-(k+\mu)r'} \right) dr' = \]  

\[ = \frac{m\beta}{i\hbar^2 \vec{k}} \left( \frac{1}{\mu - i\vec{k}} - \frac{1}{\mu + i\vec{k}} \right) = \]  

\[ = -\frac{2m\beta}{\hbar^2} \frac{1}{\mu^2 + \vec{k}^2}. \]  

(371)
As another example, consider the Coulomb potential,

\[ V(r) = \frac{q_1 q_2}{4\pi\varepsilon_0 r}, \quad (372) \]

which is equivalent to the Yukawa potential with

\[ \beta = \frac{q_1 q_2}{4\pi\varepsilon_0}, \quad \mu = 0. \quad (373) \]

Thus, we immediately see that the scattering amplitude equals

\[ f(\theta) = -\frac{m q_1 q_2}{2\pi\varepsilon_0 \hbar^2 k^2}. \quad (374) \]

The differential scattering cross section computed from this,

\[ \frac{\partial \sigma}{\partial \Omega} = |f(\theta)|^2, \quad (375) \]

describes Rutherford scattering, and is identical to the formula derived classically, if we make the identification \( \hbar k = p \).

### 16.1 Low energy scattering off a hard sphere

In this case, the potential has a hard core,

\[ V(r) = \begin{cases} \infty, & r < a \\ 0, & r > a \end{cases}, \quad (376) \]

so that the wavefunction vanishes at the boundary:

\[ \psi(a) = 0. \quad (377) \]

At low energies, the scattering amplitude is approximately a constant,

\[ f(\theta) \approx \text{const.} \equiv f_0, \quad (378) \]

and the wavefunction takes the form

\[ \psi(\vec{r}) = e^{i\vec{k} \cdot \vec{r}} + f_0 \frac{e^{ikr}}{r}. \quad (379) \]

Since

\[ (\nabla^2 + k^2) \left( \frac{e^{ikr}}{r} \right) = -4\pi \delta^3(\vec{r}) = 0 \text{ outside the sphere}, \quad (380) \]

the wavefunction we constructed above is actually an exact solution away from the origin.

At low energy, \( ka \ll 1 \), so that the exponential can be approximated as

\[ e^{ikr} \approx 1, \quad (381) \]

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at \( r = a \); the wavefunction then takes the form
\[
\psi(r = a) = 1 + f_0 \frac{e^{ika}}{a},
\] (382)
which, together with the condition in Eq. 377, implies that
\[
f_0 = -a \Rightarrow \frac{\partial \sigma}{\partial \Omega} = |f_0|^2 = a^2.
\] (383)
Integrating over all solid angles, we find that the total cross section equals
\[
\int \frac{\partial \sigma}{\partial \Omega} d\Omega = 4\pi a^2,
\] (384)
which should be compared with the cross sectional area of a sphere, \( \pi a^2 \).

As the wavevector increases, this cross section decreases, and for very high momenta, the cross section tends to the classical value \( \sigma_{\text{class}} = \pi a^2 \). Finally, note that if \( f_0 \) is constant, the wavefunction is rotationally symmetric around the origin \( (l = 0, \text{s-wave}) \).

### 16.2 Partial wave expansion

Decompose the wavefunction in spherical harmonics, by using the following expansion for the plane wave in terms of the spherical harmonics:
\[
e^{ik\hat{r} \cdot \hat{r}} = e^{ikz} = \sum_l Y_l(\theta)R_l(kr); \quad (385)
\]
the above expression is somewhat simplified with respect to the general case, because of the rotational invariance about the \( z \)-axis \( (m = 0) \). Also, the radial functions have to come from solving the differential equation
\[
(\nabla^2 + k^2) \psi = 0,
\] (386)
for the hard sphere potential.

If we consider only the s-wave, the solution is simply
\[
Y_0(\theta)R_0(kr) = \frac{e^{\pm ikr}}{r},
\] (387)
so that for general angular momentum the expansion can be written as
\[
\sin(kr) \frac{kr}{k} \quad \text{waves with } l > 0.
\] (388)
All the waves with \( l > 0 \) must satisfy
\[R_l(0) = 0, \quad (389)\]
since
\[ e^{ikr}|_{r=0} = 1, \quad \lim_{r \to 0} \frac{\sin(kr)}{kr} = 1, \quad (390) \]

For low energy, which means long wavelength, the quantity \( ka \) is small and so
\[ R_l(ka) \to 0, \quad (391) \]
for \( l > 0 \); this allows us to focus on the s-wave. In the more general case, it can be shown that \( R_l(kr) \) can be expressed in terms of the spherical Bessel functions,
\[ R_l(kr) \approx i^l j_l(kr). \quad (392) \]

Now, suppose we look only at the s-wave, so that the wavefunction looks like
\[
\psi_{\text{s-wave}}(r) = \frac{\sin(kr)}{kr} + f_0 e^{i kr} r = \frac{e^{i kr}}{r} \left( \frac{1}{2ik} + f_0 \right) - e^{-i kr} \frac{2ikr}{2ikr}; \quad (393)
\]
the first term corresponds to the “outgoing wave”, while the second term describes the “incoming wave”. In order to conserve the number of particles, the amplitude of these two waves must be the same,
\[
\left| \frac{1}{2ik} + f_0 \right|^2 = \left| \frac{1}{2ik} \right|^2 , \quad (394)
\]
which implies that
\[
|f_0| \leq \frac{1}{k}. \quad (395)
\]