Problems in Quantum Mechanics

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Stern-Gerlach Analyzers

1.1 **Projection probabilities**

Consider the following combination of Stern-Gerlach analyzers.



(The dashed line with an arrowhead points in the positive z direction.) Atoms leaving the rightmost + port are in state $|\phi+\rangle$, atoms leaving the rightmost – port are in state $|\phi-\rangle$. Show that the projection probability from $|z-\rangle$ to $|\phi+\rangle$ is $\sin^2(\phi/2)$.

1.2 Multiple analyzers

An atom of state $|z+\rangle$ is shot into the following line of three Stern-Gerlach analyzers.



What is the probability that it emerges from the + output of analyzer C? From the - output? Why don't these probabilities sum to one?

1.3 Quantum mechanics is not statistical mechanics

Find the projection probabilities from state $|z+\rangle$ to states $|30^{\circ}+\rangle$, $|30^{\circ}-\rangle$, $|x+\rangle$, and $|x-\rangle$. Find the projection probabilities from states $|30^{\circ}+\rangle$ and $|30^{\circ}-\rangle$ to $|x-\rangle$. Denote the projection probability from $|A\rangle$ to $|B\rangle$ by $PP(|A\rangle, |B\rangle)$. If we use the phrase "the probability that a system in state $|A\rangle$ is in state $|B\rangle$ " for the more precise phrase "the projection probability from $|A\rangle$ to $|B\rangle$ ", then it seems reasonable that

$$PP(|z+\rangle, |x-\rangle) = PP(|z+\rangle, |30^{\circ}+\rangle) PP(|30^{\circ}+\rangle, |x-\rangle) + PP(|z+\rangle, |30^{\circ}-\rangle) PP(|30^{\circ}-\rangle, |x-\rangle).$$

Use your numerical results to show that this expectation is wrong.

1.4 What is a basis state?

Mr. van Dam claims that a silver atom has three, not two, basic magnetic dipole states. To back up his claim, he has constructed the following "Stern-Gerlach-van Dam" analyzer out of a z Stern-Gerlach analyzer and an x Stern-Gerlach analyzer.



(The output of the x analyzer is piped to output holes A and B using atomic pipes that do not affect the magnetic dipole state.) Show that the set of exit states $\{|A\rangle, |B\rangle, |C\rangle\}$ is complete, but that $|B\rangle$ is not orthogonal to $|C\rangle$.

1.5 Analyzer loop



Atoms in state $|z+\rangle$ are injected into an analyzer loop tilted an angle θ to the z direction. The output atoms are then fed into a z Stern-Gerlach analyzer. What is the probability of the atom leaving the + channel of the last analyzer when:

- a. Branches a and b are both open?
- b. Branch b is closed?
- c. Branch a is closed?

1.6 Three analyzer loops

Atoms in state $|z+\rangle$ are passed through three analyzer loops as shown.



If all branches are open, 100% of the incoming atoms exit from the output. What percent of the incoming atoms leave from the output if the following branches are closed? (The atoms are not observed as they pass through the analyzer loops.)

 a. 1b
 d. 2a
 g. 1b and 3b

 b. 3a
 e. 2b
 h. 1b and 3a

 c. 3b
 f. 2a and 3b
 i. 1b and 3a and 2a

(Note that in going from part (h.) to part (i.) you get more output from increased blockage.)

1.7 Representations

Suppose that the representation of $|\psi\rangle$ in the $\{|z+\rangle, |z-\rangle\}$ basis is

$$\left(\begin{array}{c}\psi_+\\\psi_-\end{array}\right)$$

(i.e., $\psi_+ = \langle z + |\psi\rangle$, $\psi_- = \langle z - |\psi\rangle$). If ψ_+ and ψ_- are both real, show that there is an axis upon which the projection of μ has a definite, positive value, and find the angle between that axis and the z axis in terms of ψ_+ and ψ_- .

Photon Polarization

In lecture I have developed the principles of quantum mechanics using a particular system, the magnetic moment of a silver atom (a so-called "spin- $\frac{1}{2}$ " system), which has two basis states. Another system with two basis states is polarized light. I did not use this system mainly because photons are less familiar than atoms. This chapter develops the quantum mechanics of photon polarization much as the lectures developed the quantum mechanics of spin- $\frac{1}{2}$.

One cautionary note: There is always a tendency to view the photon as a little bundle of electric and magnetic fields, a "wave packet" made up of these familiar vectors. This view is completely incorrect. In quantum electrodynamics, in fact, the electric field is a classical macroscopic quantity that takes on meaning only when a large number of photons are present.

2.1 Classical description of polarized light



When a beam of unpolarized light passes through a sheet of perfect polarizing material (called "Polaroid" and represented by the symbol



where the arrow shows the polarizing axis), the emerging beam is of lower intensity and it is "polarized", i.e. the electric field vector undulates but points only parallel or antiparallel to the polarizing axis. When a beam of vertically polarized light (an "x-polarized beam") is passed through a sheet of ideal Polaroid with polarizing axis oriented at an angle θ to the vertical, the beam is reduced in intensity and emerges with an electric field undulating parallel to the sheet's polarizing axis (a " θ -polarized beam"). Polaroid sheet performs these feats by absorbing any component of electric field perpendicular to its polarizing axis. Show that if the incoming x-polarized beam has intensity I_0 , then the outgoing θ polarized beam has intensity $I_0 \cos^2 \theta$. Show that this expression gives the proper results when θ is 0°, 90°, 180° or 270°.

2.2 Quantal description of polarized light: Analyzers

In quantum mechanics, a photon state is described by three quantities: 1) energy, 2) direction of motion, 3) polarization. We ignore the first two quantities. There is an infinite number of possible polarization states: the photons in an x-polarized beam are all in the $|x\rangle$ state, the photons in a θ -polarized beam $(0^{\circ} \leq \theta < 180^{\circ})$ are all in the $|\theta\rangle$ state, etc. In the quantum description, when an $|x\rangle$ photon encounters a polarizing sheet oriented at an angle θ to the vertical, then either it is absorbed (with probability $\sin^2 \theta$) or else it is changed into a $|\theta\rangle$ photon (with probability $\cos^2 \theta$). A polarizing sheet is thus not an analyzer: instead of splitting the incident beam into two (or more) beams, it absorbs one of the beams that we would like an analyzer to emit. An analyzer can be constructed out of any material that exhibits double refraction. It is conventional to use a simple calcite crystal:



What are the projection probabilities $|\langle x|\theta\rangle|^2$, $|\langle x|\theta+90^\circ\rangle|^2$? Show that the states $\{|\theta\rangle, |\theta+90^\circ\rangle\}$ constitute a basis.

2.3 Interference

As usual, two analyzers (one inserted backwards) make up an analyzer loop.



Invent a series of experiments that demonstrates quantum interference. Show that the results of these experiments, and the results of problem 2.2, are consistent with the amplitudes

2.4 Circular polarization

Just as it is possible to analyze any light beam into x- and y-polarized beams, or θ - and $\theta + 90^{\circ}$ polarized beams, so it is possible to analyze and beam into right- and left-circularly polarized beams. You might remember from classical optics that any linearly polarized beam splits half-and-half into right- and left-circularly polarized light when so analyzed.



Quantum mechanics maintains that right- and left-circularly polarized beams are made up of photons in the $|R\rangle$ and $|L\rangle$ states, respectively. The projection amplitudes thus have magnitudes

$$\begin{aligned} |\langle R|\ell p\rangle| &= 1/\sqrt{2} \\ |\langle L|\ell p\rangle| &= 1/\sqrt{2} \end{aligned}$$
(2.2)

where $|\ell p\rangle$ is any linearly polarized state. By building an RL analyzer loop you can convince yourself that

$$\langle \theta | R \rangle \langle R | x \rangle + \langle \theta | L \rangle \langle L | x \rangle = \langle \theta | x \rangle = \cos \theta.$$
(2.3)

Show that no real valued projection amplitudes can satisfy both relations (2.2) and (2.3), but that the complex values

are satisfactory!

Matrix Mathematics

3.1 The trace

For any $N \times N$ matrix A (with components a_{ij}) the *trace* of A is defined by

$$tr(A) = \sum_{i=1}^{N} a_{ii}$$

Show that tr(AB) = tr(BA), and hence that tr(ABCD) = tr(DABC) = tr(CDAB), etc. (the socalled "cyclic invariance" of the trace). However, show that tr(ABC) does not generally equal tr(CBA)by constructing a counterexample. (Assume all matrices to be square.)

3.2 The outer product

Any two complex N-tuples can be multiplied to form an $N \times N$ matrix as follows: (The star represents complex conjugation.)

$$x = (x_1 \ x_2 \dots x_N)$$
$$y = (y_1 \ y_2 \dots y_N)$$
$$x \otimes y = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_N \end{pmatrix} (y_1^* \ y_2^* \dots y_N^*) = \begin{pmatrix} x_1 y_1^* & x_1 y_2^* & \dots & x_1 y_N^* \\ x_2 y_1^* & x_2 y_2^* & \dots & x_2 y_N^* \\ \vdots \\ x_N y_1^* & x_N y_2^* & \dots & x_N y_N^* \end{pmatrix}.$$

This so-called "outer product" is quite different from the familiar "dot product" or "inner product"

$$x \cdot y = (x_1^* \ x_2^* \dots x_N^*) \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{pmatrix} = x_1^* \ y_1 + x_2^* \ y_2 + \dots + x_N^* \ y_N.$$

Write a formula for the *i*, *j* component of $x \otimes y$ and use it to show that $tr(y \otimes x) = x \cdot y$.

3.3 Pauli matrices

Three important matrices are the *Pauli matrices*:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

a. Show that the four matrices $\{I, \sigma_1, \sigma_2, \sigma_3\}$, where

$$I = \left(\begin{array}{cc} 1 & 0\\ 0 & 1 \end{array}\right),$$

constitute a basis for the set of 2×2 matrices, by showing that any matrix

$$A = \left(\begin{array}{cc} a_{11} & a_{12} \\ a_{21} & a_{22} \end{array}\right)$$

can be written as

$$A = z_0 I + z_1 \sigma_1 + z_2 \sigma_2 + z_3 \sigma_3.$$

Produce formulas for the z_i in terms of the a_{ij} .

b. Show that

i.
$$\sigma_1^2 = \sigma_2^2 = \sigma_3^2 = I^2 = I$$

ii. $\sigma_i \sigma_j = -\sigma_j \sigma_i$ for $i \neq j$
iii. $\sigma_1 \sigma_2 = i\sigma_3$ (a)
 $\sigma_2 \sigma_3 = i\sigma_1$ (b)
 $\sigma_3 \sigma_1 = i\sigma_2$ (c)

Note: Equations (b) and (c) are called "cyclic permutations" of equation (a), because in each equation, the indices go in the order

and differ only by starting at different points in the "merry-go-round."

c. Show that for any complex numbers c_1, c_2, c_3 ,

$$(c_1\sigma_1 + c_2\sigma_2 + c_3\sigma_3)^2 = (c_1^2 + c_2^2 + c_3^2)I.$$

3.4 More on Pauli matrices

- a. Find the eigenvalues and corresponding (normalized) eigenvectors for all three Pauli matrices.
- b. Define exponentiation of matrices via

$$e^M = \sum_{n=0}^{\infty} \frac{M^n}{n!}.$$

Show that

$$e^{\sigma_i} = \cosh(1)I + \sinh(1)\sigma_i$$
 for $i = 1, 2, 3$

and that

$$e^{(\sigma_1 + \sigma_3)} = \cosh(\sqrt{2})I + \frac{1}{\sqrt{2}}\sinh(\sqrt{2})(\sigma_1 + \sigma_3).$$

(Hint: Look up the series expansions of sinh and cosh.)

c. Prove that $e^{\sigma_1}e^{\sigma_3} \neq e^{(\sigma_1+\sigma_3)}$.

3.5 Hermitian operators

- a. Show that if \hat{A} is a linear operator and $(a, \hat{A}a)$ is real for all vectors a, then \hat{A} is Hermitian. (Hint: Employ the hypothesis with a = b + c and a = b + ic.)
- b. Show that any operator of the form

$$\hat{A} = c_a |a\rangle \langle a| + c_b |b\rangle \langle b| + \dots + c_z |z\rangle \langle z|,$$

where the c_n are real constants, is Hermitian.

c. You know that if an operator is Hermitian then all of its eigenvalues are real. Show that the converse is false by producing a counterexample. (Hint: Try a 2×2 upper triangular matrix.)

3.6 Unitary operators

Show that all the eigenvalues of a unitary operator have square modulus unity.

3.7 Commutator algebra

Prove that

$$\begin{split} &[\hat{A}, b\hat{B} + c\hat{C}] &= b[\hat{A}, \hat{B}] + c[\hat{A}, \hat{C}] \\ &[a\hat{A} + b\hat{B}, \hat{C}] &= a[\hat{A}, \hat{C}] + b[\hat{B}, \hat{C}] \\ &[\hat{A}, \hat{B}\hat{C}] &= \hat{B}[\hat{A}, \hat{C}] + [\hat{A}, \hat{B}]\hat{C} \\ &[\hat{A}\hat{B}, \hat{C}] &= \hat{A}[\hat{B}, \hat{C}] + [\hat{A}, \hat{C}]\hat{B} \\ &[\hat{A}, [\hat{B}, \hat{C}]] &+ [\hat{C}, [\hat{A}, \hat{B}]] + [\hat{B}, [\hat{C}, \hat{A}]] = 0 \quad (\text{the "Jacobi identity"}). \end{split}$$

The Density Matrix

4.1 **Definition**

Consider a system in quantum state $|\psi\rangle$. Define the operator

$$\hat{\rho} = |\psi\rangle\langle\psi|,$$

called the *density matrix*, and show that the expectation value of the observable associated with operator \hat{A} in $|\psi\rangle$ is

 $tr\{\hat{\rho}\hat{A}\}.$

4.2 Statistical mechanics

Frequently physicists don't know exactly which quantum state their system is in. (For example, silver atoms coming out of an oven are in states of definite μ projection, but there is no way to know which state any given atom is in.) In this case there are two different sources of measurement uncertainty: first, we don't know what state they system is in (statistical uncertainty, due to our ignorance) and second, even if we did know, we couldn't predict the result of every measurement (quantum uncertainty, due to the way the world works). The density matrix formalism neatly handles both kinds of uncertainty at once.

If the system could be in any of the states $|a\rangle$, $|b\rangle$,..., $|i\rangle$,... (not necessarily a basis set), and if it has probability p_i of being in state $|i\rangle$, then the density matrix

$$\hat{\rho} = \sum_i p_i |i\rangle \langle i||$$

is associated with the system. Show that the expectation value of the observable associated with \hat{A} is still given by

 $tr\{\hat{\rho}\hat{A}\}.$

4.3 A one-line proof (if you see the right way to do it) Show that $tr\{\hat{\rho}\} = 1$.

Neutral K Mesons

You know that elementary particles are characterized by their mass and charge, but that two particles of identical mass and charge can still behave differently. Physicists have invented characteristics such as "strangeness" and "charm" to label (not explain!) these differences. For example, the difference between the electrically neutral K meson K^0 and its antiparticle the \bar{K}^0 is described by attributing a strangeness of +1 to the K^0 and of -1 to the \bar{K}^0 .

Most elementary particles are completely distinct from their antiparticles: an electron never turns into a positron! Such a change is prohibited by charge conservation. However this prohibition does not extend to the neutral K meson precisely because it is neutral. In fact, there is a time-dependent amplitude for a K^0 to turn into a \bar{K}^0 . We say that the K^0 and the \bar{K}^0 are the two basis states for a two-state system. This two-state system has an observable strangeness, represented by an operator, and we have a K^0 when the system is in an eigenstate of strangeness with eigenvalue +1, and a \bar{K}^0 when the system is in an eigenstate of strangeness with eigenvalue +1. When the system is in other states it does not have a definite value of strangeness, and cannot be said to be "a K^{0} " or "a \bar{K}^{0} ". The two strangeness eigenstates are denoted $|K^0\rangle$ and $|\bar{K}^0\rangle$.

5.1 Strangeness

Write an outer product expression for the strangeness operator \hat{S} , and find its matrix representation in the $\{|K^0\rangle, |\bar{K}^0\rangle\}$ basis. Note that this matrix is just the Pauli matrix σ_3 .

5.2 Charge Parity

Define an operator \widehat{CP} that turns one strangeness eigenstate into the other:

$$\widehat{CP}|K^0\rangle = |\overline{K}^0\rangle, \quad \widehat{CP}|\overline{K}^0\rangle = |K^0\rangle.$$

(CP stands for "charge parity", although that's not important here.) Write an outer product expression and a matrix representation (in the $\{|K^0\rangle, |\bar{K}^0\rangle\}$ basis) for the \widehat{CP} operator. What is the connection between this matrix and the Pauli matrices? Show that the normalized eigenstates of CP are

$$|K_U\rangle = \frac{1}{\sqrt{2}} (|K^0\rangle + |\bar{K}^0\rangle),$$

$$|K_S\rangle = \frac{1}{\sqrt{2}} (|K^0\rangle - |\bar{K}^0\rangle).$$

(The U and S stand for unstable and stable, but that's again irrelevant because we'll ignore K meson decay.)

5.3 The Hamiltonian

The time evolution of a neutral K meson is governed by the "weak interaction" Hamiltonian

$$\hat{H} = e\hat{1} + f\widehat{C}\widehat{P}.$$

(There is no way for you to derive this. I'm just telling you.) Show that the numbers e and f must be real.

5.4 Time evolution

Neutral K mesons are produced in states of definite strangeness because they are produced by the "strong interaction" Hamiltonian that conserves strangeness. Suppose one is produced at time t = 0 in state $|K^0\rangle$. Solve the Schrödinger equation to find its state for all time afterwards. Why is it easier to solve this problem using $|K_U\rangle$, $|K_S\rangle$ vectors rather than $|K^0\rangle$, $|\bar{K}^0\rangle$ vectors? Calculate and plot the probability of finding the meson in state $|K^0\rangle$ as a function of time.

(The neutral K meson system is extraordinarily interesting. I have oversimplified by ignoring decay. More complete treatments can be found in Lipkin, Das & Melissinos, Feynman, and Baym.)

Continuum Systems

6.1 The states $\{|p\rangle\}$ constitute a continuum basis

In lecture we showed that the inner product $\langle x|p\rangle$ must have the form

$$\langle x|p\rangle = C \ e^{i(p/\hbar)x} \tag{6.1}$$

where C may be chosen for convenience.

a. Show that the operator

$$\hat{A} = \int_{-\infty}^{\infty} dp \ |p\rangle\langle p| \tag{6.2}$$

is equal to

$$2\pi\hbar|C|^2\hat{1}\tag{6.3}$$

by evaluating

$$\langle \phi | \hat{A} | \psi \rangle = \langle \phi | \hat{1} \hat{A} \hat{1} | \psi \rangle \tag{6.4}$$

for arbitrary states $|\psi\rangle$ and $|\phi\rangle$. Hints: Set the first $\hat{1}$ equal to $\int_{-\infty}^{\infty} dx |x\rangle\langle x|$, the second $\hat{1}$ equal to $\int_{-\infty}^{\infty} dx' |x'\rangle\langle x'|$. The identity

$$\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk \ e^{ikx} \tag{6.5}$$

(see Winter eqn. (3.2-7) p. 107) for the Dirac delta function is useful here. Indeed, this is one of the most useful equations to be found anywhere!

b. Using the conventional choice $C = 1/\sqrt{2\pi\hbar}$, show that

$$\langle p|p'\rangle = \delta(p-p'). \tag{6.6}$$

The expression (6.5) is again helpful.

6.2 Peculiarities of continuum basis states

Recall that the elements of a continuum basis set are peculiar in that they possess dimensions. That is not their only peculiarity. For any ordinary state $|\psi\rangle$, the wavefunction $\psi(x) = \langle x | \psi \rangle$ satisfies

$$\int_{-\infty}^{\infty} dx \ \psi^*(x)\psi(x) = 1.$$
(6.7)

Show that the states $|x'\rangle$ and $|p\rangle$ cannot obey this normalization.

6.3 Hermiticity of the momentum operator

Show that the momentum operator is Hermitian over the space of states $|\psi\rangle$ that have wavefunction $\psi(x)$ which vanish at $x = \pm \infty$. Hint:

$$\langle \phi | \hat{p} | \psi \rangle = \int_{-\infty}^{\infty} dx \ \phi^*(x) \ \left(-i\hbar \frac{d\psi(x)}{dx} \right).$$
(6.8)

Integrate by parts.

6.4 Commutator of \hat{x} and \hat{p}

Show that $[\hat{x}, \hat{p}] = i\hbar$ by showing that $\langle \phi | [\hat{x}, \hat{p}] | \psi \rangle = i\hbar \langle \phi | \psi \rangle$ for arbitrary $| \phi \rangle$ and $| \psi \rangle$. Hints: First evaluate $\langle x|\hat{p}\hat{x}|\psi\rangle$ and $\langle x|\hat{x}\hat{p}|\psi\rangle$. It helps to define $|\chi\rangle = \hat{x}|\psi\rangle$.

6.5 Momentum representation of the Schrödinger equation You know that the Schrödinger equation

$$i\hbar \frac{d|\psi(t)\rangle}{dt} = \hat{H} |\psi(t)\rangle$$
(6.9)

has the position representation

$$i\hbar \frac{\partial \langle x|\psi(t)\rangle}{\partial t} = \langle x|\hat{H}|\psi(t)\rangle$$
(6.10)

or

$$i\hbar \ \frac{\partial\psi(x;t)}{\partial t} = -\frac{\hbar^2}{2m} \ \frac{\partial^2\psi(x;t)}{\partial x^2} + V(x) \ \psi(x;t).$$
(6.11)

In this problem you will uncover the corresponding equation that governs the time development of

$$\psi(p;t) = \langle p|\psi(t)\rangle. \tag{6.12}$$

The left hand side of equation (6.9) is no problem because

$$\langle p|i\hbar\frac{d}{dt}|\psi(t)\rangle = i\hbar \ \frac{\partial\tilde{\psi}(p;t)}{\partial t}.$$
(6.13)

To investigate the right hand side of equation (6.9) write

$$\hat{H} = \frac{1}{2m}\hat{p}^2 + \hat{V}$$
(6.14)

where \hat{p} is the momentum operator and \hat{V} the potential energy operator.

a. Use the Hermiticity of \hat{p} to show that

$$\langle p|\hat{H}|\psi(t)\rangle = \frac{p^2}{2m}\tilde{\psi}(p;t) + \langle p|\hat{V}|\psi(t)\rangle.$$
(6.15)

Now we must investigate $\langle p | \hat{V} | \psi(t) \rangle$.

b. Show that

$$\langle p|\hat{V}|\psi(t)\rangle = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dx \ e^{-i(p/\hbar)x} \ V(x)\psi(x;t)$$
(6.16)

by inserting the proper form of $\hat{1}$ at the proper location.

c. Define the (modified) Fourier transform $\tilde{V}(p)$ of V(x) by

$$\tilde{V}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dx \ e^{-i(p/\hbar)x} V(x)$$
(6.17)

$$= \int_{-\infty}^{\infty} dx \ \langle p|x \rangle V(x). \tag{6.18}$$

Note that $\tilde{V}(p)$ has funny dimensions. Show that

$$V(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dp \ e^{i(p/\hbar)x} \ \tilde{V}(p)$$
(6.19)

$$= \int_{-\infty}^{\infty} dp \langle x|p \rangle \ \tilde{V}(p).$$
(6.20)

You may use either forms (6.17) and (6.19) in which case the proof employs equation (6.5), or forms (6.18) and (6.20) in which case the proof involves completeness and orthogonality of basis states.

d. Hence show that

$$\langle p|\hat{V}|\psi(t)\rangle = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dp' \ \tilde{V}(p-p') \ \tilde{\psi}(p';t).$$
(6.21)

(Caution! Your intermediate expressions will probably involve three distinct variables that you'll want to call "p". Put primes on two of them!)

e. Put everything together to see that $\tilde{\psi}(p;t)$ obeys the integro-differential equation

$$i\hbar \ \frac{\partial\tilde{\psi}(p;t)}{\partial t} = \frac{p^2}{2m} \ \tilde{\psi}(p;t) + \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dp' \ \tilde{V}(p-p') \ \tilde{\psi}(p';t).$$
(6.22)

This form of the Schrödinger equation is particularly useful in the study of superconductivity.

The Free Particle

7.1 Energy eigenstates

In lecture we examined the behavior of a free particle in a state of definite momentum. Such states have a definite energy, but they are not the only possible states of definite energy.

a. Show that the state

$$|\rho(0)\rangle = A|p_0\rangle + B| - p_0\rangle \tag{7.1}$$

where $|A|^2 + |B|^2 = 1$ has definite energy $E(p_0) = p_0^2/2m$. (That is, $|\rho(0)\rangle$ is an energy eigenstate with eigenvalue $p_0^2/2m$).

b. Show that the "wavefunction" corresponding to $|\rho(t)\rangle$ evolves in time as

$$\rho(x;t) = \frac{1}{\sqrt{2\pi\hbar}} \left[A \ e^{i(p_0 x - E(p_0)t)/\hbar} + B \ e^{i(-p_0 x - E(p_0)t)/\hbar} \right].$$
(7.2)

I use the term wavefunction in quotes because $\rho(x;t)$ is not $\langle x | \text{normal state} \rangle$ but rather a sum of two terms like $\langle x | \text{continuum basis state} \rangle$.

c. Show that the "probability density" $|\rho(x;t)|^2$ is independent of time and given by

$$|\rho(x;t)|^{2} = \frac{1}{2\pi\hbar} [1 + 2 Re\{A^{*}B\} \cos\left(\frac{2p_{0}x}{\hbar}\right) + 2 Im\{A^{*}B\} \sin\left(\frac{2p_{0}x}{\hbar}\right)].$$
(7.3)

7.2 A useful integral

Using $\int_{-\infty}^{\infty} du \ e^{-u^2} = \sqrt{\pi}$, show that

$$\int_{-\infty}^{\infty} du \ e^{-u^2 \alpha^2/2} \ e^{iuy} = \frac{\sqrt{2\pi}}{\alpha} \ e^{-y^2/2\alpha^2}$$
(7.4)

where α may be complex, but $Re{\alpha^2} > 0$. Hint: complete the square by writing

$$-\frac{u^2\alpha^2}{2} + iuy = -\left(\frac{u\alpha}{\sqrt{2}} - i\frac{y}{\sqrt{2}\alpha}\right)^2 - \frac{y^2}{2\alpha^2}.$$

Note: If c is a real number independent of x, you know that

$$\lim_{x \to \infty} (x + c) = \infty.$$

You might think that a different limit would result if the additive constant c were complex, but in fact, that is not the case:

$$\lim_{x \to \infty} (x + ic) = \infty$$

It is not unusual for the limit of a sequence of complex numbers to be real.

7.3 A somewhat less useful integral

Given $\int_{-\infty}^{\infty} dx \ e^{-x^2} = \sqrt{\pi}$, show that

$$\int_{-\infty}^{\infty} dx \ x^2 \ e^{-x^2} = \sqrt{\pi}/2. \tag{7.5}$$

Hint: $\int_{-\infty}^{\infty} dx \ x^2 e^{-x^2} = 2 \int_{0}^{\infty} dx \ x^2 e^{-x^2}$, then integrate by parts.

7.4 Static properties of a Gaussian wavepacket

Consider the wavefunction

$$\psi(x;0) = \frac{A}{\sqrt{\sigma}} e^{-x^2/2\sigma^2} e^{i(p_0/\hbar)x}.$$
(7.6)

- a. Show that the wavefunction is properly normalized when $A = \frac{1}{\sqrt[4]{\pi}}$.
- b. Show that in this state $\langle \hat{x} \rangle = 0$ (trivial), and $\Delta x = \sqrt{\langle (\hat{x} \langle \hat{x} \rangle)^2 \rangle} = \sigma/\sqrt{2}$ (easy).
- c. Use equation (7.4) to show that

$$\tilde{\psi}(p;0) = A\sqrt{\frac{\sigma}{\hbar}} e^{-(p-p_0)^2 \sigma^2/2\hbar^2}.$$
 (7.7)

d. Hence show that $\langle \hat{p} \rangle = p_0$ and $\Delta p = \hbar/(\sqrt{2}\sigma)$.

7.5 Force-free motion of a Gaussian wavepacket

A particle with the initial wavefunction given in the previous problem evolves in time to

$$\psi(x;t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dp \ e^{i(px - E(p)t)/\hbar} \ \tilde{\psi} \ (p;0).$$
(7.8)

a. Plug in $\tilde{\psi}(p;0)$ and change the integration variable to k where $\hbar k = p - p_0$ in order to show that

$$\psi(x;t) = A \sqrt{\frac{\sigma}{2\pi}} e^{i(p_0 x - E(p_0)t)/\hbar} \int_{-\infty}^{\infty} dk \ e^{-k^2(\sigma^2 + i\frac{\hbar t}{m})/2} \ e^{ik(x - \frac{p_0}{m}t)}.$$
(7.9)

Hint: Change variable first to $p' = p - p_0$, then to $k = p'/\hbar$.

b. Define the complex dimensionless quantity

$$\beta = 1 + i \frac{\hbar t}{m\sigma^2} \tag{7.10}$$

and evaluate the integral using equation (7.4), giving

$$\psi(x;t) = A \frac{1}{\sqrt{\sigma\beta}} e^{i(p_0 x - E(p_0)t)/\hbar} e^{-(x - \frac{p_0}{m}t)^2/2\sigma^2\beta}.$$
(7.11)

c. Hence show that

$$|\psi(x;t)|^2 = \frac{A^2}{\sigma|\beta|} \ e^{-(x-\frac{p_0}{m}t)^2/(\sigma^2|\beta|^2)}.$$
(7.12)

By comparing $|\psi(x;t)|^2$ with $|\psi(x;0)|^2$, read off the results

$$\langle x \rangle = \frac{p_0}{m}t$$
, $\Delta x = \frac{\sigma|\beta|}{\sqrt{2}} = \frac{1}{\sqrt{2}} \left(\sigma^2 + \frac{\hbar^2}{\sigma^2 m^2}t^2\right)^{\frac{1}{2}}.$ (7.13)

(No computation is required!)

Potential Problems

8.1 Ground state of the simple harmonic oscillator

You may have been surprised that the lowest possible energy for the simple harmonic oscillator was $E_0 = \frac{1}{2}\hbar\omega$ and not $E_0 = 0$. This exercise attempts to explain the non-zero ground state energy in physical (semiclassical) rather than mathematical terms. It then goes on to use these ideas and the uncertainty principle to guess at a value for the ground state energy. You may abhor such non-rigorous arguments, but you must be able to do them in order to make informed guesses about the behavior of systems that are too complicated to yield to rigorous mathematical methods.

In classical mechanics the SHO ground state has zero potential energy (the particle is at the origin) and zero kinetic energy (it is motionless). However in quantum mechanics if a particle is localized precisely at the origin, and hence has zero potential energy, then it has a considerable spread of momentum values and hence a non-zero kinetic energy (or, to be precise, a non-zero expectation value for kinetic energy). The kinetic energy can be reduced by decreasing the spread of momentum values, but only by increasing the spread of position values and hence by increasing the (expected value of the) potential energy. The ground state is the state in which this trade off between kinetic and potential energies results in a minimum total energy.

Assume that the spread in position extends over some distance d about the origin (i.e. the particle will very likely be found between x = -d/2 and x = +d/2). This will result in a potential energy somewhat less than $\frac{1}{2}m\omega^2(\frac{d}{2})^2$. This argument is not intended to be rigorous, so let's forget the "somewhat less" part of the last sentence. Furthermore, a position spread of $\Delta x = d$ implies through the uncertainty principle a momentum spread of $\Delta p \ge \hbar/2d$. Continuing in our non-rigorous vein, let's set $\Delta p = \hbar/2d$ and kinetic energy equal to $\frac{1}{2m}(\frac{\Delta p}{2})^2$.

Sketch potential energy, kinetic energy and total energy as a function of d. Find the minimum value of E(d) and compare with the ground state energy $E_0 = \frac{1}{2}\hbar\omega$. (Note that if \hbar were zero, the energy minimum would be at E(d) = 0!)

8.2 Ladder operators for the simple harmonic oscillator

- a. Express \hat{x} and \hat{p} in terms of \hat{a} and \hat{a}^{\dagger} .
- b. Calculate the following simple harmonic oscillator matrix elements:

$\langle m \hat{a} n angle$	$\langle m \hat{p} n angle$	$\langle m \hat{x} \hat{p} n angle$
$\langle m \hat{a}^{\dagger} n angle$	$\langle m \hat{x}^2 n \rangle$	$\langle m \hat{p} \hat{x} n \rangle$
$\langle m \hat{x} n \rangle$	$\langle m \hat{p}^2 n \rangle$	$\langle m \hat{H} n \rangle$

- c. Show that the expectation value of the potential energy in a SHO energy eigenstate equals the expectation value of the kinetic energy in that state. (Recall that for a classical simple harmonic oscillator, the time averaged potential energy equals the time averaged kinetic energy.)
- d. Find Δx , Δp , and $\Delta x \Delta p$ for the energy eigenstate $|n\rangle$.

8.3 The infinite square well

You are no doubt familiar with the energy eigenproblem for the infinite square well, but a short review is never-the-less in order. Consider a well of width L, and place the origin at the center of the well. The mathematical problem is to find values E_n and functions $\eta_n(x)$ such that a solution to

$$-\frac{\hbar^2}{2m}\frac{d^2\eta_n}{dx^2} = E_n\eta_n(x) \tag{8.1}$$

has

$$\eta_n(-\frac{L}{2}) = \eta_n(\frac{L}{2}) = 0.$$
(8.2)

Show that the eigenvalues are

$$E_n = \frac{n^2}{2m} \left(\frac{\pi\hbar}{L}\right)^2 \quad n = 1, 2, 3, 4, \dots$$
 (8.3)

and the eigenfunctions are

$$\eta_n(x) = \begin{cases} \sqrt{\frac{2}{L}} \cos(n\pi x/L) & \text{for } n = 1, 3, 5, \dots \\ \sqrt{\frac{2}{L}} \sin(n\pi x/L) & \text{for } n = 2, 4, 6, \dots \end{cases}$$
(8.4)

Be sure to explain carefully why negative and zero values of n are not used. Note that $\eta_n(x)$ is even for n odd, odd for n even.

Bonus (research problem): I have a feeling that this problem could be solved by appropriately defined ladder operators, but I don't know how to do it. If you have a lot of time to kill, you might try to find such a solution.

8.4 Two-dimensional simple harmonic oscillator

The classical energy of a two-dimensional simple harmonic oscillator is

$$\frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{1}{2}k_x x^2 + \frac{1}{2}k_y y^2 \tag{8.5}$$

so the quantal Hamiltonian is

$$\hat{H} = \frac{\hat{p}_x^2}{2m} + \frac{1}{2}m\omega_x^2 \hat{x}^2 + \frac{\hat{p}_y^2}{2m} + \frac{1}{2}m\omega_y^2 \hat{y}^2$$

$$= \hat{H}_x + \hat{H}_y.$$

Note that any operator with subscript x commutes with any operator with subscript y. Define appropriate ladder operators \hat{a}_x , \hat{a}_x^{\dagger} , \hat{a}_y , \hat{a}_y^{\dagger} and show that a state labeled $|n, m\rangle$ is an energy eigenstate with energy

$$E_{n,m} = \hbar\omega_x \left(n + \frac{1}{2}\right) + \hbar\omega_y \left(m + \frac{1}{2}\right) \quad n, m = 0, 1, 2, 3, \dots$$
(8.6)

Show that the isotropic case $\omega_x = \omega_y$ exhibits degeneracy: there are N+1 different energy eigenstates with energy eigenvalue $\hbar\omega(N+1)$, N = 0, 1, 2, ...

Perturbation Theory for the Energy Eigenproblem

9.1 Square well with a bump

An infinite square well of width L (problem 8.3) is perturbed by putting in a bit of potential of height V and width a in the middle of the well. Find the first order energy shifts for all the energy eigenstates, and the first order perturbed wavefunction for the ground state (your result will be an infinite series). (Note: Many of the required matrix elements will vanish! Before you integrate, ask yourself whether the integrand is odd.) When a = L the perturbed problem can be solved exactly. Compare the perturbed energies with the exact energies and the perturbed ground state wavefunction with the exact ground state wavefunction.



9.2 Anharmonic oscillator

a. Show that for the simple harmonic oscillator,

$$\langle m | \hat{x}^{3} | n \rangle = \sqrt{\left(\frac{\hbar}{2m\omega}\right)^{3}} \left[\sqrt{n(n-1)(n-2)} \, \delta_{m,n-3} + 3 \sqrt{n^{3}} \, \delta_{m,n-1} \right.$$

$$+ 3 \, \sqrt{(n+1)^{3}} \, \delta_{m,n+1} + \sqrt{(n+1)(n+2)(n+3)} \, \delta_{m,n+3} \right].$$

$$(9.1)$$

b. Recall that the simple harmonic oscillator is always an approximation. The real problem always has a potential $V(x) = \frac{1}{2}kx^2 + bx^3 + cx^4 + \cdots$. The contributions beyond $\frac{1}{2}kx^2$ are called "anharmonic terms". Let us ignore all the anharmonic terms except for bx^3 . Show that to leading order the n^{th} energy eigenvalue changes by

$$-\frac{b^2}{\hbar\omega} \left(\frac{\hbar}{2m\omega}\right)^3 \quad (30n^2 + 30n + 11). \tag{9.2}$$

Note that these shifts are not "small" when n is large, in which case it is not appropriate to truncate the perturbation series at leading order. Explain physically why you don't expect the shifts to be small for large n.

9.3 Slightly relativistic simple harmonic oscillator

You know that the concept of potential energy is not applicable in relativistic situations. One consequence of this is that the only fully relativistic quantum theories possible are quantum field theories. However there do exist situations where a particle's motion is "slightly relativistic" (say, $v/c \sim 0.1$) and where the force responds quickly enough to the particle's position that the potential energy concept has approximate validity. For a mass on a spring, this situation hold when the spring's response time is much less than the period.

a. Show that a reasonable approximate Hamiltonian for such a "slightly relativistic SHO" is

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2} \, \hat{x}^2 - \frac{1}{8c^2m^3} \, \hat{p}^4.$$
(9.3)

b. Show that

$$\langle m | \hat{p}^4 | 0 \rangle = \left(\frac{m \hbar \omega}{2} \right)^2 (3 \, \delta_{m,0} - 6\sqrt{2} \, \delta_{m,2} + 2\sqrt{6} \, \delta_{m,4}).$$
 (9.4)

- c. Calculate the leading non-vanishing energy shift of the ground state due to this relativistic perturbation.
- d. Calculate the leading corrections to the ground state eigenvector $|0\rangle$.

9.4 **Two-state systems**

The most general Hamiltonian for a two state system (e.g. spin $\frac{1}{2}$, neutral K meson, ammonia molecule) is represented by

$$a_0 I + a_1 \sigma_1 + a_3 \sigma_3 \tag{9.5}$$

where a_0 , a_1 , and a_3 are real numbers and the σ 's are Pauli matrices.

- a. Assume $a_3 = 0$. Solve the energy eigenproblem. (This can be done by inspection.)
- b. Now assume $a_3 \ll a_0 \approx a_1$. Use perturbation theory to find the leading order shifts in the energy eigenvalues and eigenstates.
- c. Find the energy eigenvalues exactly and show that they agree with the perturbation theory results when $a_3 \ll a_0 \approx a_1$.

9.5 Degenerate perturbation theory in a two-state system

Consider a two state system with a Hamiltonian represented in some basis by

$$a_0 I + a_1 \sigma_1 + a_3 \sigma_3. \tag{9.6}$$

We shall call the basis for this representation the "initial basis". This exercise shows how to use perturbation theory to solve (approximately) the energy eigenproblem in the case $a_0 \gg a_1 \approx a_3$.

$$\hat{H}^{(0)} = \begin{pmatrix} a_0 & 0\\ 0 & a_0 \end{pmatrix} \quad \hat{H}' = \begin{pmatrix} a_3 & a_1\\ a_1 & -a_3 \end{pmatrix}$$
(9.7)

In this case the unperturbed Hamiltonian is degenerate. The initial basis

$$\left\{ \left(\begin{array}{c} 1\\0 \end{array}\right), \ \left(\begin{array}{c} 0\\1 \end{array}\right) \right\} \tag{9.8}$$

is a perfectly acceptable energy eigenbasis (both states have energy a_0), but the basis

$$\left\{\frac{1}{\sqrt{2}} \begin{pmatrix} 1\\1 \end{pmatrix}, \frac{1}{\sqrt{2}} \begin{pmatrix} 1\\-1 \end{pmatrix}\right\},\tag{9.9}$$

for example, is just as good.

a. Show that if the non-degenerate formula $E_n^{(1)} = \langle n^{(0)} | \hat{H}' | n^{(0)} \rangle$ were applied (or rather, misapplied) to this problem, then the formula would produce different energy shifts depending upon which basis was used!

Which, if either, are the true energy shifts? The answer comes from equation (19) of the "Derivation of Perturbation Theory" notes, namely

$$(En^{(0)} - E_m^{(0)}) \langle m^{(0)} | \bar{n}^{(1)} \rangle = \langle m^{(0)} | \hat{H}' | n^{(0)} \rangle \text{ whenever } m \neq n.$$
(9.10)

This equation was derived from the fundamental assumption that $|n(\epsilon)\rangle$ and $E_n(\epsilon)$ could be expanded in powers of ϵ . If the unperturbed states $|n^{(0)}\rangle$ and $|m^{(0)}\rangle$ are degenerate, then $E_n^{(0)} = E_m^{(0)}$ and the above equation demands that

$$\langle m^{(0)} | \hat{H} | n^{(0)} \rangle = 0$$
 whenever $m \neq n$ and $E_n^{(0)} = E_m^{(0)}$. (9.11)

If this does not apply, then the fundamental assumption must be wrong.

And this answers the question of which basis to use! Consistency demands the use of a basis in which the perturbing Hamiltonian is diagonal. (The Hermiticity of \hat{H}' guarantees that such a basis exists.)

- b. Without finding this diagonalizing basis, find the representation of \hat{H}' in it.
- c. Find the representation of $\hat{H}^{(0)}$ in the diagonalizing basis. (Trick question.)
- d. What are the energy eigenvalues of the full Hamiltonian $\hat{H}^{(0)} + \hat{H}'$? (Not "correct to some order in perturbation theory," but the exact eigenvalues!)
- e. Still without explicitly producing the diagonalizing basis, show that the states in that basis are exact energy eigenstates of the full Hamiltonian.
- f. (Optional) If you're ambitious, you may now go ahead and show that the (normalized) diagonalizing basis vectors are

$$\frac{1}{\sqrt{2}\sqrt{a_1^2 + a_3^2 - a_3\sqrt{a_1^2 + a_3^2}}} \begin{pmatrix} +a_1 \\ -a_3 + \sqrt{a_1^2 + a_3^2} \end{pmatrix} = \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix},$$
(9.12)

$$\frac{1}{\sqrt{2}\sqrt{a_1^2 + a_3^2 + a_3\sqrt{a_1^2 + a_3^2}}} \begin{pmatrix} -a_1 \\ +a_3 + \sqrt{a_1^2 + a_3^2} \end{pmatrix} = \begin{pmatrix} -\sin\theta \\ \cos\theta \end{pmatrix}, \quad (9.13)$$

where

$$\tan \theta = \frac{a_1}{a_3 + \sqrt{a_1^2 + a_3^2}}.\tag{9.14}$$

Coda: Note the reasoning of degenerate perturbation theory: We expand about the basis that diagonalizes \hat{H}' because expansion about any other basis is immediately self-contradictory, not because this basis is guaranteed to produce a sensible expansion. As usual in perturbation theory, we have no guarantee that this expansion makes sense. We do, however, have a guarantee that any other expansion does not make sense.

Perturbation Theory for the Time Development Problem

10.1 On being kicked upstairs

A particle in the ground state of an infinite square well (problem 8.3) is perturbed by a transient effect described by the Hamiltonian (in coordinate representation)

$$H'(x;t) = A_0 \sin\left(\frac{2\pi x}{L}\right)\delta(t), \qquad (10.1)$$

where A_0 is a constant with the dimensions of action. What is the probability that after this jolt an energy measurement will find the system in the first excited state?

10.2 Second-order time-dependent perturbation theory

In lecture we treated, to first order in perturbation theory, the problem of a simple harmonic oscillator in its ground state exposed to a sinusoidal external force (with frequency ω' and amplitude F_0). We concluded that the only non-vanishing first-order transition amplitudes were $c_0^{(1)}(t) = 1$ and $c_1^{(1)}(t)$. (Here the superscript (1) denotes "first-order".) Show that to second order the non-vanishing transition amplitudes are:

$$c_0^{(2)}(t) = 1 - \frac{i}{\hbar} \int_0^t H'_{01}(t') \ e^{-i\omega t'} \ c_1^{(1)}(t') dt', \qquad (10.2)$$

$$c_1^{(2)}(t) = -\frac{i}{\hbar} \int_0^t H'_{10}(t') \ e^{+i\omega t'} \ c_0^{(1)}(t') dt', \tag{10.3}$$

$$c_2^{(2)}(t) = -\frac{i}{\hbar} \int_0^t H'_{21}(t') \ e^{+i\omega t'} \ c_1^{(1)}(t') dt', \tag{10.4}$$

where

$$H'_{01}(t) = H'_{10}(t) = F_0 \sqrt{\frac{\hbar}{2m\omega}} \cos(\omega' t),$$
 (10.5)

 $\quad \text{and} \quad$

$$H_{21}'(t) = F_0 \sqrt{\frac{2\hbar}{2m\omega}} \cos(\omega' t).$$
(10.6)

The integrals for $c_0^{(2)}(t)$ and $c_2^{(2)}(t)$ are not worth working out, but it is worth noticing that $c_2^{(2)}(t)$ involves a factor of $(F_0)^2$ (where F_0 is in some sense "small"), and that $c_1^{(2)}(t) = c_1^{(1)}(t)$.

Angular Momentum

11.1 Trivial pursuit

- a. Show that if an operator commutes with two components of an angular momentum vector, it commutes with the third as well.
- b. If \hat{J}_x and \hat{J}_z are represented by matrices with pure real entries (as is conventionally the case, see problem 11.2), show that \hat{J}_y is represented by a matrix with pure imaginary entries.

11.2 Matrix representations in spin- $\frac{1}{2}$

If we are interested only in a particle's angular momentum, and not in its position, momentum, etc., then for a spin- $\frac{1}{2}$ particle the basis $\{|\frac{1}{2}, \frac{1}{2}\rangle, |\frac{1}{2}, -\frac{1}{2}\rangle\}$ spans the relevant states. These states are usually denoted simply $\{|\uparrow\rangle, |\downarrow\rangle\}$. Recall that the matrix representation of operator \hat{A} in this basis is

$$\begin{pmatrix} \langle \uparrow | \hat{A} | \uparrow \rangle & \langle \uparrow | \hat{A} | \downarrow \rangle \\ \langle \downarrow | \hat{A} | \uparrow \rangle & \langle \downarrow | \hat{A} | \downarrow \rangle \end{pmatrix},$$
(11.1)

and recall also that this isn't always the easiest way to find a matrix representation.

- a. Find matrix representations in the $\{|\uparrow\rangle, |\downarrow\rangle\}$ basis of $\hat{S}_z, \hat{S}_+, \hat{S}_-, \hat{S}_x, \hat{S}_y, \text{ and } \hat{S}^2/@$. Note the reappearance of the Pauli matrices!
- b. Find normalized column matrix representations for the eigenstates of \hat{S}_x :

$$\hat{S}_x | \rightarrow \rangle = + \frac{\hbar}{2} | \rightarrow \rangle$$
 (11.2)

$$\hat{S}_x | \leftarrow \rangle = -\frac{\hbar}{2} | \leftarrow \rangle.$$
 (11.3)

11.3 Rotations and spin- $\frac{1}{2}$

Verify explicitly that

$$| \rightarrow \rangle = e^{-i(\hat{S}_y/\hbar)(+\pi/2)} | \uparrow \rangle, \qquad (11.4)$$

$$|\leftrightarrow\rangle = e^{-i(\hat{S}_y/\hbar)(-\pi/2)}|\uparrow\rangle.$$
(11.5)

(Problems 3.3 and 3.4 are relevant here.)

11.4 Spin-1 projection amplitudes

a. (Easy.) Prove that

$$d_{m,m'}^{(j)}(\theta) = [d_{m',m}^{(j)}(-\theta)]^*.$$
(11.6)

b. Show that the $d_{m,m'}^{(j)}(\theta)$ with j = 1 are

$$\begin{array}{rcl} d_{1,1}^{(1)}(\theta) &=& +\frac{1}{2}(\cos\,\theta+1) & d_{1,0}^{(1)}(\theta) &=& -\frac{1}{\sqrt{2}}\sin\,\theta & d_{1,-1}^{(1)}(\theta) &=& -\frac{1}{2}(\cos\,\theta-1) \\ d_{0,1}^{(1)}(\theta) &=& +\frac{1}{\sqrt{2}}\sin\,\theta & d_{0,0}^{(1)}(\theta) &=& \cos\,\theta & d_{0,-1}^{(1)}(\theta) &=& -\frac{1}{\sqrt{2}}\sin\,\theta \\ d_{-1,1}^{(1)}(\theta) &=& -\frac{1}{2}(\cos\,\theta-1) & d_{-1,0}^{(1)}(\theta) &=& +\frac{1}{\sqrt{2}}\sin\,\theta & d_{-1,-1}^{(1)}(\theta) &=& +\frac{1}{2}(\cos\,\theta+1) \end{array}$$

Central Force Motion

12.1 Positronium

The "atom" positronium is a bound state of an electron and a positron. Find the allowed energies for positronium.

12.2 Operator factorization solution of the Coulomb problem

The bound state energy eigenvalues of the hydrogen atom can be found using the operator factorization method. In reduced units, the radial wave equation is

$$\left[-\frac{d^2}{d\rho^2} + \frac{\ell(\ell+1)}{\rho^2} - \frac{2}{\rho}\right] u_{n,\ell}(\rho) \equiv h_\ell \ u_{n,\ell}(\rho) = \mathcal{E}_{n,\ell} \ u_{n,\ell}(\rho).$$
(12.1)

Introduce the operators

$$D_{\pm}^{(\ell)} \equiv \frac{d}{d\rho} \mp \frac{\ell}{\rho} \pm \frac{1}{\ell}$$
(12.2)

and show that

$$D_{-}^{(\ell+1)} D_{+}^{(\ell+1)} = -h_{\ell} - \frac{1}{(\ell+1)^2}, \quad D_{+}^{(\ell)} D_{-}^{(\ell)} = -h_{\ell} - \frac{1}{\ell^2}.$$
 (12.3)

From this, conclude that

$$h_{\ell+1} D_{+}^{(\ell+1)} u_{n,\ell}(\rho) = \mathcal{E}_{n,\ell} D_{+}^{(\ell+1)} u_{n,\ell}(\rho)$$
(12.4)

whence

$$D_{+}^{(\ell+1)}u_{n,\ell}(\rho) \propto u_{n,\ell+1}(\rho)$$
(12.5)

and $\mathcal{E}_{n,\ell}$ is independent of ℓ .

Argue that for every $\mathcal{E}_{n,\ell} < 0$ there is a maximum ℓ . (Hint: examine the effective potential for radial motion.) Call this value ℓ_{\max} , and set $n = \ell_{\max} + 1$ to show that

$$\mathcal{E}_{n,\ell} = -\frac{1}{n^2}, \quad \ell = 0, \dots, n-1.$$
 (12.6)

12.3 A non-Coulombic central force

The central potential

$$V(r) = -\frac{k}{r} + \frac{c}{r^2}$$
(12.7)

is a model (albeit a poor one) for the interaction of the two atoms in a diatomic molecule. (Arnold Sommerfeld called this the "rotating oscillator" potential: see his *Atomic Structure and Spectral Lines*, 3rd ed., 1922, appendix 17.) Steven A. Klein (class of 1989) investigated this potential and found that its energy eigenproblem could be solved exactly.

- a. Sketch the potential, assuming that k and c are both positive.
- b. Following the notes "Bound State Energy Eigenproblem for Coulombic Potentials", convert the radial equation of the energy eigenproblem into

$$\left[-\frac{d^2}{d\rho^2} - \frac{2}{\rho} + \frac{\gamma + \ell(\ell+1)}{\rho^2}\right] u_{n,\ell}(\rho) = \mathcal{E}_{n,\ell} u_{n,\ell}(\rho).$$
(12.8)

where $\gamma = 2cM/\hbar^2$ and where ρ , $\mathcal{E}_{n,\ell}$, and $u_{n,\ell}(\rho)$ are to be identified.

- c. Find two values of x such that $x(x+1) = \gamma + \ell(\ell+1)$. Select whichever one will be most convenient for later use.
- d. Convince yourself that the solution described in the notes does not depend upon ℓ being an integer, and conclude that the energy eigenvalues are

$$\mathcal{E}_{n,\ell} = \frac{-1}{[n-\ell+\frac{1}{2}(-1+\sqrt{(2\ell+1)^2+4\gamma})]^2}$$
(12.9)

where n = 1, 2, 3, ... and where for each n, ℓ can take on values $\ell = 0, 1, 2, ..., n - 1$.

e. Verify that this energy spectrum reduces to the Coulomb limit when c = 0.

12.4 The quantum mechanical virial theorem

- a. Argue that, in an energy eigenstate $|\eta(t)\rangle$, the expectation value $\langle \hat{\mathbf{r}} \cdot \hat{\mathbf{p}} \rangle$ does not change with time.
- b. Hence conclude that $\langle \eta(t) | [\hat{\boldsymbol{r}} \cdot \hat{\boldsymbol{p}}, \hat{H}] | \eta(t) \rangle = 0.$
- c. Show that $[\hat{\mathbf{r}} \cdot \hat{\mathbf{p}}, \hat{\mathbf{p}}^2] = 2i\hbar \hat{\mathbf{p}}^2$, while $[\hat{\mathbf{r}} \cdot \hat{\mathbf{p}}, V(\hat{\mathbf{r}})] = -i\hbar \hat{\mathbf{r}} \cdot \nabla V(\hat{\mathbf{r}})$, where $V(\mathbf{r})$ is any scalar function of the vector \mathbf{r} . (Hint: For the second commutator, use an explicit position basis representation.)
- d. Suppose the Hamiltonian is

$$\hat{H} = \frac{1}{2m}\hat{p}^2 + V(\hat{r}) = \hat{T} + \hat{V}.$$
(12.10)

Define the force function $\mathbf{F}(\mathbf{r}) = -\nabla \mathbf{V}(\mathbf{r})$ and the force operator $\hat{\mathbf{F}} = \mathbf{F}(\hat{\mathbf{r}})$. Conclude that, for an energy eigenstate,

$$2\langle \hat{T} \rangle = -\langle \hat{\mathbf{r}} \cdot \hat{\mathbf{F}} \rangle. \tag{12.11}$$

This is the "virial theorem."

e. If $V(\mathbf{r}) = C/r^n$, show that $2\langle \hat{T} \rangle = -n \langle \hat{V} \rangle$,

$$\langle \hat{T} \rangle = \frac{n}{n-2}E, \quad \text{and} \quad \langle \hat{V} \rangle = \frac{-2}{n-2}E,$$
(12.12)

for the energy eigenstate with energy E.

12.5 Research project

Discuss the motion of wavepackets in a Coulombic potential. Does the expectation value of $\hat{\mathbf{r}}$ follow the classical Kepler ellipse? Is it even restricted to a plane? Does the wavepacket spread out in time (as with the force-free particle) or remain compact (as with the simple harmonic oscillator)?

Identical Particles

13.1 The meaning of two-particle wavefunctions

a. The wavefunction $\psi(x_A, x_B)$ describes two non-identical particles in one dimension. Does

$$\int_{-\infty}^{\infty} dx_A \int_{-\infty}^{\infty} dx_B |\psi(x_A, x_B)|^2$$
(13.1)

equal one or two? Write integral expressions for:

- i. The probability of finding particle A between x_1 and x_2 and particle B between x_3 and x_4 .
- ii. The probability of finding particle A between x_1 and x_2 , regardless of where particle B is.
- b. The wavefunction $\psi(x_A, x_B)$ describes two identical particles in one dimension. Does

$$\int_{-\infty}^{\infty} dx_A \int_{-\infty}^{\infty} dx_B \ |\psi(x_A, x_B)|^2 \tag{13.2}$$

equal one or two? Assuming that $x_1 < x_2 < x_3 < x_4$, write integral expressions for:

- i. The probability of finding one particle between x_1 and x_2 and the other between x_3 and x_4 .
- ii. The probability of finding a particle between x_1 and x_2 .
- c. Look up the definition of "configuration space" in a classical mechanics book. Does the wavefunction inhabit configuration space or conventional three-dimensional position space? For discussion: Does your answer have any bearing upon the question of whether the wavefunction is "physically real" or a "mathematical convenience"? Does it affect your thoughts concerning measurement and the "collapse of the wavepacket"?

13.2 Symmetric and close together, antisymmetric and far apart

In lecture I argued that symmetric wavefunctions describe particles that huddle together while antisymmetric wavefunctions describe particles that avoid one another.

a. Illustrate this principle as follows: Construct symmetric and antisymmetric two-particle wavefunctions out of the single-particle wavefunctions

$$\eta_1(x) = \sqrt{\frac{2}{L}}\cos(\pi \frac{x}{L}) \quad \text{and} \quad \eta_2(x) = \sqrt{\frac{2}{L}}\sin(2\pi \frac{x}{L}), \quad -\frac{L}{2} \le x \le \frac{L}{2},$$
(13.3)

which are the first and second energy eigenfunctions for the infinite square well of width L. For each (anti)symmetrized function make a plot of x_A and x_B and shade in regions of high probability density.

b. Prove that if the two wavefunctions $\psi(\mathbf{x})$ and $\phi(\mathbf{x})$ are orthogonal, then the expectation value of $(\mathbf{x}_A - \mathbf{x}_B)^2$ for the antisymmetric combination of the two wavefunctions is greater than or equal to that for the symmetric combination.

13.3 Symmetrization and antisymmetrization (mathematical)

- a. Show that any two-variable function can be written as the sum of a symmetric function and an antisymmetric function.
- b. Show that this is *not* true for functions of three variables. [Hint: Try the counterexample f(x, y, z) = g(x).]
- c. There is a function of three variables that is:
 - i. Antisymmetric under interchange of the first and second variables: f(x, y, z) = -f(y, x, z).
 - ii. Symmetric under interchange of the second and third variables: f(x, y, z) = f(x, z, y).
 - iii. Symmetric under interchange of the first and third variables: f(x, y, z) = f(z, y, x).

Find this function and show that it is unique.

Conclusion

14.1 Critique

Write a critique of this course's textbook, namely Winter's *Quantum Physics*. Compare the approach to quantum mechanics presented in this text with the approach used in lecture or by some other book (perhaps the text you used in Physics 112: Modern Physics). Be specific: cite specific topics or even specific equations to support your points. You may treat any aspect of the book: problems, pedagogy, philosophy, choice of topics, even phraseology; but you must justify your opinions. Critiques that say merely "I (dis)liked it" (regardless of the number of words used) will receive appropriate credit.

(This question is designed to encourage you to think of physics not as a set of questions with definite answers, but as a subject with room for words as well as numbers, general ideas as well as simple harmonic oscillators, and, above all, as a subject that you can have opinions about.)