PhD Qualifying Exam Fall 2011 – Quantum Mechanics Do only 3 out of the 4 problems

<u>Problem 1.</u> A spinless, non-relativistic particle of mass m moves in a three-dimensional central potential V(r), which vanishes for $r \to \infty$. The particle is in an exact energy eigenstate with wavefunction in spherical coordinates:

$$\psi(\vec{r}) = Cr^n e^{-\alpha r} \sin(\phi) \sin(2\theta),$$

where C and n and α are positive constants.

- (a) What is the angular momentum of this state? Justify your answer. [10 points]
- (b) What is the energy of the particle, and what is the potential V(r)? [30 points]

<u>Problem 2.</u> Apply the variational principle to the anharmonic oscillator having the Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + Cx^4.$$
 (1)

(a) Use as your trial wavefunction a form that is similar to the wavefunction for a harmonic oscillator:

$$\psi(x) = \left(\frac{\lambda^2}{\pi}\right)^{1/4} e^{-\frac{\lambda^2 x^2}{2}} \tag{2}$$

to determine the variational constant λ that minimizes the expectation value of \hat{H} . Note: $\int_{-\infty}^{\infty} e^{-ax^2} dx = \sqrt{\pi/a}$. [25 points]

(b) The ground state energy of the anharmonic oscillator using numerical methods is

$$E_0 = 1.060 \left(\frac{\hbar^2}{2m}\right)^{2/3} C^{1/3}.$$
(3)

What is the approximate ground state energy using the variational method? How does it compare to the numerical results? [15 points] <u>Problem 3.</u> The eigenstates of the hydrogen atom are perturbed by a constant uniform electric field E which points along the z direction. The perturbation is given by

$$H' = -eEz = -eEr\cos\theta. \tag{4}$$

The eigenstates $\psi_{nlm}(\mathbf{r})$ are n^2 -fold degenerate for a particular n. The electric field lifts this degeneracy. Let us consider n = 2.

(a) Write down the hydrogen wavefunctions for n = 2 when H' = 0. [5 points]

(b) Only two matrix elements of H' between the different states for n = 2 are nonzero. Explain why the other diagonal and off-diagonal matrix elements are zero. [5 points] (c) Evaluate the matrix elements by using the expressions for the wavefunctions below and in the formula sheet. You do not have to evaluate the integral over the radial coordinate r (or $\rho = r/a_0$, where a_0 is the Bohr radius). [15 points]

(d) Find the eigenenergies and eigenfunctions for the n = 2 levels in the electric field. [15 points]

Additional information:

For Z = 1 and n = 2, we have

$$R_{20} = \frac{1}{(2a_0)^{3/2}} (2-\rho) e^{-\rho/2} \qquad \text{and} \qquad R_{21} = \frac{1}{\sqrt{3}(2a_0)^{3/2}} \rho e^{-\rho/2}, \tag{5}$$

with $\rho = r/a_0$, where a_0 is the Bohr radius.

<u>Problem 4.</u> A free electron is at rest in a uniform magnetic field $\vec{B} = \hat{x}B$. The interaction Hamiltonian is

$$H = k\vec{S} \cdot \vec{B},$$

where k is a constant. At time t = 0, the electron's spin is measured to be pointing in the $+\hat{z}$ direction.

(a) What is the probability that at time t = T the electron's spin is measured to point in the $-\hat{z}$ direction? [25 points]

(b) What is the probability that at time t = T the electron's spin is measured to point in the $+\hat{x}$ direction? [15 points]

NIU Physics PhD Candidacy Exam – Spring 2011 – Quantum Mechanics DO ONLY THREE OUT OF FOUR QUESTIONS

Problem 1.

(a) In general, what is the first order correction to the energy of a quantum state for a one dimensional system with a time independent perturbation given by H'? [8 points]

(b) Suppose in an infinite square well between x = 0 and x = a the perturbation is given by raising one half of the floor of the well by V_0 ? What is the change in energy to the even and to the odd states? [16 points]

(c) Now suppose the perturbation is given by $\alpha\delta(x-a/2)$ where α is constant. What is the first order correction to the allowed energies for the even and odd states? [16 points]

Problem 2.

We consider scattering off a spherical potential well given by

$$V(r) = \begin{cases} -V_0 & r \le a \\ 0 & r > a \end{cases} \qquad V_0, a > 0$$

The particle's mass is m. We restrict ourselves to low energies, where it is sufficient to consider s wave scattering (angular momentum l = 0).

(a) Starting from the Schrödinger equation for this problem, derive the phase shift δ_0 . [14 points]

(b) Calculate the total scattering cross section σ assuming a shallow potential well $(a\sqrt{2mV_0/\hbar^2} \ll 1)$. [10 points]

(c) Show that the same total scattering cross section σ as in b) is also obtained when using the Born approximation. Note: part c) is really independent of parts a) and b). [16 points]

Problem 3.

For a quantum harmonic oscillator, we have the position \hat{x} and momentum \hat{p}_x operators in terms of step operators

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(a^{\dagger} + a)$$
 and $\hat{p}_x = i\sqrt{\frac{m\hbar\omega}{2}}(a^{\dagger} - a)$ (1)

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

(a) The eigenstates with energy $(n + \frac{1}{2})\hbar\omega$ in bra-ket notation are $|n\rangle$. Express the eigenstates in terms of the step operators and the state $|0\rangle$ (no need to derive). [8 points]

(b) Show that the eigenstates $|1\rangle$ and $|2\rangle$ are normalized using the fact that $|0\rangle$ is normalized (or derive the normalization factor for those states, in case your result from (a) is not normalized). [8 points]

(c) Calculate the expectation values of $\langle \hat{x}^2 \rangle$ and $\langle \hat{p}_x^2 \rangle$ for the eigenstates $|n\rangle$. [8 points]

(d) Using the result from (c), show that the harmonic oscillator satisfies Heisenberg's uncertainty principle (consider only eigenstates). [8 points]

(e) The term $H' = \gamma x^2$ is added to the Hamiltonian. Find the eigenenergies of H + H'. [8 points]

Problem 4.

(a) We want to study the spin-orbit coupling for an atomic level with l = 2. How will this level split under the interaction $\zeta \mathbf{L} \cdot \mathbf{S}$? Give also the degeneracies. [8 points]

(b) Show that for an arbitrary angular momentum operator (integer and half-integer), we can write

$$J_{\pm}|jm_{j}\rangle = \sqrt{(j \mp m_{j})(j \pm m_{j} + 1)}|jm_{j} \pm 1\rangle$$
(2)

(take $\hbar = 1$) [Hint: Rewrite $J_{\pm}J_{\mp}$ in terms of J^2 and J_z]. [10 points]

(c) Since m_j is a good quantum number for the spin-orbit coupling, we can consider the different m_j values separately. Give the matrix for $\zeta \mathbf{L} \cdot \mathbf{S}$ in the $|lm, \frac{1}{2}\sigma\rangle$ basis with $\sigma = \pm \frac{1}{2}$ for $m_j = 3/2$. Find the eigenvalues and eigenstates of this matrix. [12 points]

(d) Write down the matrix for the spin-orbit coupling in the $|jm_j\rangle$ basis for $m_j = 3/2$. [10 points]

NIU Physics PhD Candidacy Exam – Fall 2010 – Quantum Mechanics DO ONLY THREE OUT OF FOUR QUESTIONS

Problem 1.

We consider a spinless particle with mass m and charge q that is confined to move on a circle of radius R centered around the origin in the x-y plane.

(a) Write down the Schrödinger equation for this particle and solve it to find the eigenenergies and corresponding normalized eigenfunctions. Are there degeneracies? [10 points]

(b) This system is perturbed by an electric field E pointing along the x axis. To lowest nonvanishing order in perturbation theory, find the corrections to the eigenenergies of the system. [10 points]

(c) What are the corrections to the eigenfunctions due to the field E in lowest nonvanishing order? [10 points]

(d) Next we consider instead of the electric field \boldsymbol{E} the effect of a magnetic field \boldsymbol{B} pointing along the z axis. Evaluate to lowest nonvanishing order in perturbation theory the corrections to the eigenenergies of the system. [10 points]

Problem 2.

Let us consider two spins S and S' with $S = S' = \frac{1}{2}$. The z components of the spin are $S_z = \pm \frac{1}{2}$ and $S'_z = \pm \frac{1}{2}$. We can define a basis set as $|SS_z, S'S'_z\rangle$ (or simplified $|S_z, S'_z\rangle$). The spins interact with each other via the interaction

$$H = T\mathbf{S} \cdot \mathbf{S}',\tag{1}$$

where T is a coupling constant. S and S' work on the spins S and S', respectively.

(a) Rewrite the interaction in terms of S_z , S'_z and step up and down operators S_{\pm} and S'_{\pm} . [10 points]

(b) Find the eigenvalues of H when the spins are parallel. [10 points]

(c) Find the eigenvalues of H for $S_z + S'_z = 0$. [13 points]

(d) Give a physical interpretation of the eigenenergies and eigenstates of H.[7 points]

Problem 3.

Given a one-dimensional harmonic oscillator with Hamiltonian

$$H = \frac{p_x^2}{2m} + \frac{1}{2}m\omega^2 x^2$$
 (2)

and a wavefunction which is a mixture of the n = 0 and n = 1 states

$$\psi(x) = \frac{1}{\sqrt{5}} (u_0(x) - 2u_1(x)), \tag{3}$$

where u_0 and u_1 are the normalized eigenfunctions of the lowest two energy states. Note that $a^{\pm} = (\mp i p_x + m \omega x) / \sqrt{2\hbar m \omega}$.

(a) draw $\psi(x)$. [5 points]

(b) what is $\langle E \rangle$ in terms of m and ω ? [8 points]

(c) what are $\langle x \rangle$, $\langle x^2 \rangle$ and Δx ? [17 points]

(d) what is $\langle p \rangle$? [10 points]

Problem 4.

The (unnormalized) eigenfunctions for the lowest energy eigenvalues of a one-dimensional simple harmonic oscillator (SHO) are

$$\psi_0(x) = e^{-x^2/a^2}, \qquad \psi_1(x) = \frac{x}{a} e^{-x^2/a^2}, \qquad \psi_2(x) = \left(1 - \frac{4x^2}{a^2}\right) e^{-x^2/a^2},$$
$$\psi_3(x) = \left(\frac{3x}{a} - \frac{4x^3}{a^3}\right) e^{-x^2/a^2}, \qquad \psi_4(x) = \left(3 - \frac{24x^2}{a^2} + \frac{16x^4}{a^4}\right) e^{-x^2/a^2}.$$

Now consider an electron in "half" a one-dimensional SHO potential (as sketched below)

$$V(x) = \begin{cases} K x^2 & x > 0\\ \infty & x \le 0 \end{cases}$$

$$\tag{4}$$

(a) Sketch the ground and first excited state for this new potential. [6 points]

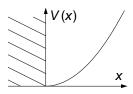
(b) Write the normalized wave function for the ground state in terms of the electron mass m and the oscillator frequency ω (corresponding to the spring constant K). [6 points]

(c) What are the energy eigenvalues for the potential V(x)? [6 points]

(d) Now we add a constant electric field \mathcal{E} in x direction. Use first-order perturbation theory to estimate the new ground state energy.[8 points]

(e) We go back to $\mathcal{E} = 0$. Now we add a second electron. Ignoring the Coulomb interaction between the electrons, write the total energy and the new two-particle wave function, assuming that the electrons are in a singlet spin state with the lowest possible energy. (You can ignore wave function normalization now.) [7 points]

(f) Repeat part (e) assuming that the electrons are instead in a triplet spin state with the lowest possible energy. [7 points]



NIU Physics PhD Candidacy Exam – Spring 2010 – Quantum Mechanics DO ONLY THREE OUT OF FOUR QUESTIONS

<u>Problem 1.</u> In many systems, the Hamiltonian is invariant under rotations. An example is the hydrogen atom where the potential V(r) in the Hamiltonian

$$H = \frac{\mathbf{p}^2}{2m} + V(r),$$

depends only on the distance to the origin.

An infinitesimally small rotation along the z-axis of the wavefunction is given by

$$R_{z,d\varphi}\psi(x,y,z) = \psi(x - yd\varphi, y + xd\varphi, z),$$

(a) Show that this rotation can be expressed in terms of the angular momentum component L_z . [10 points]

(b) Starting from the expression of L_z in Cartesian coordinates, show that L_z can be related to the derivative with respect to φ in spherical coordinates. Derive the φ -dependent part of the wavefunction corresponding to an eigenstate of L_z . [10 points]

(c) Show that if $R_{z,d\varphi}$ commutes with the Hamiltonian, then there exist eigenfunctions of H that are also eigenfunctions of $R_{z,d\varphi}$. [10 points]

(d) Using the fact that L_i with i = x, y, z commute with the Hamiltonian, show that \mathbf{L}^2 commutes with the Hamiltonian. [10 points]

<u>Problem 2.</u> To an harmonic oscillator Hamiltonian

$$H = \hbar \omega a^{\dagger} a$$

we add a term

$$H' = \lambda(a^{\dagger} + a).$$

This problem is known as the displaced harmonic oscillator. It can be diagonalized exactly by adding a constant (let us call it Δ) to the step operators.

(a) Express the constant Δ in terms of $\hbar \omega$ and λ . [8 points]

(b) The energies are shifted by a constant energy. Express that energy in terms of $\hbar\omega$ and λ . [8 points]

(c) Express the new eigenstates $|\tilde{n}\rangle$ in terms of the displaced oscillator operator \tilde{a}^{\dagger} . [8 points] (d) Calculate the matrix elements $\langle \tilde{n} | 0 \rangle$.[8 points]

(e) An harmonic oscillator is in the ground state of H. At a certain time, the Hamiltonian suddenly changes to H + H'. Plot the probability and change in energy for the final states $|\tilde{n}\rangle$ for $\tilde{n} = 0, \dots, 5$ for $\Delta = 2$. [8 points]

<u>Problem 3.</u> We consider scattering off a spherical potential well given by

$$V(r) = \begin{cases} -V_0 & r \le a \\ 0 & r > a \end{cases} \qquad V_0, a > 0$$

The particles' mass is m. We restrict ourselves to low energies, where it is sufficient to consider s wave scattering (angular momentum l = 0).

(a) Starting from the Schrödinger equation for this problem, derive the phase shift δ_0 .[14 points] (b) Calculate the total scattering cross section σ assuming a shallow potential well $(a\sqrt{2mV_0/\hbar^2} \ll 1)$. [10 points]

(c)Show that the same total scattering cross section σ as in b) is also obtained when using the Born approximation. Note: part c) is really independent of parts a) and b). [16 points]

<u>Problem 4.</u> The normalized wavefunctions for the 2s and 2p states of the hydrogen atom are:

$$\psi_{2s} = \frac{1}{\sqrt{32\pi a^3}} (N - r/a) e^{-r/2a}$$

$$\psi_{2p,0} = \frac{1}{\sqrt{32\pi a^3}} (r/a) e^{-r/2a} \cos \theta$$

$$\psi_{2p,\pm 1} = \frac{1}{\sqrt{64\pi a^3}} (r/a) e^{-r/2a} \sin \theta e^{\pm i\phi}$$

where a is the Bohr radius and N is a certain rational number.

(a) Calculate N. (Show your work; no credit for just writing down the answer.) [10 points]

(b) Find an expression for the probability of finding the electron at a distance greater than a from the nucleus, if the atom is in the 2p, +1 state. (You may leave this answer in the form of a single integral over one variable.) [10 points]

(c) Now suppose the atom is perturbed by a constant uniform electric field $\vec{E} = E_0 \hat{z}$. Find the energies of the 2s and 2p states to first order in E_0 . [20 points]

NIU Physics PhD Candidacy Exam – Fall 2009 – Quantum Mechanics DO ONLY THREE OUT OF FOUR QUESTIONS

Problem 1.

Consider the effects of the hyperfine splitting of the ground state of the Hydrogen atom in the presence of an external magnetic field $\vec{B} = B_0 \hat{z}$. Let the electron spin operator be \vec{S} and the proton spin operator be \vec{I} , and call the total angular momentum operator $\vec{J} = \vec{S} + \vec{I}$. Then the Hamiltonian for the system is:

$$H = \frac{E_{\gamma}}{\hbar^2} \vec{S} \cdot \vec{I} + 2\frac{\mu_B}{\hbar} \vec{B} \cdot \vec{S},\tag{1}$$

where E_{γ} is the energy of the famous 21 cm line and μ_B is the Bohr magneton. The states of the system may be written in terms of angular momentum eigenstates of S_z , I_z or J^2 , J_z , so clearly label which basis you are using in each of your answers.

(a) In the limit that B_0 is so large that E_{γ} can be neglected, find the energy eigenstates and eigenvalues. [12 points]

(b) In the limit that B_0 is so small that it can be neglected, find the energy eigenstates and eigenvalues. [15 points]

(c) Find the energy eigenvalues for general B_0 , and show that the special limits obtained in parts (a) and (b) follow. [13 points]

Problem 2.

A quantum mechanical spinless particle of mass m is confined to move freely on the circumference of a circle of radius R in the x, y plane.

(a) Find the allowed energy levels of the particle, and the associated wavefunctions. [16 points]

(b) Now suppose the particle has a charge q and is placed in a constant electric field which is also in the x, y plane. Calculate the shifts in energy levels to second order in the electric field, treated as a perturbation. [16 points]

(c) Show that the degeneracies are not removed to *any* order in the electric field treated as a perturbation. [8 points]

Problem 3.

Given a 2D harmonic oscillator with Hamiltonian

$$H = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{1}{2}m\omega^2(x^2 + y^2) + kmxy$$
(2)

(a) How does ⟨x⟩ change with time, that is determine d⟨x⟩/dt? [10 points]
(b) For k = 0, what are the energies of the ground state and first and second excited states? What are the degeneracies of each state? [15 points]

(c) For k > 0, using first order perturbation theory, what are the energy shifts of the ground state and the first excited states? [15 points]

Problem 4.

In many systems, the Hamiltonian is invariant under rotations. An example is the hydrogen atom where the potential V(r) in the Hamiltonian

$$H = \frac{\mathbf{p}^2}{2m} + V(r),\tag{3}$$

depends only on the distance to the origin.

An infinitesimally small rotation along the z-axis of the wavefunction is given by

$$R_{z,d\varphi}\psi(x,y,z) = \psi(x - yd\varphi, y + xd\varphi, z), \tag{4}$$

(a) Show that this rotation can be expressed in terms of the angular momentum component L_z . [10 points]

(b) Starting from the expression of L_z in Cartesian coordinates, show that L_z can be related to the derivative with respect to φ in spherical coordinates. Derive the φ -dependent part of the wavefunction corresponding to an eigenstate of L_z . [10 points]

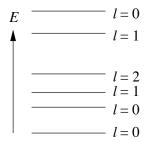
(c) Show that if $R_{z,d\varphi}$ commutes with the Hamiltonian, then there exist eigenfunctions of H that are also eigenfunctions of $R_{z,d\varphi}$. [10 points]

(d) Using the fact that L_i with i = x, y, z commute with the Hamiltonian, show that L^2 commutes with the Hamiltonian. [10 points]

2000 Spring Ph.D. Candidacy Exam, Quantum Mechanics DO ONLY 3 OUT OF 4 OF THE QUESTIONS

Problem 1.

The diagram shows the six lowest energy levels and the associated angular monenta for a spinless particle moving in a certain three-dimensional central potential. There are no "accidental" degeneracies in this energy spectrum. Give the number of nodes (changes in sign) in the radial wave function associated with each level. Justify your answer.



Problem 2.

Assume that the mu-neutrino ν_{μ} and the tau-neutrino ν_{τ} are composed of a mixture of two mass eigenstates ν_1 and ν_2 . The mixing ratio is given by

$$\begin{pmatrix} \nu_{\mu} \\ \nu_{\tau} \end{pmatrix} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} \nu_{1} \\ \nu_{2} \end{pmatrix}$$
(1)

In free space, the states ν_1 and ν_2 evolve according to

$$\begin{pmatrix} |\nu_1(x,t)\rangle \\ |\nu_2(x,t)\rangle \end{pmatrix} = e^{ipx/\hbar} \begin{pmatrix} e^{-iE_1t/\hbar} |\nu_1(0)\rangle \\ e^{-iE_2t/\hbar} |\nu_2(0)\rangle \end{pmatrix}$$
(2)

Show that the transition probability for a mu-neutrino into a tau-neutrino is given by

$$P(\mu \to \tau) = \sin^2(2\theta) \sin^2 \frac{(E_2 - E_1)t}{2\hbar}.$$
(3)

Problem 3.

Let the potential V = 0 for $r < a_0$ (the Bohr radius) and $V = \infty$ for $r > a_0$. V is a function of r only.

a) What is the energy of an electron in the lowest energy state of this potential?

b) How does that compare to the energy of the 1s state of Hydrogen?

c) What is the approximate energy of the lowest energy state with angular momentum greater than

0 (you can leave this result in integral form)?

Problem 4.

The Hamiltonian for a two-dimensional harmonic oscillator is given by

$$H_0 = (a^{\dagger}a + b^{\dagger}b + 1)\hbar\omega, \qquad (4)$$

with the coordinates given by

$$x = \sqrt{\frac{\hbar}{2m\omega}}(a^{\dagger} + a) \text{ and } y = \sqrt{\frac{\hbar}{2m\omega}}(b^{\dagger} + b).$$
 (5)

a)Give the eigenvalues of this Hamiltonian.

The Hamiltonian is perturbed by

$$H' = \alpha x y, \tag{6}$$

where α is a small constant.

b) Express H' in terms of the operators a and b and their conjugates.

c) Using degenerate perturbation theory, show how the eigenvalues are changed by H' for the states with eigenenergy $2\hbar\omega$ for H_0 .

2008 Fall Ph.D. Candidacy Exam, Quantum Mechanics DO ONLY 3 OUT OF 4 OF THE QUESTIONS

Problem 1.

We consider a system made of the orthonormalized spin states $|+\rangle$ and $|-\rangle$, where $S_z |\pm\rangle = \pm (\hbar/2) |\pm\rangle$. Initially both of these states are energy eigenstates with the same energy ϵ .

a) An interaction V couples these spin states, giving rise to the matrix elements

 $\langle 1|V|1\rangle = \langle 2|V|2\rangle = 0$ and $\langle 1|V|2\rangle = \Delta$

Give the Hamiltonian H of the interacting system.

- b) Determine the energy eigenvalues of H.
- c) Show that the states $|A\rangle$ and $|B\rangle$

$$|A\rangle = \frac{1}{\sqrt{2}} \left(|+\rangle + \frac{\Delta^*}{|\Delta|} |-\rangle \right) \quad \text{and} \quad |B\rangle = \frac{1}{\sqrt{2}} \left(|+\rangle - \frac{\Delta^*}{|\Delta|} |-\rangle \right)$$

are orthonormalized eigenstates of the interacting system.

- d) Determine the time evolution of a state $|\psi(t)\rangle$ for which $|\psi(t=0)\rangle = |+\rangle$.
- e) For the state $|\psi(t)\rangle$, calculate the probability that a measurement of S_z at time t yields $\pm \hbar/2$.

Problem 2.

A particle of mass m is constrained to move between two concentric impermeable spheres of radii r = a and r = b. There is no other potential. Find the ground state energy and normalized wave function.

Problem 3.

Given a two-dimensional oscillator with Hamiltonian

$$H = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{1}{2}m\omega^2(x^2 + y^2) + kmxy,$$
(1)

- a) What is the time dependence of $d\langle x \rangle/dt$?
- b) What is the time dependence of $d\langle p_x \rangle/dt$?

c) For k = 0, what are the energies of the ground state and the first and second excited states? What are the degeneracies of each state?

d) For k > 0, using first-order perturbation theory, what are the energy shifts of the ground state and the first excited states?

Problem 4.

a) We want to study the spin-orbit coupling for a level with l = 3. How do you expect that this level will split under the interaction $\zeta \mathbf{L} \cdot \mathbf{S}$. Give also the degeneracies.

b) Show that for an arbitrary angular momentum operator (integer and half-integer), we can write

$$J_{\pm}|jm_{j}\rangle = \sqrt{(j \mp m_{j})(j \pm m_{j} + 1)}|jm_{j}\rangle$$
⁽²⁾

(take $\hbar = 1$).

c) Since m_j is a good quantum number for the spin-orbit coupling, we can consider the different m_j values separately. Give the matrix for $\zeta \mathbf{L} \cdot \mathbf{S}$ in the $|lm, \frac{1}{2}\sigma\rangle$ basis with $\sigma = \pm \frac{1}{2}$ for $m_j = 5/2$. Find the eigenvalues and eigenstates of this matrix.

d) Write down the matrix for the spin-orbit coupling in the $|jm_i\rangle$ basis for $m_i = 5/2$.

e) Obtain the same eigenstates as in question c) by starting for the $m_j = 7/2$ state using the step operators.

2008 Spring Ph.D. Candidacy Exam, Quantum Mechanics DO ONLY 3 OUT OF 4 OF THE QUESTIONS

Problem 1.

Consider a particle with mass m confined to a three-dimensional spherical potential well

$$V(r) = \begin{cases} 0, & r \le a \\ V_0, & r > a \end{cases}$$
(1)

a) Give the Schrödinger equation for this problem.

b) Determine the explicit expressions for the ground state energy and the ground state wave function in the limit $V_0 \rightarrow \infty$.

c) For the more general case $0 < V_0 < \infty$, determine the transcendental equation from which we can obtain the eigenenergies of the particle for angular momentum l = 0.

d) Which condition must be fulfilled such that the transcendental equation derived in c) can be solved? (Hint: consider a graphical solution of the equation.) Compare this result with a particle in a one-dimensional rectangular well of depth V_0 .

Problem 2.

The ground state energy and Bohr radius for the Hydrogen atom are

$$E_1 = -\frac{\hbar^2}{2ma_B^2}, \quad a_B = \frac{4\pi\varepsilon_0\hbar^2}{e^2m}.$$
(2)

a) Calculate the ground state energy (in eV) and Bohr radius (in nm) of positronium (a hydrogenlike system consisting of an electron and a positron).

b) What is the degeneracy of the positronium ground state due to the spin? Write down the possible eigenvalues of the total spin together with the corresponding wavefunctions.

c) The ground state of positronium can decay by annihilation into photons. Calculate the energy and angular momentum released in the process and prove there must be at least two photons in the final state.

Problem 3.

A particle of mass m moves in one dimension inside a box of length L. Use first order perturbation theory to calculate the lowest order correction to the energy levels arising from the relativistic variation of the particle mass. You can assume that the effect of relativity is small. Note that the free particle relativistic Hamiltonian is $\hat{H}_{\rm rel} = \sqrt{m^2c^4 + p^2c^2} - mc^2$.

Problem 4.

a) Prove the variational theorem that states that for any arbitrary state

$$\langle \psi | H | \psi \rangle \ge E_0. \tag{3}$$

b) Consider the Hamiltonian for a particle moving in one dimension

$$\hat{H} = \frac{\hat{p}^2}{2m} + V_0 \left(\frac{\hat{x}}{a}\right)^6,$$
(4)

where m is mass, a a length scale, and V_0 an energy scale. Is the wavefunction

$$\psi(x) = C(x^2 - a^2)e^{-(x/d)^4},\tag{5}$$

where C is a normalization constant, d an adjustable parameter with dimensions of length, a good choice for the variational approximation to the ground state? Why or why not?

c) Depending on the answer of the previous part: If it is a good choice, make a rough orderof-magnitude estimate of the optimal choice for d. If it is not a good choice, propose a better variational wavefunction, including an estimate of the length scale.

2007 Fall Ph.D. Qualifier, Quantum Mechanics DO ONLY 3 OUT OF 4 OF THE QUESTIONS

Problem 1.

The spin-orbit coupling of an electron of angular momentum l and spin $s = \frac{1}{2}$ is described by the Hamiltonian

$$H = \lambda \mathbf{l} \cdot \mathbf{s},\tag{1}$$

where λ is the spin-orbit coupling parameter.

(a) Write down the matrix H and diagonalize it to show that the state is split into two states with total angular momentum $j = l \pm \frac{1}{2}$. Find the eigenenergies.

(b) Show that the eigenenergies can also be determined using the relation $\mathbf{j} = \mathbf{l} + \mathbf{s}$.

[The raising and lowering operators for l are $l_+|l, m_l\rangle = \sqrt{(l-m_l)(l+m_l+1)}|l, m_l+1\rangle$ and $l_-|l, m_l\rangle = \sqrt{(l+m_l)(l-m_l+1)}|l, m_l-1\rangle$ and similarly for s].

Problem 2.

(a) Write down the nonrelativistic Hamiltonian for a Helium atom with two electrons.

(b) Write down the ground state wavefunction (include the spin part) and give the ground state energy E_0 (in eV) in the absence of electron-electron interactions.

(c) Write down the matrix element for the lowest-order correction E_1 to the ground-state energy due to the electron-electron interaction. The 1s orbital is given by

$$\varphi_{100} = \frac{1}{\sqrt{8\pi}} \left(\frac{2Z}{a_0}\right)^{3/2} e^{-Zr/a_0} \tag{2}$$

The matrix element can be evaluated giving $\frac{5}{8} \frac{Ze^2}{4\pi\varepsilon_0 a_0}$.

(d) Find the ratio of the correction E_1 to E_0 .

The Rydberg constant is $R = \frac{Z^2 \hbar^2}{2ma_0^2}$ and the Bohr radius is $a_0 = \frac{4\pi\varepsilon_0 \hbar^2}{me^2}$.

Problem 3.

Two identical spin 1/2 fermions described by position coordinates \vec{r}_i (i = 1, 2) are bound in a three-dimensional isotropic harmonic oscillator potential

$$V(\vec{r_i}) = \frac{1}{2}m\omega^2 r_i^2.$$
 (3)

(a) Write the wave functions of the system in terms of the single-particle spin eigenstates and the one-dimensional harmonic oscillator wave functions, for each of the energy eigenstates up to and including energy $4\hbar\omega$.

(b) Assume that in addition there is a weak spin-independent interaction V between the particles:

$$V(\vec{r}_1 - \vec{r}_2) = -\lambda \delta^{(3)}(\vec{r}_1 - \vec{r}_2)$$
(4)

Find the energies of the system correct to first order in λ for each of the unperturbed states found in part (a). You may leave your results in terms of definite integrals over known functions.

Problem 4.

Consider normal 1-dimensional particle in box potential $(V(x) = \infty \text{ for } |x| > L/2 \text{ and } V(x) = 0$ inside box. Two identical particles are confined to the box (assume only orbital degrees of freedom, ignore spin).

(a) What is the normalized unperturbed ground state for

- two identical bosons of mass m confined in the box
- two identical fermions of mass m confined in the box
- And what are the unperturbed ground state energies of the two cases?

(b) Now a perturbation is applied. A small rectangular bump appears in the box between -a/2 and +a/2. This perturbation is $V_{pert} = +|V_0|$ for |x| < a/2 and is zero otherwise.

Use first-order perturbation theory to obtain the new ground state energies for the two cases.

2007 Spring Ph.D. Qualifier, Quantum Mechanics DO ONLY 3 OUT OF 4 OF THE QUESTIONS

Problem 1.

A particle moves in a 1 dimensional potential described by an attractive delta function at the origin. The potential is;

$$V(x) = -W\delta(x)$$

(a) Discuss and determine the wavefunctions valid for bound state solutions of this system.

(b) Show that there is only one bound state and determine its energy.

Problem 2.

In this problem, $|0\rangle$, $|n\rangle$ are the shorthand for the eigenstates of the 1 dimensional simple harmonic oscillator (SHO) Hamiltonian, with $|0\rangle$, denoting the ground state. The \hat{a}^{\dagger} and \hat{a} are the SHO raising and lowering operators. (sometimes termed creation and destruction (annihilation) operators).

(a) Prove that the following state vector $|z\rangle$ is an eigenstate of the lowering operator \hat{a} and that its eigenvalue is z.

$$|z\rangle = e^{z\hat{a}^{\dagger}}|0\rangle$$

The z is an arbitrary complex number. (Note, knowledge of the expansion of e^x will be useful.)

(b) Evaluate $\langle z_1 | z_2 \rangle$, where z_1 and z_2 are arbitrary complex numbers, and use this result to normalize state $|z\rangle$.

Problem 3.

Let the potential V = 0 for $r < a_0$ (the Bohr radius) and $V = \infty$ for $r > a_0$. V is a function of r only.

(a) What is the energy of an electron in the lowest energy state of this potential?

(b) How does this compare to the kinetic energy of the 1s state of Hydrogen?

(c) What is the approximate energy of the lowest energy state with angular momentum greater than 0 (you can leave this result in integral form)?

Problem 4.

In a magnetic resonance experiment a specimen containing nuclei of spin $I = \frac{1}{2}$ and magnetic moment $\mu = \hbar \gamma I$ is placed in a static magnetic field B_0 directed along the z-axis and a field B_1 which rotates in the xy-plane with angular frequency ω .

(a) Write down the Hamiltonian for the system.

(b) If the wave function is written

$$\psi(t) = c_+(t)\chi_{\frac{1}{2}} + c_-(t)\chi_{-\frac{1}{2}}$$

where $\chi_{\frac{1}{2}}$ and $\chi_{-\frac{1}{2}}$ are the spin eigenfunctions, show that

and
$$i\frac{dc_+}{dt} = \frac{1}{2}\omega_0c_+ + \frac{1}{2}\omega_1c_-e^{-i\omega t}$$
$$i\frac{dc_-}{dt} = -\frac{1}{2}\omega_0c_- + \frac{1}{2}\omega_1c_+e^{i\omega t}$$

and where $\omega_0 = \gamma B_0$ and $\omega_1 = \gamma B_1$. Assuming that the system starts in the state $\chi_{-\frac{1}{2}}$, i.e. $c_+(0) = 0$ and $c_-(0) = 1$, solve these equations to show that subsequently the probability that the system is in the state $\chi_{\frac{1}{2}}$ is

$$|c_{+}|^{2} = \omega_{1}^{2} \frac{\sin^{2} \frac{1}{2} [(\omega - \omega_{0})^{2} + \omega_{1}^{2}]^{\frac{1}{2}} t}{(\omega - \omega_{0})^{2} + \omega_{1}^{2}}$$

Ph.D. Qualifier, Quantum mechanics DO ONLY 3 OF THE 4 QUESTIONS Note the additional material for questions 1 and 3 at the end.

PROBLEM 1.

In the presence of a magnetic field $\boldsymbol{B} = (B_x, B_y, B_z)$, the dynamics of the spin 1/2 of an electron is characterized by the Hamiltonian $H = -\mu_B \boldsymbol{\sigma} \cdot \boldsymbol{B}$ where μ_B is the Bohr magneton and $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ is the vector of Pauli spin matrices.

(a) Give an explicit matrix representation for H.

In the following, we investigate the time-dependent two-component wave function $\psi(t) = \begin{pmatrix} a(t) \\ b(t) \end{pmatrix}$ characterizing the dynamics of the electron spin. (The orbital part of the electron dynamics is completely ignored.)

(b) We assume that for t < 0 the magnetic field **B** is parallel to the z axis, $\mathbf{B}(t < 0) = (0, 0, B_z)$ and constant in time. From the time-dependent Schrödinger equation, calculate $\psi(t)$ such that $\psi(t = 0) = {1 \choose 0}$.

(c) At t = 0 an additional magnetic field in x direction is switched on so that we have $\mathbf{B}(t \ge 0) = (B_x, 0, B_z)$. Solve the time-dependent Schrödinger equation for $t \ge 0$ using the ansatz

$$\psi(t) = \begin{pmatrix} a(t) \\ b(t) \end{pmatrix} = \begin{pmatrix} a_1 \cos \omega t + a_2 \sin \omega t \\ b_1 \cos \omega t + b_2 \sin \omega t \end{pmatrix}$$

Hint: The boundary condition $\psi(t=0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ simplifies the calculation of the frequency ω and the coefficients a_1, a_2, b_1 , and b_2 .

Note also that in order to get a solution $\psi(t)$ valid for all times $t \ge 0$, we may split the coupled equations into equations proportional to $\sin \omega t$ and $\cos \omega t$.

(d) Verify the normalization condition $|a(t)|^2 + |b(t)|^2 = 1$.

(e) Interpret your result for $|b(t)|^2$ by considering the limiting cases $B_x \ll B_z$ and $B_x \gg B_z$.

PROBLEM 2.

A particle experiences a one-dimensional harmonic oscillator potential. The harmonic oscillator energy eigenstates are denoted by $|n\rangle$ with $E_n = (n + 1/2)\hbar\omega$. At t = 0, the state describing the particle is

$$|\psi, t = 0\rangle = \frac{1}{\sqrt{2}} \left(|0\rangle + i|1\rangle\right)$$

(a) Calculate $\langle E(t) \rangle = \langle \psi, t | H | \psi, t \rangle$

(b) Calculate $\langle x(t) \rangle = \langle \psi, t | x | \psi, t \rangle$.

(c) Calculate the root mean squared deviation of x(t).

PROBLEM 3.

Consider a system of two *distinguishable* particles of spin $\hbar/2$. All degrees of freedom other than spin are ignored. Let $\hat{\mathbf{s}}_1$ and $\hat{\mathbf{s}}_2$ be the vector operators for spins of the particles. The Hamiltonian of this system is

$$H = A\hat{\mathbf{s}}_1 \cdot \hat{\mathbf{s}}_2$$

with A a constant.

(a) Determine the energy eigenvalues and the accompanying eigenstates of this system.

(b) A system is prepared so that particle 1 is spin up $(s_{1,z} = \hbar/2)$ and particle 2 is spin down, $(s_{1,z} = -\hbar/2)$. Express this wavefunction in terms of the eigenstates of the Hamiltonian.

PROBLEM 4.

Let us consider two orbital angular momenta $L_1 = L_2 = 1$ that interact via $H = \alpha \mathbf{L}_1 \cdot \mathbf{L}_2$. The basis set is denoted by $|L_1M_1, L_2M_2\rangle$, where M_i is the z component of L_i with i = 1, 2.

(a) Calculate the matrix element $\langle 11, 11|H|11, 11\rangle$. Is this an eigenenergy (explain)?

(b) Calculate the matrix elements $\langle 11, 10|H|11, 10 \rangle$, $\langle 10, 11|H|10, 11 \rangle$, and $\langle 11, 10|H|10, 11 \rangle$. Use these matrix elements to derive the eigenenergies and eigenfunctions for $M_1 + M_2 = 1$.

(c) An alternative way to derive the eigenenergies is to express $\mathbf{L}_1 \cdot \mathbf{L}_2$ in \mathbf{L}_1^2 , \mathbf{L}_2^2 , and \mathbf{L}^2 where $\mathbf{L} = \mathbf{L}_1 + \mathbf{L}_2$. Derive this expression and determine the eigenenergies for all possible values of \mathbf{L} .

Note:

$$L_{\pm}|LM\rangle = \sqrt{(L \mp M)(L \pm M + 1)}|L, M \pm 1\rangle$$

Additional material

For spin 1/2 particles, spin operators are $s_i = \frac{\hbar}{2}\sigma_i$

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

2006 Ph.D. Qualifier, Quantum Mechanics DO ONLY 3 OUT OF 4 OF THE QUESTIONS

Problem 1.

Consider an atomic p electron (l = 1) which is governed by the Hamiltonian $\hat{H} = \hat{H}_0 + \hat{V}$ where

$$\hat{H}_0 = \frac{b}{\hbar}\hat{L}_z + \frac{a}{\hbar^2}\hat{L}_z^2$$
 and $\hat{V} = \sqrt{2}\frac{c}{\hbar}\hat{L}_a$

(a) Show that within the basis of l = 1 states, $|1, m\rangle$, where *m* denotes the *z* component of *l*, the Hamiltonian \hat{H} reads

$$\hat{H} = \begin{pmatrix} a+b \ c & 0 \\ c & 0 \ c \\ 0 \ c \ a-b \end{pmatrix}$$

You may want to use the formula

$$\hat{L}_{\pm}|l,m\rangle = \hbar\sqrt{(l\mp m)(l\pm m+1)}|l,m\pm 1\rangle$$
 where $\hat{L}_{\pm} = \hat{L}_x \pm \hat{L}_y$

(b) We want to treat \hat{V} as a perturbation of \hat{H}_0 . What are the energy eigenvalues and eigenstates of the *unperturbed* problem?

(c) We assume $|a \pm b| \gg |c|$. Calculate the eigenvalues and eigenstates of \hat{H} in second and first order of the perturbation \hat{V} , respectively.

(d) Next we consider a = b, $|a| \gg |c|$. Calculate the eigenvalues \hat{H} in *first* order of the perturbation \hat{V} .

Problem 2.

Consider a harmonic oscillator

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

Do the following algebraically, that is, without using wave functions.

(a) Construct a linear combination $|\psi\rangle$ of the ground state $|0\rangle$ and the first excited state $|1\rangle$ such that the expectation value $\langle x \rangle = \langle \psi | x | \psi \rangle$ is as large as possible.

(b) Suppose at t = 0 the oscillator is in the state constructed in (a). What is the state vector for t > 0? Evaluate the expectation value $\langle x \rangle$ as a function of time for t > 0.

(c) Evaluate the variance $\Delta^2 x = \langle (x - \langle x \rangle)^2 \rangle$ as a function of time for the state constructed in (a). You may use

$$x = \sqrt{\frac{\hbar}{2m\omega}} (a + a^{\dagger})$$
 and $p = \sqrt{\frac{\hbar m\omega}{2}} (a - a^{\dagger})$,

where a and a^{\dagger} are the annihilation and creation operators for the oscillator eigenstates.

Problem 3.

If a hydrogen atom is placed in a strong magnetic field, its orbital and spin magnetic dipole moments precess independently about the external field, and its energy depends on the quantum numbers m_{λ} and m_s which specify their components along the external field direction. The potential energy of the magnetic dipole moments is

$$\Delta E = -(\mu_{\lambda} + \mu_s) \cdot \mathbf{B}$$

(a) For n = 2 and n = 1, enumerate all the possible quantum states $(n, \lambda, m_{\lambda}, m_s)$.

(b) Draw the energy level diagram for the atom in a strong magnetic field, and enumerate the quantum numbers and energy (the energy in terms of E_1 , E_2 , and $\mu_B B_z$) of each component of the pattern.

(c) Examine in your diagram the most widely separated energy levels for the n = 2 state. If this energy difference was equal to the difference in energy between the n = 1 and the n = 2 levels in the absence of a field, calculate what the strength of the external magnetic field would have to be. (Note: Bohr magneton is $\mu_B = 9.27 \times 10^{-24}$ Joule/Tesla). In the lab, the strongest field we can produce is on the order of 100 Tesla – how does your answer compare to this value? (Note: 1 eV=1.602×10⁻¹⁹ J).

(d) Using the dipole selection rules, draw all the possible transitions among the n = 2 and n = 1 levels in the presence of a magnetic field.

Problem 4.

A particle of mass m is in an infinite potential well perturbed as shown in Figure 1.

a) Calculate the first order energy shift for the nth eigenvalue due to the perturbation.

b) Calculate the 2nd order energy shift for the ground state.

Some useful equations:

$$\int \sin^2 x dx = \frac{x}{2} - \frac{1}{4} \sin 2x$$
$$\int \cos^2 x dx = \frac{x}{2} + \frac{1}{4} \sin 2x$$
$$2 \int \sin ax \sin bx dx = \frac{\sin(a-b)x}{a-b} - \frac{\sin(a+b)x}{a+b}$$
$$2 \int \sin ax \cos bx dx = -\frac{\cos(a-b)x}{a-b} + \frac{\cos(a+b)x}{a+b}$$
$$2 \int \cos ax \cos bx dx = \frac{\sin(a-b)x}{a-b} + \frac{\sin(a+b)x}{a+b}$$

2005 Ph.D. Qualifier, Quantum Mechanics DO ONLY 3 OUT OF 4 OF THE QUESTIONS

Problem 1.

A particle of mass m in an infinitely deep square well extending between x = 0 and x = L has the wavefunction

$$\Psi(x,t) = A\left[\sin\left(\frac{\pi x}{L}\right)e^{-iE_1t/\hbar} - \frac{3}{4}\sin\left(\frac{3\pi x}{L}\right)e^{-iE_3t/\hbar}\right],\tag{1}$$

where A is a normalization factor and $E_n = n^2 h^2 / 8mL^2$.

- (a) Calculate an expression for the probability density $|\Psi(x,t)|^2$, within the well at t = 0.
- (b) Calculate the explicit time-dependent term in the probability density for $t \neq 0$.
- (c) In terms of m, L, and h, what is the repetition period T of the complete probability density?

Problem 2.

- Let us consider the spherical harmonics with l = 1.
- (a) Determine the eigenvalues for aL_z , where a is a constant.
- (b) Determine the matrix for L_x for the basis set $|lm\rangle$ with l = 1 using the fact that

$$L_{\pm}|lm\rangle = \hbar\sqrt{(l\mp m)(l\pm m+1)}|l,m\pm 1\rangle.$$
(2)

and that the step operators are given by $L_{\pm} = L_x \pm iL_y$.

- (c) Determine the eigenvalues of aL_x for the states with l = 1.
- (d) Determine the matrix for \mathbf{L}^2 from the matrices for L_+ , L_- , and L_z .

Problem 3.

Consider a two-dimensional harmonic oscillator

$$H_0 = \hbar \omega_x a_x^{\dagger} a_x + \hbar \omega_y a_y^{\dagger} a_y \tag{3}$$

with $\hbar\omega_x \ll \hbar\omega_y$. The number of excited states is given by $N = n_x + n_y$, where $a_x^{\dagger}|n_x\rangle = \sqrt{n_x + 1}|n_x + 1\rangle$ and $a_y^{\dagger}|n_y\rangle = \sqrt{n_y + 1}|n_y + 1\rangle$ (a) Express the normalized state with N = 2 with the lowest energy in terms of the step operators

(a) Express the normalized state with N = 2 with the lowest energy in terms of the step operators and the vacuum state $|0\rangle$, i.e. the state with no oscillators excited.

The system is now perturbed by

$$H_1 = K(a_x^{\dagger}a_y + a_y^{\dagger}a_x). \tag{4}$$

(b) Calculate for the state found in (a): the correction in energy up to first order.

- (c) Express the correction in energy up to second order.
- (d) Give the lowest-order correction to the wavefunction.

NOTE: The correction term to the wavefunction is given by

$$|\psi_n^1\rangle = \sum_{m \neq n} \frac{\langle \psi_m^0 | H_1 | \psi_n^0 \rangle}{E_n^0 - E_m^0} |\psi_m^0\rangle \tag{5}$$

Problem 4.

A system has unperturbed energy eigenstates $|n\rangle$ with eigenvalues E_n (for n = 0, 1, 2, 3...) of the unperturbed Hamiltonian. It is subject to a time-dependent perturbation

$$H_I(t) = \frac{\hbar A}{\sqrt{\pi}\tau} e^{-t^2/\tau^2} \tag{6}$$

where A is a time-independent operator.

(a) Suppose that at time $t = -\infty$ the system is in its ground state $|0\rangle$. Show that, to first order in the perturbation, the probability that the system will be in its *m*th excited state $|m\rangle$ (with m > 0) at time $t = +\infty$ is:

$$P_m = a |\langle m | A | 0 \rangle|^2 e^{-b\tau^c (E_0 - E_m)^d}.$$
(7)

Calculate the constants a, b, c and d. [You may find the integral $\int_{-\infty}^{\infty} e^{-x^2} dx = \sqrt{\pi}$ to be useful.] (b) Next consider the limit of an impulsive perturbation, $\tau \to 0$. Find the probability P_0 that the system will *remain* in its ground state. Find a way of writing the result in terms of only the matrix elements $\langle 0|A^2|0\rangle$ and $\langle 0|A|0\rangle$.

Hint: the time evolution of states to first order in perturbation theory can be written as

$$|\psi(t)\rangle = \left[e^{-i(t-t_0)H_0/\hbar} - \frac{i}{\hbar}\int_{t_0}^t dt' e^{-i(t-t')H_0/\hbar}H_I(t')e^{-i(t'-t_0)H_0/\hbar}\right]|\psi(t_0)\rangle$$
(8)

where H_0 is the unperturbed time-independent Hamiltonian.

2005 Ph.D. Qualifier, Quantum Mechanics DO ONLY 3 OUT OF 4 OF THE QUESTIONS

Problem 1.

A non-relativistic particle with energy E and mass m is scattered from a weak spherically-symmetric potential:

$$V(r) = A(1 - r/a)$$
 for $(r < a)$ (1)

$$V(r) = 0 \qquad \qquad \text{for } (r \ge a), \tag{2}$$

where a and A are positive constants, and r is the distance to the origin. 1(a) In the Born approximation, for which the scattering amplitude is given by

$$f(\mathbf{k}, \mathbf{k}') = -\frac{m}{2\pi\hbar^2} \int d\mathbf{r} V(r) e^{i\mathbf{r}\cdot(\mathbf{k}-\mathbf{k}')},\tag{3}$$

find the differential cross-section for elastic scattering at an angle θ . (You may leave your result in terms of a well-defined real integral over a single real dimensionless variable.)

1(b) Show that in the low-energy limit the total scattering cross-section is proportional to a^n where n is an integer that you will find.

Problem 2.

Two distinguishable spin-1/2 fermions of the same mass m are restricted to move in one dimension, with their coordinates given by x_1 and x_2 . They have an interaction of the form

$$V(x_1 - x_2) = -g^2 \delta(x_1 - x_2) \frac{(\mathbf{S}_1 \cdot \mathbf{S}_2 + 1)}{2},$$
(4)

where S_1 and S_2 are the vector spin operators with eigenvalues of each component normalized to $\pm 1/2$. Discuss the spectrum of eigenvalues, and find the bound state wavefunctions and energy eigenvalues. Also, discuss how these results change if the particles are indistinguishable.

Problem 3

The eigenfunction for the first excited spherically symmetric state of the electron in a Hydrogen atom is given by

$$\psi(\mathbf{r}) = A(1 - Br)e^{-Br} \tag{5}$$

3a. Show that this satisfies the Schrödinger equation and deduce the value of the constant B.

3b. Determine the energy for this state.

3c. Solve for the value of A and thus obtain the expectation value of the distance r from the origin.

Assume

$$\int_0^\infty r^n e^{-\alpha r} dr = \frac{n!}{\alpha^{n+1}} \tag{6}$$

Problem 4

4(a). Let us consider an atom that can couple to Einstein oscillators of energy $\hbar\omega$. We can assume that the energy of the atom is zero. The Hamiltonian for the oscillators is given by

$$H = \hbar\omega(a^{\dagger}a + \frac{1}{2}),\tag{7}$$

where a^{\dagger} and a are the step up and step down operators. For t < 0, there is no coupling between the atom and the oscillators. Since no oscillators are excited, the system is in the ground state $|0\rangle$. At t = 0, a perturbation is created (for example, the atom is ionized) giving a coupling between the atom and the oscillators

$$H' = C(a + a^{\dagger}) \tag{8}$$

Show that the total Hamiltonian for t > 0, H + H', can be diagonalized by adding a constant shift to the step operators and determine the shift.

- 4(b). Express the energy eigenstates $|n'\rangle$ of the full Hamiltonian H + H' in a^{\dagger} and $|0\rangle$. 4(c). What are the matrix elements $\langle n'|0\rangle$, where $|0\rangle$ is the lowest eigenstate of H.
- 4(d). Assume the spectrum resulting from the sudden switching on of the perturbation is given by

$$I(E) = \sum_{n'} |\langle n'|0 \rangle|^2 \delta(E - E_{n'}).$$
(9)

Discuss the spectrum and how the spectral line shape changes as a function of $\Delta E/\hbar\omega$

 $\begin{array}{c} \mathbf{Answers} \\ 3(a) \end{array}$

$$A\frac{1}{r^2}\frac{d}{dr}\left(r^2(-B)e^{-Br}\right) = A\left(-B\frac{2}{r} + B^2\right)e^{-Br}$$
(10)

$$-A\frac{1}{r^{2}}\frac{d}{dr}\left(r^{2}\frac{d}{dr}\left[Bre^{-Br}\right]\right) = -A\frac{1}{r^{2}}\frac{d}{dr}\left(r^{2}Be^{-Br} - B^{2}r^{3}e^{-Br}\right)$$
(11)

$$= -A\left(\frac{2B}{r} - B^2 - 3B^2 + B^3r\right)e^{-Br}$$
(12)

giving

$$A\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\psi}{dr}\right) = A\left(B^2 - \frac{4B}{r}\right)(1 - Br)e^{-Br} = \left(B^2 - \frac{4B}{r}\right)\psi\tag{13}$$

For the Schrödinger Equation

$$-\frac{\hbar^2}{2m}\left(B^2 - \frac{4B}{r}\right)\psi - \frac{e^2}{r}\psi = E\psi.$$
(14)

Therefore

$$\frac{\hbar^2 B}{2mr} = \frac{e^2}{r} \qquad \Rightarrow \qquad B = \frac{me^2}{2\hbar^2} = \frac{1}{2a_0} \tag{15}$$

where $a_0 = hbar^2/me^2$ is the Bohr radius. 3(b)

$$E = -\frac{\hbar^2}{2m}B^2 = -\frac{\hbar^2}{4 \times 2ma_0^2} = -\frac{13.6}{4} \quad \text{eV}$$
(16)

PhD Candidacy Exam Fall 2004 – Quantum Mechanics Choose any 3 of 4.

<u>Problem 1.</u> (a) Planck's radiation law is given by

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

Show that the energy density u_ω in terms of wavelength becomes

$$u_{\lambda} = \frac{8\pi hc}{\lambda^5} \frac{1}{\exp\left(\frac{hc}{\lambda k_B T}\right) - 1}.$$
(2)

(b) Find the wavelength for which the energy distribution is maximum (assume that $hc/\lambda k_B T$ is large enough, so that $e^{-hc/\lambda k_B T} \rightarrow 0$). The relation $T\lambda$ =constant is known as Wien's Law. (c) Derive the Stefan-Boltzmann law from Planck's law, using

$$\int_0^\infty \frac{x^3}{e^x - 1} dx = \frac{\pi^4}{15} = 6.4938.$$
(3)

Calculate the value of the Stefan-Boltzmann constant.

<u>Problem 2.</u> (a) Let us consider the harmonic oscillator whose Hamiltonian is given by

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

By using

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

and the commutation relations of the operators

$$[a, a^{\dagger}] = 1 \tag{6}$$

show that the wavefunction $a^{\dagger}|n\rangle$ is proportional to the wavefunction $|n+1\rangle$.

(b) The wavefunctions for the harmonic oscillator are given by

$$|n\rangle = \frac{1}{\sqrt{n!}} (a^{\dagger})^n |0\rangle.$$
(7)

Determine the constant for which $a^{\dagger}|n\rangle = \text{constant}|n+1\rangle$.

(c) We can also write \hat{x} and \hat{p}_x in terms of the creation and annihilation operators

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(a^{\dagger} + a) \quad \text{and} \quad \hat{p}_x = i\sqrt{\frac{m\hbar\omega}{2}}(a^{\dagger} - a).$$
 (8)

By determining the values of $\langle \hat{x}^2 \rangle$ and $\langle \hat{p}_x^2 \rangle$, show that Heisenberg's uncertainty principle is satisfied.

<u>Problem 3.</u> (a) An electron is harmonically bound at a site. It oscillates in the x direction. The solutions of this harmonic oscillator are

$$H = \hbar\omega(a^{\dagger}a + \frac{1}{2}). \tag{9}$$

We introduce a perturbation by an electric field created by a positive point charge at a distance $R\hat{x}$. Show that the disturbing potential can be written as (you can leave out the constant energy shift from the electric field)

$$H' = P(a + a^{\dagger}) \quad \text{with} \quad P = \frac{e^2}{4\pi\epsilon_0 R^2} \sqrt{\frac{\hbar}{2m\omega}}$$
(10)

when R is much larger than the amplitude of the oscillation.

(b) Note that the Hamiltonian H + H' is not diagonal, since different values of n are coupled with each other. Show that the total Hamiltonian can be diagonalized by adding a constant shift to the step operators.

(c) What is the shift in energy as a result of the perturbation H'?

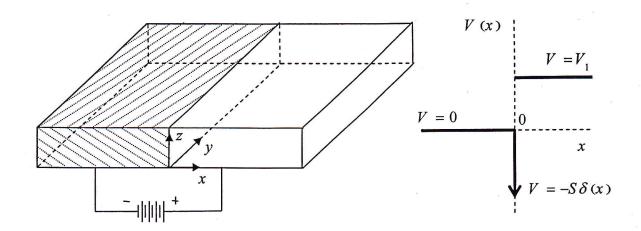
<u>Problem 4.</u> Two similar metals are separated by a very thin insulating layer along the plane x = 0. The potential energy is constant inside each metal; however, a battery can be used to establish a potential difference V_1 between the two. Assume that the electrons have a strong attraction to the material of the insulating layer which can be modeled as an attractive delta function at x = 0 for all values of y and z. A sketch of the potential energy along the x direction is shown in Figure 1. Here S and V_1 are positive.

(a) Assume that the metals extend to infinity in the y and z directions. Write down the correct three-dimensional functional form for an energy eigenfunction of a state <u>bound</u> in the x direction. Sketch its x dependence.

(b) Find the maximum value of V_1 for which a bound state can exist. Express your answer in terms of h, m, and S.

(c) Find the energy of the bound state in terms of h, m, S, and V_1 . Show that your answer is consistent with 4(b).

Fig 1:



Ph. D. Qualifying Exam

January 2004

Quantum Mechanics

Do 3 out of 4 problems

Problem 1:

The eigenfunction for the lowest spherically symmetric state of the electron in a hydrogen atom is given by

 $\psi(r) = A e^{-br}$

- (a) Sketch the radial probability distribution for this state.
- (b) Find the value of r for which the radial probability is a maximum. This gives the Bohr radius a_0 .
- (c) Show that ψ(r) satisfies the Schrödinger equation, and deduce the value of the Bohr radius in terms of ħ, m, and e. What is the ground state energy in terms of the Bohr radius?
- (d) Determine the normalization constant A in terms of the Bohr radius.
- (e) Find the value of the expectation value of r.
- (f) Find the value of the expectation value of the potential energy.
- (g) Find the value of the expectation value of the kinetic energy.

Problem 2:

A quantum mechanical particle of mass m is constrained to move in a cubic box of volume a^3 . The particle moves freely within the box.

- (a) Calculate the pressure the particle exerts on the walls of the box when the particle is in the ground state.
- (b) Suppose the volume of the box is doubled suddenly by moving one wall of the box outward. What is the probability distribution of the energy of the particle after the expansion has taken place?
- (c) What is the expectation value of the energy after the expansion?

Problem 3:

The spin-orbit coupling in hydrogen gives rise to a term in the Hamiltonian of the form $A\hat{\mathbf{L}}\cdot\hat{\mathbf{S}}/\hbar^2$ where A is a positive constant with the units of energy.

- (a) Find the zero-field splitting (separation) of the n = 3, $\ell = 2$ energy level of hydrogen due to this effect.
- (b) Assume that the hydrogen atom is in the lowest of the energy levels found in Part (a) and that it has the maximum possible value of m_j consistent with that energy. Find the probability density associated with a measurement of the z-component of the electron spin, m_s .

Problem 4:

The Hamiltonian for the harmonic oscillator in one dimension is

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

- (a) Add a perturbation of the form $\gamma \hat{x}^2$ to the Hamiltonian. The solution to this perturbed harmonic oscillator can still be solved exactly. Calculate the new exact eigenenergies (you can assume the solution of the harmonic oscillator to be known-there is no need to derive it again).
- (b) Instead of the perturbation $\gamma \hat{x}^2$, add the perturbation $\gamma \hat{x}$ to the Hamiltonian. Find the exact eigenenergies of this Hamiltonian.
- (c) Using time-independent perturbation theory, show that the first order corrections to the energy vanishes for the Hamiltonian in <u>Part (b)</u>.
- (d) Calculate the second order corrections, and show that they agree with your answer to <u>Part (b)</u> showing that the second order corrections gives the complete solution for this problem.

Information which may be useful:

$$\begin{split} \left[\hat{x}, \hat{p} \right] &= i\hbar \\ \hat{a} &= \sqrt{\frac{m\omega}{2\hbar}} \hat{x} + i\sqrt{\frac{1}{2\hbar m\omega}} \hat{p} \\ \hat{a}^{\dagger} &= \sqrt{\frac{m\omega}{2\hbar}} \hat{x} - i\sqrt{\frac{1}{2\hbar m\omega}} \hat{p} \\ \hat{x} &= \sqrt{\frac{\hbar}{2m\omega}} \left(\hat{a}^{\dagger} + \hat{a} \right) \\ \hat{p} &= i\sqrt{\frac{\hbar m\omega}{2}} \left(\hat{a}^{\dagger} - \hat{a} \right) \\ \left[\hat{a}, \hat{a}^{\dagger} \right] &= 1 \\ \hat{a} &|n\rangle &= \sqrt{n} |n-1\rangle \\ \hat{a}^{\dagger} &|n\rangle &= \sqrt{n+1} |n+1\rangle \end{split}$$

$$\hat{H} = \left(\hat{a}\hat{a}^{\dagger} + \frac{1}{2}\right)\hbar\omega$$

$$\hat{J}_{\pm}|j,m\rangle = \left(\hat{J}_{x} \pm i\hat{J}_{y}\right)|j,m\rangle = \hbar\sqrt{j(j+1) - m(m\pm 1)}|j,m\pm 1\rangle$$

The Laplacian in Spherical Coordinates is:

$$\nabla^2 F = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial F}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial F}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 F}{\partial \phi^2}$$

Useful Integrals:

$$\int_{0}^{\infty} r^{n} e^{-\alpha r} dr = \frac{n!}{\alpha^{n+1}}$$
$$\int_{0}^{\infty} e^{-ax^{2}} dx = \frac{1}{2} \sqrt{\frac{\pi}{a}}$$

Qualifying Exam

Quantum Mechanics

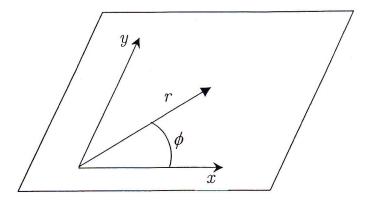
Do 3 out of 4. Problem 1:

9-2003

- (a) Find $\sigma_x^2 \sigma_p^2$ for an eigenstate, $|n\rangle$, of a harmonic oscillator with natural frequency ω . An exact expression, not a lower bound, is desired. $\sigma_x^2 \equiv \langle (x - \langle x \rangle)^2 \rangle$ is the variance associated with a measurement of the position, and $\sigma_p^2 \equiv \langle (p_x - \langle p_x \rangle)^2 \rangle$ is the variance associated with a measurement of the momentum.
- (b) Compare your answer to that which would be found for a classical harmonic oscillator of the <u>same energy</u> but undetermined phase where

$$\begin{split} x\left(t\right) &= x_0 \sin\left(\omega t + \phi\right) \\ p\left(t\right) &= p_0 \cos\left(\omega t + \phi\right). \end{split}$$

Problem 2:



Consider the "hydrogen atom problem" in two dimensions. The electron is constrained to move in a plane and feels a potential $V(r) = -Ze^2/r$ due to a charge +Ze at the origin. (This mathematical model has a physically realizable analog in the physics of semiconductors.)

(a) Find the eigenfunctions and eigenvalues for the z-component of angular momentum

$$\hat{L}_z \equiv \hat{x}\hat{p}_y - \hat{y}\hat{p}_x = -i\hbar\frac{\partial}{\partial\phi}$$

(b) The time independent Schrodinger equation for this problem is

$$\left(-\frac{\hbar^2}{2\mu}\nabla^2 + V(r)\right)\psi(r,\phi) = E\psi(r,\phi)$$

where μ is the reduced mass. Show that it is satisfied by a ψ which is a product of radial and angular functions: $\psi(r,\phi) = R(r)\Phi(\phi)$. Find $\Phi(\phi)$ and write down the equation determining R(r).

- (c) What condition must be satisfied in order for $R(r) = \alpha e^{-r/r_o}$ to be a solution of the radial equation? When this condition is satisfied find r_o and the associated energy eigenvalue E in terms of \hbar , μ , Z, and e. (α is a normalization constant which you need not find.)
- (d) Let $R(r) = r^{-\frac{1}{2}} u(r)$. Find the equation which determines u(r). Comment on the form of this equation.
- (e) A complete solution of the problem would show that the total degeneracy of the n^{th} bound state energy eigenvalue is 2n 1. Draw an energy level diagram in which the levels are separated into different angular momentum "ladders". Indicate the degeneracy and number of radial nodes associated with each of these "sub-levels" for the lowest 4 values of E.

Problem 3:

A quantum mechanical particle of mass m moves in one dimension in a potential consisting of two negative delta-function spikes, located at $x = \pm a$:

$$V(x) = -\lambda[\delta(x-a) + \delta(x+a)],$$

where λ is a positive constant.

(a) Prove that the basis of bound state wave functions can be chosen so that they are each either even or odd under reflection $x \to -x$.

(b) Derive a (transcendental) equation for the binding energy of an even bound state. By sketching the functions involved, show that there is one and only one even bound state for each value of λ .

(c) Derive the transcendental equation for an odd bound state. Show that there is a minimum value of λ for there to be an odd bound state, and determine that value.

Problem 4:

An atom that is otherwise spherically symmetric has an electron with orbital angular momentum $\ell = 2$ and spin s = 1/2.

(a) Using the raising and lowering operator formalism for general angular momenta, e.g.

$$J_{-}|j,m\rangle = (J_{x} - iJ_{y})|j,m\rangle = \sqrt{(j+m)(j-m+1)\hbar}|j,m-1\rangle,$$

construct the properly normalized linear combinations of $|\ell, m_{\ell}, s, m_s\rangle$ eigenstates that have total angular momentum eigenvalues:

(i)
$$j = 5/2$$
, $m_j = 5/2$
(ii) $j = 5/2$, $m_j = 3/2$
(iii) $j = 3/2$, $m_j = 3/2$.

(b) In an external magnetic field in the z direction of magnitude B, the magnetic interaction Hamiltonian is:

$$H_{\text{mag}} = \frac{eB}{2mc}(L_z + 2S_z).$$

What energy corrections are induced for the states of part (a), for a weak field B?

PhD Qualifying Exam January 2003 – Quantum Mechanics Choose any 3 of 4.

<u>Problem 1.</u> A system with three unperturbed states can be represented by the perturbed Hamiltonian matrix:

$$H = \begin{pmatrix} E_1 & 0 & a \\ 0 & E_1 & b \\ a^* & b^* & E_2 \end{pmatrix},$$

where $E_2 > E_1$. The quantities *a* and *b* are to be regarded as perturbations that are of the same order, and are small compared with E_1 , E_2 , and $E_2 - E_1$.

(a) Find the exact energy eigenvalues of the system.

(b) Use the second-order <u>non-degenerate</u> perturbation theory to calculate the perturbed energy eigenvalues (assuming the two degenerate energies are very slightly different). Is this procedure correct?

(c) Use the second-order <u>degenerate</u> perturbation theory to find the energy eigenvalues. Compare the three results obtained.

<u>Problem 2.</u> Consider a particle of mass m moving in the potential well:

$$V = \begin{cases} 0 & (0 < x < a) \\ \infty & \text{elsewhere} \end{cases}$$

(a) Solve the Schrödinger equation to find the energy eigenvalues E_n and the normalized wavefunctions.

(b) For the *n*th energy eigenstate with energy E_n , compute the expectation values of x and $(x - \langle x \rangle)^2$, and show that the results can be written:

$$\langle x \rangle = a/2, \langle (x - \langle x \rangle)^2 \rangle = c_1 a^2 - \frac{c_2}{mE_n},$$

where c_1 and c_2 are constant numbers that your will find. Show that in the limit of large E_n , the results agree with the corresponding classical results.

<u>Problem 3.</u> Consider a particle of mass m moving in the three-dimensional harmonic oscillator potential $V = \frac{k}{2}(x^2 + y^2 + z^2)$.

(a) Write down the Schrödinger equation for the wavefunction in rectangular coordinates. Find the allowed energy eigenvalues.

(b) What is the degeneracy of the 3rd excited energy level?

(c) Suppose the wavefunctions are found in spherical coordinates in a basis consisting of eigenstates of energy, total angular momentum, and the \hat{z} component of angular momentum, of the form:

$$\psi(r,\theta,\phi) = R(r)Y_{\ell m}(\theta,\phi),$$

where $Y_{\ell m}(\theta, \phi)$ are the spherical harmonics. Find the differential equation satisfied by R(r), for a given energy eigenvalue E and a given ℓ and m.

<u>Problem 4.</u> A particle of spin $\frac{1}{2}$ is subject to the Hamiltonian:

$$H = \frac{a}{\hbar}S_z + \frac{b}{\hbar^2}S_z^2 + \frac{c}{\hbar}S_x$$

where a, b, and c are constants.

(a) What are the energy levels of the system?

(b) In each of the energy eigenstates, what is the probability of finding $S_z = +\hbar/2$?

(c) Now suppose that a = 0, and that at time t = 0, the spin is in an energy eigenstate with $S_z = +\hbar/2$. What is the probability of finding $S_z = -\hbar/2$ at any later time t?

(d) Under the same assumptions as part (c), what is the expectation value of S_y as a function of t?

* * *

Possibly useful information:

The Pauli matrices are

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

The Laplacian in spherical coordinates is

$$\nabla^2 F = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial F}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial F}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 F}{\partial \phi^2}.$$