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 $\psi(t) = \binom{a(t)}{b(t)}$ 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 $\mathbf{B}$ 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 $\psi(t = 0) = \binom{1}{0}$.

(c) At $t = 0$ an additional magnetic field in x direction is switched on so that we have $\mathbf{B}(t \geq 0) = (B_x, 0, B_z)$. Solve the time-dependent Schrödinger equation for $t \geq 0$ 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 $\psi(t = 0) = \binom{1}{0}$ 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 $t \geq 0$, 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

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

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 $|L_1 M_1, L_2 M_2\rangle$, 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

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

(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

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

(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

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

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:

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

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

$$\Psi(x,t) = A\left[\sin\left(\frac{\pi x}{L}\right)e^{-iE_1 t/\hbar} - \frac{3}{4}\sin\left(\frac{3\pi x}{L}\right)e^{-iE_3 t/\hbar}\right], \tag{1}$$

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

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

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 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 $n = 0, 1, 2, 3 \ldots$) 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 mth excited state $|m\rangle$ (with $m > 0$) at time $t = +\infty$ is:

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

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

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

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:

$$V(r) = A(1 - r/a) \qquad \text{for } (r < a) \tag{1}$$
$$V(r) = 0 \qquad \text{for } (r \geq a), \tag{2}$$

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

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

where $\mathbf{S}_1$ and $\mathbf{S}_2$ 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

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

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

Answers

3(a)

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

$$\begin{aligned} -A\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\left[Bre^{-Br}\right]\right) &= -A\frac{1}{r^2}\frac{d}{dr}\left(r^2Be^{-Br}-B^2r^3e^{-Br}\right) &(11)\\ &= -A\left(\frac{2B}{r}-B^2-3B^2+B^3r\right)e^{-Br} &(12)\end{aligned}$$

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

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

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)

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

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

Problem 1. (a) Planck's radiation law is given by

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

Show that the energy density u_ω in terms of wavelength becomes

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

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

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

Calculate the value of the Stefan-Boltzmann constant.

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

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

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

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

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

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

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.

Problem 3. (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)

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

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' ?

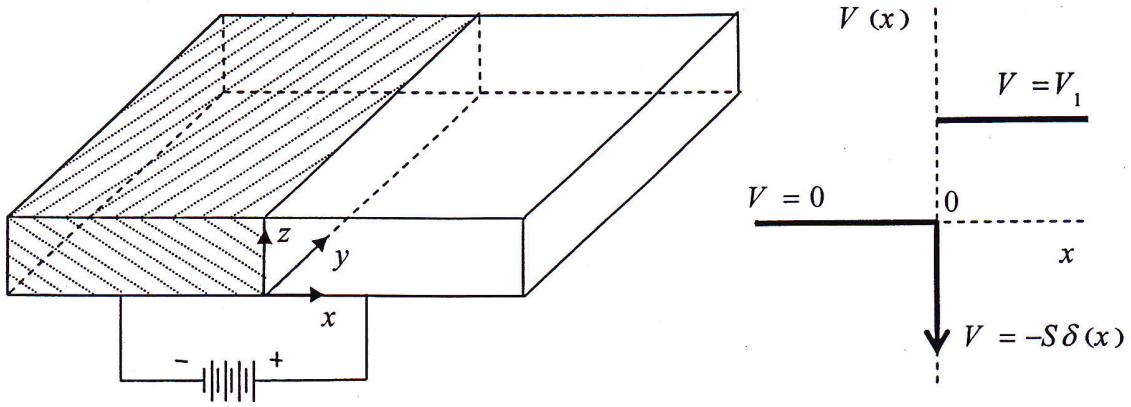
Problem 4. Two similar metals are separated by a very thin insulating layer along the plane $x = 0$. The potential energy is constant inside each metal; however, a battery can be used to establish a potential difference V_1 between the two. Assume that the electrons have a strong attraction to the material 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 bound 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 $\psi(r)$ satisfies the Schrödinger equation, and deduce the value of the Bohr radius in terms of $\hbar$, 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 Part (b).

(d) Calculate the second order corrections, and show that they agree with your answer to Part (b) showing that the second order corrections gives the complete solution for this problem.

Information which may be useful:

$$[\hat{x},\hat{p}] = i\hbar$$

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\hat{x} + i\sqrt{\frac{1}{2\hbar m\omega}}\hat{p}$$

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

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}\left(\hat{a}^\dagger + \hat{a}\right)$$

$$\hat{p} = i\sqrt{\frac{\hbar m\omega}{2}}\left(\hat{a}^\dagger - \hat{a}\right)$$

$$\left[\hat{a},\hat{a}^\dagger\right] = 1$$

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle$$

$$\hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$$

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

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

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:

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

$$\int_0^\infty e^{-ax^2}\,dx = \frac{1}{2}\sqrt{\frac{\pi}{a}}$$

9-2003

Qualifying Exam

Quantum Mechanics

Do 3 out of 4.

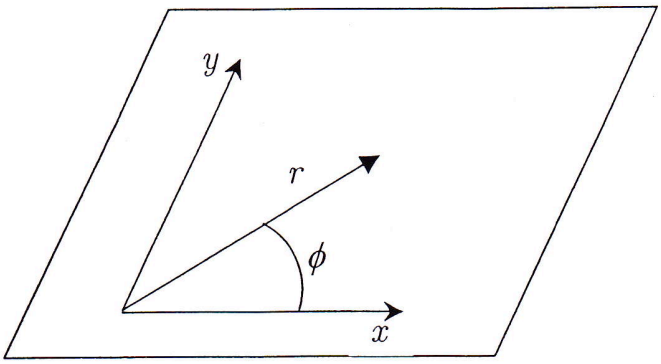
Problem 1:

(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. $\sigma_x^2 \equiv \left\langle (x - \langle x \rangle)^2 \right\rangle$ is the variance associated with a measurement of the position, and $\sigma_p^2 \equiv \left\langle \left(p_x - \langle p_x \rangle \right)^2 \right\rangle$ 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

$$x(t) = x_0 \sin(\omega t + \phi)$$
$$p(t) = p_0 \cos(\omega t + \phi).$$

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 $R(r) = r^{-1/2}u(r)$. 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 nth 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:

$$\begin{aligned} (i) \quad & j = 5/2, \quad m_j = 5/2 \\ (ii) \quad & j = 5/2, \quad m_j = 3/2 \\ (iii) \quad & j = 3/2, \quad m_j = 3/2. \end{aligned}$$

(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.

Problem 1. 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 non-degenerate 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 degenerate perturbation theory to find the energy eigenvalues. Compare the three results obtained.

Problem 2. 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 nth 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:

$$\begin{aligned} \langle x \rangle &= a/2, \\ \langle (x - \langle x \rangle)^2 \rangle &= c_1 a^2 - \frac{c_2}{m E_n}, \end{aligned}$$

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.

Problem 3. 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.

Problem 4. 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

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