Qualifying Examination
Quantum Mechanics
January 14, 2006

PROBLEM 1.
Calculate the reflection and transmission coefficients for a particle scattering of a potential $V = 0$ for $x < 0$ and $V = V_0 > 0$ for $x > 0$. Assume the energy of the particle $E > V_0$.

PROBLEM 2.
Let $\mathbf{L}$ be an angular momentum operator and let $|M\rangle$ denote a normalized eigenstate of L_z with eigenvalue M, i.e. $L_z|M\rangle = M|M\rangle$.

a) Show that

$$L_\pm|M\rangle = C_\pm(M)|M \pm 1\rangle,$$

where $L_\pm = L_x \pm iL_y$ and $C_\pm(M)$ is a constant.

b) Show that

$$\langle M|L_x|M\rangle = \langle M|L_y|M\rangle = 0, \quad \langle M|L_x^2|M\rangle = \langle M|L_y^2|M\rangle, \quad \langle M|L_xL_y + L_yL_x|M\rangle = 0.$$

PROBLEM 3A.
Consider a particle of mass m in a three-dimensional potential $V(r) = -\alpha\delta(r - a)$, where α and a are positive constants. Find wave functions (up to a normalization constant) and energies of s-states (bound states with zero angular momentum). How many s-states are there?

PROBLEM 3B.
Suppose at $t = 0$ a particle of mass m is in the ground state of an attractive δ-function potential. Let the ground state energy be E_0. For $t > 0$ the particle is subject to a periodic perturbation $V(x, t) = -xF_0 \cos\omega_0 t$. Use Fermi's golden rule to calculate the rate of transitions out of the ground state. Assume $\hbar\omega_0 \gg |E_0|$ and neglect the influence of the δ-function on the final states, i.e. take them to be plane waves.

PROBLEM 4A.
Consider a particle of mass m in a potential well

$$U(x, y, z) = \begin{cases} 0, & (x^2 + y^2)/a^2 + z^2/b^2 < 1, \\ \infty, & (x^2 + y^2)/a^2 + z^2/b^2 \geq 1, \end{cases}$$

where $|a - b| \ll b$. Note that the potential well is an ellipsoid of rotation of volume $V = 4\pi a^2 b/3$. Determine the ground state energy to the first order of perturbation theory in $\epsilon = (a - b)/b$. What is the shift in the ground state energy as compared to that for the same particle in the ground state of an infinite spherical well potential of the same volume V?

PROBLEM 4B.

Consider a spin Hamiltonian $H = A\mathbf{K}\cdot\mathbf{S} + BS_z$, where $\mathbf{S}$ is a spin 1/2, $\mathbf{K}$ is a spin K, and A and B are real parameters.

a) Show that the z-component of the total spin $\mathbf{J} = \mathbf{K} + \mathbf{S}$ is conserved. How many states are there for a given value of $J_z = m$?

b) Determine the energy levels and their degeneracies for 1) $B = 0$ 2) $A = 0$. What is the symmetry responsible for the degeneracies in each case?

c) Set $A = 1$ and determine energy levels for arbitrary B. You can use $C_\pm(M) = \sqrt{(L \mp M)(L \pm M + 1)}$, where $C_\pm(M)$ is defined in problem **B**.

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PROBLEM 1.
The solution of the Shrödinger equation describing transmission and reflection of particles with $E > V_0$ incident from the left is

$$\psi_k(x) = \begin{cases} e^{ikx} + A(k)e^{-ikx}, & x < 0 \quad (k = \sqrt{2mE/\hbar^2} > 0) \\ \\ B(k)e^{ik'x}, & x > 0 \quad (k' = \sqrt{2m(E - V_0)/\hbar^2} > 0) \end{cases}$$

The wave function and its derivative are continuous at $x = 0$. These conditions yield

$$1 + A = B, \qquad k(1 - A) = k'B$$

We obtain

$$A(k) = \frac{k - k'}{k + k'} \qquad B(k) = \frac{2k}{k + k'}$$

The reflection (R) and transmission (T) coefficients are

$$R = |A|^2 = \left(\frac{\sqrt{E} - \sqrt{E - V_0}}{\sqrt{E} - \sqrt{E - V_0}}\right)^2, \quad T = \frac{k'}{k}|B|^2 = \frac{4\sqrt{E(E - V_0)}}{(\sqrt{E} - \sqrt{E - V_0})^2}$$

PROBLEM 2.
(a) It follows from commutations relations for angular momentum components that

$$[L_z, L_\pm] = \pm L_\pm,$$

$$L_z L_\pm = L_\pm(L_z \pm 1).$$

Apply both sides of this equation to the state $|M\rangle$,

$$L_z(L_\pm|M\rangle) = L_\pm(M \pm 1)|M\rangle = (M \pm 1)(L_\pm|M\rangle).$$

We see that the state $L_\pm|M\rangle$ is either an eigenstate of L_z with eigenvalue $M \pm 1$ or zero. Therefore,

$$L_\pm|M\rangle = C_\pm(M)|M \pm 1\rangle.$$

(b) Since eigenstates with different M are orthogonal,

$$\langle M|L_\pm|M\rangle \propto \langle M|M \pm 1\rangle = 0, \quad \langle M|L_\pm^2|M\rangle = 0. \tag{1}$$

We obtain

$$\langle M|L_x|M\rangle \pm i\langle M|L_y|M\rangle = 0,$$

$$\langle M|L_x|M\rangle = \langle M|L_y|M\rangle = 0.$$

The second relation in Eq. (1) yields

$$\langle M|L_x^2 - L_y^2|M\rangle \pm i\langle M|L_xL_y + L_yL_x|M\rangle = 0.$$

Therefore,

$$\langle M|L_x^2|M\rangle = \langle M|L_y^2|M\rangle \qquad \langle M|L_xL_y + L_yL_x|M\rangle = 0.$$

PROBLEM 3A.

A substitution $\psi_E(\mathbf{r}) = \dfrac{u_{n_rl}}{r}Y_{lm}(\theta,\phi)$, where $Y_{lm}(\theta,\phi)$ is a spherical harmonic, reduces the Shrödinger equation

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right]\psi_E(\mathbf{r}) = E\psi_E(\mathbf{r}) \quad V(r) = -\alpha\delta(r-a)$$

to a one-dimensional one

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2mr^2} + V(r)\right]u_{n_rl} = Eu_{n_rl}$$

Here we are looking for s-states, i.e.

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + V(r)\right]u_{n_r0} = Eu_{n_r0}$$

Bound states have $E < 0$. Boundary conditions are $u_{n_r0}(0) = u_{n_r0}(\infty) = 0$. The solution with these boundary conditions is

$$u_{n_r0}(r) = \begin{cases} A\sinh\kappa r, & r < a, \\ Be^{-\kappa r}, & r > a, \end{cases}$$

where $\kappa = \sqrt{2m|E|/\hbar^2}$. Due to the delta function potential, the logarithmic derivative of the wave function experiences a jump at $r = a$ of magnitude $-2m\alpha/\hbar^2$

$$\frac{d\ln u_{n_r0}(a+0)}{dr} - \frac{d\ln u_{n_r0}(a-0)}{dr} = -\frac{2m\alpha}{\hbar^2}.$$

We obtain an equation determining energies of s-states

$$1 - e^{-2\kappa a} = \frac{\hbar^2\kappa}{m\alpha} = \lambda(2\kappa a), \quad \lambda = \frac{\hbar^2}{2m\alpha a}.$$

For $\lambda > 1$ there are no solutions, i.e. no s-states. For $\lambda < 1$ there is a single s-state.

The wave function is continuous at $r = a$

$$A\sinh\kappa a = Be^{-\kappa a}.$$

We obtain

$$B = \frac{A}{2}(e^{2\kappa a} - 1).$$

Thus, ($Y_{00}(\theta,\phi) = \text{const}$)

$$\psi_E(r) = \begin{cases} C\dfrac{\sinh \kappa r}{r}, & r < a, \\ \\ C(e^{2\kappa a} - 1)\dfrac{e^{-\kappa r}}{2r}, & r > a, \end{cases}$$

where C is a normalization constant.

PROBLEM 3B.
The rate of transitions (Fermi's golden rule) is

$$w = \frac{2\pi}{\hbar}\int \left|\hat{V}_{\nu 0}\right|^2 \delta(E_\nu - E_0 - \hbar\omega_0)d\nu. \tag{2}$$

Here

$$\hat{V}_{\nu 0} = \left\langle \psi_0(x) \left| \frac{xF_0}{2} \right| \psi_\nu(x) \right\rangle,$$

$\psi_0(x) = \sqrt{\kappa}e^{-\kappa|x|}$ is the ground state wave function, $\kappa = m\alpha/\hbar^2$, $E_0 = -\hbar^2\kappa^2/2m$ is the ground state energy, $\psi_\nu(x)$ and E_ν are wave functions and energies of final states, respectively.

Neglecting the influence of the δ-function on final states, we take them to be plane waves

$$\psi_\nu(x) = \frac{1}{\sqrt{2\pi}}e^{ikx}, \quad E_\nu = \frac{\hbar^2k^2}{2m}, \quad \nu \equiv k, \quad -\infty < k < \infty.$$

We find

$$\hat{V}_{\nu 0} = -\frac{F_0\sqrt{\kappa}}{2\sqrt{2\pi}}\int_{-\infty}^{\infty} x\exp[-\kappa|x| - ikx]dx = i\frac{\sqrt{2}k\kappa^{3/2}F_0}{\sqrt{\pi}(k^2+\kappa^2)^2},$$

and, using Eq. (2),

$$w = \frac{2\hbar F_0^2|E_0|^{3/2}\sqrt{\hbar\omega_0 - |E_0|}}{m(\hbar\omega_0)^4}$$

PROBLEM 4A.
In new coordinates $x' = x$, $y' = y$, and $z' = az/b = (1+\epsilon)z$ the Shrödinger equation and the boundary condition read

$$\hat{H}\psi \equiv -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x'^2} + \frac{\partial^2}{\partial y'^2} + (1+\epsilon)^2\frac{\partial^2}{\partial z'^2}\right)\psi = E\psi \quad \psi(r' = a) = 0$$

Now write the Hamiltonian in the form $\hat{H} = \hat{H}_0 + \hat{V}$, where

$$\hat{H}_0 = -\frac{\hbar^2}{2m}\nabla'^2, \quad \hat{V} = -\frac{\hbar^2}{2m}(2\epsilon - \epsilon^2)\frac{\partial^2}{\partial z'^2}. \tag{3}$$

The unperturbed Hamiltonian $\hat{H}_0$ describes a particle in a spherical box. Its ground state is

$$\psi_0^{(0)} = \frac{1}{\sqrt{2\pi a r}}\sin\frac{\pi r}{a}, \quad r \le a; \quad E_0^{(0)} = \frac{\pi^2\hbar^2}{2ma^2}.$$

(here and below primes are dropped for simplicity).

According to Eq. (3), to evaluate the first order correction in ϵ to the ground state energy, we need to compute the average $\langle \partial^2/\partial z^2 \rangle$ in the unperturbed ground state. Due to spherical symmetry of the latter

$$\langle \partial^2/\partial x^2 \rangle = \langle \partial^2/\partial y^2 \rangle = \langle \partial^2/\partial z^2 \rangle = \frac{1}{3}\langle \nabla^2 \rangle = -\frac{2m}{3\hbar^2}\langle \hat{H}_0 \rangle = -\frac{2m}{3\hbar^2}E_0^{(0)}.$$

Therefore,

$$E_0^{(1)} = \frac{2\epsilon}{3}E_0^{(0)} \quad E_0 \approx E_0^{(0)} + E_0^{(1)} = \left(1 + \frac{2\epsilon}{3}\right)\frac{\pi^2\hbar^2}{2ma^2} \tag{4}$$

The radius R of a sphere of the same volume as the ellipsoid is determined by

$$\frac{4\pi}{3}R^3 = \frac{4\pi}{3}a^2 b \approx \frac{4\pi}{3}a^3(1-\epsilon)$$

We find $R \approx a(1-\epsilon/3)$. Therefore,

$$E_0 \approx \frac{\pi^2\hbar^2}{2mR^2},$$

i.e. there is no shift as compared to a sphere of the same volume. To the first order in ϵ, the ground state energy depends only on the volume of the ellipsoid.

PROBLEM 4B.

a) The quantity $\mathbf{K}\cdot\mathbf{S}$ is a scalar product of two vectors. As such it is rotationally invariant, i.e. it commutes with all components of $\mathbf{J}$

$$[\mathbf{J}, \mathbf{K}\cdot\mathbf{S}] = 0.$$

In particular, it commutes with J_z. Since S_z also commutes with $J_z = K_z + S_z$,

$$[J_z, H] = 0$$

Eigenvalues of J_z are

$$m = -K - 1/2, -K + 1/2, \ldots, K - 1/2, K + 1/2$$

Let us use the tensor product basis $|K_z, S_z\rangle$ of simultaneous eigenstates of operators K_z and S_z. Since S_z has only two eigenvalues $\pm 1/2$, there are two states $|m - 1/2, 1/2\rangle$ and $|m + 1/2, -1/2\rangle$ for each $m \neq \pm(K + 1/2)$. There is only one state $|\pm K, \pm 1/2\rangle$ for $m = \pm(K + 1/2)$.

b) 1) $B = 0$. Use

$$\mathbf{K}\cdot\mathbf{S} = \frac{\mathbf{J}^2 - \mathbf{K}^2 - \mathbf{S}^2}{2} = \frac{J(J+1) - K(K+1) - S(S+1)}{2}$$

Total spin takes values $J = K \pm 1/2$. There are two energy levels

$$E_1\left(J = K + \frac{1}{2}\right) = \frac{A}{2}\left[\left(K + \frac{1}{2}\right)\left(K + \frac{3}{2}\right) - K(K+1) - \frac{1}{2}\left(\frac{1}{2} + 1\right)\right] = \frac{AK}{2},$$

$$E_2\left(J=K-\frac{1}{2}\right)=-\frac{A(K+1)}{2}.$$

Each level is $(2J+1)$-fold degenerate. The symmetry responsible for the degeneracy is rotational invariance.

2) $A=0$. We have $H=BS_z$. There are two energy levels

$$E_{1,2}\left(S_z=\pm\frac{1}{2}\right)=\pm\frac{B}{2}$$

Each level is $(2K+1)$-fold degenerate with respect to eigenvalues of K_z. For $A=0$ the Hamiltonian commutes with all components of $\mathbf{K}$, i.e. it is invariant with respect to arbitrary rotations in the subspace of spin $\mathbf{K}$.

c) Let us use the basis $|K_z, S_z\rangle$. Since $[J_z, H]=0$, matrix elements of the Hamiltonian between states with different m vanish. Thus, in this basis the Hamiltonian is block-diagonal. The size of blocks for $m\neq\pm(K+1/2)$ is 2×2, because there are two states for each m. Writing the Hamiltonian ($A=1$) in the form

$$H=K_zS_z+\frac{1}{2}(K_-S_++K_+S_-)+BS_z,$$

we compute

$$H\left|m+\frac{1}{2},-\frac{1}{2}\right\rangle=-\frac{1}{2}\left[\left(m+\frac{1}{2}\right)+B\right]\left|m+\frac{1}{2},-\frac{1}{2}\right\rangle+\frac{1}{2}\sqrt{\left(K+m+\frac{1}{2}\right)\left(K-m+\frac{1}{2}\right)}\left|m-\frac{1}{2},\frac{1}{2}\right\rangle,$$

$$H\left|m-\frac{1}{2},\frac{1}{2}\right\rangle=\frac{1}{2}\left[\left(m-\frac{1}{2}\right)+B\right]\left|m-\frac{1}{2},\frac{1}{2}\right\rangle+\frac{1}{2}\sqrt{\left(K+m+\frac{1}{2}\right)\left(K-m+\frac{1}{2}\right)}\left|m+\frac{1}{2},-\frac{1}{2}\right\rangle.$$

Taking inner products with states $|m\pm 1/2,\mp 1/2\rangle$, we find the corresponding block of the Hamiltonian

$$H_m=-\frac{1}{4}I+\frac{1}{2}\begin{pmatrix}-m-B & \sqrt{\left(K+\frac{1}{2}\right)^2-m^2}\\ \sqrt{\left(K+\frac{1}{2}\right)^2-m^2} & m+B\end{pmatrix},$$

where I is 2×2 identity matrix. Eigenvalues (energies) are

$$E_{1,2}(m)=-\frac{1}{4}\pm\frac{1}{2}\sqrt{\left(K+\frac{1}{2}\right)^2+2mB+B^2}.$$

Finally, consider $m=\pm(K+1/2)$. States $|\pm K,\pm 1/2\rangle$ are eigenstates of the Hamiltonian,

$$H\left|\pm K,\pm\frac{1}{2}\right\rangle=\frac{K\pm B}{2}\left|\pm K,\pm\frac{1}{2}\right\rangle,$$

with eigenvalues

$$E\left(m=\pm\left(K+\frac{1}{2}\right)\right)=\frac{K\pm B}{2}.$$