Qual Review, Meeting 5: Quantum Mechanics

1a. Prove the following: If $\langle\psi|\psi_0\rangle = 0$, then $\langle\psi|H|\psi\rangle \geq E_1$, where E_1 is the energy of the first excited state, ψ_0 is the ground state, and ψ is any other state (not necessarily an eigenstate). You may assume the eigenstates are nondegenerate and orthonormal.

1b. Find the best bound on the first excited state of the one-dimensional harmonic oscillator using the trial function $\psi(x) = Axe^{-bx^2}$.

2. Consider a particle moving in a square well potential $V(x) = V_0$ for $0 \leq x \leq a$ and ∞ everywhere else.

2a. Derive the energy eigenvalues E_n and their corresponding eigenfunctions $\psi_n(x)$.

2b. A small perturbation $V_1 = aU\delta(x - a/2)$ is added, where U is a constant with the dimensions of energy. Calculate the energy shifts of all the levels E_n to first order in U.

2c. Find the ground state energy to second order in U. You may find the identity $\sum_{j=1}^{\infty} \frac{1}{j(j+1)} = 1$ useful.

3. Consider a potential of the form $V(x) = -\alpha\delta(x)$, where $\delta(x)$ is the usual Dirac delta function.

3a. Find all bound states ($E < 0$) of this (one-dimensional) potential and their energies. (*Hint:* What is the condition on the derivative of the wavefunction at $x = 0$?)

3b. A beam of particles represented by the plane wave Ae^{ikx} is incident on the delta function from the left. Find the fraction of the particles transmitted and the fraction of the particles reflected.

4. Consider the hyperfine splitting of the Hydrogen atom in a uniform magnetic field B. Assume the Zeeman shift is of the same order as the hyperfine shift. Take the perturbation to be $A\mathbf{S}_e \cdot \mathbf{S}_p - \mu_e \cdot \mathbf{B}$, where $\mu_e = \frac{e\mathbf{S}_e}{mc}$. Find the energy shift of all four $n = 1$, $l = 0$ levels. You do not need to work out the new eigenstates created by lifting the degeneracy.

5. Consider a particle constrained to move in a circle of radius b. Concentric with the circle is a long cylindrical solenoid of radius $a < b$, with magnetic field B inside.

5a. Find the vector potential (in the Coulomb gauge $\nabla \cdot \mathbf{A} = 0$) outside the solenoid.

5b. Write down the Hamiltonian for this system. Find its eigenfunctions and their energies. The gradient in cylindrical coordinates is

$$\nabla = \hat{r}\frac{\partial}{\partial r} + \hat{\phi}\frac{1}{r}\frac{\partial}{\partial \phi} + \hat{z}\frac{\partial}{\partial z}.$$

Quantum Sols.

a) $|\psi\rangle = \sum_{n=0}^{\infty} a_n |\psi_n\rangle$ ← eigenstates of H.

$$H|\psi\rangle = \sum_{n=0}^{\infty} a_n E_n |\psi_n\rangle.$$

So $\langle\psi|H|\psi\rangle = \sum_{n=0}^{\infty} a_n E_n \langle\psi|\psi_n\rangle = \sum_{n=1}^{\infty} a_n E_n \langle\psi|\psi_n\rangle$,

since $\langle\psi|\psi_0\rangle = 0$.

Now, $\langle\psi|\psi_n\rangle = \sum_{m=0} a_m^* \langle\psi_m|\psi_n\rangle$, so

$$\langle\psi|H|\psi\rangle = \sum_{n=1}^{\infty} a_n E_n \sum_{m=0}^{\infty} a_m^* \langle\psi_m|\psi_n\rangle = \sum_{n=1}^{\infty} a_n E_n \sum_{m=0}^{\infty} a_m^* \delta_{mn}.$$

$$= \sum_{n=1}^{\infty} |a_n|^2 E_n.$$

But since E_1 is the lowest energy, $E_n \geq E_1 \ \forall n \geq 1$.

$$\Rightarrow \langle\psi|H|\psi\rangle \geq E_1 \sum_{n=1}^{\infty} |a_n|^2 \geq E_1 \sum_{n=0}^{\infty} |a_n|^2 = E_1$$

$$\Rightarrow \boxed{\langle\psi|H|\psi\rangle \geq E_1}$$

A nice corollary to the variational principle.

b]

$$\langle\psi|H|\psi\rangle = \int_{-\infty}^{\infty} A^2 x e^{-bx^2}\left(\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega^2 x^2\right) x e^{-bx^2}\,dx$$

$$= \int_{-\infty}^{\infty} A^2 x e^{-bx^2}\left(\frac{-\hbar^2}{2m}\left(-6bxe^{-bx^2} + 4b^2x^3e^{-bx^2}\right) + \frac{1}{2}m\omega^2 x^2 x e^{-bx^2}\right)dx$$

Now, $\int x^2 e^{-bx^2} = \frac{1}{2}\frac{\sqrt{\pi}}{b^{3/2}}$, $\int x^4 e^{-bx^2} = \frac{3}{4}\frac{\sqrt{\pi}}{b^{5/2}}$

$$\Rightarrow \langle\psi|H|\psi\rangle = A^2\left[\int_{-\infty}^{\infty} \frac{+6bx^2e^{-2bx^2}\hbar^2}{2m}dx - \int_{-\infty}^{\infty}\frac{4\hbar^2b^2}{2m}x^4e^{-2bx^2} + \int_{-\infty}^{\infty}\frac{1}{2}m\omega^2x^4e^{-2bx^2}\right]$$

$$= A^2\left[\frac{6b\hbar^2}{2m}\cdot\frac{1}{2}\frac{\sqrt{\pi}}{(2b)^{3/2}} - \frac{4\hbar^2b^2}{2m}\cdot\frac{3}{4}\frac{\sqrt{\pi}}{(2b)^{5/2}} + \frac{1}{2}m\omega^2\frac{3}{4}\frac{\sqrt{\pi}}{(2b)^{5/2}}\right]$$

$$= A^2\left[\frac{3\cancel{6}\hbar^2\sqrt{\pi}}{2\cancel{4}m2^{3/2}\sqrt{b}} - \frac{\cancel{4}\hbar^2\cdot 3}{2\cancel{8}m2^{5/2}\sqrt{b}} + \frac{3m\omega^2\sqrt{\pi}}{82^{5/2}b^{5/2}}\right]$$

$$= A^2\left[\frac{3\hbar^2\sqrt{\pi}}{m\sqrt{b}}\left(\frac{1}{2^{5/2}} - \frac{1}{2^{7/2}}\right) + \frac{3m\omega^2\sqrt{\pi}}{8\cdot 2^{5/2}b^{5/2}}\right]$$

Take $\frac{d}{db}\langle H\rangle = 0$, plug in, etc.

2a] $V = \begin{cases} V_0 & 0 \le x \le a \\ \infty & \text{elsewhere.} \end{cases}$

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi_n}{\partial x^2} + V_0 \psi_n = E\psi_n \Rightarrow \frac{\partial^2 \psi_n}{\partial x^2} = -\frac{2m}{\hbar^2}(E-V)\psi_n$$

$$\Rightarrow \boxed{\psi_n = A\sin(kx) \Rightarrow \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)} \Rightarrow \boxed{E = \frac{\hbar^2 n^2 \pi^2}{2ma^2} + V_0}$$

b] $E_{n,1} = \langle \psi_n | V_1 | \psi_n \rangle$

$$= \int_0^a \frac{2}{a}\sin^2\left(\frac{n\pi x}{a}\right) \cdot a U \delta\left(x - \frac{a}{2}\right) dx$$

$$= 2U\sin^2\left(\frac{n\pi}{2}\right) \Rightarrow E_{n,1} = \begin{cases} 2U & n \text{ odd} \\ 0 & n \text{ even.} \end{cases}$$

c] $E_{n,2} = \sum_{m \ne n} \frac{|\langle \psi_m^0 | V_1 | \psi_n^0 \rangle|^2}{E_n^0 - E_m^0} = \sum_{m \ne n} \frac{\left|\int \frac{2}{a}\sin\left(\frac{m\pi}{a}x\right)\sin\left(\frac{n\pi}{a}x\right) a U \delta\left(x-\frac{a}{2}\right)dx\right|^2}{E_n^0 - E_m^0}$

$$= \sum_{m \ne n} \frac{\left(2U\sin\left(\frac{m\pi}{2}\right)\sin\left(\frac{n\pi}{2}\right)\right)^2}{\frac{\hbar^2\pi^2}{2ma^2}(n^2 - m^2)} \Rightarrow$$

This is 0 if n is even. If we look only at the ground state, with $n=1$,

$$E_{1,2} = \sum_{m\neq 1} \frac{4U^2 \sin^2\left(\frac{m\pi}{2}\right)}{\frac{\hbar^2\pi^2}{2ma^2}(1-m^2)} = \sum_{\substack{m\ odd \\ m\neq 1}} \frac{4U^2 \cdot 2ma^2}{\hbar^2\pi^2(1-m^2)}$$

$$= \sum_{n=1}^{\infty} \frac{8mU^2a^2}{\hbar^2\pi^2} \frac{1}{(1-(2n+1)^2)}$$

$$= \frac{8mU^2a^2}{\hbar^2\pi^2} \sum_{n=1}^{\infty} \frac{-1}{4n^2+4n}$$

$$= \frac{-2mU^2a^2}{\hbar^2\pi^2} \sum_{n=1} \frac{1}{n(n+1)} = \boxed{\frac{-2mU^2a^2}{\hbar^2\pi^2}}$$

3a) Sch. Equ: $\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi$

Outside of $x=0$, we'll just get exponentials:

$$\psi(x) = \begin{cases} Ae^{kx} & x<0 \\ Ae^{-kx} & x>0, \end{cases} \quad k = \frac{-2mE}{\hbar^2} \quad (E<0, \text{ so } k>0).$$

coeff. same to make $\psi(x)$ continuous.

on normalize: $\int_{-\infty}^{0} A^2 e^{2kx}dx + \int_{0}^{\infty} A^2 e^{-2kx}dx = 1 \Rightarrow A^2\left(\frac{1}{2k}\cdot 2\right) = 1 \Rightarrow A = \sqrt{k}$

Now, to get E (ie k), need to impose another condition.

Trick: integrate Sch. Equ

$$\int_{-\varepsilon}^{+\varepsilon} \frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2}dx + \underbrace{\int_{-\varepsilon}^{+\varepsilon} V(x)\psi(x)\,dx}_{-\alpha\psi(0)} = \cancel{\int_{-\varepsilon}^{+\varepsilon} E\psi(x)\,dx} \rightarrow 0 \text{ as } \varepsilon \to 0.$$

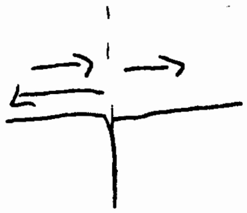
$$\frac{-\hbar^2}{2m}\Delta\left(\frac{d\psi}{dx}\right)$$

$$\Rightarrow \Delta\left(\frac{d\psi}{dx}\right) = \frac{-2m\alpha}{\hbar^2}\psi(0)$$

But $\left.\frac{d\psi}{dx}\right|_{+} = -kA$, $\left.\frac{d\psi}{dx}\right|_{-} = kA$, so $\cancel{2}k\cancel{A} = \frac{\cancel{2}m\alpha\cancel{A}}{\hbar^2} \Rightarrow k = \frac{m\alpha}{\hbar^2}$

$$\Rightarrow \boxed{E = \frac{-\hbar^2 k^2}{2m} = -\frac{m\alpha^2}{2\hbar^2} \quad \psi(x) = \frac{\sqrt{m\alpha}}{\hbar}e^{-m\alpha|x|/\hbar^2}}$$

3b]



Incoming: Ae^{ikx}

Reflected: Be^{-ikx}

Transmitted: Ce^{ikx}

B.C.'s: $\psi(x)$ continuous @ 0.

$$\Delta\left(\frac{\partial \psi(x)}{\partial x}\right) = -\frac{2m\alpha}{\hbar^2}\psi(0).$$

$A+B=C$, from b.c. #1.

$$\left.\frac{\partial \psi(x)}{\partial x}\right|_{x=0} = \begin{cases} ik(A-B) & \text{as } x\to 0^- \\ ikC & \text{as } x\to 0^+ \end{cases}$$

$$\Rightarrow \Delta\left(\frac{\partial\psi}{\partial x}\right) = ik(C-A+B) = -\frac{2m\alpha}{\hbar^2}\psi(0) = -\frac{2m\alpha}{\hbar^2}(A+B)$$

$$\Rightarrow \quad ikC = A\left(ik - \frac{2m\alpha}{\hbar^2}\right) + B\left(-ik - \frac{2m\alpha}{\hbar^2}\right)$$

$$\Rightarrow C = A\left(1 + \frac{2im\alpha}{\hbar^2}\right) - B\left(1 - \frac{2im\alpha}{\hbar^2}\right) = A+B$$

$$\text{So } B = \frac{(2im\alpha/\hbar^2)A}{2 - 2im\alpha/\hbar^2} = \left(\frac{im\alpha/\hbar^2}{1 - im\alpha/\hbar^2}\right)A$$

$$\& \; C = \frac{1}{1 - im\alpha/\hbar^2}A \Rightarrow$$

Reflected: $\frac{|B|^2}{|A^2|} = \frac{(m\alpha/\hbar^2)^2}{1+(m\alpha/\hbar^2)^2}$

Tr... $\frac{|C|^2}{\ldots} = \frac{1}{\ldots}$

t] $V = A\,\underset{\sim}{S_e}\cdot\underset{\sim}{S_p} - \underset{\sim}{\mu_e}\cdot\underset{\sim}{B} = A\,\underset{\sim}{S_e}\cdot\underset{\sim}{S_p} - \frac{e\underset{\sim}{B}}{mc}\cdot\underset{\sim}{S_e}$

Usual trick: $\underset{\sim}{J} = \underset{\sim}{S_e} + \underset{\sim}{S_p} \Rightarrow J^2 = S_e^2 + S_p^2 + 2\underset{\sim}{S_e}\cdot\underset{\sim}{S_p}$

$$\Rightarrow V = \frac{A}{2}(J^2 - S_e^2 - S_p^2) - \frac{eB}{mc}S_{ez}$$

$$= \frac{A\hbar^2}{2}\left(j(j+1) - \frac{3}{2}\right) - \frac{eB}{mc}S_{e,z}$$

$E_1 = \langle V \rangle$, but need to pick basis.

Can use either $|j\,m\rangle$ or $|m_e\,m_p\rangle$, here let's use the first.

$|j\,m\rangle$: $|0\,0\rangle$, $|1\,-1\rangle$, $|1\,0\rangle$, $|1\,1\rangle$

$|m_e\,m_p\rangle$: $|+-\rangle$, $|++\rangle$, $|--\rangle$, $|-+\rangle$

$|1\,1\rangle = |++\rangle$, $|1\,-1\rangle = |--\rangle$.

$$\Rightarrow J_-|1\,1\rangle = (S_{e-} + S_{p-})|1\,1\rangle = (|-+\rangle + |+-\rangle)\cdot c$$

$$\Rightarrow \frac{1}{\sqrt{2}}(|-+\rangle + |+-\rangle) = |1\,0\rangle$$

So $|0\,0\rangle = \frac{1}{\sqrt{2}}(|+-\rangle - |-+\rangle)$. to make 'em orthogonal

So the perturbation matrix is: $\langle j\, m | V | j' m' \rangle$

$$
\begin{array}{c|cccc}
 & |00\rangle & |11\rangle & |10\rangle & |1-1\rangle \\
\langle 0 0| & -\frac{3A\hbar^2}{4} & 0 & \hbar eB/2mc & 0 \\
\langle 1 1| & 0 & \frac{A\hbar^2}{4}+\frac{\hbar eB}{2mc} & 0 & 0 \\
\langle 1 0| & \hbar eB/2mc & 0 & A\hbar^2/4 & 0 \\
\langle 1 -1| & 0 & 0 & 0 & \frac{A\hbar^2}{4}-\frac{\hbar eB}{2mc}
\end{array}
$$

b/c $\langle 00 | S_{e,z} | 00 \rangle = \langle 00 | S_e \left(\frac{1}{\sqrt{2}} (|+-\rangle - |-+\rangle \right)$

$= \langle 00 | \frac{1}{\sqrt{2}} \left(\frac{\hbar}{2} |+-\rangle + \frac{\hbar}{2} |-+\rangle \right. = 0.$

$S_{e,z} |11\rangle = \frac{\hbar}{2} |++\rangle = \frac{\hbar}{2} |11\rangle$

$S_e |10\rangle = \frac{\hbar}{2} (|+-\rangle - |+-\rangle)$, etc.

Diagonalize to get shifts $\frac{A\hbar^2}{4} + \frac{\hbar eB}{2mc}$, for $|11\rangle$

$\frac{A\hbar^2}{4} - \frac{\hbar eB}{2mc}$, for $|1-1\rangle$

and $-\frac{A\hbar^2}{4} \pm \sqrt{\frac{A^2\hbar^4}{4} + \frac{\hbar^2 e^2 B^2}{4m^2c^4}}$ for

some combination of $|10\rangle$ & $|00\rangle$.

5.

a) $\underset{\sim}{B} = B\hat{z}$.

$\nabla \times \underset{\sim}{A} = \underset{\sim}{B} \Rightarrow \int \nabla \times \underset{\sim}{A} \cdot d\underset{\sim}{a} = \int \underset{\sim}{B} \cdot da$

$$\int \underset{\sim}{A} \cdot d\underset{\sim}{l} = \int \underset{\sim}{B} \cdot d\underset{\sim}{a} = \Phi$$

$$\Rightarrow \boxed{A = \frac{\Phi}{2\pi r}\hat{\phi}}$$ Checks: $\nabla \times \underset{\sim}{A} = 0$.

b) $H = \frac{1}{2m}\left(\underset{\sim}{p} - \frac{e\underset{\sim}{A}}{c}\right)^2 = \frac{1}{2m}\left(\frac{\hbar}{i}\nabla - \frac{e\underset{\sim}{A}}{c}\right)^2$

$$= \frac{1}{2m}\left(-\hbar^2\nabla^2 - \frac{e\hbar}{ic}\underset{\sim}{A}\cdot\nabla - \frac{e\hbar\underset{\sim}{\nabla}\cdot\underset{\sim}{A}}{ic} + \frac{e^2A^2}{c^2}\right)$$

$$= \frac{1}{2m}\left(-\hbar^2\nabla^2 + \frac{e^2A^2}{c^2} + \frac{2e\hbar i}{c}\underset{\sim}{A}\cdot\nabla\right)$$

$\Rightarrow H\psi = E\psi$, with $\psi = \psi(\phi)$ (r, θ fixed).

$$\frac{1}{2m}\left(-\hbar^2\nabla^2 + \frac{e^2\Phi^2}{4\pi^2b^2c^2} + \frac{\cancel{2}e\hbar i}{c}\frac{\Phi}{\cancel{2}\pi b}\left(\frac{1}{b}\frac{\partial}{\partial\phi}\right)\right)\psi = E\psi$$

$$\Rightarrow \frac{1}{2m}\left(-\frac{\hbar^2}{b^2}\frac{\partial^2\psi}{\partial\phi^2} + \left(\frac{e\Phi}{2\pi bc}\right)^2\psi + i\frac{\hbar e\Phi}{c\pi b^2}\frac{\partial\psi}{\partial\phi}\right) = E\psi$$

$$\Rightarrow \frac{\partial^2 \psi}{\partial \phi^2} - 2i\beta \frac{\partial \psi}{\partial \phi} + \varepsilon \psi = 0, \quad \beta = \frac{e\Phi}{2\pi\hbar c}, \quad \varepsilon = \frac{2mb^2 E}{\hbar^2} - \beta^2.$$

$$\Rightarrow \boxed{\psi = A e^{i\lambda\phi}, \quad \lambda = \beta \pm \sqrt{\beta^2 + \varepsilon} = \beta \pm \frac{b}{\hbar}\sqrt{2mE}.}$$

B.C.: $\psi(\phi + 2\pi) = \psi(\phi) \Rightarrow \lambda \in \mathbb{Z}$.

$$\beta \pm \frac{b}{\hbar}\sqrt{2mE} = n$$

$$\Rightarrow \boxed{E_n = \frac{\hbar^2}{2mb^2}\left(n - \frac{e\Phi}{2\pi\hbar c}\right)^2, \quad n = 0, \pm 1, \pm 2, \dots}$$

Magnetic field lifts the degeneracy!