

S-08

Jan-2008

Problem 1: The Infinite Square Well: (10 Points)

A single particle is in a one dimensional infinitely deep potential well of width L where $V(x)$ is given by:

$$V(x) = \begin{cases} 0, & \text{if } 0 \leq x \leq L \\ \infty, & \text{otherwise} \end{cases}$$

1. Find the allowed energies (E_n) and the normalized eigenfunctions ($\Psi(x)$) to Schrodinger's Equation for this potential. Show all your work. (2 Points)
2. Sketch the wave functions for the first three stationary states for this potential. (2 Points)
3. Now, if four spin-1/2 identical particles of mass m are placed in this potential, calculate the three lowest values for the total energy of the system of particles. (3 Points)
4. Determine the degeneracy for each of the three energy states found in part 3. (3 Points)

I think it's right
but need to check!

5-α Need to figure out

Problem 2: The Harmonic Oscillator (10 Points):

The normalized wave functions for the one-dimensional quantum harmonic oscillator can be written as,

$$\Psi_n(x) = \left(\frac{\sqrt{\alpha}}{2^n n! \sqrt{\pi}} \right)^{1/2} e^{-\alpha x^2/2} H_n(\sqrt{\alpha}x),$$

where n is the principle quantum number of the oscillator, H_n is the n^{th} order Hermite polynomial, $\alpha = \omega m/\hbar$, ω is the oscillator frequency, and m is its mass. The following equations may be useful,

$$\Rightarrow \underline{H_{n+1}(q)} + 2nH_{n-1}(q) - 2qH_n(q) = 0$$

$$\Rightarrow \underline{\frac{dH_n(q)}{dq}} = 2nH_{n-1}(q)$$

$$q = \sqrt{\alpha} x$$

and

<

$$\int \langle H_n | q | H_{n+1} \rangle dq \Rightarrow \int H_n^*(q) q (2q H_n(q) - 2n H_{n-1}(q)) dq$$

$$= \int H_n^*(q) q H_{n+1}(q) dq \Rightarrow \langle H_n | q H_n \rangle = 0 \quad 2 \int H_n^*(q) q^2 H_n(q) - 2n \int H_n^*(q) q H_{n-1}(q)$$

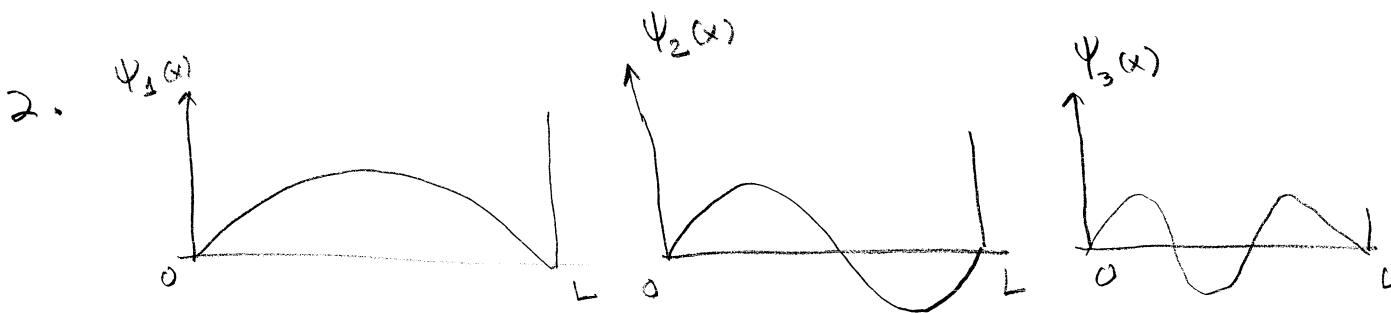
$$\Rightarrow \langle H_n | q H_{n-1} \rangle = 2^{n-1} n! \sqrt{\pi} \quad 2 \int H_n^*(q) q^2 H_n(q) = 2^{n-1} n! \sqrt{\pi} + 2^n (n+1)! \sqrt{\pi}$$

1. Calculate the expectation value of x and x^2 for the n^{th} state of the harmonic oscillator, where x is the position. (2 Points)
2. Calculate the expectation value of p and p^2 for the n^{th} state of the harmonic oscillator, where p is the momentum. (2 Points)
3. Calculate Δx and Δp for the n^{th} state. What is the uncertainty product ($\Delta x \Delta p$) for the oscillator? (2 Points)
4. Calculate the expectation value of the kinetic energy and the potential energy of the n^{th} state of the oscillator. Show that the sum of the expectation value of the kinetic and potential energies are equal to the total energy of the n^{th} state. (2 Points)
5. How does the uncertainty principle relate to the fact that the energy is not zero in the ground state? Explain and interpret your answer to receive credit. (2 Points)

P1.

1. $E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$

$\Psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right)$



3. 4 spin-1/2 identical particles each particle has the same eigenfunc $\Psi_n(x)$

So, we think of as a equivalent 4 decoupled particles

with $E_n = E_1 + E_2 + E_3 + E_4$

$= \frac{\pi^2 \hbar^2}{2mL^2} (n_1^2 + n_2^2 + n_3^2 + n_4^2)$

$= \frac{n^2 \pi^2 \hbar^2}{2mL^2}$

$n_1=1$
 $n_2=2$
 $n_3=3$
 $n_4=4$
fermion!

2. $n=4 \quad E_1 = \frac{4\pi^2 \hbar^2}{2mL^2}$

$n=5 \quad E_2 = \frac{5\pi^2 \hbar^2}{2mL^2}$

$n=6 \quad E_3 = \frac{6\pi^2 \hbar^2}{2mL^2}$

4. $n=4 \quad \Psi_{1111} = \text{non degenerate}$

$n=5 \Rightarrow \Psi_{2111} \Psi_{1211} \Psi_{1121} \Psi_{1112}$

$n=6 \Rightarrow \Psi_{2211} \Psi_{1122} \Psi_{2121} \Psi_{1212}$

Prb2

$$1) \langle \hat{x} \rangle = \langle \psi_n | \hat{x} | \psi_n \rangle$$

$$= \int_{-\infty}^{+\infty} \psi_n^*(x) x \psi_n(x) dx$$

$$q = \sqrt{\alpha} x$$

$$\Rightarrow q^2 = \alpha x^2$$

$$x = \frac{1}{\sqrt{\alpha}} q \Rightarrow dx = \frac{1}{\sqrt{\alpha}} dq$$

$$= \underbrace{\left(\frac{\sqrt{\alpha}}{2^n n! \sqrt{\pi}} \right)}_{\beta} \int_{-\infty}^{+\infty} \left[e^{-\alpha x^2/2} H_n(\sqrt{\alpha} x) \right]^* x \left[e^{-\alpha x^2/2} H_n(\sqrt{\alpha} x) \right] dx$$

$$= \beta \int_{-\infty}^{+\infty} e^{-2\alpha x^2/2} H_n^*(\sqrt{\alpha} x) x H_n(\sqrt{\alpha} x) dx$$

$$= \frac{\beta}{\alpha} \int_{-\infty}^{+\infty} e^{-q^2} H_n^*(q) q H_n(q) dq$$

$$= \frac{\beta}{\alpha} \int_{-\infty}^{+\infty} \underbrace{e^{-q^2} H_n^*(q) q H_n(q) dq}_{du} + 2 \int$$

$$= \underbrace{e^{-q^2} \int_{-\infty}^{+\infty} H_n^*(q) q H_n(q) dq}_{=0} + 2 \int$$

$$H_{n+1}(q) = 2q H_n(q) - 2n H_{n-1}$$

$$u dv = uv - \int u dv$$

$$\int u v dx = u \int v dx - \int$$

$$dv = e^{-q^2}$$

$$v = \int e^{-q^2} dq$$

$$= \sqrt{\pi}$$

$$uv - \int v du$$

$$\int u v dx = uv - \int v du$$

$$u = e^{-q^2}$$

$$\Rightarrow du = -2q e^{-q^2}$$

$$v du = uv - \int u dv$$

$$\langle x^2 \rangle = \frac{\beta}{2^{3/2}} \int_{-\infty}^{+\infty} \underbrace{e^{-q^2}}_u \underbrace{H_n^*(q) q^2 H_n(q)}_{dv} dq$$

$$du = -(2q) e^{-q^2} dq$$

$$= e^{-q^2} \int_{-\infty}^{+\infty} H_n^*(q) q^2 H_n(q) dq = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} H_n^*(q) q^2 H_n(q) dq (-2q e^{-q^2} dq)$$

$$= \frac{e^{-q^2}}{2} (2^{n-1} n! \sqrt{\pi} + 2^n (n+1)! \sqrt{\pi}) + (2^{n-1} n! \sqrt{\pi} + 2^n (n+1)! \sqrt{\pi}) \int_{-\infty}^{+\infty} q e^{-q^2} dq$$

$$= \frac{e^{-q^2} - e^{q^2}}{2} (2^{n-1} n! \sqrt{\pi} + 2^n (n+1)! \sqrt{\pi})$$

$$= 2^n \sqrt{\pi} \frac{e^{-q^2} - e^{q^2}}{2} \left[\frac{n!}{2} + (n+1)! \right]$$

$$q^2 = u$$

$$\Rightarrow 2q dq = du$$

$$= \frac{1}{2} \int_{-\infty}^{+\infty} e^{-u} du$$

$$= -\frac{e^{-u}}{2}$$

$$= -\frac{e^{-q^2}}{2}$$

$$2. \langle p^2 \rangle = \langle n | p^2 | n \rangle = \int_{-\infty}^{+\infty} \psi_n^*(x) \hat{p}^2 \psi_n(x) dx$$

$$q = \sqrt{\alpha} x \\ q^2 = \alpha x^2$$

$$= \left(\frac{\sqrt{\alpha}}{2^n n! \sqrt{\pi}} \right) \int_{-\infty}^{+\infty} e^{-\alpha x^2/2} H_n(\sqrt{\alpha} x) \hat{p}^2 e^{-\alpha x^2/2} H_n(\sqrt{\alpha} x) dx \quad dq = \sqrt{\alpha} dx$$

$$= -\frac{\hbar^2}{2m} \left(\frac{\sqrt{\alpha}}{2^n n! \sqrt{\pi}} \right) \int_{-\infty}^{+\infty} e^{-q^2/2} H_n(q) \underbrace{\frac{d^2}{dx^2}}_{\frac{1}{\alpha} \frac{d^2}{dq^2}} e^{-q^2/2} H_n(q) \frac{1}{\sqrt{\alpha}} dq$$

$$\frac{d^2}{dq^2} \left\{ e^{-q^2/2} H_n(q) \right\} = \frac{d}{dq} \left\{ \left(-\frac{1}{2} \right) 2q e^{-q^2/2} H_n(q) + H_n'(q) e^{-q^2/2} \right\}$$

$$= \frac{d}{dq} \left\{ -H_n q e^{-q^2/2} + 2n H_{n-1}(q) e^{-q^2/2} \right\}$$

$$= -H_n' q e^{-q^2/2} + q^2 H_n e^{-q^2/2} + 2n H_{n-1}'(q) e^{-q^2/2} - q 2n H_{n-1}(q) e^{-q^2/2}$$

$$= -2n H_{n-1}(q) q e^{-q^2/2} + \underbrace{q^2 H_n(q) e^{-q^2/2}}_{-q 2n H_{n-1}(q) e^{-q^2/2}} + 2n(n-1) H_{n-2}(q) e^{-q^2/2}$$

$$\langle p^2 \rangle = -\frac{1}{(\alpha)^{3/2}} \frac{\hbar^2}{2m} \left(\right) \int_{-\infty}^{+\infty} H_n(q) q^2 H_n(q) dq$$

Problem 3: The Variational Principle: (10 Points)

If the case where you would like to calculate the ground state energy (E_g) for a system described by the Hamiltonian H but you are unable to solve the Schrodinger equation, the variational principle will give you an upper bound for the ground state energy.

For any normalized function Ψ , the variational principle states:

$$E_g \leq \langle \Psi | H | \Psi \rangle$$

1. (2 Points) Prove the variational principle. i.e show that

$$E_g \leq \langle \Psi | H | \Psi \rangle$$

Hint (Write $\Psi = \sum_n c_n \phi_n$ where ϕ_n are the (unknown) eigenfunctions of H)

Now consider a specific case:

In the x -basis, a one-dimensional operator

$$\Omega = -\frac{d^2}{dx^2} + |x|$$

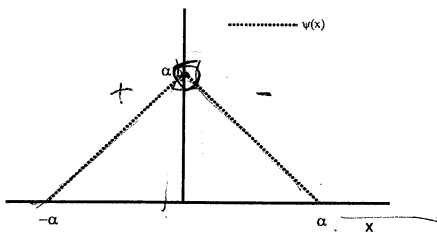
has an eigenvalue λ and an eigenfunction $\psi(x)$ with $\psi(x) \rightarrow 0$ for $|x| \rightarrow \infty$.

Let us choose an *unnormalized* trial function

$$\psi(x) = \langle x | \psi \rangle = \begin{cases} \alpha - |x|, & \text{for } |x| \leq \alpha, \text{ and} \\ 0, & \text{for } |x| > \alpha \end{cases}$$

$\Rightarrow -\alpha < x < \alpha$
 $\Rightarrow x < \alpha$
 $\Rightarrow x > -\alpha$

where α is the variational parameter.



$x > \alpha$
 $x < -\alpha$

$+E$

\int
 $-E$

Rt
 $-E \rightarrow 0$

2. (2 Points) Find $\langle \psi | \psi \rangle$.

3. (3 Points) Find the expectation value of the operator Ω .

4. (3 Points) Determine the best bound on the lowest eigenvalue (λ) of the operator Ω with the trial function $\psi(x)$. (Note your answer cannot depend on α .)

↓
doesn't work

$$\langle \Omega \rangle = \frac{\alpha}{4}$$

I have to do it

Problem 4: Measurement of Hermitian Observables: (10 Points)

Consider a system with three Hermitian observables that are represented in a three-dimensional Hilbert space using the orthonormal basis $|e_1\rangle$, $|e_2\rangle$ and $|e_3\rangle$

with

$$|e_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, |e_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, |e_3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

and

$$A = \begin{pmatrix} 2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, B = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 2i \\ 0 & -2i & 1 \end{pmatrix}, C = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

The system at time $t=0$ is in the state:

$AB = \begin{pmatrix} 2 & 0 & 0 \\ 0 & 1 & 2i \\ 0 & -2i & 1 \end{pmatrix}$ $BA = \begin{pmatrix} 2 & 0 & 0 \\ 0 & 1 & 2i \\ 0 & -2i & 1 \end{pmatrix}$

$$|\Psi(0)\rangle = \frac{1}{\sqrt{6}}|e_1\rangle - \frac{1}{\sqrt{6}}|e_2\rangle + \sqrt{\frac{2}{3}}|e_3\rangle$$

1. Find the eigenvalues and normalized eigenvectors of B and C . (1 Point)
2. Find the probability of measuring B at time $t = 0$ with the eigenvalue $b = 1$, and then immediately measuring C and finding the eigenvalue $c = 1$, i.e. find $P_{|\Psi(0)\rangle}(b = 1, c = 1)$. (2 Points)
3. Now find the probability if these measurements are performed in reverse order at $t = 0$, i.e. find $P_{|\Psi(0)\rangle}(c = 1, b = 1)$. (2 Points)
4. Are the probabilities obtained in part 1. and part 2. the same or different? Explain in detail. (2 Points)
5. Use the Generalized Uncertainty Principle to determine a lower bound on $\Delta B \Delta C$ for the system in the initial state $|\Psi(0)\rangle$. Discuss your results. (2 Points)
6. Discuss in detail, the conditions that would result in obtaining a lower bound of zero when using the Generalized Uncertainty Principle. Would you expect to get zero for a particular pair of the observables, A , B , and C in this problem? Or for other conditions? (1 Point)

$$BC = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 2i \\ -2i & 0 & 1 \end{pmatrix} \quad CB = \begin{pmatrix} 0 & 1 & 2i \\ 1 & 0 & 0 \\ 0 & -2i & 1 \end{pmatrix}$$

P3

$$1) \Psi = \sum_n c_n \phi_n$$

$$\begin{aligned} \langle \Psi | H | \Psi \rangle &= \sum_n |c_n|^2 \langle \phi_n | H | \phi_n \rangle \\ &= \sum_n |c_n|^2 E_n \geq \underline{E_1} \\ &= |c_1|^2 \underline{E_1} + \sum_{n=2} |c_n|^2 E_n \end{aligned}$$

$$\langle \Psi | H | \Psi \rangle = E_1 + \sum_{n=2} E_n$$

2.

$$\langle \Psi | \Psi \rangle = \int_{-\infty}^{+\infty} \psi^*(x) \psi(x) dx$$

$$= \int_{-\alpha}^0 (\alpha+x)(\alpha+x) dx + \int_0^{\alpha} (\alpha-x)(\alpha-x) dx$$

$$= \int_{-\alpha}^0 (\alpha^2 + 2\alpha x + x^2) dx + \int_0^{\alpha} (\alpha^2 - 2\alpha x + x^2) dx$$

$$= \left. \alpha^2 x + \alpha x^2 + \frac{x^3}{3} \right|_{-\alpha}^0 + \left. \alpha^2 x - \alpha x^2 + \frac{x^3}{3} \right|_0^{\alpha}$$

$$= \left[- \left(-\alpha^3 + \alpha^3 + \frac{-\alpha^3}{3} \right) \right] + \left[\alpha^3 - \alpha^3 + \frac{\alpha^3}{3} \right]$$

$$= \frac{2}{3} \alpha^3$$

$$\langle \Omega \rangle = \int_{-\infty}^{+\infty} \Psi^*(x) \Omega \Psi(x) dx = \int_{-\infty}^{+\infty} \Psi^*(x) \left[-\frac{d^2}{dx^2} + |x| \right] \Psi(x) dx$$

$$= \underbrace{-\int_{-\infty}^{+\infty} \Psi^*(x) \frac{d^2}{dx^2} \Psi(x) dx}_{=0} + \int_{-\infty}^{+\infty} \Psi^*(x) |x| \Psi(x) dx$$

= 0 Since, $\Psi(x)$ is 1st order
in x \therefore we are taking
 \Rightarrow 2nd derivative

$$= \int_{-\alpha}^0 (x+\alpha)(-x)(x+\alpha) dx + \int_0^{\alpha} (x-\alpha)x(x-\alpha) dx$$

$$= -\int_{-\alpha}^0 (x^3 + 2\alpha x^2 + \alpha^2 x) dx + \int_0^{\alpha} (x^3 - 2\alpha x^2 + \alpha^2 x) dx$$

$$= -\left[\frac{x^4}{4} + \frac{2}{3}\alpha x^3 + \frac{1}{2}\alpha^2 x^2 \right]_{-\alpha}^0 + \left[\frac{x^4}{4} - \frac{2}{3}\alpha x^3 + \frac{1}{2}\alpha^2 x^2 \right]_0^{\alpha}$$

$$= \left[+ \left(\frac{\alpha^4}{4} - \frac{2}{3}\alpha^4 + \frac{1}{2}\alpha^4 \right) \right] + \left[\frac{\alpha^4}{4} - \frac{2}{3}\alpha^4 + \frac{1}{2}\alpha^4 \right]$$

$$= 2\alpha^4 \left(\frac{1}{4} - \frac{2}{3} + \frac{1}{2} \right)$$

$$= \frac{2\alpha^4}{12} = \frac{\alpha^4}{6}$$

$$\langle \Omega \rangle = \frac{\langle \Psi | \Omega | \Psi \rangle}{\langle \Psi | \Psi \rangle} = \frac{\alpha^4}{6} \times \frac{3}{2\alpha^3} = \frac{1}{4} \alpha$$

$$4. \frac{d\langle \Omega \rangle}{d\alpha} = 0$$

P4

$$A = \begin{pmatrix} 2 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad B = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 2i \\ 0 & -2i & 1 \end{pmatrix} \quad C = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

For C

$$\begin{vmatrix} 0-\lambda & 1 & 0 \\ 1 & 0-\lambda & 0 \\ 0 & 0 & 1-\lambda \end{vmatrix} = \begin{vmatrix} -\lambda & 1 & 0 \\ 1 & -\lambda & 0 \\ 0 & 0 & 1-\lambda \end{vmatrix} = (1-\lambda)(\lambda^2-1) = 0$$

$$\lambda = 1, 1, -1$$

• $\lambda = -1$

$$\begin{pmatrix} +1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \Rightarrow \begin{cases} a_1 + a_2 = 0 \\ a_1 + a_2 = 0 \\ a_3 = 0 \end{cases} \Rightarrow a_2 = -a_1$$

$$|\lambda = -1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}$$

• $\lambda = 1$

$$\begin{pmatrix} -1 & 1 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix} = 0 \Rightarrow \begin{cases} -b_1 + b_2 = 0 \\ b_1 - b_2 = 0 \end{cases} \Rightarrow b_1 = b_2$$

$$\Rightarrow b_3 \text{ arbitrary}$$

$$|\lambda = 1\rangle = \frac{1}{\sqrt{2|b_1|^2 + |b_3|^2}} \begin{pmatrix} b_1 \\ b_1 \\ b_3 \end{pmatrix}$$

$$|\lambda = 1, 1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}$$

$$\langle \lambda = 1, 2 | \lambda = 1, 1 \rangle = 0 \Rightarrow (b_1, b_1, b_3) \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} = 0 \Rightarrow 2b_1 = 0 \Rightarrow b_1 = 0$$

$$|\lambda = 1, 2\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

For B

$$\begin{vmatrix} 1-\lambda & 0 & 0 \\ 0 & 1-\lambda & 2i \\ 0 & -2i & 1-\lambda \end{vmatrix} = 0 \Rightarrow (1-\lambda) \{ (1-\lambda)^2 - 4 \} = 0$$
$$\Rightarrow (1-\lambda)(1-\lambda+2)(1-\lambda-2) = 0$$
$$\Rightarrow (1-\lambda)(3-\lambda)(\lambda+1) = 0$$
$$\Rightarrow \lambda = 1, -1, 3$$

$\lambda = 1$

$$\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 2i \\ 0 & -2i & 0 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = 0 \Rightarrow \begin{cases} 0 = 0 \Rightarrow a_1 \text{ arbitrary} \\ 2i a_3 = 0 \Rightarrow a_3 = 0 \\ -2i a_2 = 0 \Rightarrow a_2 = 0 \end{cases}$$

$$|\lambda=1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

$\lambda = -1$

$$\begin{pmatrix} 2 & 0 & 0 \\ 0 & 2 & 2i \\ 0 & -2i & 2 \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix} = 0 \Rightarrow \begin{cases} 2b_1 = 0 \Rightarrow b_1 = 0 \\ 2b_2 + 2ib_3 = 0 \\ -2ib_2 + 2b_3 = 0 \end{cases} \Rightarrow b_3 = ib_2$$

$$|\lambda=-1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ i \end{pmatrix}$$

$\lambda = 3$

$$\begin{pmatrix} -2 & 0 & 0 \\ 0 & -2 & 2i \\ 0 & -2i & -2 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = 0 \Rightarrow \begin{cases} -2c_1 = 0 \Rightarrow c_1 = 0 \\ -2c_2 + 2ic_3 = 0 \\ -2ic_2 - 2c_3 = 0 \end{cases} \Rightarrow c_2 = ic_3$$

$$|\lambda=3\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ i \\ 1 \end{pmatrix} \neq$$

2.

$$|b=1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = |e_1\rangle$$

$$P(b=1) = |\langle b=1 | \Psi(0) \rangle|^2 = \frac{1}{6}$$

$$|c=1\rangle = \alpha |c=1,1\rangle + \beta |c=1,2\rangle = \frac{1}{\sqrt{2}} [|e_1\rangle + |e_2\rangle] + |e_3\rangle$$

$$\langle c=1 | c=1 \rangle = \alpha^2 + \beta^2 = 1$$

$$* \langle c=-1 | c=1 \rangle = 0$$

$$\Rightarrow \frac{1}{\sqrt{2}} (1 \ -1 \ 0) \frac{\alpha}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} + \frac{1}{\sqrt{2}} (1 \ -1 \ 0) \frac{\beta}{\sqrt{2}} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = 0$$

$$\Rightarrow \frac{\alpha}{2} (1-1) + \frac{\beta}{2} (0) \quad */$$

$$\begin{aligned} P(c=1)_{|b=1\rangle} &= |\langle c=1 | b=1 \rangle|^2 \\ &= |\langle c=1,1 | b=1 \rangle|^2 + |\langle c=1,2 | b=1 \rangle|^2 \\ &= \frac{1}{2} \end{aligned}$$

$$\leadsto P(b=1, c=1) = P(b=1) P(c=1) = \frac{1}{12}$$

$$\begin{aligned} 3. \quad P(c=1) &= |\langle c=1 | \Psi(0) \rangle|^2 = \left| \frac{1}{\sqrt{12}} - \frac{1}{\sqrt{12}} + \left| \frac{\sqrt{2}}{3} \right|^2 \right|^2 \\ &= \frac{2}{3} \end{aligned}$$

$$P(b=1)_{|c=1\rangle} = |\langle b=1 | c=1 \rangle|^2 = \left| \frac{1}{\sqrt{2}} \right|^2 = \frac{1}{2}$$

$$\leadsto P(c=1 \ b=1) = \frac{1}{3}$$

4. Lets check the commutation of B & C

$$BC = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 2i \\ -2i & 0 & 1 \end{pmatrix} \quad CB = \begin{pmatrix} 0 & 1 & 2i \\ 1 & 0 & 0 \\ 0 & -2i & 1 \end{pmatrix}$$

$$[B, C] \neq 0$$

So, $P(b=1, c=1) \neq P(B=1, b=1)$ is expected
which is what we got

5.

Problem 5: Perturbation Theory: (10 Points)

A single particle is in a one dimensional infinite well of length L . The potential $V(x)$ is given by:

$$V(x) = \begin{cases} 0, & \text{if } 0 \leq x \leq L \\ \infty, & \text{otherwise} \end{cases}$$

Suppose the potential energy inside the well is changed to

$$V(x) = \epsilon \sin \frac{\pi x}{L}$$

when $0 \leq x \leq L$.

Note you may use your results from Problem 1 for this problem.

1. Calculate the energy shifts for the perturbed well to first order in ϵ . **(2 Points)**
2. Which energy level is shifted the most to first order in ϵ ? **(1 Point)**
3. Calculate the second order (in ϵ) correction to the ground state energy **(2 Points)**
4. Calculate the corrections to the ground state wavefunction to first order in ϵ . **(2 Points)**
5. Suppose that ϵ is larger than the energy of the first excited state. Carefully sketch the wavefunction versus x for the ground state and for the first excited state. How many nodes, maxima, and minima does the wavefunction have in each state. **(2 Points)**
6. Suppose the wavefunction is a linear combination of the ground state and the first excited state from part 5. Describe how the maximum of the probability density depends on time. **(1 Point)**

S-08

Problem 6: Spherically Symmetric States: (10 Points)

Consider eigenfunctions of the Hamiltonian of a particle in a three-dimensional central potential. In particular, consider those eigenfunctions that depend only on the electron's radial coordinate r , that is $\Psi_E = \Psi_E(r)$. States represented by such eigenfunctions are called "spherically symmetric states".

Couldn't
do it

1. Derive an equation for a function $\chi_E(r)$ defined by:

$$\Psi_n(r) \equiv \frac{1}{r} \chi_n(r),$$

where n is the principle quantum number. (2 Points)

The remainder of this problem concerns a hydrogen atom in the approximation that we neglect all interactions except the Coulomb interaction and treat the proton as an infinitely massive point particle at the origin.

2. Sketch $\chi_n(r)$ for the lowest three spherical bound states of the hydrogen atom. Justify the qualitative features of each function. (2 Points)
3. (2 Points). Consider the eigenfunction for the ground state. Prove that to be physically admissible this function must decay exponentially as r becomes infinite.

$$\chi_1(r) \rightarrow e^{-\alpha r}, \text{ when } r \rightarrow \infty$$

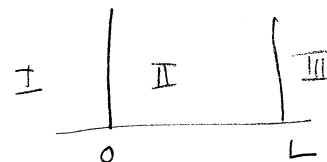
where α is a constant, and that therefore $\chi_1(r)$ must have the form.

$$\chi_1(r) = f(r)e^{-\alpha r}.$$

4. Use $f(r) = r$. Justify why this is an appropriate choice and show that the above equation is a solution of the equation you derived for $\chi_1(r)$ and determine the corresponding eigenvalue E_1 . (2 Points)
5. Derive an expression for the constant α in terms of fundamental constants. (2 Points)

P5.

$$V(x) = \begin{cases} 0 & \text{if } 0 \leq x \leq L \\ \infty & \text{otherwise} \end{cases}$$



• Region I

$$\Psi_I(x) = 0$$

• Region III

$$\Psi_{III}(x) = 0$$

• Region II

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right] \Psi_{II}(x) = E \Psi_{II}(x)$$

$$\Rightarrow \frac{d^2 \Psi_{II}(x)}{dx^2} + \frac{2mE}{\hbar^2} \Psi_{II}(x) = 0 \quad K^2 = \frac{2mE}{\hbar^2} \Rightarrow E = \frac{\hbar^2 K^2}{2m}$$

$$\Rightarrow \frac{d^2 \Psi_{II}(x)}{dx^2} + K^2 \Psi_{II}(x) = 0$$

$$\Rightarrow \lambda = \pm iK$$

$$\Psi_{II}(x) = A \cos Kx + B \sin Kx$$

Matching the boundary

$$\Psi_I(0) = \Psi_{II}(0)$$

$$\Rightarrow 0 = A$$

$$\Psi_{II}(L) = \Psi_{III}(L)$$

$$\Rightarrow B \sin KL = 0$$

$$\Rightarrow \sin KL = 0$$

$$\Rightarrow K = \frac{n\pi}{L}$$

$$\Psi_{II}(x) = B \sin\left(\frac{n\pi}{L}x\right)$$

$$|B|^2 \int_0^L \sin^2\left(\frac{n\pi}{L}x\right) dx = 1 \Rightarrow |B|^2 \frac{L}{2} = 1$$

$$\Rightarrow B = \sqrt{2/L}$$

$$\Psi_{II}(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right)$$

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$$

$$E_n^{(4)} = \langle n^{(0)} | H' | n^{(0)} \rangle$$

$$= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \langle n^{(0)} | x \rangle \langle x | H' | y \rangle \langle y | n^{(0)} \rangle dx dy$$

$$= \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \psi^*(x) H' \delta(x-y) \psi(y) dx dy$$

$$= \int_{-\infty}^{+\infty} \psi^*(x) H' \psi(x) dx$$

$$= \int_0^L \psi_{II}^*(x) \sin\left(\frac{\pi x}{L}\right) \psi_{II}(x) dx$$

$$= \frac{2}{L} \int_0^L \sin^2\left(\frac{n\pi x}{L}\right) \sin\left(\frac{\pi x}{L}\right) dx$$

$$= \frac{1}{L} \int_0^L \left\{ 1 - \cos\left(\frac{2n\pi}{L}x\right) \right\} \sin\left(\frac{\pi}{L}x\right) dx$$

$$= \frac{1}{L} \int_0^L \sin\left(\frac{\pi}{L}x\right) dx - \frac{1}{L} \int_0^L \cos\left(\frac{2n\pi}{L}x\right) \sin\left(\frac{\pi}{L}x\right) dx$$

$$= \frac{1}{L} \left[-\frac{L}{\pi} \cos\left(\frac{\pi}{L}x\right) \right]_0^L - \frac{1}{L} \left[-\frac{\cos\left\{\frac{(2n-1)\pi}{L}x\right\}}{2 \frac{(1-2n)\pi}{L}} - \frac{\cos\left\{\frac{(2n+1)\pi}{L}x\right\}}{2 \frac{(2n+1)\pi}{L}} \right]_0^L$$

$$= \frac{1}{L} \left[+\frac{L}{\pi} + \frac{L}{\pi} \right] - \frac{1}{L} \left[+\frac{L}{(1-2n)\pi} + \frac{L}{(2n+1)\pi} \right] = \frac{2}{\pi} + \frac{2n+1+1-2n}{(2n+1)(1-2n)\pi}$$

$$= \frac{2}{\pi} + \frac{4 \cdot 2}{(2n+1)(1-2n)\pi}$$

$$\cos 2x - 1 = \cos^2 x - \sin^2 x - 1$$

$$\Rightarrow = -2\sin^2 x$$

$$\Rightarrow \sin^2 x = \frac{1}{2}(1 - \cos 2x)$$

$$\begin{aligned} \therefore \text{The energy shift} &= \frac{2}{\pi} + \frac{2}{(2n+1)(1-2n)\pi} \\ &= \frac{2}{\pi} + \frac{2}{(1-4n^2)\pi} \end{aligned}$$

2. For $n=1$ the 2nd term is max, so the ground state is shifted most

$$3. E_1 = \frac{\pi^2 \hbar^2}{2mL^2} \quad \Psi_1(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi}{L}x\right)$$

$$E_n^{(2)} = \sum_{n \neq m} \frac{|\langle m^{(0)} | H' | n^{(0)} \rangle|^2}{E_n^{(0)} - E_m^{(0)}}$$

I think I hv to find the 1st order correction for wave func

$$|n\rangle = \sum_m \lambda^m |n^{(m)}\rangle$$

$$E_n = \sum_m \lambda^m E_n^{(m)}$$

$$H|n\rangle = E|n\rangle$$

$$\Rightarrow (H_0 + \lambda H') \left(\sum_m \lambda^m |n^{(m)}\rangle \right) = \left(\sum_m \lambda^m E_n^{(m)} \right) \left(\sum_m \lambda^m |n^{(m)}\rangle \right)$$

$$\Rightarrow H_0 |n^{(0)}\rangle + \lambda (H_0 |n^{(1)}\rangle + H' |n^{(0)}\rangle) + \lambda^2 (H_0 |n^{(2)}\rangle + H' |n^{(1)}\rangle)$$

$$= E_n^{(0)} |n^{(0)}\rangle + \lambda (E_n^{(0)} |n^{(1)}\rangle + E_n^{(1)} |n^{(0)}\rangle)$$

$$+ \lambda^2 (E_n^{(0)} |n^{(2)}\rangle + E_n^{(1)} |n^{(1)}\rangle + E_n^{(2)} |n^{(0)}\rangle)$$

0th order in λ

$$H_0 |n^{(0)}\rangle = E_n^{(0)} |n^{(0)}\rangle \quad (1)$$

$$H_0 |n^{(1)}\rangle + H' |n^{(0)}\rangle = E_n^{(0)} |n^{(1)}\rangle + E_n^{(1)} |n^{(0)}\rangle \quad (2)$$

$$H_0 |n^{(2)}\rangle + H' |n^{(1)}\rangle = E_n^{(0)} |n^{(2)}\rangle + E_n^{(1)} |n^{(1)}\rangle + E_n^{(2)} |n^{(0)}\rangle$$

$$(2) \Rightarrow \langle m^{(0)} | H_0 |n^{(1)}\rangle + \langle m^{(0)} | H' |n^{(0)}\rangle = \langle m^{(0)} | E_n^{(0)} |n^{(1)}\rangle \\ \neq \langle m^{(0)} | E_n^{(1)} |n^{(0)}\rangle$$

$$\Rightarrow E_m^{(0)} \langle m^{(0)} | n^{(1)}\rangle + \langle m^{(0)} | H' |n^{(0)}\rangle = E_n^{(0)} \langle m^{(0)} | n^{(1)}\rangle \\ + E_n^{(1)} \langle m^{(0)} | n^{(0)}\rangle$$

$$\langle m^{(0)} | H' |n^{(0)}\rangle = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \langle m^{(0)} | x \rangle \langle x | H' | y \rangle \langle y | n^{(0)} \rangle dx dy \\ = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \psi_m^*(x) H' \delta(x-y) \psi_n(x) dx dy \\ = \int_{-\infty}^{+\infty} \psi_m^*(x) H' \psi_n(x) dx$$

For groundstate.

$$\langle m^{(0)} | H' |n^{(0)}\rangle = \int_0^L \left(\frac{\sqrt{2}}{L}\right)^2 \sin\left(\frac{m\pi x}{L}\right) \sin\left(\frac{\pi x}{L}\right) \sin\left(\frac{\pi}{L}\right) x dx \\ = \frac{2}{L} \int_0^L \sin\left(\frac{m\pi}{L}\right) x \sin^2\left(\frac{\pi}{L}\right) x dx$$

$$= \frac{2}{L} \int_0^L \frac{1}{2} \sin\left(\frac{m\pi}{L}\right)x \left\{ 1 - \cos\left(\frac{2\pi}{L}\right)x \right\} dx$$

$$= \frac{1}{L} \int_0^L \sin\left(\frac{m\pi}{L}\right)x dx - \frac{1}{L} \int_0^L \sin\left(\frac{m\pi}{L}\right)x \cos\left(\frac{2\pi}{L}\right)x dx$$

$$= \frac{1}{L} \left[\frac{L}{m\pi} \left\{ -\cos\left(\frac{m\pi}{L}\right)x \right\} \right]_0^L - \underbrace{\hspace{10em}} \begin{cases} = 0, & m+2 \text{ even} \\ = 2m/(m^2-4) & m+2 \text{ odd} \end{cases}$$

$$= \frac{1}{m\pi} \left\{ -(-1)^m + 1 \right\} - \begin{cases} 0, & m+2 \text{ even} \\ 2m/(m^2-4) & m+2 \text{ odd} \end{cases}$$

the term to
be nonzero
m odd \rightarrow m+2 also odd

$$a. \quad \frac{d^2 \psi(r)}{dr^2} - \frac{2m}{\hbar^2} V(r) \psi(r) = -\frac{2mE}{\hbar^2} \psi(r)$$

$$\Rightarrow \frac{d^2 \psi(r)}{dr^2} + \frac{2m}{\hbar^2} [E - V(r)] \psi(r) = 0$$

$$\psi_n(r) = 1$$

