

KING FAHD UNIVERSITY of PETROLIUM and MINERALS
Physics Department
Quantum Mechanics I (Phys-401)
Spring 2008

Instructor: Prof. Dr. Ibraheem Nasser

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1- Write down the function $\psi(x) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}$ in Dirac's notation.

2- If the initial wave function of a harmonic oscillator is given by

$$\psi(x, 0) = \sqrt{\frac{1}{3}}\psi_0(x) + \sqrt{\frac{2}{3}}\psi_2(x)$$

where $\psi_0(x)$ and $\psi_2(x)$ are the eigen function for the ground state and the second excited states, respectively.

a) Calculate the wave function at any time.

b) Calculate the expectation value of x and E in the state $\psi(x, 0)$.

3- Find the probability of finding the ground state harmonic oscillator outside the

classical limits. Use $\psi_0(x) = \left(\frac{1}{x_o \sqrt{\pi}}\right)^{1/2} e^{-\frac{1}{2}x^2/x_o^2}$

4- Calculate the following brackets:

$$[\hat{x}, \hat{p}_x], [\hat{x}, \hat{p}_x^2], [\hat{x}^2, \hat{p}_x], [\hat{p}_x, \hat{V}] \text{ where } V(x) = a_0 + a_1x + a_2x^2 + \dots$$

5- Prove the following:

$$a) \quad \left[[\hat{x}, \hat{p}_x^2], \hat{x} \right] = 2\hbar^2 \quad b) \quad \hat{B}^{-1} [\hat{A}, \hat{B}] \hat{B}^{-1} = -[\hat{A}, \hat{B}^{-1}]$$

$$c) \quad [\hat{x}^3, \hat{p}_x] = 3i\hbar\hat{x}^2 \quad d) \quad [\hat{H}, \hat{x}] = \left[\frac{\hat{p}^2}{2m} + V(x), \hat{x} \right] = \frac{-2i\hbar}{2m} \hat{p}$$

In the following problem, it is recommended to also use any software packages (Mathematica, Maple, Matlab, etc...)

6- Using the normalized, linear harmonic oscillator wave functions perform the necessary integrations to verify the following:

a) That ψ_0 and ψ_1 are normalized.

- b) That ψ_0 and ψ_1 are orthogonal.
- c) That $\langle \psi_0 | x^2 | \psi_0 \rangle = \frac{1}{2}$.
- d) That $\langle \psi_1 | x^2 | \psi_1 \rangle = \langle \psi_1 | p_x^2 | \psi_1 \rangle = \frac{3}{2}$.
- e) That $\langle \psi_0 | x | \psi_1 \rangle = \langle \psi_1 | x | \psi_0 \rangle = \frac{\sqrt{2}}{2}$.
- f) Carry out the necessary differentiations and integrations to find the following expectation values for the first excited state of the harmonic oscillator: $\langle x \rangle$, $\langle x^2 \rangle$, $\langle p_x \rangle$, $\langle p_x^2 \rangle$.
- g) Using the results of (f), find $\langle T \rangle$, $\langle V \rangle$, and $\langle E \rangle$ for the same state.
- h) Calculate the minimum uncertainty product $\Delta x \cdot \Delta p_x$ for this state.

$$[\text{Use: } \hat{H} = \frac{p_x^2}{2m} + \frac{1}{2} m \omega^2 \hat{x}^2, \psi_n(x) = \left(\frac{\sqrt{\alpha}}{2^n n! \sqrt{\pi}} \right)^{1/2} e^{-\alpha x^2/2} H_n(\sqrt{\alpha} x)]$$

1- Use the notation:

$$\psi(x) = \langle x | \psi \rangle = \sum_{n=1}^{\infty} \langle x | n \rangle \langle n | \psi \rangle = \sum_{n=1}^{\infty} \langle n | \psi \rangle \langle x | n \rangle,$$

Then $c_n = \langle n | \psi \rangle$, $\langle x | n \rangle = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}$

1- a- Remember $E_n = (n + \frac{1}{2})\hbar\omega$

$$\begin{aligned} \psi(x, t) &= \sqrt{\frac{1}{3}}\psi_0(x)e^{-iE_0t/\hbar} + \sqrt{\frac{2}{3}}\psi_2(x)e^{-iE_2t/\hbar} \\ &= \sqrt{\frac{1}{3}}\psi_0(x)e^{-i\omega t/2} + \sqrt{\frac{2}{3}}\psi_2(x)e^{-i5\omega t/2} \end{aligned}$$

b-

$$\langle x \rangle = 0,$$

$$\langle E \rangle = \frac{1}{3}E_0 + \frac{2}{3}E_2 = \frac{1}{3}(\frac{1}{2}\hbar\omega) + \frac{2}{3}(\frac{5}{2}\hbar\omega) = \frac{11}{6}\hbar\omega$$

3- The turning points are defined by $E = U$, i.e. $\frac{1}{2}\hbar\omega = \frac{1}{2}m\omega^2x_o^2 \Rightarrow x_o = \pm\sqrt{\frac{\hbar}{m\omega}}$. The probability of finding the oscillator within the range of turning points is:

$$\int_{-x_o}^{x_o} |\psi_0(x)|^2 dx = \frac{1}{x_o\sqrt{\pi}} \int_{-x_o}^{x_o} e^{-x^2/x_o^2} dx = \frac{2}{\sqrt{\pi}} \int_0^1 e^{-y^2} dy = \frac{2}{\sqrt{\pi}} \frac{\sqrt{\pi}}{2} \text{Erf}[1] = 0.843$$

Hence the probability of finding the ground state harmonic oscillator outside the classical limits (classical forbidden zone) $= 1 - 0.843 = 0.157$

4-

$$\begin{aligned} [\hat{x}, \hat{D}_x] f(x) &= x \frac{d}{dx} [f(x)] - \frac{d}{dx} [xf(x)] \\ &= x \frac{d}{dx} f(x) - \left(x \frac{d}{dx} f(x) + f(x) \frac{d}{dx} x \right) \\ &= -f(x) \\ &\Rightarrow \boxed{[\hat{x}, \hat{D}_x] = -1} \end{aligned}$$

$$\begin{aligned}
[\hat{x}^2, \hat{D}_x]f(x) &= x^2 \frac{d}{dx}[f(x)] - \frac{d}{dx}[x^2 f(x)] \\
&= x^2 \frac{d}{dx}f(x) - \left(x^2 \frac{d}{dx}f(x) + f(x) \frac{d}{dx}x^2 \right) \\
&= -2xf(x). \\
\Rightarrow \boxed{[\hat{x}^2, \hat{D}_x] = -2x}
\end{aligned}$$

$$[\hat{x}, \hat{p}_x] = \left[\hat{x}, \frac{\hbar}{i} \frac{\partial}{\partial x} \right] = \frac{\hbar}{i} \left[\hat{x}, \frac{\partial}{\partial x} \right] = -\frac{\hbar}{i} \left[\frac{\partial}{\partial x}, \hat{x} \right] = -\frac{\hbar}{i} = i\hbar,$$

$$[\hat{x}, \hat{p}_x^2] = [\hat{x}, \hat{p}_x] \hat{p}_x + \hat{p}_x [\hat{x}, \hat{p}_x] = i\hbar \frac{\hbar}{i} \frac{\partial}{\partial x} + \frac{\hbar}{i} \frac{\partial}{\partial x} i\hbar = 2\hbar^2 \frac{\partial}{\partial x} = 2i\hbar \hat{p}_x$$

$$[\hat{x}^2, \hat{p}_x] = [\hat{x}\hat{x}, \hat{p}_x] = \hat{x} [\hat{x}, \hat{p}_x] + [\hat{x}, \hat{p}_x] \hat{x} = 2i\hbar x$$

$$[\hat{p}_x, \hat{x}^2] = [\hat{p}_x, \hat{x}\hat{x}] = [\hat{p}_x, \hat{x}] \hat{x} + \hat{x} [\hat{p}_x, \hat{x}] = -i\hbar(2x) = -i\hbar \frac{d}{dx}(x^2)$$

$$[\hat{p}_x, \hat{x}^3] = [\hat{p}_x, \hat{x}^2 \hat{x}] = [\hat{p}_x, \hat{x}] \hat{x}^2 + \hat{x} [\hat{p}_x, \hat{x}^2] = -i\hbar(3x^2) = -i\hbar \frac{d}{dx}(x^3)$$

By inspection:

$$[\hat{p}_x, \hat{x}^n] = -i\hbar \frac{d}{dx}(x^n)$$

Then,

$$[\hat{p}_x, \hat{V}] = -i\hbar \left\{ a_1 + a_2 \frac{dx^2}{dx} + a_3 \frac{dx^3}{dx} + \dots \right\} = -i\hbar \frac{d}{dx}V(x)$$

Using MATHEMATICA and the following wave function:

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

You can check the following results:

$$\hat{x}_{mm} = \langle \psi_m(x) | x | \psi_m(x) \rangle = \int_{-\infty}^{\infty} \psi_m(x) x \psi_m(x) dx = \begin{cases} 0, & \text{if } m \neq n \pm 1 \\ \frac{1}{\alpha} \sqrt{\frac{n+1}{2}}, & \text{if } m = n+1 \\ \frac{1}{\alpha} \sqrt{\frac{n}{2}}, & \text{if } m = n-1 \end{cases}$$

$$\hat{x}_{nn}^2 = \langle \psi_n(x) | x^2 | \psi_n(x) \rangle = \int_{-\infty}^{\infty} \psi_n(x) x^2 \psi_n(x) dx = \frac{2n+1}{2\alpha},$$

$$\langle \hat{p}_x \rangle = \langle \psi_n(x) | -i\hbar \frac{\partial}{\partial x} | \psi_n(x) \rangle = -i\hbar \int_{-\infty}^{\infty} \psi_n(x) \left(\frac{\partial}{\partial x} \psi_n(x) \right) dx = 0,$$

$$\langle \hat{p}_x^2 \rangle = \langle \psi_n(x) | -\hbar^2 \frac{\partial^2}{\partial x^2} | \psi_n(x) \rangle = -\hbar^2 \int_{-\infty}^{\infty} \psi_n(x) \left(\frac{\partial^2}{\partial x^2} \psi_n(x) \right) dx = \hbar^2 \alpha \left(\frac{2n+1}{2} \right),$$

$$\langle T \rangle = \frac{1}{2m} \langle \hat{p}_x^2 \rangle = \frac{\omega \hbar}{2} \left(n + \frac{1}{2} \right),$$

$$\langle V \rangle = \frac{m\omega^2}{2} \langle \hat{x}^2 \rangle = \frac{\omega \hbar}{2} \left(n + \frac{1}{2} \right),$$

$$\langle E \rangle = \langle T \rangle + \langle V \rangle = \left(n + \frac{1}{2} \right) \hbar \omega$$