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1. Wave Function
 - a) What are the fundamental behaviors of the wave function?
 - b) How can you determine wave function of a quantum particle
 - c) What is the expectation value and eigenvalue of an operator? When they are the same?

a) Fundamental behaviors of the wave function

A wave function $\Psi(x, t)$ must be

- Single valued: A single-valued function is function that, for each point in the domain, has a unique value in the range.
- Continuous: The function has finite value at any point in the given space.
- Differentiable: Derivative of wave function is related to the flow of the particles.
- Square integrable: The wave function contains information about where the particle is located, its square being probability density. Therefore $\int_{-\infty}^{\infty} |\Psi(x, t)|^2 dx < \infty$

b) The wave function can be determined by solving Schrödinger equation: $i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi + V(x, y, z) \Psi$

c) Expectation value of an operator is defined as $\langle A \rangle = \int_{-\infty}^{\infty} \psi^* A \psi dx$. When ψ is eigen function of A then expectation value and eigenvalues of the operator is the same.

2. Under what condition the function $\psi(x) = A \cos kx$ is eigenfunction of the operator $H = \frac{p^2}{2m} + V_0$ where $p = -i\hbar \frac{d}{dx}$ is momentum operator, if its eigenvalue is twice of the constant potential V_0 .

Solution

$$\begin{aligned}
 H\psi &= E\psi \\
 -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} A \cos kx + V_0 A \cos kx &= 2V_0 A \cos kx \\
 \frac{\hbar^2}{2m} k^2 + V_0 &= 2V_0 \text{ or } k^2 = \frac{2m}{\hbar^2} V_0
 \end{aligned}$$

3. Miscellaneous problems
 - a) Show that the function e^{-3ikx} is eigenfunction of momentum and kinetic energy operators.
 - b) Generalized uncertainty between two observable is given by:

$$\Delta A \Delta B \geq \frac{1}{2i} \langle [A, B] \rangle$$

Calculate the uncertainty relation between the observables, *momentum, energy, position and time.*

c) Show that, if the eigenvalue equation

$$Q\psi = q\psi$$

then expectation value of the operator is equal to eigenvalues of the operator.

Solution

a) Momentum operator is given by $p = -i\hbar \frac{d}{dx}$; the eigenvalue equation can be written as $p\psi = \alpha\psi$, then we obtain:

$$-i\hbar \frac{d}{dx} e^{-3ikx} = -3\hbar k e^{-3ikx}$$

With the eigenvalue $\alpha = -3\hbar k$.

Similarly kinetic energy operator can be written as: $K = \frac{p^2}{2m} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2}$ we can write eigenvalue equation

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} e^{-3ikx} = \frac{9\hbar^2 k^2}{2m} e^{-3ikx}$$

With the eigenvalues $\frac{9\hbar^2 k^2}{2m}$.

b) Using the operator relations of the observables $p = -i\hbar \frac{d}{dx}$, $E = -i\hbar \frac{d}{dt}$, $x = x$ and $t = t$, we obtain the commutation relation:

$$[p, x] = [E, t] = -i\hbar, \text{ and } [p, t] = [E, x] = [x, t] = 0$$

The uncertainties are $\Delta p \Delta x \geq \frac{\hbar}{2}$; $\Delta E \Delta t \geq \frac{\hbar}{2}$, Others are zero.

c) Expectation value can be defined as: $\langle Q \rangle = \int_{-\infty}^{\infty} \psi^* Q \psi dx$ substituting $Q\psi = q\psi$ and using normalization condition we obtain:

$$\langle Q \rangle = \int_{-\infty}^{\infty} \psi^* Q \psi dx = \int_{-\infty}^{\infty} \psi^* q \psi dx = q \int_{-\infty}^{\infty} \psi^* \psi dx = q$$

4. What is the postulates, secondary postulates and principles of quantum mechanics?

5. **Problem 1.** A particle in the harmonic oscillator potential starts out in the state

$$\Psi(x, 0) = A(3\psi_0 + 4\psi_1)$$

a) Determine A.

b) Construct $\Psi(x, t)$.

c) Find $\langle x \rangle$ and $\langle p \rangle$.

d) Verify that $\frac{d\langle p \rangle}{dt} = -\langle \frac{dV}{dx} \rangle$.

e) If you measure the energy what values you get and with what probabilities.

Solution1

a) Using the normalization conditions:

$$1 = A^2(9\langle \psi_0 | \psi_0 \rangle + 16\langle \psi_1 | \psi_1 \rangle) = 25A^2, \text{ then } A = \frac{1}{5}$$

b) It is easy to construct time dependent wave function:

$$\Psi(x, t) = \frac{1}{5} \left(3\psi_0 e^{-\frac{iE_0 t}{\hbar}} + 4\psi_1 e^{-\frac{iE_1 t}{\hbar}} \right) = \frac{1}{5} \left(3\psi_0 e^{-i\frac{\omega t}{2}} + 4\psi_1 e^{-i\frac{3\omega t}{2}} \right)$$

Using energy values $E_0 = \frac{1}{2}\hbar\omega$ and $E_1 = \frac{3}{2}\hbar\omega$, we obtain

$$|\Psi(x, t)|^2 = \frac{1}{25} (9\psi_0^2 + 16\psi_1^2 + 24\psi_0\psi_1 \cos(\omega t))$$

c) We can use integral relations or operators to obtain expectation values. Here let us use operators

The ladder operators

$$a_{\pm} = \frac{1}{\sqrt{2\hbar\omega m}} (\mp ip + m\omega x)$$

Then we can obtain the relations

$$x = \frac{\sqrt{2\hbar\omega m}}{2m\omega} (a_+ + a_-) \text{ and } p = \frac{\sqrt{2\hbar\omega m}}{2i} (a_- - a_+)$$

with the action of the operators $a_+ \psi_n = \sqrt{n+1} \psi_{n+1}$ and $a_- \psi_n = \sqrt{n} \psi_{n-1}$

$$\begin{aligned} \langle x \rangle = \frac{1}{25} \sqrt{\frac{\hbar}{2\omega m}} & (9\langle \psi_0 | (a_+ + a_-) | \psi_0 \rangle + 16\langle \psi_1 | (a_+ + a_-) | \psi_1 \rangle + 12e^{i\omega t} \langle \psi_1 | (a_+ + a_-) | \psi_0 \rangle \\ & + 12e^{-i\omega t} \langle \psi_0 | (a_+ + a_-) | \psi_1 \rangle) \end{aligned}$$

$$\langle x \rangle = \frac{1}{25} \sqrt{\frac{\hbar}{2\omega m}} (9 \times 0 + 16 \times 0 + 24 \cos(\omega t)) = \frac{24}{25} \sqrt{\frac{\hbar}{2\omega m}} \cos(\omega t)$$

Similarly

$$\begin{aligned} \langle p \rangle = \frac{1}{25} \frac{\sqrt{2\hbar\omega m}}{2i} & (9\langle \psi_0 | (a_- - a_+) | \psi_0 \rangle + 16\langle \psi_1 | (a_- - a_+) | \psi_1 \rangle + 12e^{i\omega t} \langle \psi_1 | (a_- - a_+) | \psi_0 \rangle \\ & + 12e^{-i\omega t} \langle \psi_0 | (a_- - a_+) | \psi_1 \rangle) \end{aligned}$$

$$\langle p \rangle = \frac{1}{25} \frac{\sqrt{2\hbar\omega m}}{2} (9 \times 0 + 16 \times 0 - 24 \sin(\omega t)) = -\frac{24}{25} \sqrt{\frac{\hbar\omega m}{2}} \sin(\omega t)$$

It is obvious that the classical relation $\langle p \rangle = m \frac{d}{dt} \langle x \rangle = -\frac{24}{25} \sqrt{\frac{\hbar\omega m}{2}} \sin(\omega t)$.

d) Potential is given by

$$V = \frac{1}{2} m \omega^2 x^2 \text{ then } \frac{dV}{dx} = m \omega^2 x \text{ therefore } \left\langle \frac{dV}{dt} \right\rangle = m \omega^2 \langle x \rangle = \frac{24}{25} \sqrt{\frac{\hbar}{2\omega m}} m \omega^2 \cos(\omega t)$$

We can verify that $\frac{d}{dt} \langle p \rangle = -\left\langle \frac{dV}{dt} \right\rangle$ (This is the Ehrenfest theorem!)

e) Energy $E_0 = \frac{\hbar\omega}{2}$ with probability $c_0 = \frac{9}{25}$ and $E_1 = \frac{3\hbar\omega}{2}$ with $c_1 = \frac{16}{25}$.

6. Find the eigenfunctions of the operators $\frac{d}{dx}$, $\frac{d^2}{dx^2}$.

Solution.

Eigenvalue equation can be written as $A\psi = a\psi$ where A is operator a is its eigenvalue and ψ is eigenfunction of A . Then

$$\frac{d}{dx} \psi = a\psi \Rightarrow \frac{d\psi}{\psi} = a dx$$

Integrating both sides yields

$$\psi = C e^{ax}$$

Similarly

$$\frac{d^2}{dx^2} \psi = a\psi \Rightarrow \frac{d^2\psi}{dx^2} = a\psi$$

Solution of the differential equation yields

$$\psi = C_1 e^{\sqrt{a}x} + C_2 e^{-\sqrt{a}x}$$

7. Find the eigenfunctions of the operators $a = \frac{d}{dx} + x$ and $a^+ = -\frac{d}{dx} + x$ have the same eigenfunction.

Solution. Let us find eigenfunction of a

$$\left(\frac{d}{dx} + x\right)\psi = a\psi \Rightarrow \frac{d\psi}{\psi} = (a - x)dx$$

Solving the equation, we obtain

$$\psi = C e^{ax - \frac{x^2}{2}}$$

You can calculate eigenfunction of a^+ .

8. Calculate commutator of a and a^+

Solution

$$\begin{aligned} [a, a^+] &= \left(\frac{d}{dx} + x\right)\left(-\frac{d}{dx} + x\right) - \left(-\frac{d}{dx} + x\right)\left(\frac{d}{dx} + x\right) \\ &= -\frac{d^2}{dx^2} + \frac{d}{dx}x - x\frac{d}{dx} + x^2 + \frac{d^2}{dx^2} + \frac{d}{dx}x - x\frac{d}{dx} - x^2 \\ &= 2\frac{d}{dx}x - 2x\frac{d}{dx} = 2 \\ [a, a^+] &= 2 \end{aligned}$$

9. Show that whenever a solution $\Psi(x; t)$ of the TDSE separates into a product $\Psi(x; t) = f(x)\phi(t)$ then $f(x)$ must satisfy the corresponding TISE and $\phi(t)$ must be proportional to $e^{-i\frac{E}{\hbar}t}$.

10. Show that e^{+ikx} and e^{-ikx} satisfy the TISE with $V(x) = 0$ and determine the value of E for each.

11. For the SHO, $\psi_0(x) = A \exp\left(-\frac{x^2}{2}\right)$. What is E_0 ?

12. By applying the appropriate operators, show that $\psi(x) = e^{+ikx}$ is an eigenstate of energy and momentum for a free particle (for which $V(x) = 0$).