BLDE Association's

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Roll No. : 05 **R.C.U. Exam Seat No.** P15KM23S103004.

Subject Code : B420010.

Subject : Quantum Mechanics - I.

Test	Maximum Marks	Marks Obtained
First Test	20	16 04/04

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2 a) Ehrenfest theorem:

Statement: It states that, the Schrodinger equations leads to classical laws of motion for the

$$\langle P_x \rangle = m\frac{d\langle x\rangle}{dt} \quad \text{or} \quad \langle P \rangle = m\frac{d\langle r\rangle}{dt}$$

and.

$$\langle F \rangle = \langle -\nabla V \rangle.$$

Proof:

Consider the x-component of velocity, then its time derivative is given by,

$$\frac{d\langle x\rangle}{dt} = \frac{d}{dt}\int \psi^* x\, \psi\, dx$$

$$\frac{d}{dt}\langle x\rangle = \int \psi^* x \frac{\partial \psi}{\partial t} dx + \int \frac{\partial \psi^*}{\partial t} x\, \psi\, dx \quad \text{--- (1)}$$

Consider the Schrodinger time dependent wave equation,

i.e.

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V\psi$$

$$\Rightarrow \frac{\partial \psi}{\partial t} = \frac{1}{i\hbar}\left[-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V\psi\right] \quad \text{--- (2)}$$

Its conjugate is given by,

$$\frac{\partial \psi^*}{\partial t} = \frac{-1}{i\hbar}\left[-\frac{\hbar^2}{2m}\frac{\partial^2 \psi^*}{\partial x^2} + V\psi^*\right] \quad \text{--- (3)}$$

Now substitute eq^n (2) & (3) in (1), we get

$$\frac{d\langle x\rangle}{dt} = \int \psi^* x\left(\frac{1}{i\hbar}\left(-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi\right)\right)dx + \int \frac{-1}{i\hbar}\left(-\frac{\hbar^2}{2m}\frac{\partial^2\psi^*}{\partial x^2} + V\psi^*\right)x\,\psi\, dx$$

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$$\frac{d}{dt}\langle x\rangle = \frac{1}{i\hbar}\frac{-\hbar^2}{\partial m}\left[\int \psi^* x \frac{\partial^2 \psi}{\partial x^2}dx - \int \frac{\partial^2 \psi^*}{\partial x^2} x\psi\, dx\right] \quad \text{--- (4)}$$

$$= \frac{i\hbar}{\partial m}\left[x\frac{\partial}{\partial x}\left(\int \psi^* \frac{\partial \psi}{\partial x}dx - \int \frac{\partial \psi^*}{\partial x}\psi\, dx\right)\right] \text{ ---}$$

$$= \frac{i\hbar}{\partial m}\left[x\frac{\partial}{\partial x}\left(\int \psi^* \frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x}\psi\, dx\right)\right] \quad \text{--- (5)}$$

Integrating eq^n (5) by parts from $-\infty$ to ∞

$$\frac{d}{dt}\langle x\rangle = -\frac{i\hbar}{\partial m}\left[\int_{-\infty}^{\infty}\psi^*\frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x}\psi\, dx\right]$$

$$\frac{d}{dt}\langle x\rangle = -\frac{i\hbar}{\partial m}\int_{-\infty}^{\infty}\psi^*\frac{\partial \psi}{\partial x}dx + \frac{i\hbar}{\partial m}\int_{-\infty}^{\infty}\frac{\partial \psi}{\partial x}\psi\, dx \quad \text{--- (6)}$$

Integrating eq^n (6) of II term.

$$\therefore \frac{d}{dt}\langle x\rangle = -\frac{i\hbar}{\partial m}\int_{-\infty}^{\infty}\psi^*\frac{\partial \psi}{\partial x}dx - \frac{i\hbar}{\partial m}\int_{-\infty}^{\infty}\psi^*\frac{\partial \psi}{\partial x}dx$$

$$= -\frac{\cancel{2}i\hbar}{\cancel{2}m}\int_{-\infty}^{\infty}\psi^*\frac{\partial \psi}{\partial x}dx$$

$$m\frac{d}{dt}\langle x\rangle = -i\hbar\int_{-\infty}^{\infty}\psi^*\frac{\partial \psi}{\partial x}dx$$

$$= \int_{-\infty}^{\infty}\psi^*\left(-i\hbar\frac{\partial}{\partial x}\right)\psi\, dx$$

$$\therefore \int_{-\infty}^{\infty}\psi^* P_x \psi\, dx = m\frac{d}{dt}\langle x\rangle$$

$$\boxed{\therefore \langle P_x\rangle = m\frac{d}{dt}\langle x\rangle}$$

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In general,

$$\left[\langle P \rangle = m \frac{d}{dt} \langle x \rangle \right]_{//}$$

The time derivative of $\langle P_x \rangle$ is given by:

$$\frac{d}{dt}\langle P_x \rangle = \frac{d}{dt} \int_{-\infty}^{\infty} \psi^* \left(-i\hbar \frac{\partial}{\partial x} \right) \psi \, dx .$$

$$= -i\hbar \frac{d}{dt} \int_{-\infty}^{\infty} \psi^* \frac{\partial \psi}{\partial x} dx .$$

$$= -i\hbar \left[\int_{-\infty}^{\infty} \left(\psi^* \frac{\partial}{\partial t}\left(\frac{\partial \psi}{\partial x} \right) + \frac{\partial \psi}{\partial x} \frac{\partial \psi^*}{\partial t} \right) dx \right].$$

$$= -i\hbar \int_{-\infty}^{\infty} \psi^* \frac{\partial}{\partial x}\left(\frac{\partial \psi}{\partial t} \right) dx - i\hbar \int_{-\infty}^{\infty} \frac{\partial \psi}{\partial x} \frac{\partial \psi^*}{\partial t} dx \quad \text{--- (7)}$$

From Schrodinger time dependent eq^n, equation (7) becomes,

$$\frac{d}{dt}\langle P_x \rangle = -i\hbar \left[\int_{-\infty}^{\infty} \psi^* \frac{\partial}{\partial x} \left(\frac{1}{i\hbar} \left(\frac{-\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V\psi \right) \right) - \frac{\partial \psi}{\partial x} \left(\frac{-1}{i\hbar} \left(\frac{-\hbar^2}{2m} \frac{\partial^2 \psi^*}{\partial x^2} + V\psi^* \right) \right) \right]$$

$$= -i\hbar \int_{-\infty}^{\infty} \left(\psi^* \frac{\partial}{\partial x}(V\psi) - \frac{\partial \psi}{\partial x} (V\psi^*) \right) dx \quad \text{--- (8)}$$

On solving eq^n (8) we get,

$$\langle F_x \rangle = \int_{-\infty}^{\infty} \psi^* \left(-\frac{\partial}{\partial x} V \right) \psi \, dx .$$

Thus,

$$\left[\langle F \rangle = \langle -\nabla V \rangle \right]_{//}$$

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1 a) Schrodinger time independent wave equation

Let us consider the wave function $\psi(r,t)$ given by,

$$\psi = A e^{-2\pi i/h (Et - Px)} \quad \text{--- (1)}$$

$$= A e^{-2\pi i/h (Et)} \cdot e^{2\pi i/h (Px)}$$

$$\psi = \psi_0 e^{-2\pi i/h (Et)} \quad \text{--- (2)}$$

Differentiate equation (2) wrt 't'.

$$\frac{\partial \psi}{\partial t} = \psi_0 e^{-2\pi i/h (Et)} \left(-\frac{2\pi i}{h} E \right).$$

$$\frac{\partial \psi}{\partial t} = \psi E \left(-\frac{2\pi i}{h} \right) \quad \text{--- (3)}$$

Differentiate equation (1) wrt 'x' twice.

$$\frac{\partial^2 \psi}{\partial x^2} = A e^{-2\pi i/h (Et - Px)} \left(\frac{2\pi i P}{h} \right)^2.$$

$$\frac{\partial^2 \psi}{\partial x^2} = \psi \left(\frac{2\pi i P}{h} \right)^2. \quad \text{--- (4)}.$$

Total energy is given by,

$$E = \frac{P^2}{2m} + V \quad \text{--- (5)}$$

Substitute eqn (3) & (4) in (5).

$$\frac{1}{\psi} \left(\frac{-h}{2\pi i} \right) \frac{\partial \psi}{\partial t} = \frac{1}{2m} \frac{1}{\psi} \left(\frac{h^2}{4\pi^2 i^2} \right) \frac{\partial^2 \psi}{\partial x^2} + V$$

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Multiply ψ on both side then,

$$i\hbar \frac{\partial \psi}{\partial t} = \frac{-\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V\psi \quad \text{---} (6)$$

Again substitute equation (3) in (6), we get

$$\boxed{E\psi = \frac{-\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V\psi}$$

This is 1-dimensional Schrodinger time independent wave equation.

$\therefore$ The 3-dimensional equation is given by,

$$\boxed{E\psi = \frac{-\hbar^2}{2m} \nabla^2 \psi + V\psi}$$

(1) b)

i) $[X, P_z]$

$\rightarrow$ $[x, P_z] = [X P_z - P_z X]$

$$= \left[X\left(-i\hbar \frac{\partial}{\partial z}\right) - \left(-i\hbar \frac{\partial}{\partial z}\right) X \right]$$

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$$= -X i\hbar \frac{\partial}{\partial z}(1) + i\hbar \frac{\partial}{\partial z} X$$

$[x, P_z] = 0$

Hence X & P_z are commute with each other.

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① b) ii) $[x^n, P_x]$

To solve $[x^n, P_x]$, lets first solve,

- $[x, P_x] = [xP_x - P_x x]$

$$= \left[x\left(-i\hbar\frac{\partial}{\partial x}\right) - \left(-i\hbar\frac{\partial}{\partial x}\right)x\right]$$

$$[x, P_x] = i\hbar$$

- lets consider,

$$[x^2, P_x] = x[x, P_x] + [x, P_x]x$$

$$= x(i\hbar) + (i\hbar)x$$

$$= 2xi\hbar$$

- lets consider,

$$[x^3, P_x] = x[x^2, P_x] + [x^2, P_x]x$$

$$= x(2xi\hbar) + (2xi\hbar)x$$

$$= 2x^2i\hbar + 2x^2i\hbar$$

$$= 3x^2i\hbar$$

Thus as we solve so on, the general equation is given by,

$$\boxed{[x^n, P_x] = nx^{n-1}i\hbar}$$ //

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