Quantum Mechanics

Lecture # 3

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Probability density/Probability current density:

Probability density / Probability Current density

" The probability of finding the particle per unit volume per unit length"

or

" The probability of finding a particle at particular point"

i-e

$$P_{(x,t)}dx = \psi^{*}_{(x)}\psi_{(x)}dx$$

or

$$P_{(x,t)}dx = |\psi|^2 dx$$

⇒ This gives the probability density in the interval $[x, x+dx]$.

•Probability current density in quantum:

* Probability current density in quantum:-

According to S.W.E

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

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

Taking conjugate of (i)

$$-\frac{\hbar^2}{2m}\nabla^2\psi^* + V\psi^* = -i\hbar\frac{\partial\psi^*}{\partial t} \quad \text{—— (ii)}$$

Multiplying (i) by 'ψ^*' and (ii) by 'ψ'

$$-\frac{\hbar^2}{2m}\psi^*\nabla^2\psi + \psi^* V\psi = i\hbar\psi^*\frac{\partial\psi}{\partial t} \quad \text{—— (iii)}$$

Cont.

$$-\frac{\hbar^2}{2m}\psi\nabla^2\psi^* + \psi V\psi^* = -i\hbar\psi\frac{\partial\psi^*}{\partial t} \quad \text{—— (iv)}$$

By (iii) − (iv)

$$-\frac{\hbar^2}{2m}\left(\psi^*\nabla^2\psi - \psi\nabla^2\psi^*\right) = i\hbar\left(\psi^*\frac{\partial\psi}{\partial t} + \psi\frac{\partial\psi^*}{\partial t}\right)$$

$$-\frac{\hbar}{2im}\left(\psi^*\nabla^2\psi - \psi\nabla^2\psi^*\right) = \frac{\partial}{\partial t}(\psi\psi^*)$$

$$\Rightarrow \frac{\partial}{\partial t}(\psi\psi^*) + \vec{\nabla}\cdot\frac{\hbar}{2im}\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right) = 0$$

$$\Rightarrow \frac{\partial}{\partial t}\rho + \vec{\nabla}\cdot\vec{S} = 0 \quad \text{—— (v)}$$

where $S = \frac{\hbar}{2im}\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right)$

Eq. (v) is known as "eq. of continuity". where 'ρ' is the "probability density" and 'S' is "probability current density" or "particle current density."

" This eq. states the "conservation of particle/charge" by saying that the time derivative of particle density ρ, plus the divergence of particle density is 'zero.'

let

$$\psi^*\nabla\psi = Z = x + iy$$

$$\psi\nabla\psi^* = Z^* = x - iy$$

Cont.

Now $\quad Z - Z^* = 2iy$

$= 2i\,\mathrm{Im}(Z)$

$= 2i\,\mathrm{Im}(\psi^* \nabla \psi)$

So,

$$S = \frac{\hbar}{2im} \cdot 2i\,\mathrm{Im}(\psi^* \nabla \psi)$$

$$\boxed{S = \frac{\hbar}{m}\,\mathrm{Im}(\psi^* \nabla \psi)}$$

•Theorem#1:

Theorem:- Prove that $\left[x, \frac{d}{dx}\right] = -1$ where x and $\frac{d}{dx}$ are operators

Consider

$$\left[x, \frac{d}{dx}\right]\psi$$

$$= \left[x\frac{d}{dx} - \frac{d}{dx}x\right]\psi$$

$$= \left[x\frac{d\psi}{dx} - \frac{d}{dx}x\psi\right]$$

$$= x\frac{d\psi}{dx} - x\frac{d\psi}{dx} - \psi\frac{dx}{dx}$$

$$\left[x, \frac{d}{dx}\right]\psi = -\psi$$

$$\left[x, \frac{d}{dx}\right] = -1$$

Hence proved.

•Theorem#2

Theorem :-

Prove that $\psi^*(x,y,z,t)\cdot\psi(x,y,z,t)$ is necessarily real or either positive or zero.

We know that any complex fn. such as $\psi(x,y,z,t)$ can be written as

$$\psi(x,y,z,t) = K(x,y,z,t) + iM(x,y,z,t) \qquad \because z = a + ib$$

where

$K(x,y,z,t)$ and $M(x,y,z,t)$ are real.

Also

$$\psi^*(x,y,z,t) = K(x,y,z,t) - iM(x,y,z,t)$$

Now

$$\psi^*(x,y,z,t)\psi(x,y,z,t) = \{K(x,y,z,t) - iM(x,y,z,t)\}\{K(x,y,z,t) + iM(x,y,z,t)\}$$

$$\psi^*(x,y,z,t)\psi(x,y,z,t) = K^2 - i^2M^2$$

$$= K^2 + M^2 \qquad \because i^2 = -1$$

This is equal to sum of squares of two real functions. Therefore, $\psi^*(r,t)\psi(r,t)$ is real and is either positive or zero.

Hence proved.

Constant of Motion:

"Constant of Motion"

⇒ Following are two conditions for a constant of motion :

- It should be independent of time.
- It should commute with hamiltonian of the system.

Considering an operator related to an observable A. Its expectation value is

$$\langle A \rangle = \int \psi^* \alpha \psi \, d\tau$$

→ where 'α' is the operator associated with observable 'A'.

→ Time rate of change of $\langle A \rangle$ is

$$\frac{d\langle A \rangle}{dt} = \int \left[\psi^* \frac{\partial \alpha}{\partial t} \psi + \psi^* \alpha \frac{\partial \psi}{\partial t} + \frac{\partial \psi^*}{\partial t} \alpha \psi \right] d\tau \quad \text{—— (i)}$$

The state function must satisfy S.W.E

$$i\hbar \frac{\partial \psi}{\partial t} = H\psi$$

$$\Rightarrow \quad \frac{\partial \psi}{\partial t} = \frac{1}{i\hbar} H\psi$$

$$\frac{\partial \psi}{\partial t} = -\frac{i}{\hbar} H\psi \quad \text{—— (ii)}$$

Also

$$\frac{\partial \psi^*}{\partial t} = \frac{i}{\hbar} H\psi^* \quad \text{—— (iii)}$$

Cont.

Applying this condition in eq. (iv)

$$\frac{d\langle A\rangle}{dt} = 0$$

$\Rightarrow \langle A\rangle = \text{Constant}$

Hence A is called a constant of motion.

Cont.

Put (ii) and (iii) in (i)

$$\frac{d\langle A\rangle}{dt} = \int\left[\psi^*\frac{\partial\alpha}{\partial t}\psi + \psi^*\alpha\left(-\frac{i}{\hbar}H\psi\right) + \frac{i}{\hbar}(H\psi)^*\alpha\psi\right]d\tau$$

$\because H^* = H$

$$\frac{d\langle A\rangle}{dt} = \int\left[\psi^*\frac{\partial\alpha}{\partial t}\psi - \frac{i}{\hbar}\psi^*\alpha H\psi + \frac{i}{\hbar}H\psi^*\alpha\psi\right]d\tau$$

$$= \int\left[\psi^*\frac{\partial\alpha}{\partial t}\psi\, d\tau + \frac{i}{\hbar}\left[H\psi^*\alpha\psi - \psi^*\alpha H\psi\right]d\tau\right.$$

$$= \int\psi^*\left[\frac{\partial\alpha}{\partial t} + \frac{i}{\hbar}\left[H\alpha - \alpha H\right]\right]\psi\, d\tau$$

$$= \int\psi^*\left[\frac{\partial\alpha}{\partial t} + \frac{i}{\hbar}\left[H,\alpha\right]\right]\psi\, d\tau$$

$$\frac{d\langle A\rangle}{dt} = \frac{\partial\alpha}{\partial t} + \frac{i}{\hbar}\left[H,\alpha\right] \quad \text{———} \quad (iv)$$

For the observable $\langle A\rangle$ to be a constant of motion, there are following two conditions

i) $\dfrac{\partial\alpha}{\partial t} = 0$

ii) $[H, \alpha] = 0$