ABESIT Ghaziabad (290)

Course: Engg. Physics (KAS 201T)

Unit-III

Quantum Mechanics

Faculty Name : Dr. Anchala

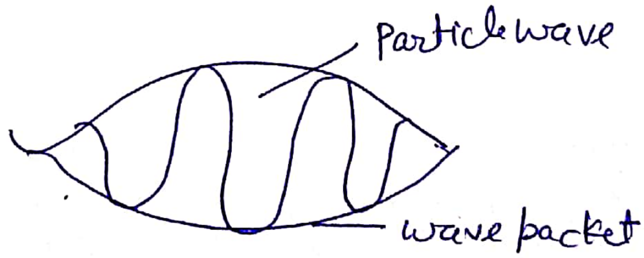
Lecture 31 - Time-dependent Schrodinger equation

outcome: Describe the Schrodinger time dependent wave equation

Schrodinger Time-dependent wave equation :-

The Schrodinger wave equation is the fundamental equation of wave mechanics in the same sense as the Newton's law of classical mechanics.

In wave mechanics a material particles is equivalent to a wave packet. Schrodinger equation is used to locate the position of the particle in the wave packet.



The general differential equation of a wave travelling in +x direction with velocity v having wave function ψ is

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 \psi}{\partial t^2} \quad \text{—— (1)}$$

The general solution of equation (1) is

$$\psi = A e^{i(kx - \omega t)} \quad \text{——— (2)}$$

We know that $k = \frac{2\pi}{\lambda}$ and $\lambda = \frac{h}{p}$

$$k = \frac{2\pi p}{h} = \frac{p}{\hbar} \qquad \left(\because \hbar = \frac{h}{2\pi}\right)$$

and $E = h\nu = 2\pi\hbar \times \frac{\omega}{2\pi} = \hbar\omega$

$$\omega = \frac{E}{\hbar} \quad \text{——— (4)}$$

Substituting (3) and (4) in equation (2)

$$\psi = A e^{i\left(\frac{px}{\hbar} - \frac{E}{\hbar}t\right)}$$

$$\psi = A e^{\frac{i}{\hbar}(px - Et)} \quad \text{——— (5)}$$

Now, differentiating equation (5) with respect to t

$$\frac{\partial \psi}{\partial t} = A e^{\frac{i}{\hbar}(px - Et)} \left(-\frac{i}{\hbar}E\right)$$

$$\frac{\partial \psi}{\partial t} = \left(\frac{-i}{\hbar}E\right)\psi = \left(\frac{-i}{\hbar}\right)E\psi$$

$$E\psi = -\frac{\hbar}{i}\frac{\partial \psi}{\partial t}$$

$$E\psi = i\hbar\frac{\partial \psi}{\partial t} \quad \text{——— (6)}$$ (multiplying and divide by i)

Differentiating equation (5) with respect to 'x' twice

$$\frac{\partial \psi}{\partial x} = A e^{\frac{i}{\hbar}(px - Et)} \left(\frac{i}{\hbar}p\right)$$

$$\frac{\partial^2 \psi}{\partial x^2} = A e^{\frac{i}{\hbar}(px - Et)} \left(\frac{i}{\hbar}p\right)\left(\frac{i}{\hbar}p\right)$$

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{i^2}{\hbar^2}p^2\psi = -\frac{p^2}{\hbar^2}\psi$$

$$p^2\psi = -\hbar^2 \frac{\partial^2\psi}{\partial x^2} \quad \text{——— (7)}$$

Total energy of the particle

$$E = K.E + P.E$$

$$E = \frac{p^2}{2m} + V$$

multiplying both sides by ψ

$$E\psi = \frac{p^2}{2m}\psi + V\psi \quad \text{——— (8)}$$

Substituting equation (6) and (7) in equation (8)

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

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

This is time-dependent Schrodinger wave equation.

When the particle is moving in 3-dimensional space the equation becomes

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2}\right) + V\psi = i\hbar\frac{\partial\psi}{\partial t}$$

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

where $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$