WAVE FUNCTION

A variable quantity which characterizes de Broglie waves is known as wave function and is denoted by the symbol Ψ . The value of the wave function associated with a moving particle at point (x,y,z) and time ‘t’ gives the probability of finding the particle at that time and at that point.

PHYSICAL SIGNIFICANCE OF WAVE FUNCTION

- The wave function has **no physical meaning.**
- It is a **complex quantity** representing the matter **wave of a particle**.
- $|\psi|^2$ is **real and positive**, amplitude may be positive or negative but the intensity(square of amplitude) is always real and positive.
- $|\psi|^2$ represents the probability density or probability of **finding the particle in the given region.**
- For a given volume $d\tau$, probability $\mathbf{P = \int\int\int |\psi|^2 d\tau}$ where $d\tau = dx\, dy\, dz$
- The **probability value** lies between **0 and 1.**
- $\int\int\int |\psi|^2 d\tau = 1$, this wave function is called **normalized wave function**.

SCHROEDINGER'S WAVE EQUATION

- Austrian scientist, **Erwin Schroedinger**
- describes the wave nature of a particle , derived in **mathematical form**
- connected the expression of **De-Broglie wavelength** with **classical wave equation**
- two forms of **Schroedinger's wave equation**
- Time **Independent** wave equation
- Time **dependent** wave equation

SCHROEDINGER'S TIME INDEPENDENT WAVE EQUATION

- Let us consider a system of stationary wave associated with a **moving particle.** Let ψ be the wave function of the particle along x, y and z coordinates axes at any time t.

The differential wave equation of a progressive wave with wave velocity 'u' can be written in terms of Cartesian coordinates as,

$$\frac{d^2\psi}{dx^2}+\frac{d^2\psi}{dy^2}+\frac{d^2\psi}{dz^2}=\frac{1}{v^2}\frac{d^2\psi}{dt^2} \qquad \frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}=\frac{1}{v^2}\frac{\partial^2\psi}{\partial t^2}\ldots(1)$$

The solution of eqn(1) is $\psi=\psi_0 e^{-i\omega t}$

Differentiating the above equation with respect to time 't' twice,

$$\frac{\partial\psi}{\partial t}=-i\omega\psi_0 e^{-i\omega t}=-i\omega\psi \qquad \frac{\partial^2\psi}{\partial t^2}=-\omega^2\psi\ldots..(2)$$

Substituting (2) in (1) $$\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}=\frac{-\omega^2\psi}{V^2}$$

SCHROEDINGER'S TIME INDEPENDENT WAVE EQUATION

$$\omega = 2\pi\nu$$

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} = \frac{-4\pi^2\nu^2\psi}{V^2}$$

$$substituting\ V = \nu\lambda$$

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} = \frac{-4\pi^2\nu^2\psi}{\nu^2\lambda^2}$$

$$\lambda = \frac{h}{mV}$$

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} = \frac{-4\pi^2 m^2 V^2\psi}{h^2}$$

$$total\,energy\,E = \frac{1}{2}mV^2 + V$$

$$2m(E - V) = m^2V^2$$

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} = \frac{-8\pi^2 m(E-V)\psi}{h^2}$$

$$\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} = \nabla^2, where\ \nabla\ is\ Laplacian\ Operator$$

$$\nabla^2\psi = \frac{-8\pi^2 m(E-V)\psi}{h^2} \Rightarrow \frac{-2m}{\hbar^2}(E-V)\psi$$

$$since\ \hbar = \frac{h}{2\pi}$$

$$\nabla^2\psi + \frac{2m}{\hbar^2}(E-V)\psi = 0 \ (Time\ independent\ Schroedinger\ wave\ eqn)$$

SCHROEDINGER'S TIME DEPENDENT WAVE EQUATION

The solution of the classical differential eqn. of wave system is, $\psi = \psi_0 e^{-i\omega t}$

Differentiating the above equation with respect to time 't' ,

$$\frac{\partial \psi}{\partial t} = -i\omega\psi_0 e^{-i\omega t} = -i\omega\psi$$

Substituting E=hν $\omega = 2\pi\nu$

$$\frac{\partial \psi}{\partial t} = -i2\pi\nu\psi = -i2\pi\left(\frac{E}{h}\right)\psi$$

$$\frac{\partial \psi}{\partial t} = -i2\pi\nu\psi = -i\left(\frac{E}{\hbar}\right)\psi = -i^2\left(\frac{E}{i\hbar}\right)\psi \quad \sin ce\, \hbar = \frac{h}{2\pi}$$

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

$$\nabla^2\psi + \frac{2m}{\hbar^2}(E - V)\psi = 0 (Time independent\ Schroedinger\ wave\ eqn)$$

$$\nabla^2\psi + \frac{2m}{\hbar^2}E\psi - \frac{2m}{\hbar^2}V\psi = 0$$

SCHROEDINGER'S TIME DEPENDENT WAVE EQUATION

$$\nabla^2\psi + \frac{2m}{\hbar^2} i\hbar \frac{\partial \psi}{\partial t} - \frac{2m}{\hbar^2} V\psi = 0$$

$$multiply\ throughout\ by\ \frac{\hbar^2}{2m}$$

$$\frac{\hbar^2}{2m}\nabla^2\psi + E\psi - V\psi = 0$$

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi (Time dependent Schroedinger\ wave\ eqn)$$

$$The\ Hamiltonian\ operator$$

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

$$H\psi = E\psi$$

$$E = energy\ operator$$