

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 ψ 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 , probability $P = \iiint |\psi|^2 d$ where $d = dx dy dz$
- The **probability value** lies between **0 and 1**.
- $\iiint |\psi|^2 d = 1$, 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,

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

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

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

$$\frac{\partial\psi}{\partial t} = -i\omega\psi_0 e^{-i\omega t} = -i\omega\psi \quad \frac{\partial^2\psi}{\partial t^2} = -\omega^2\psi \dots(2)$$

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

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

substituting $V = v\lambda$

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

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

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

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

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} = -\frac{8\pi^2m(E - V)\psi}{h^2} \quad \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} = \nabla^2, \text{ where } \nabla^2 \text{ is Laplacian Operator}$$

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

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

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 $E = h\omega$ $\omega = 2\pi\nu$

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

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

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

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

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

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 $\frac{\hbar^2}{2m}$

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

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

The Hamiltonian operator

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

$$H\psi = E\psi$$

E = energy operator