

SCHRODINGER WAVE EQUATION

- Time dependent wave equation
- Time independent equation

Assumptions.

- (i) de Broglie wavelength can be applied for the matter waves for any field of force. Based on this, the total energy of a particle can be written as,

$$T.E = P.E + K.E \quad \text{or} \quad E = V + \left(\frac{1}{2}\right)mv^2$$

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

Since $p = mv$

$$p = [2m(E - V)]^{1/2} \quad (1)$$

But from de Broglie wavelength,

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

$$\lambda = \frac{h}{[2m(E - V)]^{1/2}} \quad (2)$$

(ii) The wave function associated with the material particles, with function of time 't' can be written as,

$$\psi = \psi_0 e^{-i\omega t} \quad (3)$$

Where ψ_0 is the amplitude of the wave at the point (x, y, z) and $\omega = 2\pi\nu$ where ν is the frequency of radiation.

(i) Schrodinger time independent 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 coordinate axes at any time t.

The differential wave equation of a progressive wave with wave velocity u can be written as in terms of Cartesian coordinate.

$$\frac{d^2\psi}{dx^2} + \frac{d^2\psi}{dy^2} + \frac{d^2\psi}{dz^2} = \frac{1}{u^2} \times \frac{d^2\psi}{dt^2} \quad (4)$$

The solution for the equation (4) is equation (3)

Differentiating equation (3) w.r.t. t twice, we get,

$$\begin{aligned} \frac{d\psi}{dt} &= -i\omega\psi_0 e^{-i\omega t} = -i\omega\psi \\ \frac{d^2\psi}{dt^2} &= -\omega^2\psi \end{aligned} \quad (5)$$

Substituting $\frac{d^2\psi}{dt^2}$ value in equation (4), we get,

$$\begin{aligned}\frac{d^2\psi}{dx^2} + \frac{d^2\psi}{dy^2} + \frac{d^2\psi}{dz^2} &= -\frac{\omega^2}{u^2}\psi \\ &= -\frac{(2\pi\nu)^2}{u^2}\psi\end{aligned}\quad (6)$$

Where $\omega = 2\pi\nu$

$$\frac{d^2\psi}{dx^2} + \frac{d^2\psi}{dy^2} + \frac{d^2\psi}{dz^2} = -\frac{4\pi^2\nu^2}{u^2}\psi$$

Substituting the wave velocity $u (= \nu\lambda)$, we get,

$$\frac{d^2\psi}{dx^2} + \frac{d^2\psi}{dy^2} + \frac{d^2\psi}{dz^2} = -\frac{4\pi^2\nu^2}{\lambda^2\nu^2}\psi \quad (7)$$

Substituting wavelength value from equation (2) in equation (7)

$$\frac{d^2\psi}{dx^2} + \frac{d^2\psi}{dy^2} + \frac{d^2\psi}{dz^2} = -\frac{4\pi^2}{h^2} \times 2m(E - V)\psi \quad (8)$$

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

Where ∇^2 is the Laplacian operator.

Equation (8) can be written as,

$$\nabla^2\psi = -\frac{8\pi^2}{h^2} m(E - V)\psi \quad (9)$$

$$= -\frac{2m}{\hbar^2} (E - V)\psi$$

$$\text{Where } \hbar = \frac{h}{2\pi}$$

$$\text{Therefore, } \nabla^2\psi + \frac{2m}{\hbar^2} (E - V)\psi = 0 \quad (10)$$

Equation (9) or (10) is known as *Schrodinger time independent equation*.

(ii) Schrodinger time dependent equation

From the Schrodinger second assumption, differentiating Equation (3) w.r.t. t , we get,

$$\frac{d\psi}{dt} = -i\omega\psi = -i2\pi\nu\psi$$

Substituting $E = h\nu$ we get

$$= \frac{-i2\pi E}{h} \psi = -i \frac{E}{h} \psi$$

$$E\psi = -\frac{\hbar}{i} \frac{d\psi}{dt}$$

$$E\psi = i\hbar \frac{d\psi}{dt} \quad (12)$$

From Schrodinger time independent equation (10)

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

Substituting $E\psi$ value, we get,

$$\nabla^2\psi + \frac{2m}{\hbar^2} i\hbar \times \frac{d\psi}{dt} - \frac{2m}{\hbar^2} V\psi = 0 \quad (13)$$

Multiplying equation (13) by $\hbar^2/2m$, we get,

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

Or

$$-\frac{\hbar^2}{2m} \nabla^2\psi + V\psi = i\hbar \frac{d\psi}{dt} \quad (14)$$

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V = H \quad (15)$$

Where H is an operator known as *Hamiltonian operator*.
Therefore,

$$H\psi = E\psi \quad (16)$$

Where $E\psi = i\hbar \times \frac{d\psi}{dt}$ is an energy operator

Equations (14) or (16) is called as *Schrodinger time dependent wave equation*.

Physical significance of ψ

- It relates the particles and wave nature of matter statistically.
- It is a complex quantity and hence we cannot measure it.
- It's square is a measure of the probability of finding the particle at a particular position. It cannot predict the exact location of the particle
- The wave function is a complex quantity, whereas the probability is a real and positive quantity. Therefore, a term called position probability density $P(r, t)$ is introduced. It is defined as the product of the wave function and its complex conjugate as,

$$P(r, t) = |\psi(r, t)|^2$$

- The probability of finding the particle within a volume $d\tau$ is

$$P = \int |\psi|^2 d\tau$$

Where $d\tau = dx \, dy \, dz$

- If a particle is definitely present then its probability value is one.

i.e.
$$P = \int_{-\infty}^{+\infty} |\psi|^2 d\tau = 1$$

- In optics, the amount of light is expressed in terms of its intensity rather than its amplitude, since intensity is a measurable physical quantity. Similarly, the wave function ψ has no physical meaning, whereas the probability density has physical meaning.