

4.5 Schrodinger wave equation

4.5.1 Schrodinger Time Independent wave equation

Consider a wave associated with a moving particle. Let x, y, z be the coordinate of the particle and Ψ is a wave function for de – Broglie at any instant of time t .

The classical differential equation for wave motion is given by

$$\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} = \frac{1}{v^2} \frac{\partial^2 \Psi}{\partial t^2} \text{-----(1)}$$

$$\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right] = \frac{1}{v^2} \frac{\partial^2 \Psi}{\partial t^2}$$

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

$$(1) \quad \text{gives} \quad \nabla^2 \Psi = \frac{1}{v^2} \frac{\partial^2 \Psi}{\partial t^2} \text{-----(2)}$$

The solution of equation (2) becomes

$$\Psi(x, y, z, t) = \Psi_0(x, y, z)e^{-i\omega t} \text{-----(3)}$$

Differentiating (3) twice w.r.t time 't'

$$\frac{\partial \Psi}{\partial t} = -i \Psi_0 e^{-i\omega t}$$

$$\frac{\partial^2 \Psi}{\partial t^2} = (-i\omega)(-i\omega)\Psi_0 e^{-i\omega t} \text{-----(4)}$$

$$\frac{\partial^2 \Psi}{\partial t^2} = -\omega^2 \Psi \text{-----(5)}$$

Substitute (5) in (2)

$$\nabla^2 = -\frac{1}{v^2}(\omega^2 \psi)$$

$$\nabla^2 = -\frac{\omega^2}{v^2} \psi \text{-----(6)}$$

w.k.t

$$\omega = 2\pi\nu \quad ; \text{ but } v = \nu\lambda$$

$$\omega = 2\pi\frac{\nu}{\lambda} \quad \nu = \frac{v}{\lambda}$$

$$\frac{\omega}{v} = \frac{2\pi}{\lambda}$$

$$\frac{\omega^2}{v^2} = \frac{4\pi^2}{\lambda^2} \text{-----(7)}$$

Sub (7) in (6)

$$\nabla^2 \psi = -\frac{4\pi^2}{\lambda^2} \psi$$

$$\nabla^2 \psi + \frac{4\pi^2}{\lambda^2} \psi = 0 \text{-----(8)}$$

$$\text{According to De-Broglie's theory } \lambda = \frac{h}{mv} \text{-----(9)}$$

Where m - mass of particle

v - velocity

sub (9) in (8)

$$\nabla^2 \psi + \frac{4\pi^2}{\left(\frac{h}{mv}\right)^2} \psi = 0$$

$$\nabla^2 \psi + \frac{4\pi^2 v^2 m^2}{h^2} \psi = 0 \text{-----(10)}$$

Taking $\hbar = \frac{h}{2\pi}$; $\frac{1}{\hbar} = \frac{2\pi}{h}$

$$\frac{1}{\hbar^2} = \frac{4\pi^2}{h^2} \text{-----(11)}$$

Sub (11) in (10)

$$\nabla^2 \psi + \frac{v^2 m^2}{h^2} \psi = 0 \text{-----(12)}$$

Total Energy $E = V + \frac{1}{2}mv^2$

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

Multiply 'm' on both sides

$$2m(E-V) = m^2 v^2 \text{-----(13)}$$

Sub (13) in (12)

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

This is the final expression of Schrodinger time independent wave equation.

4.5.2 Schrodinger Time dependent wave equation:

The differential equation for wave motion is given by

$$\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} = \frac{1}{v^2} \frac{\partial^2 \Psi}{\partial t^2}$$

$$\nabla^2 \Psi = \frac{1}{v^2} \frac{\partial^2 \Psi}{\partial t^2} \text{-----(1)}$$

The solution of equation (1) becomes

$$\Psi(x, y, z, t) = \Psi_0(x, y, z)e^{-i\omega t} \text{-----(2)}$$

Differentiating (2) twice w.r.t time 't'

$$\frac{\partial \Psi}{\partial t} = -i \Psi_0 e^{-i\omega t}$$

$$\frac{\partial \Psi}{\partial t} = (-i \omega \Psi) \text{-----(3)}$$

w.k.t

$$\omega = 2\pi\nu \quad ; \text{ but } E = h\nu \quad ; \quad \nu = \frac{E}{h}$$

$$\omega = 2\pi \frac{E}{h} \text{-----(4)}$$

Substitute (4) in (3)

$$\frac{\partial \Psi}{\partial t} = \frac{-i2\pi E\Psi}{h} = \frac{-i2\pi E\Psi}{ih} \text{ (multiply \& divide by i)}$$

$$\frac{\partial \Psi}{\partial t} = \frac{-2\pi E \Psi}{ih} = \frac{E \Psi}{i\hbar}$$

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

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

Substitute $E \Psi$ in time independent wave equation

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

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

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

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

$$\frac{-\hbar^2}{2m} \nabla^2 + V\Psi = E\Psi \text{-----(6)}$$

Substitute (5) in (6)

$$\frac{-\hbar^2}{2m} \nabla^2 + V\Psi = i\hbar \frac{\partial \Psi}{\partial t} \text{-----(7)}$$

$$\left[\frac{-\hbar^2}{2m} \nabla^2 + V \right] \Psi = i\hbar \frac{\partial \Psi}{\partial t} \text{-----(8)}$$

(8) is the Schrodinger Time dependent wave equation

Here

$$\text{Hamiltonian operator } H = \left[\frac{-\hbar^2}{2m} \nabla^2 + V \right]$$

$$\text{Energy operator } E = i\hbar \frac{\partial \Psi}{\partial t}$$

$$(8) \text{ gives } H \Psi = E \Psi$$

