

- Schrödinger's Equations:

1- Time – dependent Schrödinger equation (TDSE):

A free particle moving along x- axis with a defined momentum is described by the an infinite plane wave

$$\Psi (x, t)=A e^{i(K_x x-\omega t)} \quad \dots\dots\dots (1)$$

$$K_x=\frac{p_x}{\hbar} \quad \text{and} \quad \omega = \frac{E}{\hbar} \quad \dots\dots\dots (2)$$

$$K = \frac{2\pi}{\lambda} = \frac{2\pi}{h/p} = \frac{2\pi p}{h} = \frac{p}{\hbar}$$

$$\omega = 2\pi\nu, \quad E = h\nu, \quad \nu = \frac{E}{h}$$

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

Substituting Eqn. (2) in (1) we get:

$$\Psi (x, t)=A e^{\frac{i}{\hbar}(p_x x-Et)} \quad \dots\dots\dots (3)$$

Differentiation of Eqn. (3) with respect to time gives:

$$\frac{\partial \Psi}{\partial t} = A e^{\frac{i}{\hbar}(p_x x-Et)} \cdot \left(-\frac{i}{\hbar} E \right)$$

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

بالضرب في $i\hbar$

$$i\hbar \frac{\partial \Psi}{\partial t} = E \Psi (x, t) \quad \dots\dots\dots (4)$$

Successive differentiation of Eqn. (3) with respect to x leads to:

$$\frac{\partial \Psi}{\partial x} = A e^{\frac{i}{\hbar}(p_x x-Et)} \cdot \left(\frac{i}{\hbar} p_x \right)$$

$$\frac{\partial \Psi}{\partial x} = \frac{i}{\hbar} p_x \Psi(x, t)$$

بالمضرب في $-i\hbar$

$$-i\hbar \frac{\partial \Psi}{\partial x} = p_x \Psi(x, t) \dots\dots\dots 5$$

$$\frac{\partial^2 \Psi}{\partial x^2} = A e^{\frac{i}{\hbar}(p_x x - Et)} \cdot \left(\frac{i}{\hbar} p_x\right) \cdot \left(\frac{i}{\hbar} p_x\right)$$

$$\frac{\partial^2 \Psi}{\partial x^2} = -\frac{p_x^2}{\hbar^2} \Psi(x, t)$$

بضرب الطرفين بالمقدار $-\frac{\hbar^2}{2m}$

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} = \frac{p_x^2}{2m} \Psi(x, t) \dots\dots\dots 6$$

Classically for a free nonrelativistic particle

$$E = \frac{p_x^2}{2m} + V(x, t) \dots\dots\dots 7$$

Hence from Eqns. (4) and (7) we may write:

$$i\hbar \frac{\partial \Psi}{\partial t} = E \Psi(x, t) = \left[\frac{p_x^2}{2m} + V(x, t) \right] \Psi(x, t)$$

$$= \frac{p_x^2}{2m} \Psi(x, t) + V(x, t) \Psi(x, t)$$

Substituting Eqn. (6) in above Eqn. we get:

$$\therefore \boxed{i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V(x, t) \Psi(x, t)} \dots\dots\dots 8$$

Eqn. (8) is the **1-dimensional time-dependent Schrödinger equation**. For a free particle, $V(x, t) = 0$

In 3- dimensions Eqn. (8) becomes:

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi + V(r, t) \Psi(r, t) \dots\dots\dots 9$$

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

The operator for the Hamiltonian (H) of the system is:

$$H = -\frac{\hbar^2}{2m} \nabla^2 + V(r, t)$$

Hence Eqn. (9) can be written in the form:

$$i\hbar \frac{\partial \Psi}{\partial t} = H \Psi(r, t) \dots\dots\dots 10$$

So eqns. (4) and (5) written in the form

$$\begin{aligned} (i\hbar \frac{\partial}{\partial t}) \Psi &= E \Psi & \therefore E &= i\hbar \frac{\partial}{\partial t} \\ (-i\hbar \frac{\partial}{\partial x}) \Psi &= p_x \Psi & \therefore p_x &= -i\hbar \frac{\partial}{\partial x} \end{aligned}$$

In 3 – dimensions

$$E = i\hbar \frac{\partial}{\partial t} \quad \text{and} \quad p = -i\hbar \nabla$$