Schrodinger's Wave Equation:

We expect the wave function to describe the dynamical state of a system (or a particle). Since, Ψ is a wave amplitude (Probability amplitude) and we have seen that Ψ is expected to have a role similar to standing waves. It is, therefore, required to have wave equation for the wave function $\Psi(x, y, z, t)$. It was the genius of Erwin Schrödinger who utilized this idea and proposed an equation called Schrodinger's Wave Equation in 1926. This equation is fundamental in quantum mechanics as Newton's equation of motion in classical mechanics and Maxwell's equation in electromagnetism.

Schrodinger's time independent Wave Equation:

According to de-Broglie theory, a particle of mass 'm' is always associated with a wave. If the particle has wave properties, it is expected that there should be some sort of wave equation which describes the behavior of the particle. Consider a system of stationary waves associated with a particle. Let x, y, z be the coordinates of the particle and Ψ, the wave displacement for the de Broglie at any time *t*.

Schrodinger decided that if electron or any particle is expected to show wave nature, its wave equation also should be similar to the general wave equation (similar for water waves wind waves or any waves), which is written as follows.

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

Where, $\Psi -$ is amplitude of waves; $v -$ is velocity of waves; $t -$ is time.

$$\Psi = \Psi_0 e^{-i\omega t} ----2$$

Eqn 2, is the general solution of the wave equation, which is eqn 1.

If we include electron's (or particle's) parameters such as wavelength, mass, momentum, total energy, potential energy etc., in the general wave equation then we can call it as the wave equation of electron (or of any particle).

For that purpose, if we differentiate wave function $\Psi = \Psi_0 e^{-i\omega t}$, two times with respect to time, then we can replace $\frac{\partial^2\Psi}{\partial t^2}$ term in the general wave equation. Now we will have (particle's) ω^2also in the general wave equation.

$$\frac{\partial\Psi}{\partial \mathrm{t}} = \Psi_0 e^{-i\omega t} \times (-i\omega)$$

$$= -i\omega\Psi$$

$$\frac{\partial^2\Psi}{\partial t^2} = -\omega^2\Psi$$

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

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

$$\nabla^2\Psi = -\frac{\omega^2}{v^2}\Psi$$

Now we have chance to include electron's wavelength as follows,

$$\omega = 2\pi\vartheta = 2\pi(v/\lambda) \qquad [\because \vartheta = v/\lambda]$$

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

$$\nabla^2\Psi + \frac{4\pi^2}{\lambda^2}\Psi = 0$$

Based on De broglie's suggestion wavelength of particle is correlated with its momentum as follows,

$$\lambda = \frac{\mathrm{h}}{\mathrm{mv}}$$

$$\nabla^2\Psi + \frac{4\pi^2 \mathrm{m}^2 \mathrm{v}^2}{\mathrm{h}^2}\Psi = 0$$

After looking at m^2v^2, term we find that we have chance to include Kinetic, potential and total energies of the particle as follows,

$$\text{E (e}^{-}\text{s total energy)} = \text{V (potential energy)} + \frac{1}{2}\text{mv}^2\text{(kinetic energy)}$$

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

$$E - V = \frac{1}{2}mv^2$$

$$E - V = \frac{1}{2}mv^2$$

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

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

$\nabla^2\Psi + \frac{8\pi^2 m}{h^2}(E - V)\Psi = 0$ (Schrodinger's time independent equation for electron or any particle)

$$\nabla^2\Psi + \frac{2m}{\hbar^2}(E - V)\Psi = 0; \rightarrow\rightarrow\rightarrow \quad \left[\because \hbar = \frac{h}{2\pi}\right]$$

$$\text{For a free particle, as } V = 0;\ \text{thus,} \quad \nabla^2\Psi + \frac{2mE}{\hbar^2}\Psi = 0$$

Schrödinger's time independent equation can also be expressed in the following way,

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

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

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

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

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

$$\hat{H}\,\Psi = \boldsymbol{E}\,\Psi$$

Here, $\hat{H} = \left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)$ is known as Hamiltonian Operator

For a one dimensional motion, the Schrodinger time independent equation is as follows,

$$\frac{d^2\Psi}{dx^2} + \frac{8\pi^2 m}{h^2}(E - V)\Psi = 0$$

<u>Schrodinger's time dependent Wave Equation:</u>

If the time independent wave equation is included with the parameter, then that equation will become a time dependent one. By eliminating E in the Schrodinger's time independent Wave Equation, we can easily get the Schrodinger time dependent wave equation. Keeping that in mind, we notice that the first order differentiation of $\Psi = \Psi_0 e^{-i\omega t}$, will include ω term as follows,

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

Here we have chance to write ω term in terms of E as follows

$$= -(i2\pi\vartheta)\Psi_0 e^{-i\omega t} = -(i2\pi\vartheta)\Psi; \rightarrow\rightarrow\rightarrow \quad [\because \omega = 2\pi\vartheta]$$

$$= -\left(i2\pi\frac{E}{h}\right)\Psi; \rightarrow\rightarrow\rightarrow \quad [\because E = h\vartheta \text{ or } \vartheta = E/h]$$

$$= -i\frac{E}{\hbar}\Psi; \rightarrow\rightarrow\rightarrow \quad \left[\because \hbar = \frac{h}{2\pi}\right]$$

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

Now we have chance to include $\frac{\partial\Psi}{\partial t}$, term which contain time factor by replacing EΨ, in the time independent wave equation. Then finally we are able to write the time dependent Schrodinger's wave equation as follows,

$$\nabla^2\Psi + \frac{2m}{\hbar^2}\left(i\hbar\frac{\partial\Psi}{\partial t} - V\Psi\right) = 0$$

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

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

$\left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\Psi = i\hbar\frac{\partial\Psi}{\partial t}$ (Schrodinger's time dependent equation for electron or any particle)

where $\left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)$ is called as Hamiltonian operator and its symbol is H and $E\Psi = i\hbar\frac{\partial\Psi}{\partial t}$ is called energy operator. Then we can write the Schrodinger's time dependent wave equation as follows,

$$H\Psi = E\Psi$$