Engineering Physics

(PHY1701)

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- Wave function (AB 182-184 & 190-195), &
- **Schrödinger equation (time dependent & independent)** (AB 187 -190 & 195-197).

❖ Concepts of Modern Physics, Arthur Beiser et al., Sixth Edition, Tata McGraw Hill (2013) (AB)

Introduction of Schroedinger's Wave Equation

- Classical mechanics fails to explain the microscopic system of particles due to uncertainty principle.
- Therefore, classical mechanics, which assumed both the entities have definite values at all instants – not valid for atomic systems.
- According to de Broglie theory, a material particle is associated with a matter wave ; $\lambda = h/mv$
- So, finally, Schroedinger did mathematical reformation using a wave function associated with matter waves.
- Schroedinger described the amplitude of matter wave by $\Psi(x,y,z,t)$ known as wave function or state of the system.

[Erwin Schrödinger]

Schroedinger's Time independent Wave Equation

- Let us consider a particle of mass m, moving with a velocity v associated with standing waves.
- Let Ψ be the wave function of a particle along x, y, and z coordinate axes at time t.
- The classical differential equation of a progressive wave, moving with a wave velocity v can be given by,

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

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

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

- 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).

Time independent Wave Equation

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

$$= -i\omega\Psi$$

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

Now we will have (particle's) ω^2also in the general wave equation. Substituting these value in Equation 1 we get,

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

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

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

Time independent Wave Equation

Now we can include electron's wavelength as follows,

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

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

If we substitute in this equation, $\nabla^2\Psi = -\frac{\omega^2}{v^2}\Psi$

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

According to de Broglie wave equation,

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

$$\nabla^2\Psi + \frac{4\pi^2\mathrm{m}^2\mathrm{v}^2}{\mathrm{h}^2}\Psi = 0 \text{--------- eq. 3}$$

Time independent Wave Equation

- If we consider the $\mathbf{m^2v^2}$ term, we can include Kinetic, potential and total energies of the particle as follows,

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

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

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

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

$$2(\text{E} - \text{V}) = \text{mv}^2$$

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

$$\boxed{\nabla^2\Psi + \frac{8\pi^2\text{m}}{\text{h}^2}(\text{E} - \text{V})\Psi = 0} \text{ -------- eq. 4}$$

(Shroedinger's time independent equation for electron or any particle)

Time independent Wave Equation

$$\left[\because \hbar = \frac{h}{2\pi}\right] \quad \nabla^2\Psi + \frac{2m}{\hbar^2}(E - V)\Psi = 0; \quad \text{---------- eq. 5}$$

For a free particle, V=0, thus,

$$\boxed{\nabla^2\Psi + \frac{2mE}{\hbar^2}\Psi = 0}$$

(Shroedinger's time independent equation for free particle)

Eq. 8 can also be expressed in the following way,

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

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

Time independent Wave Equation

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

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

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

$$\boxed{\hat{\mathbf{H}}\,\Psi = \mathbf{E}\,\Psi}$$

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

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

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

Schroedinger's Time dependent Wave Equation

Schrodinger's time dependent equation may be obtained from time independent equation by eliminating the term E.

$$\Psi = \Psi_0 e^{-i\omega t} \quad \text{------- eq. 1}$$

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

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

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

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

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

$$E\Psi = i\hbar\frac{\partial \Psi}{\partial t} \quad \text{------- eq. 2}$$

Wave Function

Substituting the value of E Ψ in Schrodinger time independent eq., we get

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

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

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

$$\boxed{\left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\Psi = i\hbar\frac{\partial\Psi}{\partial t}} \quad \text{------- eq. 3}$$

(Shroedinger's time dependent equation for any particle)

Equation 4 can be written as,

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

$$\boxed{\hat{\mathbf{H}}\,\Psi = \mathbf{E}\,\Psi}$$

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

- The connection to the Schrodinger equation can be made by examining wave and particle expressions for energy:

$$\frac{1}{2}mv^2 = \frac{p^2}{2m} \xleftarrow{\text{particle}} E \xrightarrow{\text{wave}} h\nu = \hbar\omega$$

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