

The origin of Schrodinger equation

Total energy

*= Kinetic Energy(KE)
+ Potential energy (V)*

$$E = KE + V \dots \dots \dots (3.1)$$

$$KE = \frac{1}{2} mv^2 = \frac{m^2v^2}{2m} = \frac{P^2}{2m}$$

$$\therefore E = \frac{P^2}{2m} + V \text{ and } E\psi$$

$$= \frac{P^2}{2m} \psi + V\psi \dots \dots (3.2)$$

- $\psi = e^{\frac{i}{\hbar}(xp_x - Et)}$
- $\frac{\partial \psi}{\partial x} = \frac{i}{\hbar} p_x e^{\frac{i}{\hbar}(xp_x - Et)}$
- $\frac{\partial \psi}{\partial x} = \frac{i}{\hbar} p_x \psi$
- $\frac{\partial^2 \psi}{\partial x^2} = \left(\frac{i}{\hbar} p_x\right)^2 \psi = -\frac{p_x^2}{\hbar^2} \psi$
- $\therefore p_x^2 = -\hbar^2 \frac{\partial^2}{\partial x^2}$ *sub. in (3.2)*

$$E\psi = \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi + V\psi \quad \text{Time Independent Schrodinger}$$

Equation (TISE)

- $\psi = e^{\frac{i}{\hbar}(xp_x - Et)}$ *wavefunction*
- $\frac{\partial \psi}{\partial t} = \frac{-i}{\hbar} E e^{\frac{i}{\hbar}(xp_x - Et)}$
- $\frac{\partial \psi}{\partial t} = \frac{-i}{\hbar} E \psi$
- $-\frac{\hbar}{i} \frac{\partial \psi}{\partial t} = E \psi$
- $\therefore E_{op} = -\frac{\hbar}{i} \frac{\partial}{\partial t}$
- $E_{op} = i\hbar \frac{\partial}{\partial t}$
- $\therefore -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V\psi = i\hbar \frac{\partial \psi}{\partial t} \dots\dots(3.3)$
- Time Dependent Schrodinger equation (TDSE)

- ***Test your understanding**
- start with $E = \hbar\omega$ to find TDSE
- Then we have different formula of Schrodinger equation(S.E.)
- $-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V\psi = E\psi$ (TISE) in one dimension (1DTISE)
- $-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V\psi = i\hbar \frac{\partial \psi}{\partial t}$ (TDSE) in on dimension
- $-\frac{\hbar^2}{2m} \nabla^2 \psi_{(x,y,z)} + V\psi(x, y, z) = E\psi(x, y, z)$ (3DTISE)
- $-\frac{\hbar^2}{2m} \nabla^2 (x, y, z, t) + V\psi(x, y, z, t) = i\hbar \frac{\partial \psi}{\partial t}$ (3D.TDSE)
- The simplest formula of S.E. is:
- $H\psi = E\psi$
- $H = T = KE + V$
- H : Hamiltonian

- **3.2 Probability current Density**

- The idea of probability current comes from the multiplication (product)
- of $\dot{\psi}^*(x, t)\psi(x, t)$
- This relation leads to the term of probability current, if we examine the principles of classical physics, we can find the concepts of density and of current.
- The change in the electrical charge density with time within a certain is zone leading to transfer the electrical current outside the surrounding surface and the same concept is applied on material, heat,.....etc.

- $-\frac{d\rho}{dt} = \frac{ds}{dx} \dots \dots \dots (3.4)$

- Where ρ is the density of the electrical charge, t is time, S is the output current and x is the surrounding surface. However the negative (-) sign means decreasing the density inside the enclosure volume.
- This idea can be generalized to the principle of probability density of quantum mechanics.
- Let $\psi(x, t)$ is the variation with time and the probability density $-\frac{d\rho}{dt}$ variation with time, the probability density reducing with time, this agrees

- with equation(3.4) then the leakage current is found and to describe this leakage starting by Schrodinger equation.

- $$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + v(x)\psi = -\frac{\hbar}{i} \frac{d\psi}{dt} \dots \dots \dots (3.5)$$

- And the conjugate equation

- $$-\frac{\hbar^2}{2m} \frac{d^2\psi^*}{dx^2} + v(x)\psi^* = \frac{\hbar}{i} \frac{d\psi^*}{dt} \dots \dots \dots (3.6)$$

- Multiple equation (3.5) by ψ^* & equation (3.6) by ψ and Subtract them

- we will get the following

- $$-\frac{\hbar^2}{2m} \left(\psi^* \frac{d^2\psi}{dx^2} - \psi \frac{d^2\psi^*}{dx^2} \right) = \frac{\hbar}{i} \left(\dot{\psi}^* \frac{d\psi}{dt} + \psi \frac{d\dot{\psi}^*}{dt} \right)^*$$
- $$-\frac{\hbar}{2} \left[mi \frac{d}{dx} \left(\psi^* \frac{d\psi}{dx} - \psi \frac{d\psi^*}{dx} \right) \right] = \frac{d}{dt} (\dot{\psi}^* \psi) \dots (3.7)$$

- By comparing equation(3.7) and equation (3.4) we can conclude that the term $\psi^* \psi$ representing the probability density and corresponding to ρ .
- Thus, the probability current density equation can be written in the following form .S

$$= -\frac{\hbar}{2m\lambda} \left[\psi^* \frac{d\psi}{dx} - \psi \frac{d\psi^*}{dx} \right] \dots \dots \dots (3.8)$$
- Equation (3.8) is called continuous equation ; by using the above equation can be determine the current probability density for any wave equation or wave function.

- **3.3 Applications of Schrodinger equation**

- **3.3.1 Free particle**

- Free particle means no force effect on particle then the potential energy is equal to =zero.

- $$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V\psi = E\psi \text{ TISE....(A)}$$

- $$V = -\int_{x_1}^{x_2} Fdx = 0, \text{ since } F = 0$$

- The TISE

- $$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = E\psi \dots \dots \dots \dots \dots \dots (B)$$

- $\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0 \dots\dots\dots (C)$
- $E = T + V$ & $T = \frac{P^2}{2m}, v = 0$
- Then
- $p^2 = 2mE, P = \hbar k$
- $\hbar^2 k^2 = 2mE$
- $\therefore k^2 = \frac{2mE}{\hbar^2}$ sub in eq (C)
- $\frac{d^2\psi}{dx^2} + k^2 \psi = 0$

- $\frac{d^2\psi}{dx^2} + k^2 \psi = 0$
- The solution :
- $\psi = Ae^{ikx}$ represents the particle that is move to the right side, with momentum equals $P = \hbar k$.
- $\psi_{(x)} = Be^{-ikx}$ represents the particle that is moved to the left side, with momentum equals $P = \hbar k$.
- The probability Density of free particle at any point equals
- $\psi^*_{(x)}\psi_{(x)} = A^* e^{ikx} Ae^{-ikx} = A^* A = \text{Constant}$
- The probability density of free particle in any point equals to the P.D. in any other points this means the uncertainty $\Delta x = \infty$. The result agrees with the Heisenberg uncertainty principle.

- The particle moved with the momentum of $P = \hbar k$ means $\Delta P = 0$
- $\Delta x \cdot \Delta P \geq \hbar$
- $\Delta x = \infty$ when $\Delta P_x = 0$

Thank You For Listening