

11/11/24

Time dependent SE :-

(V = potential energy)

(i) 1-D

along x axis :
$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \left(\frac{\partial^2 \psi}{\partial x^2} \right) + (V\psi)$$

along y axis :
$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \left(\frac{\partial^2 \psi}{\partial y^2} \right) + (V\psi)$$

along z axis :
$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \left(\frac{\partial^2 \psi}{\partial z^2} \right) + (V\psi)$$

(ii) 2-D

along xy plane :
$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} \right) + V\psi$$

along yz plane :
$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \left(\frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} \right) + V\psi$$

along zx plane :
$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \left(\frac{\partial^2 \psi}{\partial z^2} + \frac{\partial^2 \psi}{\partial x^2} \right) + V\psi$$

(iii) 3-D

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} \right) + V\psi$$

(or)

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

For free particle $V = 0$

Time independent SE :-

(E - total energy)

(i) 1D

along x axis:
$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2m}{\hbar^2} (E - V) \psi = 0$$

along y axis:
$$\frac{\partial^2 \psi}{\partial y^2} + \frac{2m}{\hbar^2} (E - V) \psi = 0$$

along z axis:
$$\frac{\partial^2 \psi}{\partial z^2} + \frac{2m}{\hbar^2} (E - V) \psi = 0$$

(ii) 2D

along xy plane:
$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{2m}{\hbar^2} (E - V) \psi = 0$$

along yz plane:
$$\frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} + \frac{2m}{\hbar^2} (E - V) \psi = 0$$

along xz plane:
$$\frac{\partial^2 \psi}{\partial z^2} + \frac{\partial^2 \psi}{\partial x^2} + \frac{2m}{\hbar^2} (E - V) \psi = 0$$

(iii) 3D

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} + \frac{2m}{\hbar^2} (E - V) \psi = 0$$

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

for free particle: $V = 0$

Applications of Schrodinger Wave Equation :-

- (i) 1-Dimensional potential step
- (ii) 1-Dimensional potential well or particle in a box
- (iii) potential barrier

All applications are based on time independent SE in 1-Dimensional.

1. Potential STEP :-

When 2 regions are separated by a potential then it constitutes a potential step problem.

for $E > V$

the potential distribution for V the step problem

$V(x) = 0, x < 0$, Region-I

$V(x) = V_0, x > 0$, Region-II

Region-I

Region-II
 $V = V_0$

$V = 0$

The Schrodinger Equations are :

$$1. \frac{\partial^2 \psi}{\partial x^2} + \frac{2mE}{\hbar^2} \psi = 0, \text{ Region - I} \quad \text{--- (2)}$$

$$2. \frac{\partial^2 \psi}{\partial x^2} + \frac{2m(E - V_0)}{\hbar^2} \psi = 0, \text{ Region - II} \quad \text{--- (3)}$$

$$\left. \begin{aligned} \text{let } \frac{2mE}{\hbar^2} &= k_1^2 \Rightarrow k_1 = \frac{\sqrt{2mE}}{\hbar} \\ \frac{2m(E - V_0)}{\hbar^2} &= k_2^2 \Rightarrow k_2 = \frac{\sqrt{2m(E - V_0)}}{\hbar} \end{aligned} \right\} \text{--- (4)}$$

$$\therefore \frac{\partial^2 \psi_1}{\partial x^2} + k_1^2 \psi_1 = 0 \text{ and } \frac{\partial^2 \psi_2}{\partial x^2} + k_2^2 \psi_2 = 0 \quad \text{--- (5)}$$

The solⁿ of Eqⁿ (5) is given by,

$$\left. \begin{array}{l} \text{Reg-I, } \psi_1 = A e^{ik_1 x} + B e^{-ik_1 x} \\ \text{Reg-II, } \psi_2 = C e^{ik_2 x} + \boxed{D e^{-ik_2 x}} \end{array} \right\} \quad (6)$$

↓
not valid

$\psi_i = \text{incident wave} = A e^{ik_1 x}$

$\psi_r = \text{reflected wave} = B e^{-ik_1 x} \quad (7)$

$\psi_t = \text{transmitted} = C e^{ik_2 x}$

Reflection co-efficient - (R_c)

It is defined as the no. of particles reflect,

$$R_c = \frac{[\sqrt{E} - \sqrt{E - V_0}]^2}{[\sqrt{E} + \sqrt{E - V_0}]^2} \quad (8)$$

Transmission coefficient - (T_c)

It is defined as the no. of particles transmitted into the second region.

$$T_c = \frac{4\sqrt{E} \times \sqrt{E - V_0}}{[\sqrt{E} + \sqrt{E - V_0}]^2} \quad (9)$$

$$\boxed{R_c + T_c = 1}$$

This shows the $E > V_0$ then according to quantum ~~mechanics~~ mechanics few particles are reflected or few particles are transmitted.

Q. Let in a step problem, $E = 16 \text{ eV}$, $V_0 = 7 \text{ eV}$ find R_c and T_c .

$$R_c = \frac{(\sqrt{16} - \sqrt{16-7})^2}{(\sqrt{16} + \sqrt{16-7})^2} = \frac{(4-3)^2}{(4+3)^2} = \frac{1}{49} = 0.02 \approx 2\%$$

$$T_c = 1 - R_c = 1 - 0.02 = 0.98 \approx 98\%$$

Q. $E = 25 \text{ eV}$, $V_0 = 9 \text{ eV}$

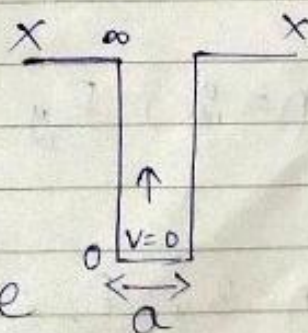
$$R_c = \frac{(\sqrt{25} - \sqrt{25-9})^2}{(\sqrt{25} + \sqrt{25-9})^2} = \frac{(5-4)^2}{(5+4)^2} = \frac{1}{81} = 0.01 \approx 1\%$$

$$T_c = 1 - R_c = 1 - 0.01 = 99\%$$

2. Potential Well - (a particle in a box) :-
When a particle is trapped by infinite barriers then it constitutes a potential well problem.

Potential distribution is given by

$$V(x) = 0, \quad 0 < x < a \quad \text{--- (1)}$$



The Schrodinger eqⁿ for the particle in the well is given by

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2mE}{\hbar^2} \psi = 0 \quad \text{--- (2)}$$

$$\text{let } k = \frac{\sqrt{2mE}}{\hbar} \quad \text{--- (3)}$$

$$\therefore \frac{\partial^2 \psi}{\partial x^2} + k^2 \psi = 0 \quad \text{--- (4)}$$

$$\text{Sol}^n \quad \psi = Ae^{ikx} + Be^{-ikx}$$

$$\text{or } \psi = C \sin kx + D \cos kx \quad \text{--- (5)}$$

For boundary - I, $x=0 \Rightarrow \psi=0 \Rightarrow D=0$

$$\psi = C \sin kx$$

boundary II, $x=a, \psi=0 \Rightarrow \sin ka = 0 \Rightarrow \sin n\pi$

$$ka = n\pi$$

$$\Rightarrow k^2 a^2 = n^2 \pi^2$$

$$\Rightarrow \frac{2mE}{\hbar^2} a^2 = n^2 \pi^2$$

$$\Rightarrow E_n = \frac{n^2 \hbar^2 \pi^2}{2ma^2} \quad (\because n = 1, 2, \dots)$$

Where a = width of the well

For $n=1, E_1 = \frac{\hbar^2 \pi^2}{2ma^2} \rightarrow \text{ground state energy}$

$n=2, E_2 = 4E_1 \rightarrow 1^{\text{st}} \text{ Excited state energy}$

$n=3, E_3 = 9E_1 \rightarrow 2^{\text{nd}} \text{ Excited state energy}$

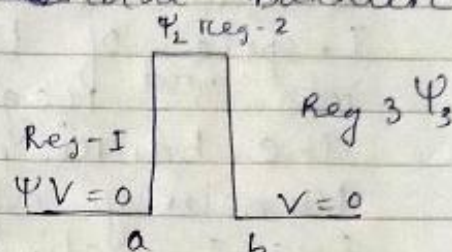
Potential Barrier :-

when 2 regions are separated by a barrier then it constitutes a potential barrier problem.

$$V(x) = 0, x < 0$$

$$V(x) = V_0, 0 < x < b$$

$$V(x) = 0, x > b$$



For $E < V_0$

Here energy is less and potential is high. The Schrodinger Equations are :-

$$\text{Reg-I} = \frac{\partial^2 \Psi_1}{\partial x^2} + \frac{2mE}{\hbar^2} \Psi_1 = 0$$

$$\text{Reg-II} = \frac{\partial^2 \Psi_2}{\partial x^2} - \frac{2m(V_0 - E)}{\hbar^2} \Psi_2 = 0$$

$$\text{Reg-III} = \frac{\partial^2 \Psi_3}{\partial x^2} + \frac{2mE}{\hbar^2} \Psi_3 = 0$$

Solⁿ - $\Psi_1 = A e^{ikx} + B e^{-ikx}$
 $\Psi_2 = C e^{\alpha x} + D e^{-\alpha x}$
 $\Psi_3 = F e^{ikx} + \boxed{G e^{-ikx}} \rightarrow \text{not valid}$

Transmission probability / Flux :-

$$\boxed{T_c = e^{-2\alpha b}}$$

$$\alpha = \frac{2m}{\hbar^2} (V_0 - E)$$

b = width of barrier

Conclusion :-

Quantum Tunneling :-

In spite of low energy particles transmits into 3rd region by making tunnels in the barrier this phenomenon is called tunneling effect.

Ex:- Tunneling diodes, tunneling microscopes, Josephson diode.