

## Particle in a box (Infinite Square well Potential):

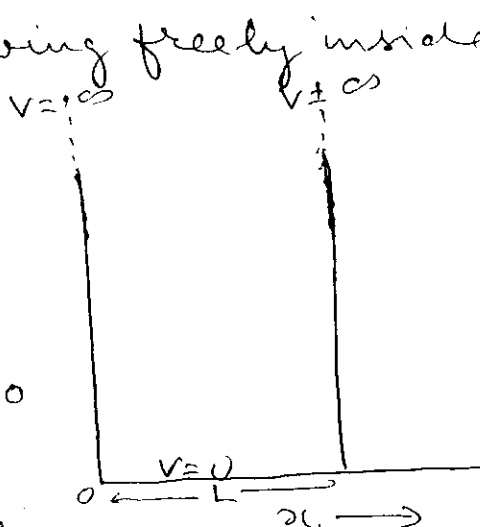
Consider a particle moving freely inside a box along  $x$ -axis

$L$  = length of the box

for  $x > 0$  and  $x < L$   $V = 0$

$\Rightarrow V = 0$  for  $0 < x < L$

and  $V = \infty$  for  $x > L$  and  $x \leq 0$



This means that particle cannot exist outside the box

$\therefore$  outside the box  $\psi = 0$

and inside the box

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2m}{\hbar^2} E \psi = 0 \quad \text{--- (1)}$$

$$\frac{\partial^2 \psi}{\partial x^2} + K^2 \psi = 0 \quad \text{--- (2) where } K^2 = \frac{2mE}{\hbar^2} \Rightarrow K = \frac{\sqrt{2mE}}{\hbar} \quad \text{--- (3)}$$

General solution of this = n is

$$\psi = A \sin Kx + B \cos Kx \quad \text{--- (4)}$$

Using boundary conditions

$$\psi = 0 \text{ at } x = 0 \Rightarrow 0 = B.$$

$$\Rightarrow \psi = A \sin Kx \quad \text{--- (5)}$$

Also  $\psi = 0$  at  $x = L$

$$\Rightarrow 0 = A \sin KL$$

Since  $\psi$  is finite  $A \neq 0$

$$\therefore \sin KL = 0 = \sin n\pi \quad n = 1, 2,$$

$$KL = n\pi$$

$$K = \frac{n\pi}{L} \quad \text{--- (6)}$$

$$\therefore (3) \& (6) \Rightarrow \frac{n^2 \pi^2}{L^2} = \frac{2mE}{\hbar^2}$$

$$E_n = \frac{n^2 \hbar^2 \pi^2}{2mL^2} = \frac{n^2 h^2}{8mL^2}$$

$$E_n = \frac{n^2 h^2}{8mL^2} \quad \text{--- (7)}$$

$n = 1, 2, 3, \dots$

This shows that particle inside a box can have only discrete energies  $\frac{h^2}{8mL^2}$ ,  $\frac{4h^2}{8mL^2}$ ,  $\frac{9h^2}{8mL^2}$  ...

Each permitted energy is called energy eigen value. of the particle and constitutes energy level. corresponding function is called energy eigen function

$$\Psi_n = A \sin \frac{n\pi x}{L} \quad \left( \because k = \frac{n\pi}{L} \right)$$

To find A, let us apply normalisation condition

$$\int_{-\infty}^{+\infty} |\Psi_n|^2 dx = 1 \Rightarrow \int_0^L |\Psi_n|^2 dx = 1$$

$$\Rightarrow A^2 \int_0^L \sin^2 kx dx = 1$$

$$\Rightarrow A^2 \int_0^L \frac{(1 - \cos 2kx)}{2} dx = 1.$$

$$\Rightarrow \frac{A^2}{2} \int_0^L 1 dx - \frac{A^2}{2} \int_0^L \cos 2kx dx = 1$$

$$\Rightarrow \frac{A^2 L}{2} - \frac{A^2}{2} \left| \frac{\sin 2 \frac{n\pi x}{L}}{2k} \right|_0^L = 1 \Rightarrow \frac{A^2 L}{2} - 0 = 1$$

$$\Rightarrow \frac{A^2 L}{2} = 1$$

$$\Rightarrow A = \sqrt{\frac{2}{L}}$$

$$\therefore \underline{\underline{\Psi_n = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}}}$$

Although  $\Psi_n$  may be +ve or -ve  $|\Psi_n|^2$  is always +ve. Also since  $\Psi_n$  is normalised, its value at a given  $x$  gives the probability density of finding the particle there.