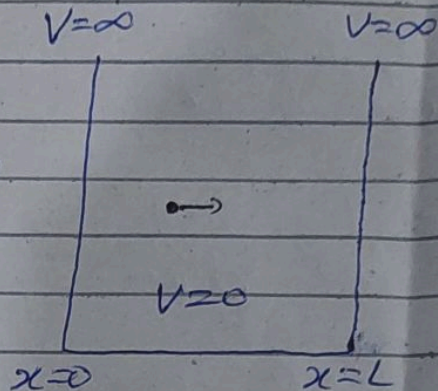


Schrodinger Wave equation for a particle in one-dimensional Box

Consider a particle that is constrained to move only in  $x$  direction from  $x=0$  to  $x=L$



Schrodinger wave eq: in operator form

$$\hat{H}\psi = E\psi \rightarrow \textcircled{1}$$

( $\hat{H}$  = hamiltonian operator in  $x$ -direction)

$$\hat{H} = \frac{-\hbar^2}{8\pi^2 m} \frac{d^2}{dx^2} + V$$

Putting value in eq ①

$$\frac{-\hbar^2}{8\pi^2 m} \frac{d^2\psi}{dx^2} + V\psi = E\psi$$

$$\frac{-\hbar^2}{8\pi^2 m} \frac{d^2\psi}{dx^2} + V\psi = E\psi = 0$$

$$\frac{\hbar^2}{8\pi^2 m} \frac{d^2\psi}{dx^2} (E - V)\psi = 0$$

Multiplying throughout by  $\frac{8\pi^2 m}{\hbar^2}$

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

Outside the box  $V = \infty$   $x < 0$  or  $x > L$

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m}{\hbar^2} (E - \infty)\psi = 0$$

This is possible ~~only~~ only when  $\psi = 0$   
i.e. particle is not outside the box

$$\frac{d^2\psi}{dx^2} + (-\infty)\psi = 0$$

$$\psi = \frac{1}{\infty} \frac{d^2\psi}{dx^2} = 0$$

Inside the box  $U=0$   $0 < x$  or  $x < L$

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

$$\frac{d^2\psi}{dx^2} + \left( \frac{8\pi^2m}{h^2} \right) E\psi = 0 \quad \text{2nd } \psi$$

$$\rightarrow k^2$$

$$k^2 = \frac{2mE}{h^2}$$

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \quad \text{2nd order differential equation}$$

Wave function can be represented in the term of the trigonometric functions

$$\psi(x) = A \sin kx + B \cos kx$$

(A, B = arbitrary constant)

when  $x=0$

$$\psi(0) = 0$$

$$0 = A \sin 0 + B \cos 0$$

$$\left( \begin{array}{l} \sin 0 = 0 \\ \cos 0 = 1 \end{array} \right)$$

$$0 = 0 + B$$

$$B = 0$$

When  $x=L$

$$\psi(L) = 0$$

$$0 = A \sin KL + B \cos KL \quad \therefore B = 0$$

$$0 = A \sin KL + 0$$

$$A \sin KL = 0 \quad \therefore KL = n\pi$$

$$\sin KL = 0 = \sin n\pi$$

By comparing

$$KL = n\pi$$

$$k = \frac{n\pi}{L} \quad \text{or} \quad k^2 = \frac{n^2\pi^2}{L^2} \quad \therefore k^2 = \frac{2mE}{\hbar^2}$$

Now

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

$$E = \frac{\hbar^2 n^2 \pi^2}{2mL^2}$$

$$\hbar = \frac{h}{2\pi}$$

$$E = \frac{\hbar^2 n^2 \pi^2}{4\pi^2 2mL^2}$$

$$\hbar^2 = \frac{h^2}{4\pi^2}$$

$$\boxed{E = \frac{h^2 n^2}{8mL^2}}$$

$$\therefore n = 1x, 4x, 9x, 16x, \dots$$

So energy of a particle in one dimensional is quantised

When  $n=1$

$$E_1 = \frac{h^2}{8ml^2}$$

$n=2$

$$E_2 = \frac{4h^2}{8ml^2}$$

$n=3$

$$E_3 = \frac{9h^2}{8ml^2}$$

$n=4$

$$E_4 = \frac{16h^2}{8ml^2}$$

The probability of finding the particle in a small space between  $x$  and  $x+dx$  is given by

$$\psi^2(x) dx$$

$$\int_0^L \psi^2 dx = 1$$

$$\therefore \psi = A \sin\left(\frac{n\pi x}{L}\right)$$

$$A^2 \int_0^L \sin^2\left(\frac{n\pi x}{L}\right) dx = 1$$

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

$$\psi(x) = \frac{2}{L} \sin \frac{n\pi x}{L}$$