Particle in a 1D (1 dimensional) Box :

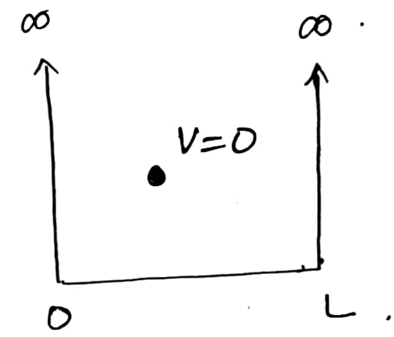
Consider a particle moving horizontally along x-axis.

mass of the particle is $\underline{m}$.

Particle is under the influence of potential V, which is of the form of

$$V(x) = \begin{cases} 0 & 0 < x < L. \\ \infty & x < 0;\ x > L \end{cases}$$

The potential is like infinite deep well from which particle can't escape.



Solution of this problem gives possible wave function & energy values, the particle can possess.

Consider time independent Schrödinger equation

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

from 0 to L $V=0$.

$\Rightarrow$ The particle possess kinetic energy alone & behaves like a free particle.

hence above equation can be written as,

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} E\psi = 0.$$

or $$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \quad \text{—(1)} \qquad \left[\because \frac{2mE}{\hbar^2} = k^2\right] \text{—(2)}$$

above eq'n (1) is a second order differential eqn.
The solution for equation (1) is —

$$\psi(x) = A \sin kx + B \cos kx \quad \text{—(3)}$$

A & B are arbitrary constants

Now, consider boundary conditions

(i) At $x = 0$ $\psi(x) = 0$ [$\because$ at walls ψ vanishes]

$\therefore$ (2) becomes

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

$$0 = B$$

(ii) At $x = L$ $\psi(x) = 0$ [$\because$ at walls ψ vanishes]

$\therefore$ (2) becomes

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

$$0 = A \sin kL \qquad [\text{ as } B = 0 \text{ from (i)}]$$

A can't be 0 $\therefore$ $\sin kL = 0$.

$\Rightarrow \quad kL = n\pi$ [$\because$ $\sin 0$, $\sin 180$, $\sin 360^\circ$ ---- $= 0$] i.e $\sin 0, \pi, 2\pi, 3\pi, \ldots = 0$

or $k = \dfrac{n\pi}{L}$ — (4)

Substituting $B = 0$ & $k = \dfrac{n\pi}{L}$ in (2) we get,

$$\boxed{\psi(x) = A \sin \frac{n\pi}{L} x} \quad \text{— (5)}$$

where $A = \sqrt{\frac{2}{L}}$ [proof given at end]

To determine energy of the particle –

$k^2 = \dfrac{2mE}{\hbar^2}$ [from eqn 2]

or $k^2 = \dfrac{2mE}{(h/2\pi)^2} = \dfrac{8mE\pi^2}{h^2}$.

from eq'n (4) we can write

$$\frac{n^2\cancel{\pi^2}}{L^2} = \frac{8mE\cancel{\pi^2}}{h^2}$$

$$\boxed{\frac{n^2h^2}{8mL^2} = E_n} \quad \text{— (6)}$$

$\psi(x)$ is the eigen function with E_n as eigen value.

Energy levels of an electron

Consider equation (6)

for $n=1$ $\qquad E_1 = \frac{h^2}{8mL^2}$

$n=2$ $\qquad E_2 = \frac{4h^2}{8mL^2} = 4E_1$.

$n=3$ $\qquad E_3 = \frac{9h^2}{8mL^2} = 9E_1$

⋮

In general, $E_n = n^2 E_1$

$\Rightarrow$ Energy levels are discrete.

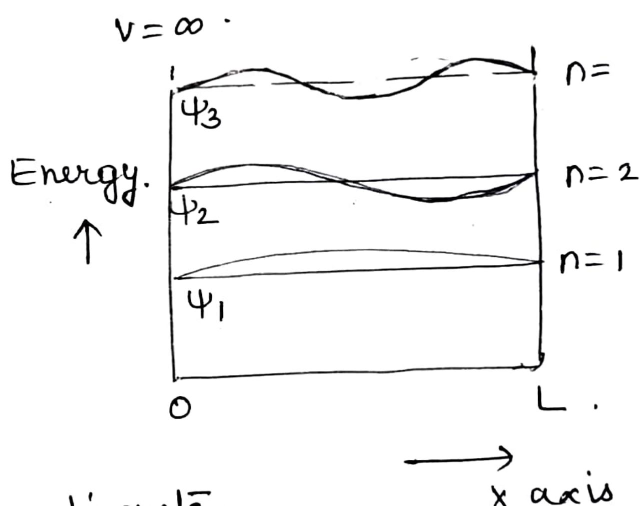


Figure represents various eigen functions & their eigen values of a particle enclosed in a 1D box.

The energy values are discrete.

No of nodes : $(n+1)$

No of antinodes : n

Eg $n=2$ $\quad \psi_2$ has 2 anti nodes

3 nodes

↳ where amplitude is 0

To find normalization constant A,

$$\int_0^L \psi^* \psi \, dx = 1 .$$

$$\therefore \quad \int_0^L A^2 \sin^2 \frac{n\pi x}{L} \, dx = 1.$$

$$\text{or} \quad \frac{1}{2}\int_0^L A^2 \left(1 - \cos 2\frac{n\pi x}{L}\right) dx = 1$$

$$\text{or} \quad \left(\frac{A^2}{2}\int_0^L dx - \frac{A^2}{2}\int_0^L \cos 2\frac{n\pi x}{L} \, dx \right) = 1$$

$$\text{or} \quad \frac{A^2}{2}[L] - \left(\frac{A^2}{2}\left[\sin 2\frac{n\pi x}{L}\right] \times \frac{L}{2n\pi} \right)_0^L = 1 .$$

$$\text{or} \quad \frac{A^2}{2}[L] - \frac{A^2}{2}\left[\underbrace{\sin 2n\pi - \sin 0}_{0} \right] = 1 .$$

$$\text{or} \quad \frac{A^2}{2}[L] = 1 \implies A = \sqrt{\frac{2}{L}}$$

$$\therefore \quad \boxed{\psi = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}}$$