Infinite square well / Particle in a box

$V(x) = 0 \quad 0<x<L$
$\quad\;\; = \infty \quad |x|>L$

Consider a particle moving along the x-axis between $x=0$ and $x=L$ where L is the length of the box. Inside the box the particle is free. At the endpoints, it experiences strong forces that contain it. Simple example is a ball bouncing elastically between two impenetrable walls.

$\psi = 0$ for $x \leq 0$ and $x \geq L$

Our task is to find ψ within the box i.e; $x=0$ & $x=L$

TISE becomes

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

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

$$\therefore \frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0$$

Let $k^2 = \frac{2mE}{\hbar^2}$

$$\therefore \frac{d^2\psi}{dx^2} + k^2\psi = 0$$

Soln:- $\psi(x) = A\sin kx + B\cos kx$ for $0<x<L$

[Since $\cos 0 = 1$, the second term cannot describe the particle because it does not vanish at $x=0$. Hence we conclude that $B=0$
Since $\sin 0 = 0$, the sine term always yields $\psi = 0$ at $x = 0$]

Boundary Conditions

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

$\psi(0) = B = 0$ [continuity at $x=0$]

$\psi(L) = A\sin kL = 0$.

$\therefore kL = n\pi$

$\therefore k = \frac{n\pi}{L}$ where n = any +ve integer $= 1, 2, 3, \ldots$

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

$\therefore \frac{2mE}{\hbar^2} = \frac{n^2\pi^2}{L^2} \Rightarrow \boxed{E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}}$ $n = 1, 2, 3, \ldots$

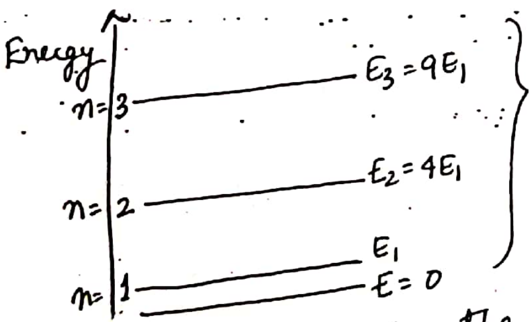
for $n = 1$, $E_1 = \frac{\pi^2\hbar^2}{2mL^2}$ (gr. state energy is non zero)

$n = 2$, $E_2 = n^2E_1 = 4E_1$

$n = 3$, $E_3 = 9E_1$

$n = 4$, $E_4 = 16E_1$

excited state energies.



Allowed energies for a particle in a box

$E = 0$ is not allowed, the particle can never be at rest. The least energy the particle can have is E_1 which is called the zero pt. energy. In classical physics, all values of energy including $E = 0$ are allowed.

wavefn for a particle in a box $= \psi_n(x) = A \sin \frac{n\pi x}{L}$ for $0 < x < L$ and $n = 1, 2, 3$.

These eigenfunctions meet all the requirements. For each quantum no. 'n', ψ_n is finite, single valued fn of x and ψ_n and $\frac{\partial \psi_n}{\partial x}$ are continuous (except at the ends of the box;

Also integral of $|\psi_n|^2$ over all space is finite

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

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

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

$$\Rightarrow A^2\left(\frac{L}{2}\right) = 1 \Rightarrow A = \sqrt{\frac{2}{L}}$$

$\therefore$ The normalized wavefn's of the particle are

$$\psi_n(x) = \sqrt{\frac{2}{L}}\sin\frac{n\pi x}{L} \quad \text{where } n = 1, 2, 3, \ldots$$

<u>Nodes</u> :- $\sin\frac{n\pi x}{L} = 0$

$$\Rightarrow \frac{n\pi x}{L} = m\pi \quad [m = 0, 1, 2, \ldots n]$$

$$\Rightarrow x = m\left(\frac{L}{n}\right).$$

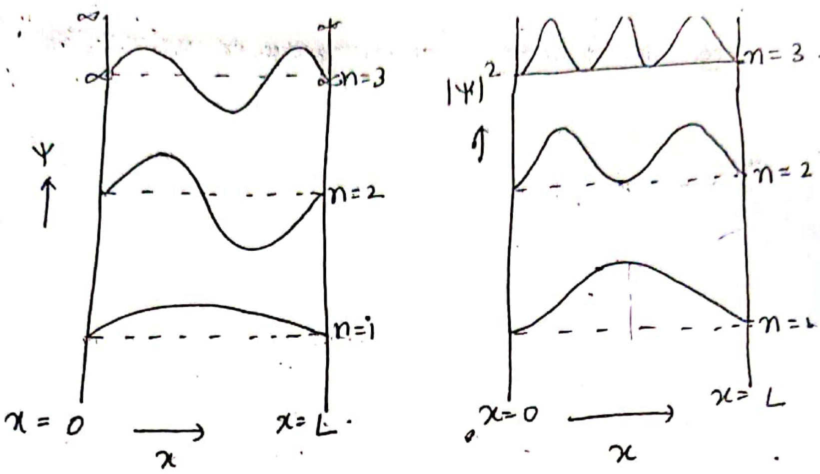
nodes occur at $x = 0, \frac{L}{n}, \frac{2L}{n}, \ldots \frac{nL}{n}$.

<u>Antinodes</u> :- $\sin\frac{n\pi x}{L} = 1$

$$\Rightarrow \frac{n\pi x}{L} = (2m+1)\pi/2$$

$$\Rightarrow x = \left(\frac{2m+1}{2n}\right)L$$

Antinodes occur at $\frac{L}{2n}, \frac{3L}{2n}, \ldots$



<u>IMP points to remember</u>

→ $E = 0$ is not allowed because that makes $\Psi = 0$.

→ $E_1 = \frac{\pi^2\hbar^2}{2mL^2}$ = zero pt. energy

→ Accr. to classical physics, free particle in a box can have any value of energy from 0 to ∞. But accr. to Q.Mech only discrete values of energy & momentum are possible.

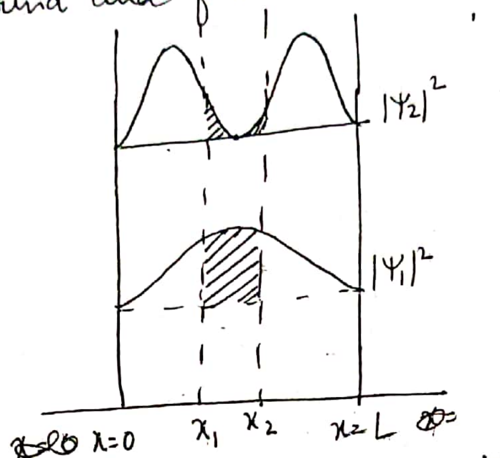
→ Classically the particle is equally likely to be found at any point within the box from 0 to L. But Q.Mech says probability of finding the particle is maxm at antinodes and minm at the nodes.

$$\Psi_n(x,t) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}x\right)e^{-i\omega t}$$

$$= \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}x\right)e^{-i\frac{E}{\hbar}t}$$

$$= \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)e^{-\frac{i}{\hbar}\cdot\frac{n^2\pi^2\hbar^2}{2mL^2}t} = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)e^{-i\frac{n^2\pi^2}{2m\ldots}}$$

* Find the probability that a particle trapped in a box L wide can be found between 0.45L and 0.55L for the ground and first excited state.



This part of the box is $\frac{L}{10}$ of box width & is centered on the middle of the box. Classically we would expect the particle to be in this region 10% of the time.

Accr. to Q. Mech

$$P_{x_1, x_2} = \int_{x_1}^{x_2} |\psi_n|^2 dx = \frac{2}{L}\int_{x_1}^{x_2} \sin^2 \frac{n\pi x}{L} dx$$

$$= \left[\frac{x}{L} - \frac{1}{2n\pi} \sin \frac{2n\pi x}{L}\right]_{x_1}^{x_2}$$

$x_1 = 0.45L$ & $x_2 = 0.55L$.

$P_{x_1, x_2} = 0.198 = 19.8$ percent for $n=1$ (gr. state)

$P_{x_1, x_2} = 0.0065 = 0.65$ " for $n=2$ (first excited state)

Q. Prove the orthogonality of eigenfunction for particle in 1-D infinite square well.

Q. Completeness of condition of eigenfunction

Comparison with classical Mechanics

(a) There is a minimum energy

In classical mechanics, there is no restriction on minimum energy. We can put the particle at rest in the box giving zero energy. But Q. Mech does not allow the particle to have energy less than the ground state energy E_1. The reason for this can be traced to the uncertainty principle. As the particle can be found in the range $0<x<L$, the uncertainty Δx in its position is of the order of L. The linear momentum is then uncertain by at least by an amount $\frac{\hbar}{L}$. This means that we cannot say that the particle is at rest. So there should be a min^m energy.

(b) Energy values are discrete

→ The allowed energies of a particle in a deep potential well are seen to be discrete. The energies are E_1, E_2, E_3 and so on. Classically the energy can take any value but quantum mechanically not all values are allowed.

(c) Nodes in eigen fn.s.

Zero node in gr. state

one node in 1st excited state

two nodes in 2nd excited state.

(d)
$$\frac{E_{n+1}-E_n}{E_n} = \frac{(n+1)^2-n^2}{n^2} = \frac{2n+1}{n^2}$$

In the classical limit, $n \to \infty$

$$\lim_{n\to\infty} \frac{E_{n+1}-E_n}{E_n} = \lim_{n\to\infty} \frac{2n+1}{n^2} = \frac{\frac{2}{n}+\frac{1}{n^2}}{1} = 0$$

Thus the levels become so close together that they are practica[lly] indistinguishabl[e]