UNIT 2: QUANTUM MECHANICS

INFINITE POTENTIAL WELL

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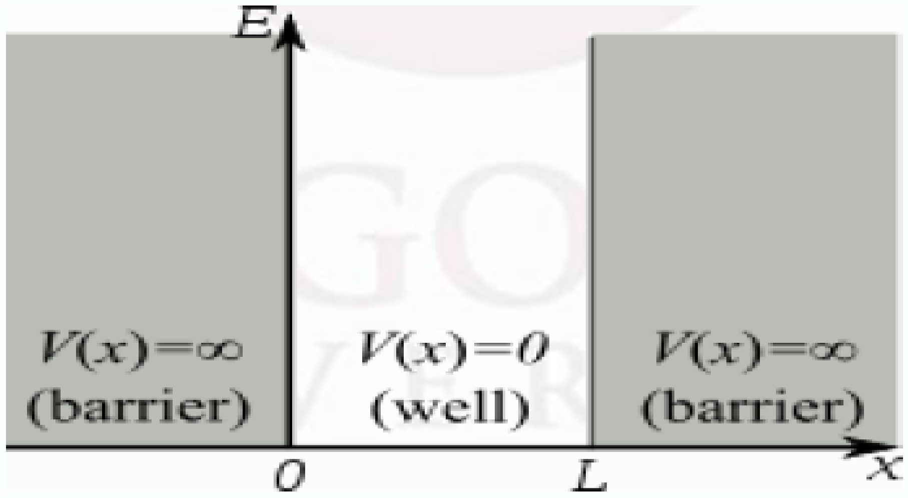
Particle in a One-Dimensional Box with infinitely hard walls (InfinitePotential Well)

Consider a particle of mass m moving along x-axis between the two rigid walls x=0 & x=L. The particle is free to move between the walls. The potential energy of the particle between the two walls is zero and no force is acting on the particle. The particle does not loose energy when it strikes back and forth in the potential well because the walls are infinitely rigid. Let $U(x)$ is the potential energy function. Then $U(x)$ can be represented mathematically as $U(x) = 0$ for $0 < x < L$

$U(x) = \infty$ for $x \leq 0$ and $x \geq L$



The wave function for the particle can be determined by solving the Schrodinger equation, i.e.

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

Since U=0 inside the box, we get $\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0$

The general solution of this equation is $\psi(x) = A\sin(kx) + B\cos(kx)$

Where A and B are arbitrary constants to be determined from the boundary conditions and k is given by

$k = \sqrt{\frac{2mE}{\hbar^2}}$. The boundary conditions are ψ(x) = 0, at x = 0 and at x = L.

For x = 0, $\psi(x) = A\sin(kx) + B\cos(kx) \Rightarrow B = 0$

Thus the wave function becomes $\psi_n = A\sin(kx)$

Further ψ(x) = 0, at x = L gives

$$\sin(kL) = 0 \Rightarrow kL = n\pi$$

Since A cannot be zero as this will make the wave function zero everywhere.

$$k = \frac{n\pi}{L}, \quad n = 1, 2, 3\ etc$$

The wave function becomes $\psi_n = A\sin\left(\frac{n\pi}{L}\right)x$

The subscript n in ψ_n means that the wave-function depends on n. The allowed energies are obtained using

$$k = \frac{n\pi}{L} \Rightarrow k^2 = \frac{n^2\pi^2}{L^2} \Rightarrow \frac{2mE_n}{\hbar^2} = \frac{n^2\pi^2}{L^2} \Rightarrow E_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2$$

$$\boxed{E_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2 \Rightarrow E_n \propto n^2}$$

Each value of the energy E_n for n=1, 2, 3 etc is called an ***energy Eigen value*** and corresponding wave function is called ***Eigen function.*** Thus inside the box, the particle can only have the discrete energy values. The allowed wave functions and the allowed energy values E_n exist only for integral values of n. The number n is called the quantum number. Hence energy spectrum consists of discrete energy levels where the spacing between the levels is determined by the values of n and L.

Wave Functions: The constant A can be determined by using this information that the probability of finding an electron somewhere inside the box is unity, i.e.

$$\int_0^L \psi_n^* \psi_n dx = 1$$

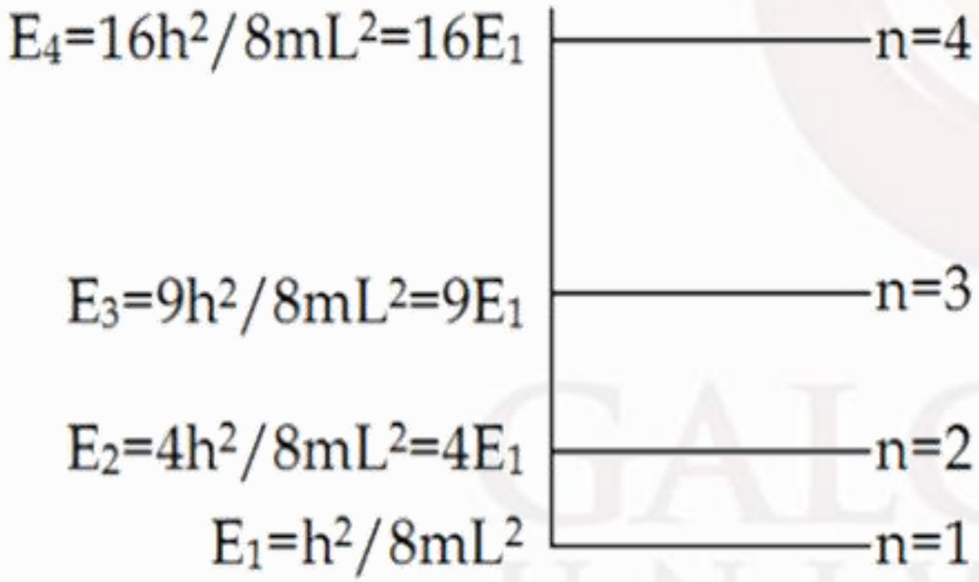
This is called as normalisation condition. We get,

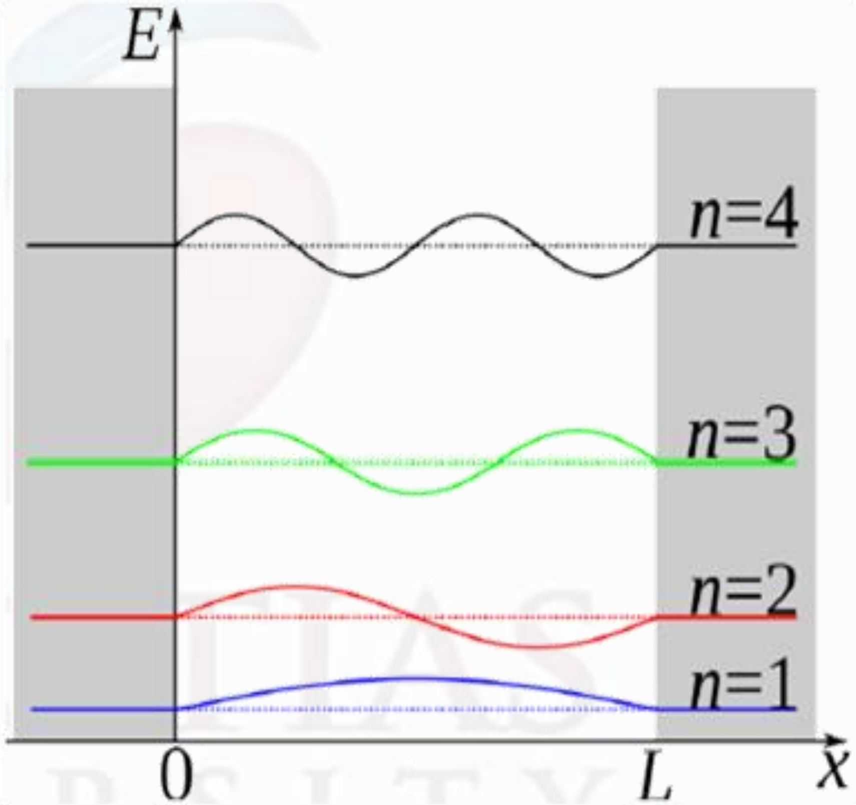
$$A^2 \int_0^L \sin^2\left(\frac{n\pi}{L}x\right) dx = 1 \Rightarrow A^2 \int_0^L 1 - \cos\left(\frac{2n\pi}{L}x\right) dx = 2 \Rightarrow A^2 \int_0^L dx = 2 \Rightarrow A = \sqrt{\frac{2}{L}}$$

Thus the normalized wave function is given by

$$\boxed{\psi_n = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right)}$$

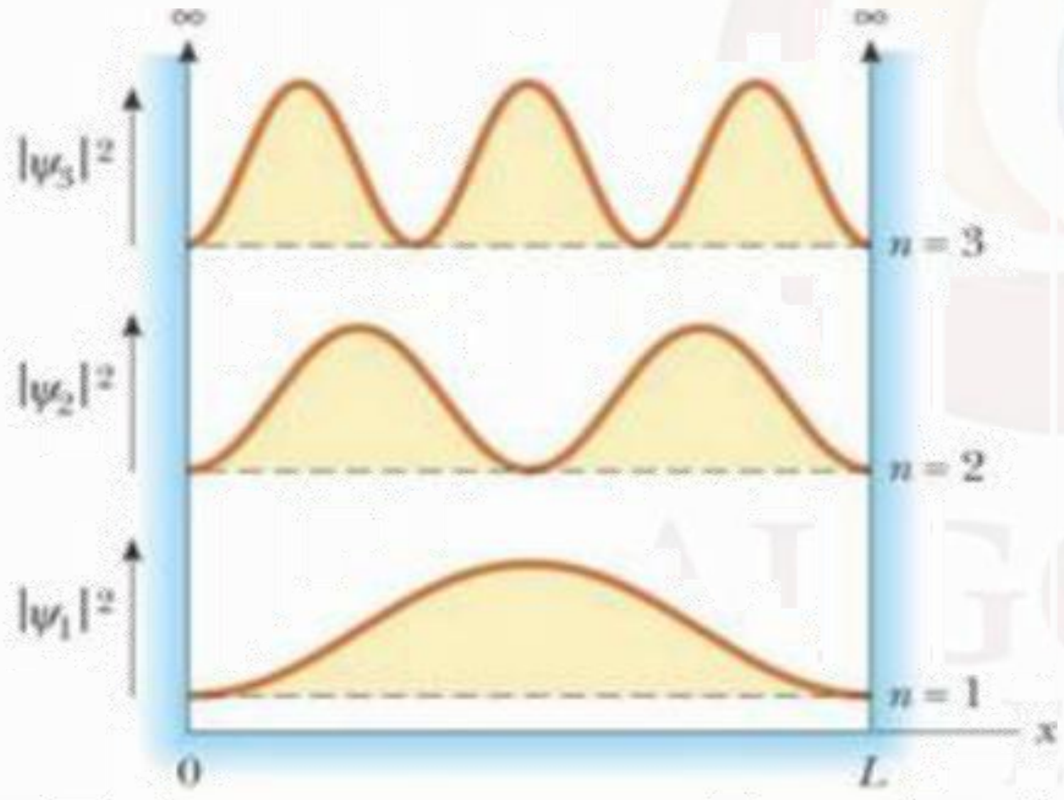
The energy levels and the wave functions corresponding to n=1, 2, 3, and 4 are shown below;





PROBABILITY VS X PLOT

The probabilities of finding the particle are given by $|\psi|^2$ and are shown below for first three wave functions.



REFERENCES

- CONCEPTS OF MODERN PHYSICS, ARTHUR BEISER, MCGRAW-HILL.
- INTRODUCTION TO MODERN PHYSICS, RICH MEYER, KENNARD, COOP, TATA MCGRAW HILL
- INTRODUCTION TO QUANTUM MECHANICS, DAVID J. GRIFFITH, PEARSON EDUCATION.