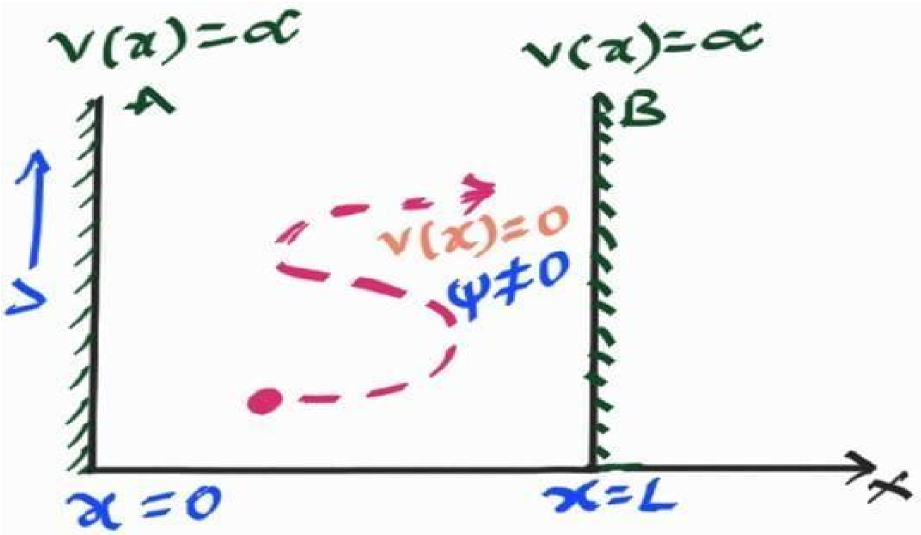
10.PARTICLE IN ONE DIMENSIONAL BOX

Introduction:

The "particle in a one-dimensional potential box" is a fundamental concept in quantum physics(mechanics), and the solutions to the Schrodinger equation for this model was developed by Erwin Schrödinger.

- Let us consider a particle of mass 'm' moving along the x-axis enclosed in a 1-D potential box as shown in figure.



- Since the walls have infinite potential, the particle does not penetrate out from the box. **i.e.**, Potential energy of the particle V=∞ at the walls of the box.
- But the particle is free to move between the walls A & B at x=0 & x=L.

Boundary conditions:

- The potential energy of particle is:

  $V(x) = 0$ for $0 < x < L$---------------(1)

  $V(x) = \infty$ for $0 \geq x \geq L$---------------(2)

- The **TISWE** for a free particle is

  $\partial^2\psi/\partial x^2 + 8\pi^2 m(E/h^2)\,\psi = 0$ ------ - --- (3)

- **Let** $8\pi^2 mE/h^2 = k^2$ ----------------- (4)
- **From (2) & (3)** => $\partial^2\psi/\partial x^2 + k^2\psi = 0$ ------- (5)
- **The general solution** for **(4)** is

  $\psi(x) = A \sin kx + B \cos kx$ --- (6)

Where*:* A, B -> Two constants

k -> wave vector (or) wave no.

Boundary condition (i): $\psi(x) = 0$ at $x = 0$

- **From (5)** => $0 = A \sin k(0) + B \cos k(0)$

$0 = 0 + B \Rightarrow B = 0$ ($\because \sin 0 = 0, \cos 0 = 1$)

$\therefore \psi(x) = A\sin kx$ (or) $\psi_n = A\sin kx$ --- (7)

Boundary condition (ii): $\psi(x) = 0$ at $x = L$

- **From (6)** => $0 = A \sin kL$
- **Since**, $A \neq 0 \Rightarrow \sin kL = 0$

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

$KL = n\pi$

$\Rightarrow K = n\pi/L$

$\Rightarrow K^2 = n^2\pi^2/L^2$ -------------- (8)

- **From (7)** => $\psi(x) = A \sin(n\pi x/L)$ ------------- (9)

Energy of the particle:

- From (3) & (7) => $8\pi^2 mE/h^2 = n^2\pi^2/L^2$

$\Rightarrow E = n^2h^2/8mL^2$ ---------------(10)

Energy levels of the particle:

For energy level 1, n=1 => $E1 = h^2/8mL^2$

For energy level 2, n=2 => $E2 = 2^2h^2/8mL^2 = 2^2E_1$

For energy level 3, n=3 => $E3 = 3^2h^2/8mL^2 = 3^2E_1$

$\therefore$ The general equation for energy levels is

$E_n = n^2E_1$ ----------------(11)

- **From (10),** Energy levels of an electron are discrete.

Evaluation of A:

- To find A value by applying the normalization conditions over the integral "0 to L"

$\int_0^L |\psi(x)|^2 \, dx = 1$ ----------------(12)

- **From (8)** => $\psi(x) = A \sin(n\pi x/L)$

$\therefore \int_0^L A^2 \sin^2(n\pi x/L) \, dx = 1$

$A^2 \int_0^L \sin^2(n\pi x/L) \, dx = 1$

$$A^2 \int_0^L 1dx \; - \; A^2 \int_0^L \cos(2n\pi x/L))/2 \, dx = 1$$

$$A^2 [x/2]_0^L - A^2 [\cos(2n\pi x/2L)] = 1$$

$$A^2 (L/2) - A^2 [0] = 1$$

$$A^2 (L/2) = 1$$

$$A^2 = 2/L$$

$$A = \sqrt{(2/L)} \text{ ------------------(13)}$$

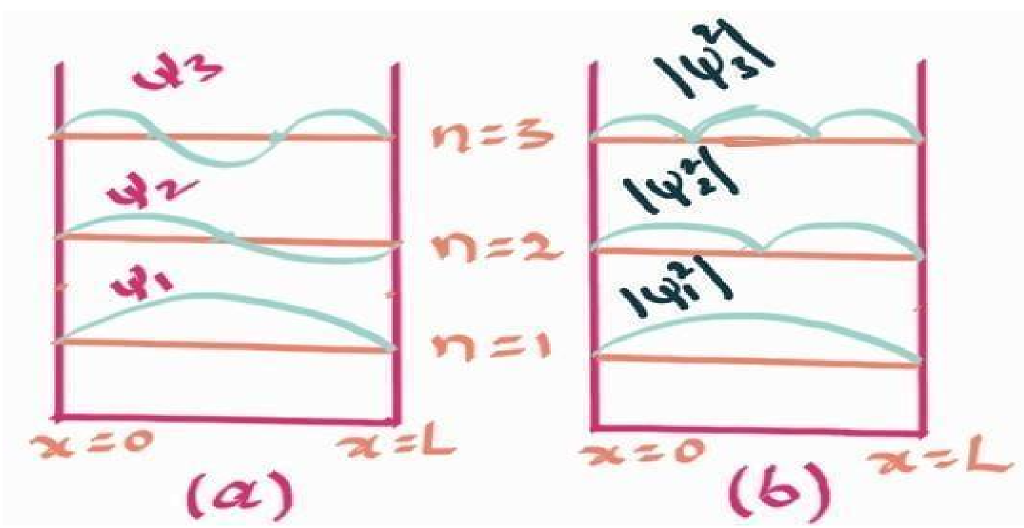
- **The normalized wave function** of the particle

$$\psi_n = \sqrt{(2/L)} \sin(n\pi x/L) \text{ ---------------(14)}$$

(or)

$$\psi(x) = \sqrt{(2/L)} \sin(n\pi x/L) \text{ --------------(15)}$$

- The normalized wave functions $\boldsymbol{\psi_1}$, $\boldsymbol{\psi_2}$, and $\boldsymbol{\psi_3}$ in (fig a) represent the *normalized wave functions* of a particle in a one-dimensional box of length L and each $\boldsymbol{\psi_n}$ corresponds to a *quantum state* with quantum number n=1,2,3,........



  - **Number of Nodes:** As **'n'** increases, the number of *nodes* (points where $\psi = 0$ inside the box) also increases like $\boldsymbol{\psi_1}$ has **no nodes**, $\boldsymbol{\psi_2}$ has **one node**, $\boldsymbol{\psi_3}$ has **two nodes**, and so on.
  - **Probability Density ($|\psi_n|^2$):** The plots on the right (fig b) show $|\psi_n|^2$, which gives the *probability distribution* of finding the particle at different positions and higher **n** values give *more oscillations*, meaning the particle has *more regions* of high & low probability inside the box.