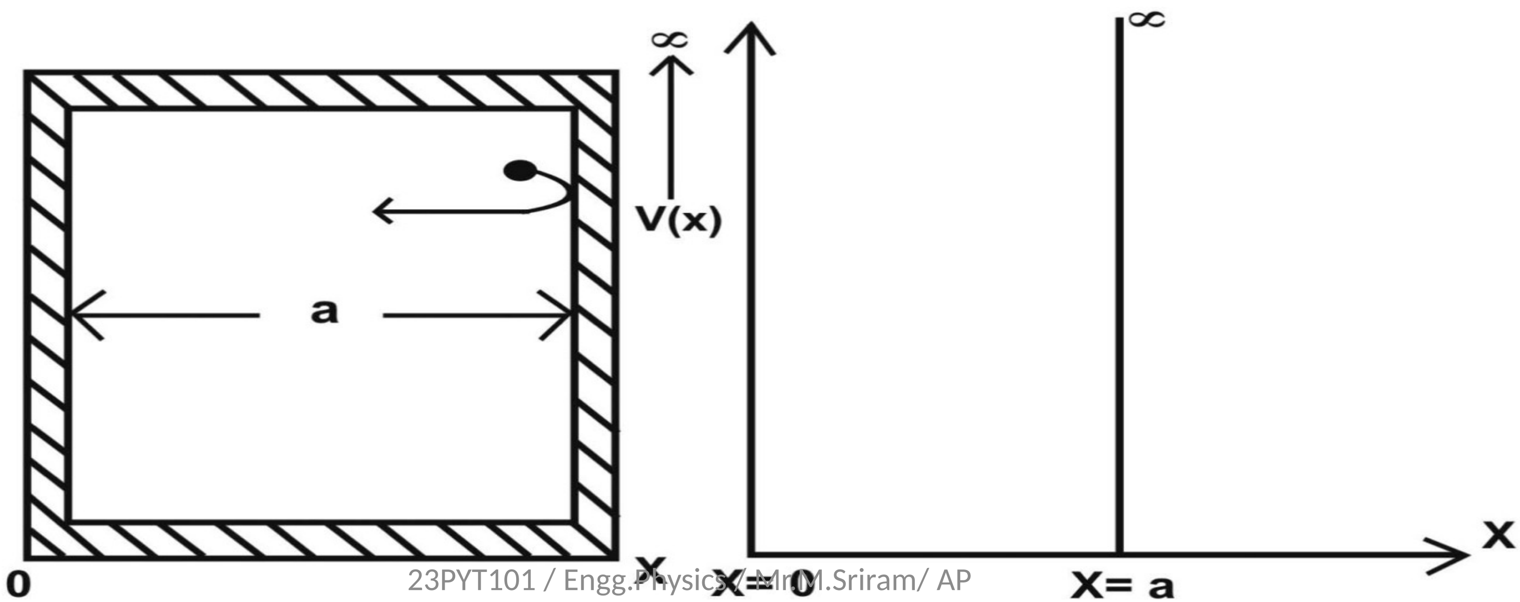
PARTICLE IN A ONE DIMENSIONAL BOX

Boundary conditions:

- *V(x) = 0   when 0   x   a*
- *V(x) =   when 0   x   a*

To find the wave function of a particle with in a box of width “a”, consider a Schrodinger’s one dimensional time independent wave eqn.



PARTICLE IN A ONE DIMENSIONAL BOX

$$\nabla^2\psi + \frac{2m}{\hbar^2}(E - V)\psi = 0 (Time\ independent\ Schroedinger\ wave\ eqn)...(1)$$

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

Since the potential energy inside the box is zero (V=0). The particle has kinetic energy alone and thus it is named as a free particle or free electron. For a free electron the schroedinger wave equation is given by

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m}{h^2}E\psi = 0...(3)$$

$$\frac{d^2\psi}{dx^2} + K^2\psi = 0..(4) \qquad Let\ K^2 = \frac{8\pi^2 mE}{h^2}$$

Eqn (3) is a second order differential equation, the solution of the equation (3) is given by

$$\psi(x) = A\ sin\ kx + B\ Cos\ kx \ldots\ldots\ldots.(5)$$

PARTICLE IN A ONE DIMENSIONAL BOX

Applying Boundary conditions

(I) When x = 0, (x) =0   (ii) when x = a, (x) =0

0 = B   0 = ASinKa

Sin n = SinKa

i.e., n =Ka

then, K = n /a:

But

$$Let\ K^2 = \frac{8\pi^2 mE}{h^2}$$

$$also K^2 = \frac{n^2\pi^2}{a^2}$$

$$comparing\ both\ K^2$$

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

$$E_n = \frac{n^2 h^2}{8ma^2}$$

$$\Psi_n = A\ sin\ \frac{n\pi}{a} x$$

PARTICLE IN A ONE DIMENSIONAL BOX

$$Energy\ of\ an\ electron = E_n = \frac{n^2 h^2}{8ma^2}$$

When n = 1

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

When n = 2

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

When n = 3

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

For each value of n,(n=1,2,3..) there is an energy level.

Each energy value is called **Eigen value** and the corresponding wave function is called **Eigen function.**

PARTICLE IN A ONE DIMENSIONAL BOX

Normalization of the wave function

- Normalization is the process by which the probability of finding the particle is done. If the particle is definitely present in a box, then P=1

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

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

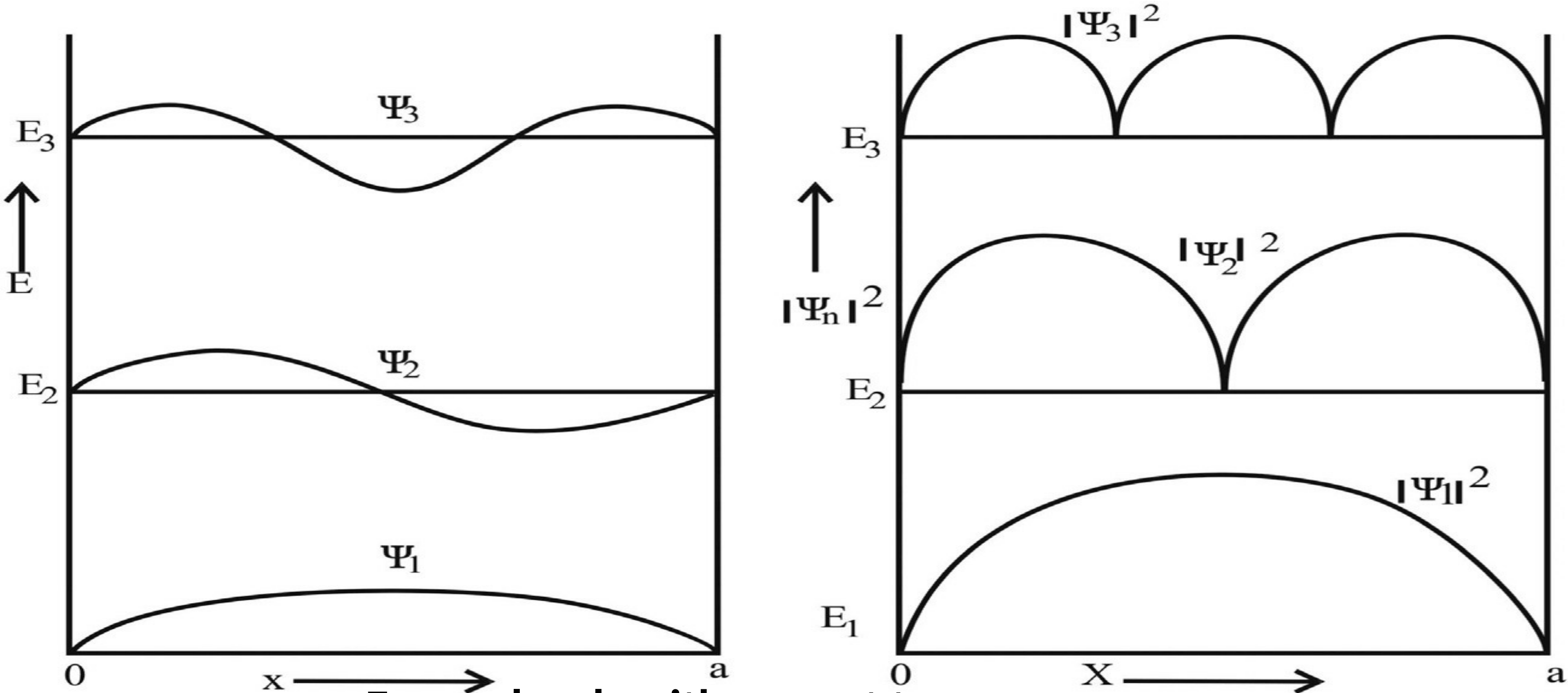
$$\frac{A^2}{2} \int_0^a 1 - \cos\left(\frac{2n\pi x}{a}\right) dx = 1$$

$$\frac{A^2}{2} \left\{ \int_0^a dx - \int_0^a \cos\left(\frac{2n\pi x}{a}\right) dx \right. = 1$$

$$\frac{A^2}{2} \{ a - 0 \} = 1$$

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

PARTICLE IN A ONE DIMENSIONAL BOX



Energy levels with respect to
(a) wave functions and (b) probability density

Therefore, the normalized wave function is given as,

$$\Psi_n = \sqrt{\frac{2}{a}}\, sin\, \frac{n\pi}{a} x$$

PARTICLE IN A ONE DIMENSIONAL BOX

- **En** is known as normalized Eigen function. The energy E

$$E_n = \frac{n^2 h^2}{8ma^2}$$

- normalized wave functions n are indicated in the above figure.

$$\Psi_n = \sqrt{\frac{2}{a}}\, sin\, \frac{n\pi}{a} x$$

ELECTRON IN A CUBICAL METAL PIECE

$$\Psi_{(n_x n_y n_z)} = \sqrt{\frac{2}{a}}\, sin\, \frac{n_x \pi}{a} x \sqrt{\frac{2}{a}}\, sin\, \frac{n_y \pi}{a} y \sqrt{\frac{2}{a}}\, sin\, \frac{n_z \pi}{a} z$$

$$\Psi_{(n_x n_y n_z)} = \sqrt{\frac{8}{a^3}}\, sin\, \frac{n_x \pi x}{a}\, sin\, \frac{n_y \pi y}{a}\, sin\, \frac{n_z \pi z}{a}$$

$$E_n = \frac{n_x^2 h^2}{8ma^2} + \frac{n_y^2 h^2}{8ma^2} + \frac{n_z^2 h^2}{8ma^2}$$

$$= \frac{h^2}{8ma^2} (n_x^2 + n_y^2 + n_z^2)$$