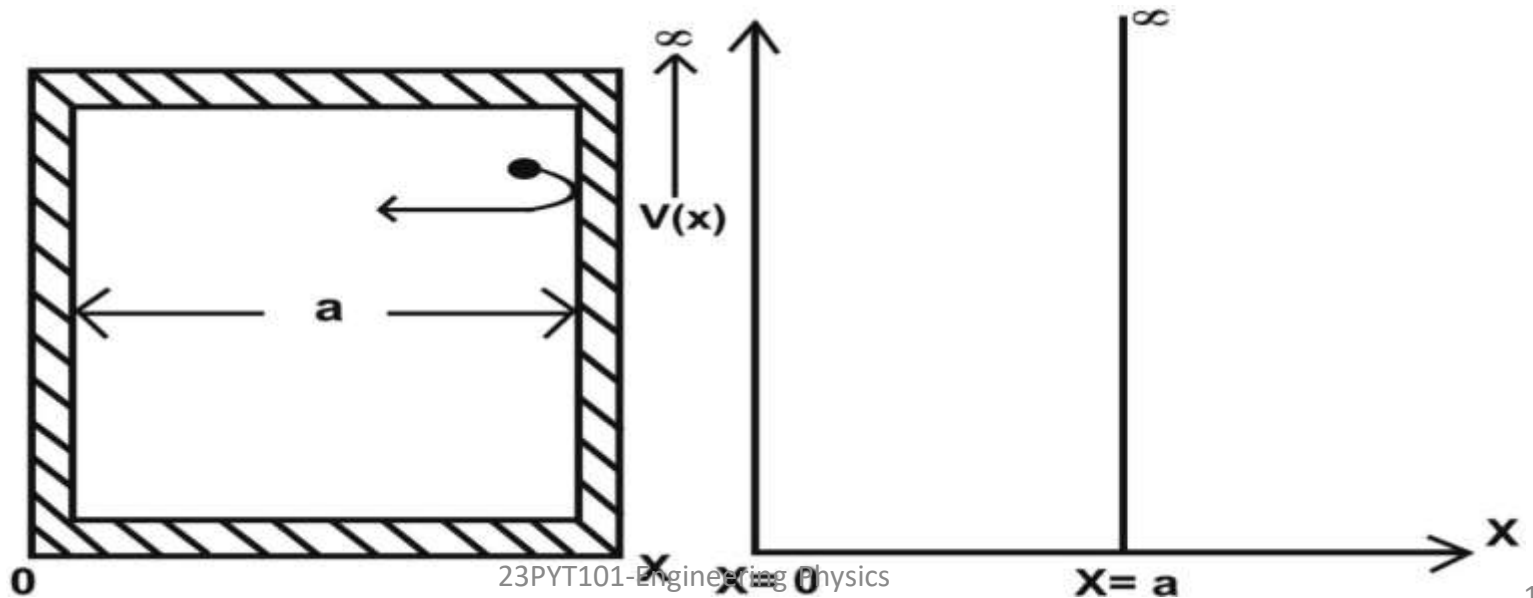


# PARTICLE IN A ONE DIMENSIONAL BOX

## Boundary conditions:

- $V(x) = 0$  when  $0 < x < a$
- $V(x) = \infty$  when  $0 \geq x \geq a$

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

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

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

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

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

$$\frac{d^2 \psi}{dx^2} + K^2 \psi = 0 \dots (4) \quad \text{Let } K^2 = \frac{8\pi^2 m E}{h^2}$$

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

$$\psi(x) = A \sin kx + B \cos kx \dots \dots \dots (5)$$

# PARTICLE IN A ONE DIMENSIONAL BOX

## Applying Boundary conditions

(i) When  $x = 0$ ,  $\psi(x) = 0$

$$0 = B$$

(ii) when  $x = a$ ,  $\psi(x) = 0$

$$0 = A \sin Ka$$

$$\sin n\pi = \sin Ka$$

$$\text{i.e., } n\pi = Ka$$

then,  $K = n\pi/a$ :

But

*comparing both  $K^2$*

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

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

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

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

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

# PARTICLE IN A ONE DIMENSIONAL BOX

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

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  $P=1$

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

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

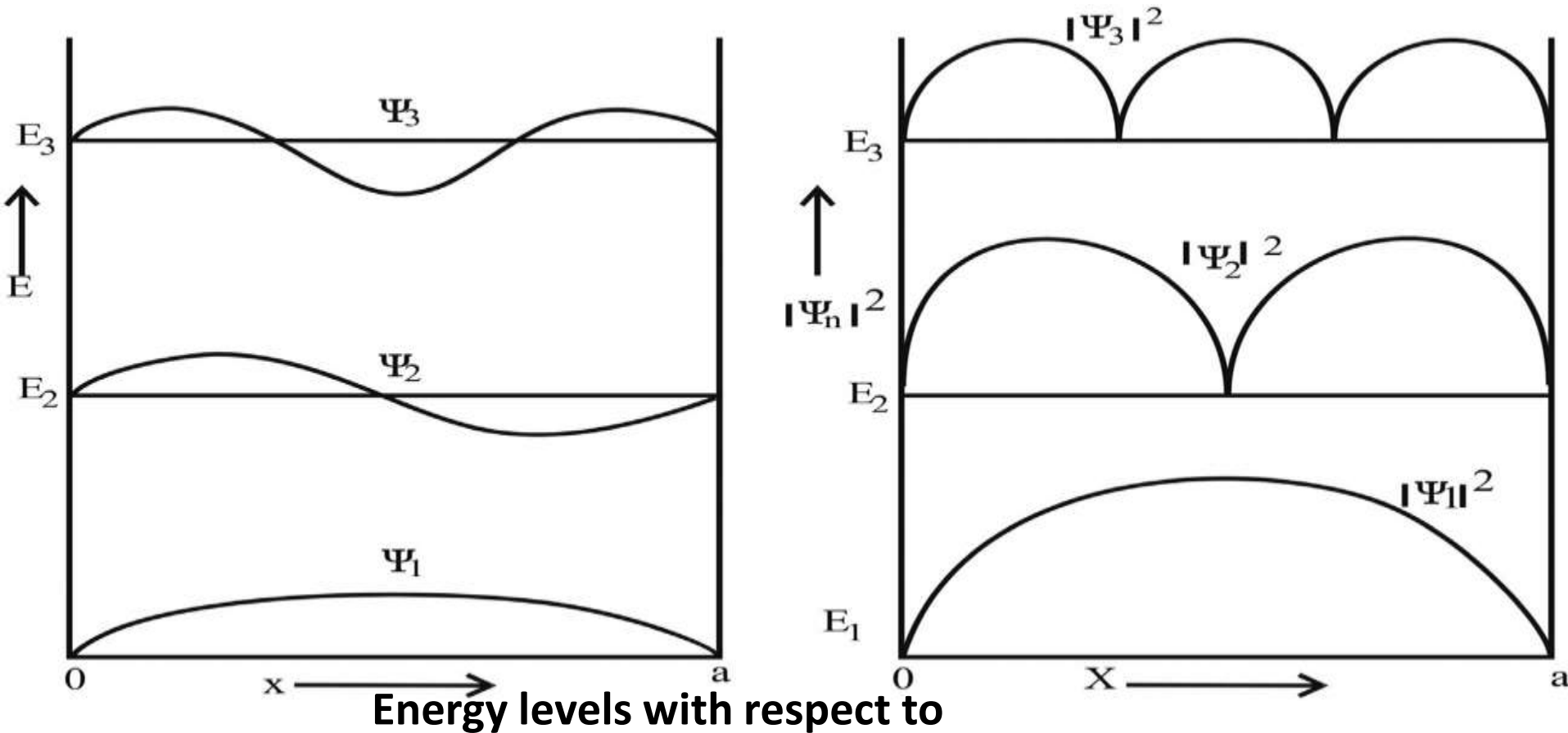
$$\frac{A^2}{2} \int_0^a 1 - \cos\left(\frac{2n\pi x}{a}\right) dx = 1$$

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

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

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

# 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,

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

23PY1101-Engineering Physics  
Dr.V.Manikandan / AP / Physics

# PARTICLE IN A ONE DIMENSIONAL BOX

- $E_n$  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

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

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

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

