4.1. PARTICLE IN A BOX

(Particle in one dimensional infinite potential well)

Consider a free particle of mass m confined to move in one dimensional rectangular box of length L i.e. the particle moves only along a straight line say along x-axis. Let the walls of the box be rigid, elastic and non-penetrable. Let the particle can travel along x-axis between $x = 0$ and $x = L$.

Let the collision of the particle with the walls be elastic so it does not loose energy. Let us represent this by an infinite square well potential as shown in figure 4.1.

The potential V is defined as

$$V_{(x)} = \begin{cases} 0 & \text{for } 0 < x < L \\ \infty & \text{for } x < 0 \text{ and } x > L \end{cases}$$

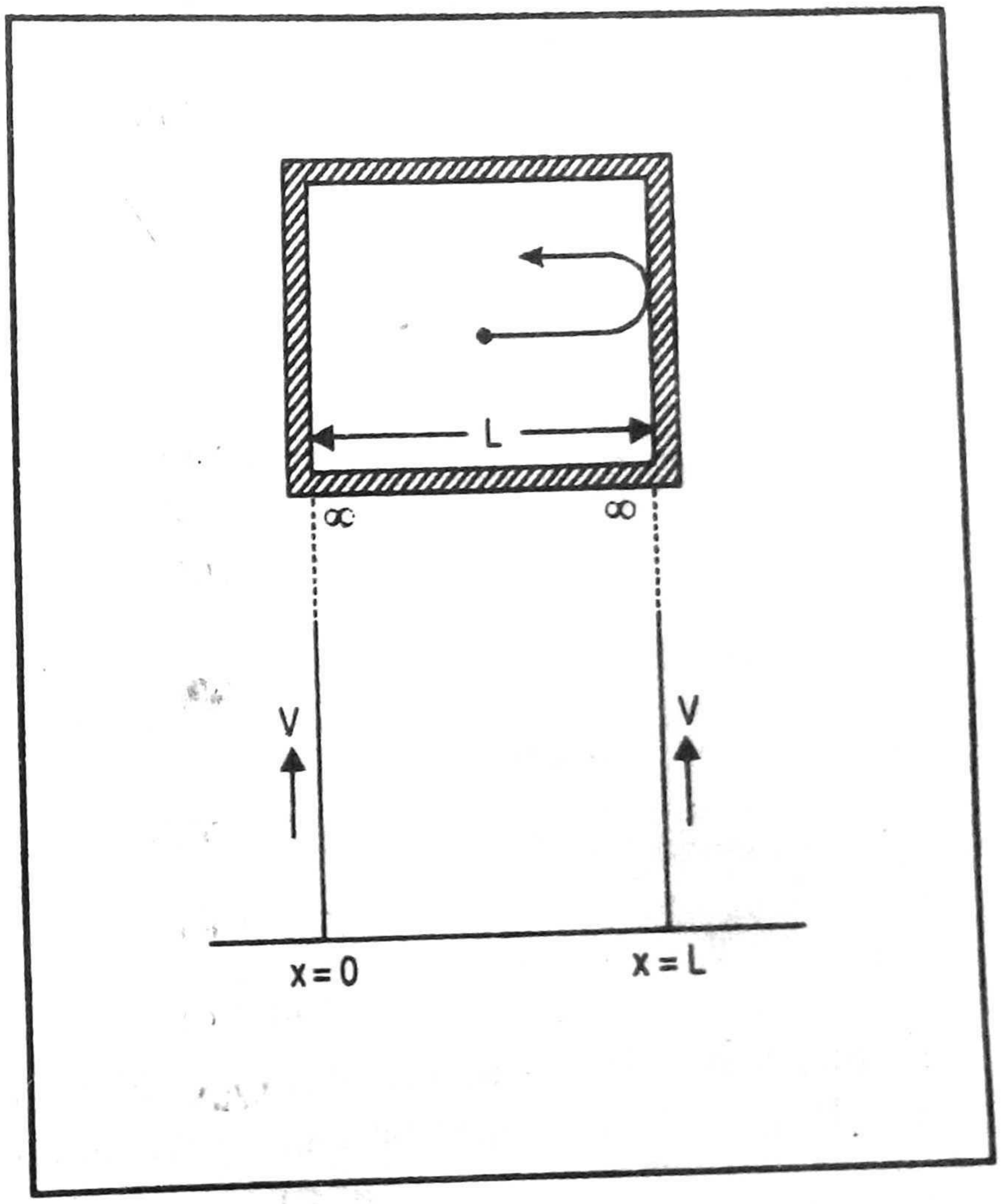

Fig. 4.1

Classical view

Classically, the particle can have any value of energy. If E = 0, the particle will be at rest inside the box and if E > 0, the particle will move along x-axis and at $x = 0$ and $x = L$, it will experience a force

$F = -\dfrac{dV}{dx}$ (since $V = \infty$, so $F = \infty$) in the direction opposite to its motion and is reflected from the walls and thus moves back and forth along x-axis.

Quantum mechanical view

The Schrodinger wave equation for the wave function of a particle moving along a straight line in the presence of external field is given by

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

For a free particle inside the well V = 0, so the above equation becomes

$$\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0 \qquad \text{....(1)}$$

or

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0, \qquad \text{....(2)}$$

where

$$k^2 = \frac{2mE}{\hbar^2} \qquad \text{....(3)}$$

The general solution Eq. (2) may be written as

$$\psi(x) = Ae^{ikx} + Be^{-ikx}, \qquad \text{.....(4)}$$

where A and B are the constants to be determined by the boundary conditions.

Boundary Conditions

The wave function $\psi = 0$ at $x = 0$ and at $x = L$

(*i*) At $x = 0$, $\psi = 0$, So Eq. (4) becomes

$$A + B = 0$$

or

$$B = -A \quad \text{....(5)}$$

So Eq. (4) becomes

$$\psi(x) = Ae^{ikx} - A\,e^{-ikx} = A[e^{ikx} - e^{-ikx}]$$

$$= 2iA\frac{e^{ikx} - e^{-ikx}}{2i}$$

or

$$\psi(x) = 2iA \sin kx$$

$$= C \sin kx, \quad \text{...(6)}$$

where $C = 2iA$

(*ii*) At $x = L$, $\psi = 0$. So Eq. (6) becomes

$$0 = C \sin kL$$

or

$$\sin kL = 0$$

or

$$kL = n\pi, \ (n = 0, 1, 2, ...)$$

or

$$k = \frac{n\pi}{L} \quad \text{...(7)}$$

or

$$k^2 = \frac{n^2\pi^2}{L^2} \quad \text{.....(8)}$$

Using Eq. (3), we get

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

or

$$E = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

where *n* is called quantum number. Since E depends on *n* so let us denote the energy of the particle by E_n. Hence above equation can be written as

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} \quad \text{....(9)}$$

Thus $E_n \propto n^2$, $\quad E_n \propto \frac{1}{L^2}$, $\quad E_n \propto \frac{1}{m}$.

Energy level diagram (*or Eigen values of energy*)

For $n = 1$, the value of E_n will be minimum and is given by

$$E_1 = \frac{\pi^2\hbar^2}{2mL^2} \quad \text{....(10)}$$

This is called *ground level energy* and the state is called *ground state*. The energy corresponds to higher states is called *excited energy* and the states are called excited states. These are given by

$$E_2 = \frac{2^2\pi^2\hbar^2}{2mL^2} = 4E_1$$

$$E_3 = \frac{3^2\pi^2\hbar^2}{2mL^2} = 9E_1$$

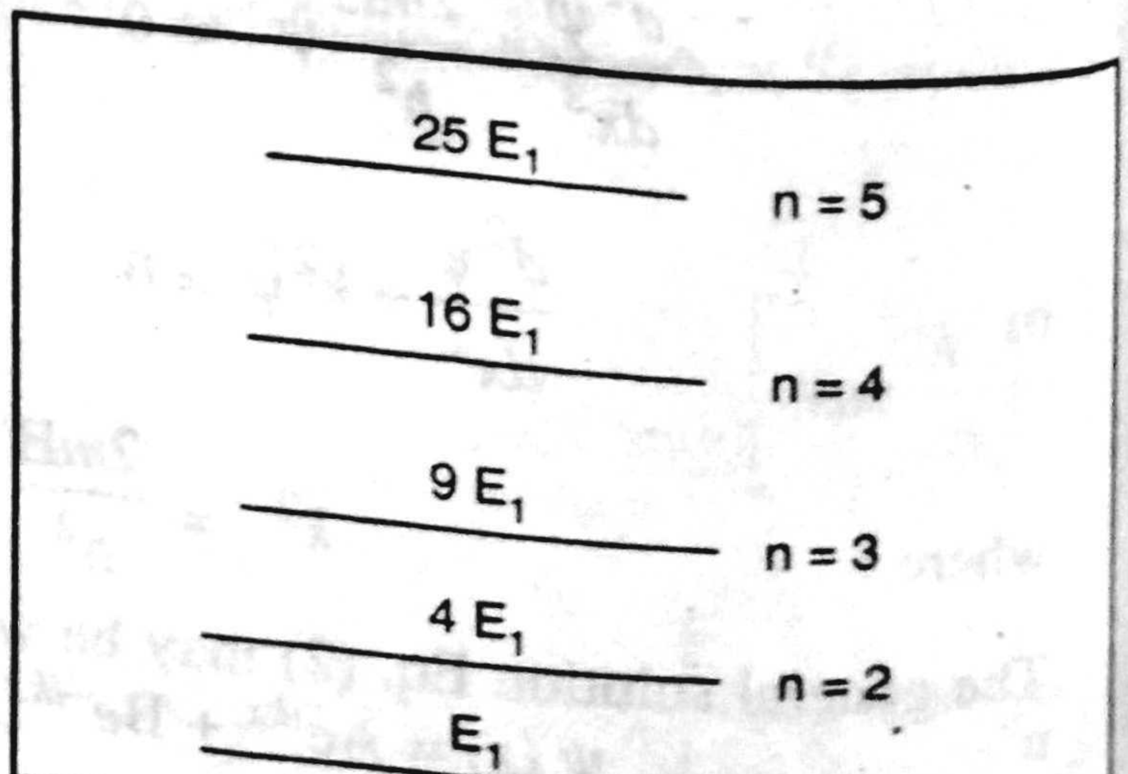

Fig. 4.2

$$E_4 = \frac{4^2\pi^2\hbar^2}{2mL^2} = 16E_1$$

and so on.

Thus we find that the particle can have any value of energy given by E_1, $4E_1$, $9E_1$, $16E_1$,......Hence ergy is quantised. These allowed values of energies of the particle are called *energy levels* or *eigen lues of energy*, shown in fig 4.2, and are not equally spaced.

Eigen values of momentum

The linear momentum of any one of the allowed value E_n is given by

$$p_n^2 = 2mE_n \qquad \left[\because E_n = \frac{p_n^2}{2m}\right]$$

Using Eq. (8), we get

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

or
$$p_n = \frac{n\pi\hbar}{L}, \quad (n = 0, 1, 2,.....) \qquad .....(11)$$

Thus momentum is also quantized into discrete allowed values. Hence the momentum of a particle side the box is

(*i*) directly proportional to the quantum number n *i.e.* $p_n \propto n$

(*ii*) inversely proportional to the length L of the box *i.e.* $p_n \propto \frac{1}{L}$

(*iii*) independent of the mass of the particle.

Zero point energy

The minimum possible energy possessed by the particle inside the box is called zero point energy.

The energy of the particle inside will be minimum at $n = 1$

So zero point energy

$$E_1 = \frac{\pi^2\hbar^2}{2mL^2} \qquad \text{(see Eq. (9))}$$

Since $E = 0$ is not allowed because if $E = 0$, then $\psi = 0$ everywhere inside the box and then probability ensity in the box $|\psi|^2 = 0$ i.e. the particle is not in the box, hence $E \neq 0$.

Hence, the particle can not have zero total energy inside the box, so it cannot be at rest in the box quantum mechanically).

Wave function.

From Eq. (6), the wave function $\psi(x)$ of the particle inside the box is given by

$$\psi(x) = C \sin kx. \qquad ......(12)$$

Using Eq. (7), we get

$$\psi(x) = C \sin\left(\frac{n\pi x}{L}\right)$$

$\therefore$ Probability density

$$P = \psi^*(x)\,\psi(x) = C \sin\left(\frac{n\pi x}{L}\right) . C \sin\frac{n\pi x}{L}$$

or

$$\psi^* \psi = C^2 \sin^2 \frac{n\pi x}{L}$$

Since the probability density between $x = 0$ and $x = L$ is 1, because the particle is somewhere within this boundary.

i.e. $$\int_0^L \psi^* \psi dx = 1$$

or $$C^2 \int_0^L \sin^2 \frac{n\pi x}{L} dx = 1$$

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

or $$\frac{C^2}{2}\left[\int_0^L dx - \int_0^L \cos\frac{2n\pi x}{L} dx\right] = 1$$

or $$\frac{C^2}{2}[L - 0] = 1 \qquad \left[\because \int_0^L \cos\frac{2\pi nx}{L} dx = 0\right]$$

or $$C^2 = \frac{2}{L}$$

or $$C = \sqrt{\frac{2}{L}}$$

Thus normalized wave function of the particle inside the well is given by

$$\psi = \sqrt{\frac{2}{L}} \sin\frac{n\pi x}{L} \qquad ...(13)$$

The normalized wave functions ψ_1, ψ_2 and ψ_3 together with the probability densities $|\psi_1|^2$, $|\psi_2|^2$ and $|\psi_3|^2$ are plotted in fig. 4.3 (a & b). Although ψ_n may be positive as well as negative but $|\psi_n|^2$ is

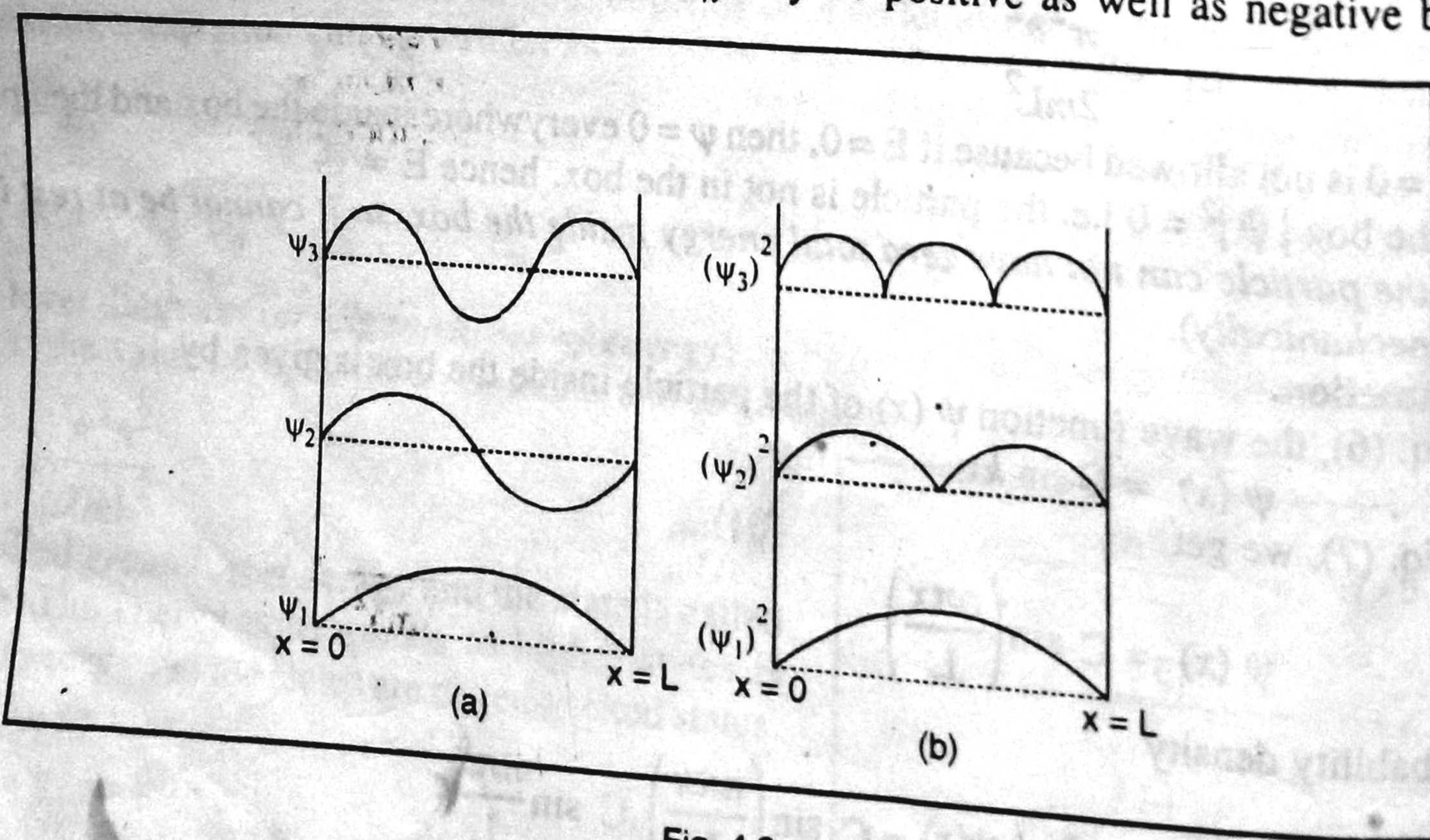

Fig. 4.3

always positive and since ψ_n is normalized, its value at a given x is equal to the probability density of finding the particle there. In every case $|\psi_n|^2 = 0$ at $x = 0$ and $x = L$, the boundaries of the box.