5.4. PARTICLE IN A FINITE POTENTIAL WELLS (Qualitative)

- Consider a particle of mass m moving with velocity v along the x-direction between $x = 0$ and $x = a$.
- The walls of the box are not rigid. Hence it is represented by a potential well of finite depth.

Step I: Let E be the total energy of particle inside the box and V be its P.E. The potential energy which is assumed to be zero within the box and its value outside the box is finite say V_o and $V_o > E$.

The variation of potential with x is shown in fig.

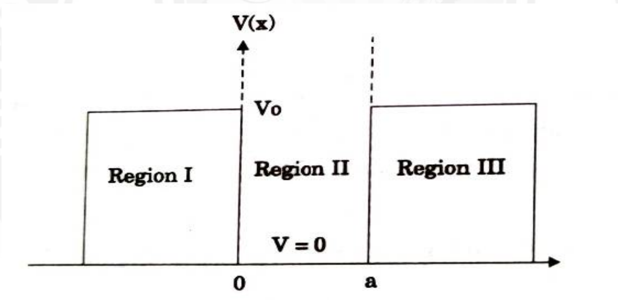


Fig. 5.11 Particle in a finite potential well with potential $V = 0$ in the Region II enclosed between the Regions I and III with $V = V_o$ of finite height

$V(x) = V_0 x \leq 0$ Region I

$V(x) = 00 < x < a$ Region II

and $V(x) = V_0 x \geq a$ Region III

Classically, the particle with energy $E < V_0$ cannot be present in regions I and III outside the box.

Consider the quantum mechanical picture of the particle in one dimension. If ψ is the wave function associated with the particle then Schrodinger's time independent equation for it is,

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

Step II: Consider the three regions I, II, III separately and let $\psi_{\mathrm{I}}, \Psi_{\mathrm{II}}, \Psi_{\mathrm{III}}$ be the wave functions in them respectively.

We have for region I.

$$\frac{d^2\psi_I}{dx^2} + \frac{2m}{\hbar^2}(E-V_0)\Psi_I = 0$$

For region II,

$$\frac{d^2\psi_{\mathrm{II}}}{dx^2} + \frac{2mE}{\hbar^2}\psi_{\mathrm{II}} = 0$$

$$(\because V = 0)$$

and for region III,

$$\frac{d^2\psi_{\mathrm{III}}}{dx^2} + \frac{2m(E-Vo)}{\hbar^2}\psi_{\mathrm{III}} = 0$$

$\frac{2mE}{\hbar^2} = k^2$ and $\frac{2m(E-Vo)}{\hbar^2} = -k^2$ (as $E < Vo$)

Then the equation in the three regions is written as,

$$\frac{d^2\psi_1}{dx^2} - k^2\psi_1 = 0$$

$$\frac{d^2\psi_{1I}}{dx^2} + k^2\psi_{II} = 0$$

$$\frac{d^2\psi_{III}}{dx^2} - k'^2\psi_{III} = 0$$

Step III: The solutions of these equations are of the form.

$\psi_1 = Ae^{k'x} + Be^{-k'x}$ for $x < 0$

$\psi_{II} = P \cdot e^{ikx} + Q \cdot e^{-ihx}$ for $0 < x < a$

$\psi_{III} = C \cdot e^{k'x} + De^{-k'x}$ for $x > a$

Step IV: As $x \to \pm\infty, \psi$ should not become infinite. Hence $B = 0$ and $C = 0$.

Hence the wave functions in three regions are

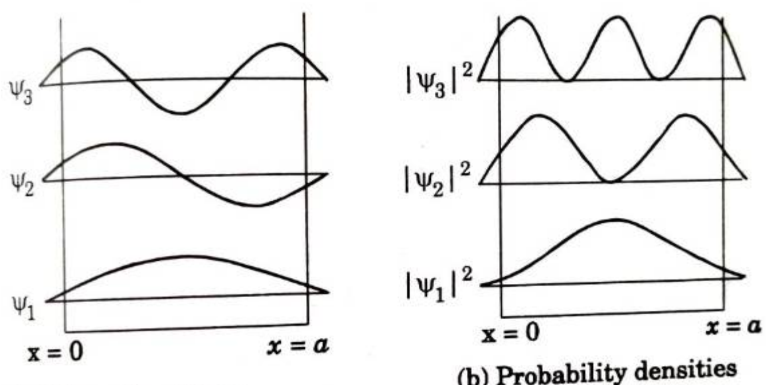
$$\psi_I = Ae^{k'x}$$
$$\psi_{II} = P \cdot e^{ikx} + Q \cdot e^{-ikx}$$
$$\psi_{III} = D \cdot e^{-k'x}$$

Step V: The constants A, P, Q and D can be determined by applying the boundary conditions. The wave function ψ and its derivative $\frac{d\psi}{dx}$ should be continuous in the region where ψ is defined.

$$\Psi_1(0) = \psi_{\text{II}}(0)$$

$$\left[\frac{d\psi_1}{dx}\right]_{x=0} = \left[\frac{d\psi_{\text{II}}}{dx}\right]_{x=0}$$
$$\psi_{\text{II}}(a) = \psi_{\text{III}}(a)$$
$$\left[\frac{d\psi_{\text{II}}}{dx}\right]_{x=a} = \left[\frac{d\psi_{\text{III}}}{dx}\right]_{x=a}$$

- Using these four conditions, we get four equations from which the four constants A, P, Q, D can be determined. Thus the wave functions can be known completely.
- The first three wave functions and probability densities when plotted against x are as shown in fig.



(a) Wave functions

(b) Probability densities inside non - rigid box

- The eigen functions are similar in appearance to those of infinite well except that they extend a little outside the box.
- Even though the particle energy **E** is less than the P.E. V_0, there is a definite probability that the particle is found outside the box.
- The particle energy is not enough to break through the walls of the box but it can penetrate the walls and leak out.
- This shows penetration of the particle into the classically forbidden region.
- The energy levels of the particle are still discrete but there are a finite number of them. Such a limit exists because, soon the particle energy becomes equal to V_0.

  For energies higher than this the particle energy is not quantised but may have any value above V_0.
- These predictions are unique in quantum mechanics and shows different behaviour from that expected in classical physics.