B.Sc. (Semester - 6)
Subject: Physics
Course: US06CPHY21
Quantum Mechanics
UNIT- I Stationary States and Energy Spectra

Stationary States and Energy Spectra:

The state of a quantum mechanical system is specified by giving its wave function Ψ. If a particle moving in a static or time-independent potential, then the solution of the wave equation are describe as a stationary states. In these states, the position probability density $|\Psi|^2$ at every point $\vec{X}$ in space remains independent of time.

When a particle is described by such a wave function its energy has a perfectly definite value. The energy spectrum i.e. the set of energy values associated with the various stationary states is discrete. These energy states are described as a energy spectra.

The Time-Independent Schrodinger Equation:

Let us consider a particle moving in a time-independent potential $V(x)$. By the method of separation of variable, we can write the wave function

$$\Psi(\vec{X},t) = u(\vec{X})\, f(t) \qquad \text{... (1.1)}$$

Substituting this value in

$$i\hbar\, \frac{\partial \Psi(\vec{X},t)}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi(\vec{X},t) + V(\vec{X},t)\Psi(\vec{X},t)$$

$$i\hbar\, \frac{\partial}{\partial t}\left[u(\vec{X})\, f(t)\right] = -\frac{\hbar^2}{2m}\nabla^2\left[u(\vec{X})\, f(t)\right] + V(\vec{X},t)\left[u(\vec{X})\, f(t)\right]$$

Dividing throughout by $u(\vec{X})\, f(t)$, we get

$$\frac{1}{f}\, i\hbar \frac{df}{dt} = -\frac{\hbar^2}{2m}\frac{\nabla^2 u}{u} + V(\vec{X},t) \qquad \text{... (1.2)}$$

The R.H.S is independent of t and L.H.S is independent of $\vec{X}$. Their equality implies that both the sides must be equal to a constant.

$$\therefore\ \frac{1}{f}\, i\hbar \frac{df}{dt} = E$$

$$\therefore\ i\hbar \frac{df(t)}{dt} = E(t) \qquad \text{... (1.3)}$$

And,

$$\left[-\frac{\hbar^2}{2m}\frac{\nabla^2 u}{u} + V(\vec{X})\right] = E$$

$$\therefore\ \left[-\frac{\hbar^2}{2m}\frac{\nabla^2 u}{u} + V(\vec{X})\right] u(\vec{X}) = E u(\vec{X}) \qquad \text{... (1.4)}$$

This is time independent Schrodinger equation.

The solution of equation (1.3) is

$$\frac{df}{f} = \frac{E}{i\hbar}\, dt$$

Integration gives,

$$logf = \frac{E}{i\hbar}t = \frac{-iEt}{\hbar}$$

$$\therefore f = exp\left(\frac{-iEt}{\hbar}\right) \qquad \dots (1.5)$$

The solution of equation (1.4) is depends on the value of E. Hence we can write as $u_E(\vec{X})$.

Hence, equation (1.1) becomes

$$\Psi(\vec{X},t) = u_E(\vec{X})\, e^{-iEt/\hbar} \qquad \dots (1.6)$$

The wave function Ψ would be vanish as $t \to \infty\ or - \infty$. The value of E has to be real. Hence, the probability density becomes

$$\left|\Psi(\vec{X},t)\right|^2 = \left|u_E(\vec{X})\right|^2 \qquad \dots (1.7)$$

Therefore, the probability density is time independent. Expectation value must also be time independent.

Equation (1.4) states that the action of the Hamiltonian operator of the particle on the wave function $u_E(\vec{X})$ is simplify to reproduce the same wave function multiplied by the constant E. $u_E(\vec{X})$ is called *energy eigen function* and E is called *energy eigen value*. The energy eigen values refer as energy levels of the system.

A Particle in a Square Well Potential:

Consider a particle whose potential energy function has the shape of well with vertical sides defined by

$$\left.\begin{array}{lll} V(x) = 0 & for\ x < -a & (Region - I) \\ V(x) = -V_0 & for\ -a < x < a & (Region - II) \\ V(x) = 0 & for\ x > a & (Region - III) \end{array}\right\} \qquad \dots (1.8)$$

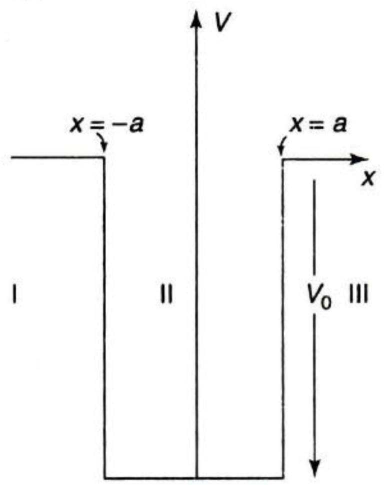

Fig: 1.1

The kinetic energy $(E - V)$ can never be negative. Since, $V = 0$ for $|x| > a$, $(E - V)$ can be positive in this region if $E > 0$. Hence, any particle with $E < 0$ can not enter in the region I and III. It will stay within the potential well between $x = a$ and $x = -a$. Hence, the particle bound by the potential.

The time independent Schrodinger equation for two regions becomes

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dx^2} = Eu, \quad for\ |x| > a \qquad ...(1.9)$$

And

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dx^2} - V_0 u = Eu, \quad for\ |x| < a \qquad ...(1.10)$$

- **Bound States in a Square Well: $(E < 0)$**

(a) Admissible solutions of wave equation:

For $E < 0$, we write equations (1.9) & (1.10) as follows:

$$\frac{d^2u}{dx^2} + \frac{2mE}{\hbar^2}u = 0, \quad for\ |x| > a\ \ (Region: I\ \&\ III) \qquad ...(1.11)$$

$$and \qquad \frac{d^2u}{dx^2} + \frac{2m}{\hbar^2}V_0 u + \frac{2mE}{\hbar^2}u = 0$$

$$\therefore \frac{d^2u}{dx^2} + \frac{2m(E + V_0)}{\hbar^2}u = 0, \quad for\ |x| < a\ \ (Region: II) \qquad ...(1.12)$$

Equations (1.11) & (1.12) can be written as

$$\frac{d^2u}{dx^2} - \alpha^2 u = 0, \quad for\ |x| > a\ \ (Region: I\ \&\ III) \qquad ...(1.13)$$

$$and \qquad \frac{d^2u}{dx^2} + \beta^2 u = 0, \qquad for\ |x| < a\ \ (Region: II) \qquad ...(1.14)$$

Where $-\alpha^2 = \frac{2mE}{\hbar^2}$ and $\beta^2 = \frac{2m(E+V_0)}{\hbar^2}$ are positive constants.

The general solution of equation (1.14) is

$$u^{II}(x) = A\ cos\beta x + B\ sin\beta x \qquad ...(1.15)$$

Where A and B are constants.

This is the solution in region- II.

The general solution of equation (1.13) in the region- I & III is the linear combination of $e^{\alpha x}$ and $e^{-\alpha x}$.

- **For region $- \ I$: $\ -\infty < x < a$**

In this region, as $x \to -\infty$, then $e^{-\alpha x} \to \infty$.

Therefore, the admissible solution in region- I must be of the form

$$u^{I}(x) = C\ e^{\alpha x} \qquad ...(1.16)$$

- **For region $- \ III$: $\ a < x < \infty$**

In this region, as $x \to \infty$, then $e^{\alpha x} \to \infty$.

Therefore, the admissible solution in region- III must be of the form

$$u^{III}(x) = D\ e^{-\alpha x} \qquad ...(1.17)$$

C and D are constants.

The solution $u(x)$ and its first derivative $\frac{du}{dx}$ must be continuous. At the point $x = -a$ where regions I & III meet, we should have

$$u^{I} = u^{II} \quad and \quad \frac{du^{I}}{dx} = \frac{du^{II}}{dx} \quad at \quad (x = -a)$$

$$\therefore C\ e^{-\alpha a} = A\ cos\beta a - B\ sin\beta a \qquad ...(1.18)$$

And

$$-C\,e^{-\alpha a}\alpha = -A\,\sin\beta a\,\beta - B\,\cos\beta a\,\beta$$

$$\therefore C\,\alpha\,e^{-\alpha a} = A\beta\,\sin\beta a + B\beta\,\cos\beta a \qquad \dots(1.19)$$

Similarly, at $x = a$

$$u^{II} = u^{III} \quad and \quad \frac{du^{II}}{dx} = \frac{du^{III}}{dx}$$

$$D\,e^{-\alpha a} = A\,\cos\beta a + B\,\sin\beta a \qquad \dots(1.20)$$

$$and \qquad -D\alpha\,e^{-\alpha a} = -A\beta\,\sin\beta a + B\beta\,\cos\beta a \qquad \dots(1.21)$$

Adding equations (1.18) & (1.20), we get

$$(C + D)e^{-\alpha a} = 2A\,\cos\beta a \qquad \dots(1.22)$$

Adding equations (1.19) & (1.21), we get

$$(C - D)\alpha\,e^{-\alpha a} = 2B\beta\,\cos\beta a \qquad \dots(1.23)$$

Subtracting equations (1.18) & (1.20), we get

$$(C - D)e^{-\alpha a} = -2B\,\sin\beta a$$

$$\therefore\ -(C - D)e^{-\alpha a} = 2B\,\sin\beta a \qquad \dots(1.24)$$

Subtracting equations (1.19) & (1.21), we get

$$(C + D)\alpha\,e^{-\alpha a} = 2A\beta\,\sin\beta a \qquad \dots(1.25)$$

Now, dividing equation (1.25) by (1.22), we get

$$\frac{(C + D)\alpha\,e^{-\alpha a}}{(C + D)e^{-\alpha a}} = \frac{2A\beta\,\sin\beta a}{2A\,\cos\beta a}$$

$$\therefore \alpha = \beta\,\tan\beta a \qquad \dots(1.26)$$

$$\text{unless } A = 0 \text{ and } C + D = 0 \quad i.e. \quad C = -D \qquad \dots(1.27)$$

Now, dividing equation (1.23) by (1.24), we get

$$\frac{(C - D)\alpha\,e^{-\alpha a}}{-(C - D)e^{-\alpha a}} = \frac{2B\beta\,\cos\beta a}{2B\,\sin\beta a}$$

$$\therefore -\alpha = \beta\,\cot\beta a$$

$$\therefore \alpha = -\beta\,\cot\beta a \qquad \dots(1.28)$$

$$\text{unless } B = 0 \text{ and } C - D = 0 \quad i.e. \quad C = D \qquad \dots(1.29)$$

Hence, the combination of equations (1.26) & (1.29) and (1.28) & (1.27) becomes the possible solutions.

There exist two types of admissible solutions.

(1) When, $B = 0$ and $C = D$, then from equation (1.22), we get

$$D = A\,e^{\alpha a}\cos\beta a \qquad \dots(1.30)$$

(2) When, $A = 0$ and $C = -D$, then from equation (1.24), we get

$$2De^{-\alpha a} = 2B\,\sin\beta a$$

$$D = B\,e^{\alpha a}\sin\beta a \qquad \dots(1.31)$$

Hence, we get two set of solutions

$$\left.\begin{array}{l} \alpha = \beta\,\tan\beta a \\ C = D \\ B = 0 \\ D = A\,e^{\alpha a}\cos\beta a \end{array}\right\} \qquad \dots(1.32)$$

And

$$\left.\begin{array}{l} \alpha = -\beta\,\cot\beta a \\ C = -D \\ A = 0 \\ D = B\,e^{\alpha a}\sin\beta a \end{array}\right\} \qquad \dots(1.33)$$

(b) The Energy Eigen Values: (Discrete Spectrum)

Both the types of solutions exist only for certain discrete values of the energy parameter E. We have

$$-\alpha^2 = \frac{2mE}{\hbar^2} \quad and \quad \beta^2 = \frac{2m(E+V_0)}{\hbar^2}$$

$$\therefore\ \alpha^2 + \beta^2 = -\frac{2mE}{\hbar^2} + \frac{2mE}{\hbar^2} + \frac{2mV_0}{\hbar^2}$$

$$\therefore\ \alpha^2 + \beta^2 = \frac{2mV_0}{\hbar^2}$$

Multiplying by a^2 on both the sides ,we get

$$(\alpha^2 + \beta^2)a^2 = \frac{2mV_0a^2}{\hbar^2}$$

$$\therefore (\alpha^2 + \beta^2)a^2 = \frac{V_0}{\hbar^2/_{2ma^2}}$$

$$\therefore (\alpha^2 + \beta^2)a^2 = \frac{V_0}{\Delta} \qquad \dots(1.34)$$

Where, $\Delta = \hbar^2/_{2ma^2}$ is a natural unit of energy as follow.

$$\Delta = \frac{\hbar^2}{2ma^2} = \frac{(m^2\ kg/s)^2}{kg.m^2} = \frac{m^4 kg^2}{kg.m^2 s^2} = \frac{kg\ m^2}{s^2} = Joul$$

In equation (1.34) $\frac{V_0}{\Delta}$ is a measure of strength of the potential.

Since α and β are positive constants. Hence, $\alpha/_\beta = tan\beta a$ must be positive and hence values of βa lying in the following intervals are admissible.

$$2r\frac{\pi}{2} \le \beta a \le (2r+1)\frac{\pi}{2} \qquad \dots(1.35)$$

$$Here, \quad (r = 0,1,2,\dots)$$

Now, substituting $\alpha = \beta\ tan\beta a$ in equation (1.34), we get

$$(\beta^2 tan^2\beta a + \beta^2)a^2 = \frac{V_0}{\Delta}$$

$$\therefore \beta^2 a^2(tan^2\beta a + 1) = \frac{V_0}{\Delta}$$

$$\therefore \beta^2 a^2\ sec^2\beta a = \frac{V_0}{\Delta}$$

$$\therefore\ sec^2\beta a = \frac{V_0}{\beta^2 a^2\ \Delta} \qquad \dots(1.36)$$

$$or \qquad |cos\beta a| = \left(\frac{\Delta}{V_0}\right)^{1/2} \beta a \qquad \dots(1.37)$$

The modulus sign arises because the left hand side of the equation is known to be positive.

Similarly, substituting $\alpha = -\beta\ cot\beta a$ in equation (1.34), we get

$$(\beta^2 cot^2\beta a + \beta^2)a^2 = \frac{V_0}{\Delta}$$

$$\therefore \beta^2 a^2(cot^2\beta a + 1) = \frac{V_0}{\Delta}$$

$$\therefore\ cosec^2\beta a = \frac{V_0}{\beta^2 a^2\ \Delta} \qquad \dots(1.38)$$

$$or \quad |sin\beta a| = \left(\frac{\Delta}{V_0}\right)^{1/2} \beta a \qquad \ldots (1.39)$$

Here also α and β are positive, but $^{\alpha}/_{\beta} = cot\beta a$, must be negative. Hence value of βa lying in the intervals

$$(2r-1)\frac{\pi}{2} \leq \beta a \leq 2r\frac{\pi}{2} \qquad \ldots (1.40)$$

$$Here, \quad (r = 1,2, \ldots)$$

Equations (1.37) & (1.39) can be satisfied only by certain specific discrete values of β, which can be found graphically. These values called β_n are determined by the intersections of the straight line $\left(^{\Delta}/_{V_0}\right)^{1/2} \beta a$ with the curves for $|cos\beta a|$ and $|sin\beta a|$ are shown as solid lines and dashed line respectively in fig.(1.2). The parts to be ignored are indicated by dotted lines.

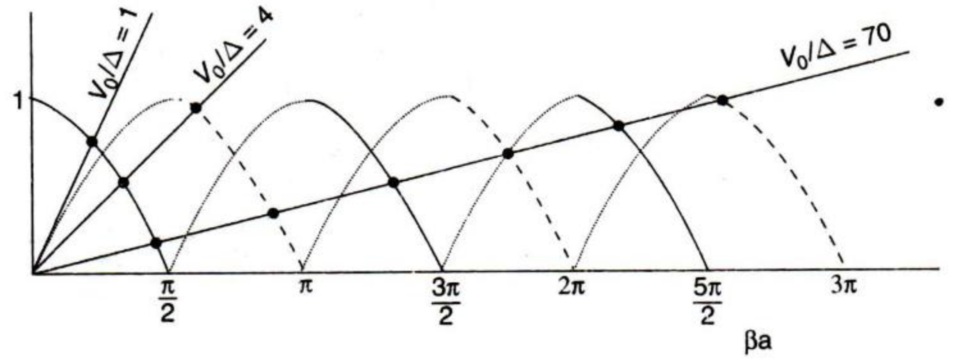

Fig:1.2

If the intersections occur at $\beta = \beta_n$ $(n = 0,1,2 \ldots)$ the corresponding allowed values of the energy are obtained as follows.

We know that,

$$\beta^2 = \frac{2m(E+V_0)}{\hbar^2}$$

For all possible values of n, we can write

$$(\beta_n)^2 = \frac{2m(E_n+V_0)}{\hbar^2}$$

$$\therefore E_n + V_0 = \frac{(\beta_n)^2\hbar^2}{2m}$$

$$\therefore E_n + V_0 = \frac{(\beta_n)^2\hbar^2}{2m} \times \frac{a^2}{a^2}$$

$$\therefore E_n + V_0 = \frac{(\beta_n a)^2\hbar^2}{2ma^2}$$

$$\therefore E_n + V_0 = (\beta_n a)^2 \times \frac{\hbar^2}{2ma^2} = (\beta_n a)^2\Delta$$

$$\therefore E_n = (\beta_n a)^2\Delta - V_0$$

$$\therefore E_n = \left[(\beta_n a)^2\frac{\Delta}{V_0} - 1\right]V_0 \qquad \ldots (1.41)$$

From fig.(1.2), if $\left(\frac{\Delta}{V_0}\right)^{1/2}\beta a \to 1$ in the interval

$$\frac{1}{2}\pi N \leq \beta a \leq \frac{1}{2}\pi(N+1)$$

then there are $(N+1)$ intersections. In other words, the number of discrete energy level is $(N+1)$ if

$$\frac{1}{2}\pi N\left(\frac{\Delta}{V_0}\right)^{1/2} \leq 1 \leq \frac{1}{2}\pi(N+1)\left(\frac{\Delta}{V_0}\right)^{1/2}$$

$$or \qquad N \leq \frac{2}{\pi}\left(\frac{V_0}{\Delta}\right)^{1/2} < (N+1) \qquad \ldots(1.42)$$

Hence, *there exists at least one bound state, however weak the potential may be.*

(c) The Energy Eigen Functions; Parity:

We have the eigen functions

$$u^I(x) = C\, e^{\alpha x}\ , \qquad x < -a \qquad \ldots(1.43)$$
$$u^{II}(x) = A\, cos\beta x + B\, sin\beta x \quad , -a < x < q \qquad \ldots(1.44)$$
$$u^{III}(x) = D\, e^{-\alpha x}, \qquad x > a \qquad \ldots(1.45)$$

Using equation (1.32), we get

$$u^I(x) = A\, e^{\alpha a} cos\beta a\, e^{\alpha x}\ , \qquad x < -a \qquad \ldots(1.46)$$
$$u^{II}(x) = A\, cos\beta x\ , \qquad -a < x < q \qquad \ldots(1.47)$$
$$u^{III}(x) = A\, e^{\alpha a} cos\beta a\, e^{-\alpha x}, \qquad x > a \qquad \ldots(1.48)$$

If we represents values of $\alpha = \alpha_n$ and $\beta = \beta_n$ then above equations becomes

$$u_n{}^I(x) = A\, e^{\alpha_n a} cos\beta_n a\, e^{\alpha_n x}\ , \qquad x < -a \qquad \ldots(1.49)$$
$$u_n{}^{II}(x) = A\, cos\beta_n x\ , \qquad -a < x < q \qquad \ldots(1.50)$$
$$u_n{}^{III}(x) = A\, e^{\alpha_n a} cos\beta_n a\, e^{-\alpha_n x}, \qquad x > a \qquad \ldots(1.51)$$
$$n = 0,1,2, \ldots$$

The nature of such functions is illustrated graphically in fig.(1.3). $u_n(x)$ is symmetric about the origin.

$$u_n(x) = u_n(-x) \qquad \ldots(1.52)$$

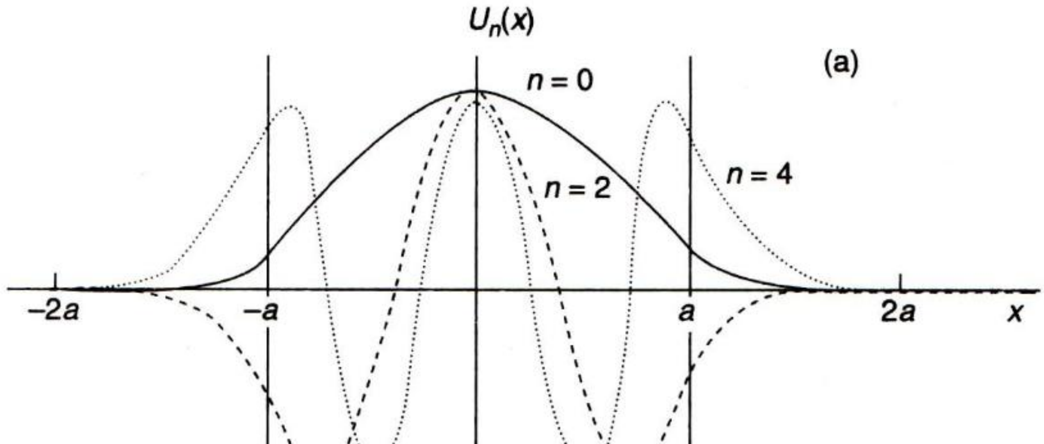

Fig: 1.3

Any wave function which has this symmetry property is said to be of *even parity*.

The eigen function corresponding to $n = 1,3,5, ...$ are characterized by equation (1.33). We have

$$u_n{}^I(x) = -(B\, e^{\alpha_n a} sin\beta_n a\,)e^{\alpha_n x}\ , \qquad x < -a \qquad ...(1.53)$$

$$u_n{}^{II}(x) = B\ sin\beta_n x\ , \qquad -a < x < q \qquad ...(1.54)$$

$$u_n{}^{III}(x) = (B\, e^{\alpha_n a} sin\beta_n a)\ e^{-\alpha_n x}, \qquad x > a \qquad ...(1.55)$$

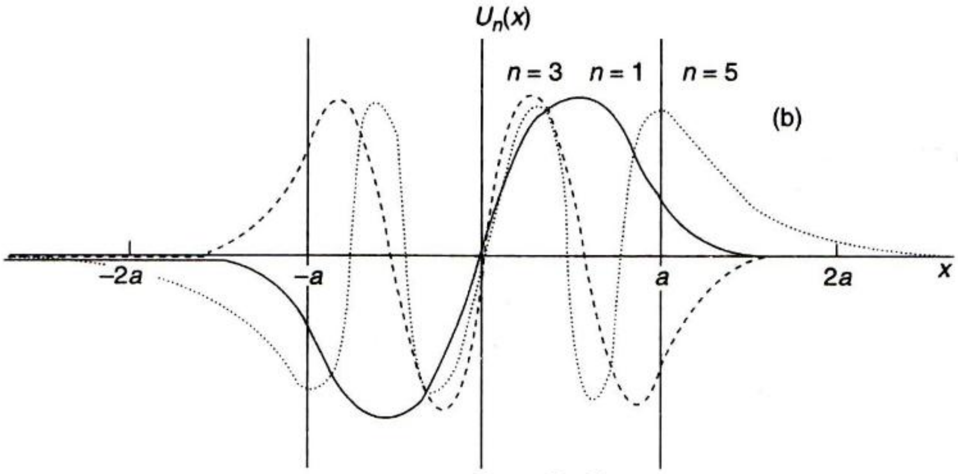

Fig: 1.4

These functions are illustrated in fig.(1.4). They are anti-symmetric with respect to the origin.

$$i.e. \qquad u_n(x) = -u_n(-x) \qquad ...(1.56)$$

Any wave function which has this property of anti-symmetric is said to be of *odd parity*.

Penetration into Classically Forbidden Regions:

We know that a classical particle of energy $E < 0$ can stay only in region-II and cannot at all entre region-I and III. However, the quantum mechanical wave functions $u_n(x)$ have non vanishing values in both these classically forbidden regions. Hence, there is probability of finding the particle in regions I & III. In this regions $|\Psi|^2 \rightarrow 0$, hence for a large value of x, the $probability \rightarrow 0$. Therefore, the particle cannot escape to infinity distance, it stay bound to the potential.

The Square Well: Non-Localized States($E > 0$) :

In this case, the Schrodinger equations can be written as,

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dx^2} = Eu,\ \ for\ \ x < -a\ \ and\, x > a\ \ \ (Region{:}\, I\ \&\ III) \qquad ...(1.57)$$

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dx^2} - V_0 u = Eu,\ \ for\ \ x < -a\ \ and\, x > a\ \ \ (Region{:}\, II) \qquad ...(1.58)$$

When, $E > 0$, $\frac{2mE}{\hbar^2}$ is positive.

Suppose $\frac{2mE}{\hbar^2} = k^2$ and $\frac{2m(E+V_0)}{\hbar^2} = \beta^2$. Hence equations (1.57) & (1.58) becomes

$$\frac{d^2u}{dx^2} + k^2u = 0, \ \ for \ \ x < -a \ \ and \ x > a \ \ \ (Region: I \ \& \ III) \qquad \dots(1.59)$$

$$\frac{d^2u}{dx^2} + \beta^2u = 0, \qquad for \ \ x < -a \ \ and \ x > a \ \ \ (Region: II) \qquad \dots(1.60)$$

The general solution of equations (1.59) & (1.60) are

$$u^I = C_+ \, e^{ikx} + C_- \, e^{-ikx} \ , \qquad x < -a \qquad \dots(1.61)$$

$$u^{III} = D_+ \, e^{ikx} + D_- \, e^{-ikx} \ , \qquad x > a \qquad \dots(1.62)$$

$$and \qquad u^{II} = A_+ \, e^{i\beta x} + A_- \, e^{-i\beta x} \ , \qquad -a < x < a \qquad \dots(1.63)$$

- **Physical Interpretation:**

In equation (1.58) the plane wave $C_+ \, e^{ikx}$ represent the motion of particle from $x = -\infty$ to $x = -a$ i.e. towards right hand side and plane wave $C_- \, e^{-ikx}$ represent the motion from $x = -a$ to $x = -\infty$ i.e. to L.H.S. Similarly $D_+ \, e^{ikx}$ and $D_- \, e^{-ikx}$ represents the wave travel towards R.H.S and L.H.S from $x = +a$ to $x = +\infty$ respectively. Similarly, we can interpreted equation (1.63) between the limits $x = -a$ to $x = +a$.

- **Boundary Conditions:**

The potential $V_0 = 0$ when $x < -a$ and $x > a$. Here, $E > 0$. Hence, the particle has a positive kinetic energy. The particle cannot stay in the region. Therefore, the boundary conditions

$$\lim_{x \to -\infty} u^I(x) \to 0 \qquad and \quad \lim_{x \to \infty} u^{III}(x) \to 0$$

are not satisfied. A particle with the wave functions (1.61), (1.62) & (1.63) is not localized. It is not confined to any finite region of space. Since $|u(x)|^2$ remains nonzero even when $x \to \pm\infty$. Such wave functions are not normalizable.

The solution and its first derivatives must be continuous at $x = -a$ and $x = +a$. Here, there is not any restrictions on k or β. Hence, any energy $E > 0$ is an eigen value. When $E > 0$, the continuity conditions gives four equations but they involve six unknowns $A_\pm, C_\pm, D_\pm$. Since, the number of equations is less than the number of unknowns. An infinite number of solutions exist. Thus, the energy eigen values from a continuous (not a discrete) set. Hence, the energy spectrum for $E > 0$ is a continuum.

The probability of reflection is given by

$$R = \left[1 + \frac{4E \ (E + V_0}{V_0^2 sin^2 \left\{ 2 \sqrt{\frac{(E+V_0)}{\Delta}} \right\}} \right]^{-1} \qquad \dots(1.64)$$

This expression is shown graphically in fig.(1.5).

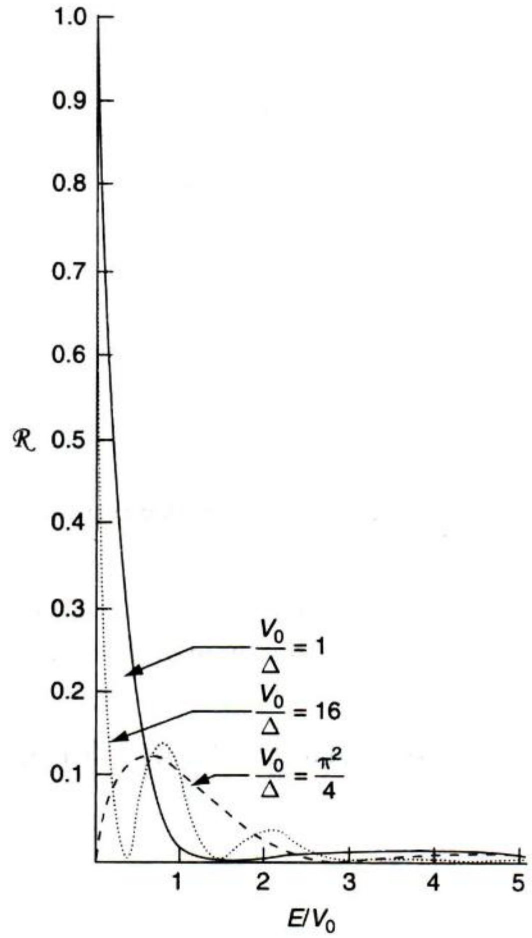

Fig: 1.5

For very low energies $E \to 0$, the reflection is almost total. As $\left(E/_{V_0}\right)$ increases, R oscillates between zero and $\left[1 + \frac{4E(E+V_0)}{V_0^2}\right]^{-1}$. This bound depends only on $\left(E/_{V_0}\right)$, not the width of the potential well.

- The frequency of oscillation depends on the parameter $\Delta = \frac{\hbar^2}{2ma^2}$, i.e. depend on width of the potential well.
- The complete transmission occurs $(R = 0)$ when the energy is such that

$$\left\{2\frac{\sqrt{(E+V_0)}}{\Delta}\right\} = sin(2\beta a) = 0$$

The Square Potential Barrier:

(a) Quantum Mechanical Tunneling:

Let us consider a potential barrier as shown in fig.(1.6). There is a effect of the penetration of the wave function into classically forbidden regions. It means there is an ability of particles to *tunnel* through barriers of height V_0.

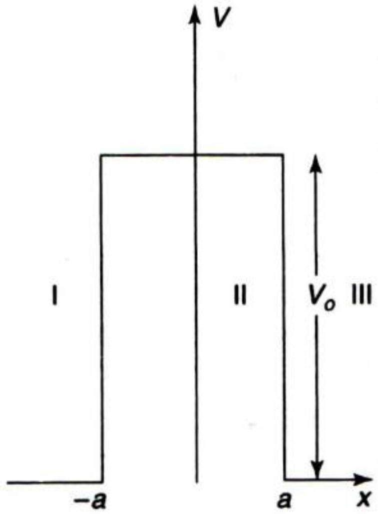

Fig: 1.6

The potential of the square well barrier is given by

$$V_0 = \begin{cases} 0\,, & x < -a \\ V_0\,, & -a < x < a \\ 0, & x > a \end{cases} \qquad \ldots(1.65)$$

The Schrodinger equations for region I and III becomes

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dx^2} = Eu, \quad for\ |x| > a$$

$$\therefore\ \frac{d^2u}{dx^2} + \frac{2mE}{\hbar^2}u = 0$$

$$\therefore\ \frac{d^2u}{dx^2} + \alpha^2 u = 0 \qquad \ldots(1.66)$$

Where, $\alpha^2 = \frac{2mE}{\hbar^2}$

The Schrodinger equation in region II is given by

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dx^2} + V_0 u = Eu, \quad for\ |x| < a$$

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

$$\therefore\ \frac{d^2u}{dx^2} - \beta^2 u = 0 \qquad \ldots(1.67)$$

Where, $\beta^2 = -\frac{2m}{\hbar^2}(E - V_0)$

The solutions of equations (1.66) are

$$u^I = A_+\, e^{i\alpha x} + A_-\, e^{-i\alpha x}\ , \qquad x < -a \qquad \ldots(1.68)$$

$$and \quad u^{III} = C_+\, e^{i\alpha x} + C_-\, e^{-i\alpha x}\ , \qquad x > a \qquad \ldots(1.69)$$

A_+, A_-, C_+ & C_- are constants.

- $A_+\, e^{i\alpha x}$ represent the particles are incident on the barrier only from the left side with positive momentum, and
- $A_-\, e^{-i\alpha x}$ represent the particles moving with momentum $-\hbar k$ away from the barrier i.e. the particles reflected by the barrier.

$$\therefore\ Amplitude\ for\ reflection = \left|\frac{A_-}{A_+}\right|$$

$$\therefore Reflection\ probability = \left|\frac{A_-}{A_+}\right|^2 \qquad ...(1.70)$$

In region III , the particles cannot moving to left, Hence $C_- = 0$

$$u^{III} = C_+ \, e^{i\alpha x} \qquad ...(1.71)$$

This wave function represent that particles moving to the right, which could come only by tunneling through the barrier from region-I.

$$\therefore The\ amplitude\ for\ tuneeling = \left|\frac{C_+}{A_+}\right|$$

$$\therefore Tunneling\ \ probability = \left|\frac{C_+}{A_+}\right|^2 \qquad ...(1.72)$$

The solution of equation (1.66) in region II is

$$u^{II} = B_+ \, e^{\beta x} + B_- \, e^{-\beta x} \qquad ...(1.73)$$

Now, the continuity conditions at $x = -a$ are

$$u^I = u^{II} \quad and \quad \frac{du^I}{dx} = \frac{du^{II}}{dx}$$

Hence, using continuity condition, we have

$$A_+ \, e^{-i\alpha a} + A_- \, e^{i\alpha a} = B_+ \, e^{-\beta a} + B_- \, e^{\beta a} \qquad ...(1.74)$$

$$and \qquad -i\alpha A_+ \, e^{-i\alpha a} + i\alpha A_- \, e^{i\alpha a} = -\beta B_+ \, e^{-\beta a} + \beta B_- \, e^{\beta a}$$

$$i\alpha A_+ \, e^{-i\alpha a} - i\alpha A_- \, e^{i\alpha a} = \beta B_+ \, e^{-\beta a} - \beta B_- \, e^{\beta a} \qquad ...(1.75)$$

Similarly, at $x = +a$

$$u^{II} = u^{III} \quad and \quad \frac{du^{II}}{dx} = \frac{du^{III}}{dx}$$

$$B_+ \, e^{\beta a} + B_- \, e^{-\beta a} = C_+ \, e^{i\alpha a} \qquad ...(1.76)$$

$$and \qquad \beta B_+ \, e^{\beta a} - \beta B_- \, e^{-\beta a} = i\alpha C_+ \, e^{i\alpha a} \qquad ...(1.77)$$

Dividing equations (1.77) by (1.76), we have

$$\frac{\beta B_+ \, e^{\beta a} - \beta B_- \, e^{-\beta a}}{B_+ \, e^{\beta a} + B_- \, e^{-\beta a}} = \frac{i\alpha C_+ \, e^{i\alpha a}}{C_+ \, e^{i\alpha a}} = i\alpha$$

$$\therefore \ i\alpha\left(B_+ \, e^{\beta a} + B_- \, e^{-\beta a}\right) = \beta B_+ \, e^{\beta a} - \beta B_- \, e^{-\beta a}$$

$$\therefore \ i\alpha \, B_- \, e^{-\beta a} + \beta B_- \, e^{-\beta a} = \beta B_+ \, e^{\beta a} - i\alpha \, B_+ \, e^{\beta a}$$

$$\therefore B_- \, e^{-\beta a}(\beta + i\alpha) = B_+ \, e^{\beta a}(\beta - i\alpha)$$

$$\therefore B_- = B_+ \, e^{2\beta a} \frac{(\beta - i\alpha)}{(\beta + i\alpha)}$$

$$\therefore B_- = B_+ \frac{\beta - i\alpha}{\beta + i\alpha} \, e^{2\beta a} \qquad ...(1.78)$$

Now, dividing equation (1.75) by (1.74), we get

$$\frac{i\alpha A_+ \, e^{-i\alpha a} - i\alpha A_- \, e^{i\alpha a}}{A_+ \, e^{-i\alpha a} + A_- \, e^{i\alpha a}} = \frac{\beta B_+ \, e^{-\beta a} - \beta B_- \, e^{\beta a}}{B_+ \, e^{-\beta a} + B_- \, e^{\beta a}}$$

Substituting the value of B_- from equation (1.78), we get

$$\frac{i\alpha A_+ \, e^{-i\alpha a} - i\alpha A_- \, e^{i\alpha a}}{A_+ \, e^{-i\alpha a} + A_- \, e^{i\alpha a}} = \frac{\beta B_+ \, e^{-\beta a} - \beta B_+ \frac{\beta - i\alpha}{\beta + i\alpha} \, e^{2\beta a} \, e^{\beta a}}{B_+ \, e^{-\beta a} + B_+ \frac{\beta - i\alpha}{\beta + i\alpha} \, e^{2\beta a} \, e^{\beta a}}$$

$$= \frac{B_+ \, e^{\beta a} \, \beta \left\{e^{-2\beta a} - \left(\frac{\beta - i\alpha}{\beta + i\alpha}\right) e^{2\beta a}\right\}}{B_+ \, e^{\beta a} \left\{e^{-2\beta a} + \left(\frac{\beta - i\alpha}{\beta + i\alpha}\right) e^{2\beta a}\right\}}$$

$$= \frac{\beta\ \left\{e^{-2\beta a} - \left(\frac{\beta - i\alpha}{\beta + i\alpha}\right) e^{2\beta a}\right\}}{\left\{e^{-2\beta a} + \left(\frac{\beta - i\alpha}{\beta + i\alpha}\right) e^{2\beta a}\right\}}$$

$$= \frac{\beta\ \{(\beta + i\alpha)e^{-2\beta a} - (\beta - i\alpha)e^{2\beta a}\}}{\{(\beta + i\alpha)e^{-2\beta a} + (\beta - i\alpha)e^{2\beta a}\}}$$

$$= \frac{\beta\ \{\beta\, e^{-2\beta a} + i\alpha\, e^{-2\beta a} - \beta\, e^{2\beta a} + i\alpha e^{2\beta a}\}}{\{\beta\, e^{-2\beta a} + i\alpha\, e^{-2\beta a} + \beta\, e^{2\beta a} - i\alpha e^{2\beta a}\}}$$

$$= \frac{\beta\ \{-\beta\left(e^{2\beta a} - e^{-2\beta a}\right) + i\alpha\left(e^{2\beta a} + e^{-2\beta a}\right)\}}{\{\beta\ (e^{2\beta a} + e^{-2\beta a}) - i\alpha\ (e^{2\beta a} - e^{-2\beta a})\}}$$

$$= \frac{\beta\ \{-\beta\ sinh(2\beta a) + i\alpha\ cosh(2\beta a)\}}{\{\beta\ cosh(2\beta a) - i\alpha\ sinh(2\beta a)\}}$$

$$\therefore\ \left\{i\alpha A_+\, e^{-i\alpha a} - i\alpha A_-\, e^{i\alpha a}\right\}\{\beta\ cosh(2\beta a) - i\alpha\ sinh(2\beta a)\}$$
$$= \left\{A_+\, e^{-i\alpha a} + A_-\, e^{i\alpha a}\right\}\beta\ \{-\beta\ sinh(2\beta a) + i\alpha\ cosh(2\beta a)\}$$

$$\therefore\ i\alpha A_+\beta\ cosh(2\beta a)\, e^{-i\alpha a} + \alpha^2 A_+ sin\,h(2\beta a)\, e^{-i\alpha a} - i\alpha\beta A_-\, cosh(2\beta a)\, e^{i\alpha a}$$
$$- \alpha^2 A_- sin\,h(2\beta a)\, e^{i\alpha a}$$
$$= \beta\ i\alpha A_+\ cosh(2\beta a)\, e^{-i\alpha a} - \beta^2 A_+ sin\,h(2\beta a)\, e^{-i\alpha a}$$
$$+ i\alpha\beta A_-\ cosh(2\beta a)\, e^{i\alpha a} - \beta^2 A_- sin\,h(2\beta a)\, e^{i\alpha a}$$

$$\therefore\ A_+\left\{i\alpha\beta\ cosh(2\beta a)\, e^{-i\alpha a} + \alpha^2 sin\,h(2\beta a)\, e^{-i\alpha a} - i\alpha\beta A_-\ cosh(2\beta a)\, e^{i\alpha a}\right.$$
$$\left. + \beta^2 sin\,h(2\beta a)\, e^{-i\alpha a}\right\}$$
$$= A_-\left\{i\alpha\beta\ cosh(2\beta a)\, e^{i\alpha a} + \alpha^2 sin\,h(2\beta a)\, e^{i\alpha a} + i\alpha\beta\ cosh(2\beta a)\, e^{i\alpha a}\right.$$
$$\left. - \beta^2 sin\,h(2\beta a)\, e^{i\alpha a}\right\}$$

$$\therefore\ A_+(\alpha^2 + \beta^2) sin\,h(2\beta a)\, e^{-i\alpha a}$$
$$= A_-\left\{2i\alpha\beta\ cosh(2\beta a)\, e^{i\alpha a} + (\alpha^2 - \beta^2) sin\,h(2\beta a)\, e^{i\alpha a}\right\}$$

$$\therefore\ \frac{A_-}{A_+} = \frac{(\alpha^2 + \beta^2) sin\,h(2\beta a)\, e^{-i\alpha a}}{\{(\alpha^2 - \beta^2) sin\,h(2\beta a)\, e^{i\alpha a} + 2i\alpha\beta\ cosh(2\beta a)\, e^{i\alpha a}\}}$$

$$\therefore\ \frac{A_-}{A_+} = \frac{-i(\alpha^2 + \beta^2)\ e^{-2i\alpha a}\ sin\,h(2\beta a)}{-i(\alpha^2 - \beta^2) sin\,h(2\beta a) + 2\alpha\beta\ cosh(2\beta a)} \qquad \dots(1.79)$$

Now,

$$\frac{C_+}{A_+} = \frac{C_+}{B_+}\frac{B_+}{A_+} \qquad \dots(1.80)$$

But, equation (1.76) is

$$B_+\, e^{\beta a} + B_-\, e^{-\beta a} = C_+\, e^{i\alpha a} \qquad \dots(1.81)$$

Substituting the value of B_- form equation (1.78), we get

$$B_+\, e^{\beta a} + B_+\, \frac{(\beta - i\alpha)}{(\beta + i\alpha)} e^{2\beta a} e^{-\beta a} = C_+\, e^{i\alpha a}$$

$$\therefore\ B_+\left\{e^{\beta a} + \frac{(\beta - i\alpha)}{(\beta + i\alpha)} e^{\beta a}\right\} = C_+\, e^{i\alpha a}$$

$$\therefore\ B_+\, e^{\beta a}\left\{\frac{(\beta + i\alpha) + (\beta - i\alpha)}{(\beta + i\alpha)}\right\} = C_+\, e^{i\alpha a}$$

$$\therefore \frac{C_+}{B_+} = \frac{e^{\beta a}(2\beta)e^{-\beta a}}{(\beta + i\alpha)} \qquad \dots(1.82)$$

Similarly, we can obtain

$$\therefore \frac{B_+}{A_+} = \frac{\{\alpha\, e^{-\beta a}\, e^{-i\alpha a}\,(\beta + i\alpha)\}}{-i(\alpha^2 - \beta^2)sin\,h(\,2\beta a) + 2\alpha\beta\,cosh(\,2\beta a)} \qquad \dots(1.83)$$

Using equations (1.82) & (1.83) in (1.80) ,we get

$$\frac{C_+}{A_+} = \frac{e^{\beta a}(2\beta)e^{-\beta a}\{\alpha\, e^{-\beta a}\, e^{-i\alpha a}\,(\beta + i\alpha)\}}{(\beta + i\alpha)\{-i(\alpha^2 - \beta^2)sin\,h(\,2\beta a) + 2\alpha\beta\,cosh(\,2\beta a)\}}$$

$$\therefore \frac{C_+}{A_+} = \frac{2\alpha\beta\, e^{-2i\alpha a}}{\{-i(\alpha^2 - \beta^2)sin\,h(\,2\beta a) + 2\alpha\beta\,cosh(\,2\beta a)\}} \qquad \dots(1.84)$$

The transmission probability is given by

$$T = \left|\frac{C_+}{A_+}\right|^2$$

$$\therefore T = \frac{4\,\alpha^2\beta^2}{\{-i(\alpha^2 - \beta^2)sin\,h(\,2\beta a) + 2\alpha\beta\,cosh(\,2\beta a)\} \times \{-i(\alpha^2 - \beta^2)sin\,h(\,2\beta a) + 2\alpha\beta\,cosh(\,2\beta a)\}}$$

$$\therefore T = \left\{\frac{(\alpha^2 - \beta^2)^2 sinh^2(2\beta a) - 4\alpha^2\beta^2 sinh^2(2\beta a) + 4\alpha^2\beta^2 cosh^2(2\beta a)}{4\,\alpha^2\beta^2}\right\}^{-1}$$

$$\therefore T = \left[1 + \frac{(\alpha^2 + \beta^2)^2 sinh^2(2\beta a)}{4\,\alpha^2\beta^2}\right]^{-1} \qquad \dots(1.85)$$

But, $\alpha^2 = \frac{2mE}{\hbar^2}$ and $\beta^2 = -\frac{2m}{\hbar^2}(E - V_0)$

$$\therefore T = \left[1 + \frac{\left\{\frac{2mE}{\hbar^2} - \frac{2mE}{\hbar^2} + \frac{2mV_0}{\hbar^2}\right\}^2 sinh^2(2\beta a)}{4\,\frac{2mE}{\hbar^2}\,\frac{2m(V_0 - E)}{\hbar^2}}\right]^{-1}$$

$$\therefore T = \left[1 + \frac{V_0^2}{4(V_0 - E)E}\, sin^2\left\{2\sqrt{\frac{(V_0 - E)}{\Delta}}\right\}\right]^{-1} \qquad (because\ (\beta a)^2 = \frac{(V_0 - E)}{\Delta}$$

- **Case: I**

If $2\sqrt{\frac{(V_0 - E)}{\Delta}} = y \gg 1$

$$\therefore T = \left[1 + \frac{V_0^2}{4(V_0 - E)E}\, sin^2 y\right]^{-1} \qquad \dots(1.86)$$

But, $y \gg 1$

$$\therefore sin\,hy = \frac{1}{2}(e^y - e^{-y}) \rightarrow \frac{1}{2}e^y$$

$$\therefore sin\,hy = \frac{1}{4}e^{2y}$$

$$\therefore T = \left[\frac{V_0^2}{4(V_0 - E)E}\,\frac{e^{4\sqrt{\frac{(V_0 - E)}{\Delta}}}}{4}\right]^{-1}$$

$$\therefore T = \frac{16(V_0 - E)E}{V_0^2}\; e^{-4\sqrt{\frac{(V_0 - E)}{\Delta}}}$$

$$\therefore T = \frac{16(V_0 - E)E}{V_0^2} \; exp\left\{-4\sqrt{\frac{(V_0 - E)}{\Delta}}\right\} \qquad \ldots (1.87)$$

Hence, if $V_0 \gg E$ then, $\ll 1$, i.e. transmission probability decreases exponentially.

- **Case: II**

If $y \ll 1$

$$sinhy = \frac{1}{2}(e^y - e^{-y}) \rightarrow \frac{1}{2}[1 + y + \cdots..-1 + y - \cdots.]$$

$$\therefore \; sinhy = y$$

Hence, equation (1.86) becomes

$$T = \left[1 + \frac{V_0^2}{4(V_0 - E)E} \; sin^2 y\right]^{-1} = \left[1 + \frac{V_0^2}{4(V_0 - E)E} \; \frac{4(V_0 - E)}{\Delta}\right]^{-1}$$

$$\therefore T = \left[1 + \frac{V_0^2}{\Delta E}\right]^{-1} \qquad \ldots (1.88)$$

The graph of transmission probability is shown in fig.(1.7)

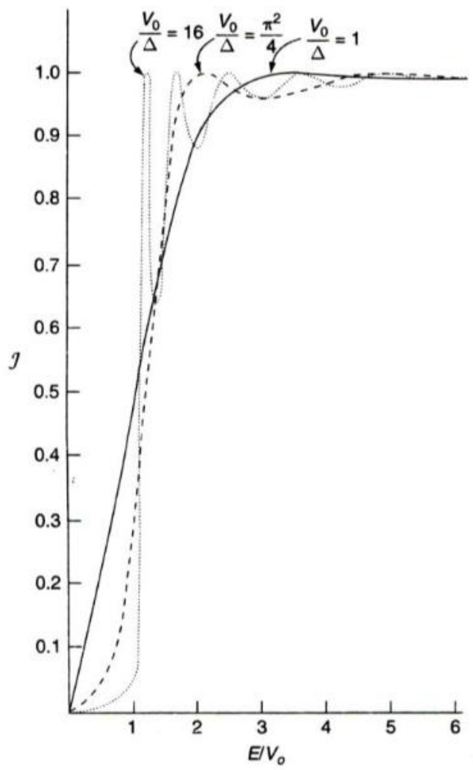

Fig: 1.7

(b) Reflection at potential barrier and well:

The reflection probability is given by

$$R = \left|\frac{A_-}{A_+}\right|^2$$

$$\therefore R = \frac{(\alpha^2 + \beta^2)^2 sinh^2(2\beta a)}{(\alpha^2 - \beta^2)^2 sinh^2(2\beta a) + 4\alpha^2\beta^2 cosh^2(2\beta a)}$$

$$\therefore R = \frac{(\alpha^2 + \beta^2)^2 sinh^2(2\beta a)}{(\alpha^2 + \beta^2)^2 sinh^2(2\beta a) - 4\alpha^2\beta^2 sinh^2(2\beta a) + 4\alpha^2\beta^2 cosh^2(2\beta a)}$$

$$\therefore R = \frac{(\alpha^2 + \beta^2)^2 sinh^2(2\beta a)}{(\alpha^2 + \beta^2)^2 sinh^2(2\beta a) + 4\alpha^2\beta^2} \quad \dots (1.89)$$

$$\therefore R + T = \frac{(\alpha^2 + \beta^2)^2 sinh^2(2\beta a)}{(\alpha^2 + \beta^2)^2 sinh^2(2\beta a) + 4\alpha^2\beta^2} + \frac{4\alpha^2\beta^2}{(\alpha^2 + \beta^2)^2 sinh^2(2\beta a) + 4\alpha^2\beta^2}$$

$$\therefore R + T = 1 \quad \dots (1.90)$$

Probability of reflection: For $E > V_0$

$$R = \frac{(\alpha^2 + \beta^2)^2 sinh^2(2\beta a)}{(\alpha^2 - \beta^2)^2 sinh^2(2\beta a) + 4\alpha^2\beta^2 cosh^2(2\beta a)}$$

But in the case of $E < V_0$, $\beta = i\beta'$

$$\therefore \ \beta^2 = -\beta'^2$$

$$\therefore R = \frac{(\alpha^2 - \beta'^2)^2 sinh^2(2i\beta' a)}{(\alpha^2 + \beta'^2)^2 sinh^2(2i\beta' a) - 4\alpha^2\beta'^2 cosh^2(2i\beta' a)}$$

$$\therefore R = \frac{(\alpha^2 - \beta'^2)^2 sin^2(2\beta' a)}{(\alpha^2 + \beta'^2)^2 sin^2(2\beta' a) - 4\alpha^2\beta'^2 cos^2(2\beta' a)}$$

$$\therefore R = \left[1 + \frac{4\alpha^2\beta'^2}{(\alpha^2 - \beta'^2)^2 sin^2(2\beta' a)}\right]^{-1} \quad \dots (1.91)$$

Substituting the value of α and β, we get

$$\therefore R = \left[1 + \frac{4E(V_0 - E)}{V_0^2 sin^2\left\{2\sqrt{\frac{(E - V_0)}{\Delta}}\right\}}\right]^{-1} \quad \dots (1.92)$$

The graph of reflection probability is shown in fig.(1.8).

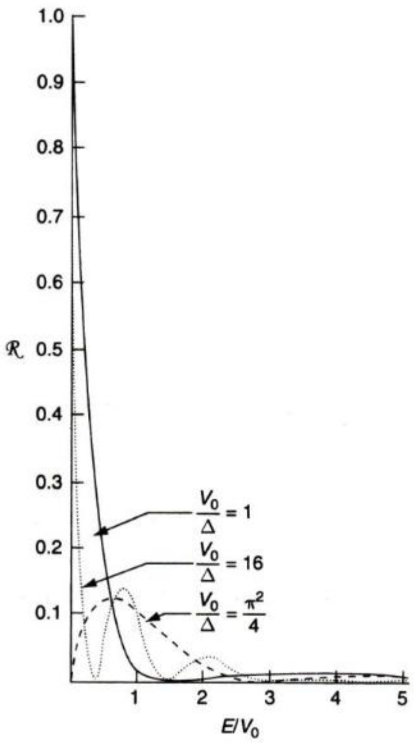

Fig: 1.8

Question Bank

Multiple choice questions:

(1) The operator operating on the wave function should always standing on _____ side

(a) Middle (b) **Right**
(c) Left (d) Upper

(2) According to the wave function and it first partial derivative should be _______ functions for all values of $\vec{X}$

(a) Zero (b) **Continuous**
(c) Infinity (d) discontinuous

(3) If the particle moving in a ______ potential then the solution of the wave equation are describe as a stationary states

(a) **time independent** (b) time dependent
(c) velocity dependent (d) velocity independent

(4) Any particle with energy _____ cannot enter in the regions I and III

(a) $E = 0$ (b) $E = \propto$
(c) $\boldsymbol{E} < 0$ (d) $E > 0$

(5) For bound state of a particle in a square well the energy is _______

(a) $E = 0$ (b) $E = \propto$
(c) $\boldsymbol{E} < 0$ (d) $E > 0$

(6) The limit of a region-I for a square well potential is __________

(a) $-\propto < x < 0$ (b) $a < x < \propto$
(c) $-a < x < a$ (d) $-\propto < x < -a$

(7) The limit of a region-II for a square well potential is __________

(a) $-\propto < x < 0$ (b) $a < x < \propto$
(c) $-\boldsymbol{a} < x < a$ (d) $-\propto < x < -a$

(8) The limit of a region-III for a square well potential is __________

(a) $-\propto < x < 0$ (b) $\boldsymbol{a} < x < \propto$
(c) $-a < x < a$ (d) $-\propto < x < -a$

(9) $\frac{V_0}{\Delta}$ is a measure the ________ of the potential

(a) Height (b) Width
(c) **Strength** (d) Length

(10) There exists at least _______ bound state, however weak the potential may be

(a) Two (b) **One**
(c) Three (d) Infinite

(11) Any wave function having symmetry property is said to be of ______ parity

(a) Zero (b) **Even**
(c) Odd (d) Infinite

(12) Any wave function having anti-symmetry property is said to be of ______ parity

(a) Zero (b) Even
(c) **Odd** (d) Infinite

(13) For non-localized states of the square well potential ________

(a) $E = 0$ (b) $E = \propto$
(c) $E < 0$ (d) $\boldsymbol{E} > 0$

(14) For $E > 0$, the particle has a ______ kinetic energy

(a) Zero (b) **Positive**
(c) Negative (d) Infinity

Short Questions:

1. Define stationary states of the wave function
2. Write the time independent Schrodinger equation
3. State the physical significance of time independent Schrodinger equation
4. Write the admissible solution for a particle in a square well potential
5. Define square well potential
6. What is the condition of the total probability of the wave function

Long Questions:

1. Describe the stationary states and energy spectra of the quantum mechanical system
2. Derive the time independent Schrodinger equation and explain their physical significance
3. Discuss the motion of a particle in a square well for bound state and derive the admissible solutions of the time independent Schrodinger equations
4. Derive the expression of energy eigen values for a particle in a square well using the admissible solutions
5. Derive the energy eigen function for a particle in a square well potential
6. Discuss the square well potential for non-localized states($E > 0$) with the physical interpretation and suitable boundary conditions