B.Sc. (Semester – 6)
Subject : Physics
Course : US06CPHY01
Title : Quantum Mechanics

Unit : 2 - 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 descrete. 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

$$\psi(\vec{x}, t) = u(\vec{x})\, f(t) \quad ----- (1)$$

substituting this value in

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

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

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

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

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.

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

$$\therefore \quad i\hbar \frac{df(t)}{dt} = Ef(t) \quad \text{--------- (3)}$$

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

$$\therefore \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{x})\right]u(\vec{x}) = Eu(\vec{x}) \quad \text{---- (4)}$$

This is time independent schrodinger equation.

The sol^n of eq^n (3) is

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

Integration gives $\quad \log f = \frac{E}{i\hbar}t = -\frac{iEt}{\hbar}$

$$\therefore \quad f = \exp\left(-iEt/\hbar\right) \quad \text{----- (5)}$$

The sol^n of eq^n (4) is depends on the value of E hence we can write as $u_E(\vec{x})$.

$\therefore$ Eq^n (1) reduces to

$$\boxed{\psi(\vec{x},t) = u_E(\vec{x})\, e^{-iEt/\hbar}} \quad \text{------ (6)}$$

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

$$|\psi(\vec{x}, t)|^2 = |u_E(\vec{x})|^2 \quad \text{------ (7)}$$

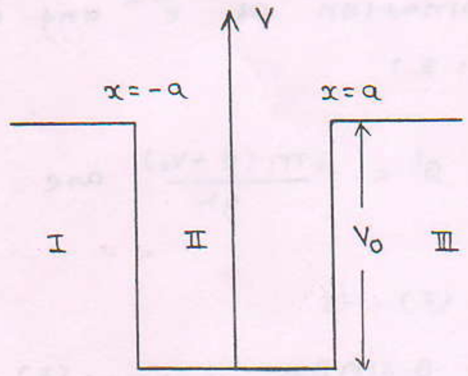
Therefore, the probability density is time independent. Expectation value must also be time independent.

Eq^n. (4) states that the action of the Hamiltonian operator of the particle on the wave function $u_E(\vec{x})$ is simply 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

$$\left.\begin{aligned} V(x) &= 0 \quad \text{for} \quad x < -a \quad (\text{Region - I}) \\ V(x) &= -V_0 \quad \text{for} \quad -a < x < a \quad (\text{Region - II}) \\ V(x) &= 0 \quad \text{for} \quad x > a \quad (\text{Region - III}) \end{aligned}\right\} \text{— (1)}$$



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 regions I & III. It will stay within the potential well between $x=a$

and $x = -a$. Hence the particle is bound by the potential.

The time independent Schrodinger eqn for two region becomes

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

and,

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dx^2} - V_0 u = Eu, \text{ for } |x| < a \quad \text{----- (3)}$$

⇒ Bound states in a square well : $(E<0)$

(a) Admissible solutions of wave equation :-

For $E < 0$, we write eqns. (2) & (3) as follows:

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

The general soln of eqns (7) is

$$u^{II}(x) = A\cos\beta x + B\sin\beta x \quad \text{------ (8)}$$

where A & B are constants.

This is the soln in region II.

The general soln of eqn. (6) in the region I & II is the linear combination of $e^{\alpha x}$ and $e^{-\alpha x}$.

dx^2

(Region: II)

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This is the soln in region II.

The general solⁿ of eqⁿ. (6) in the region I & II is the linear combination of $e^{\alpha x}$ and $e^{-\alpha x}$.

For region - I , $-\infty < x < a$.

Hence as $x \to -\infty$, $e^{-\alpha x} \to \infty$.

$\therefore$ The admissible solⁿ in region - I must be of the form

$$u^{I}(x) = C e^{\alpha x} \quad \text{-------- (9)}$$

For region - III , $a < x < \infty$.

As $x \to \infty$, $e^{\alpha x} \to \infty$. Hence, the admissible solⁿ in region III is

$$u^{III}(x) = D e^{-\alpha x} \quad \text{-------- (10)}$$

C & 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 & II meet, we should have

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

$$\therefore \boxed{C e^{-\alpha a} = A \cos\beta a - B \sin\beta a} \quad \text{------ (11)}$$

and,

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

$$\therefore \boxed{C \alpha e^{-\alpha a} = A\beta \sin\beta a + B\beta \cos\beta a} \quad \text{---- (12)}$$

similarly, at $x = a$

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

$$\boxed{D e^{-\alpha a} = A \cos\beta a + B \sin\beta a} \quad \text{----- (13)}$$

and,

$$\boxed{-D\alpha e^{-\alpha a} = -A\beta \sin\beta a + B\beta \cos\beta a} \quad \text{--- (14)}$$

Adding eqⁿˢ. (11) & (13) we get

$$\boxed{(C + D) e^{-\alpha a} = 2A \cos\beta a} \quad \text{------ (15)}$$

Adding (12) & (14) we get

$$\boxed{(C-D)\alpha e^{-\alpha a} = 2B\beta\cos\beta a} \quad \text{------ (16)}$$

Subtracting (11) & (13)

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

$$\therefore \boxed{-(C-D)e^{-\alpha a} = 2B\sin\beta a} \quad \text{---- (17)}$$

Subtracting (12) & (14)

$$\boxed{(C+D)\alpha e^{-\alpha a} = 2A\beta\sin\beta a} \quad \text{------ (18)}$$

Now, ~~Didi~~ Dividing (18) by (15) we get

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

$$\therefore \boxed{\alpha = \beta\tan\beta a} \quad \text{---- (19)}$$

unless $A=0$ and $C+D=0$ i.e $C=-D$.

Similarly dividing (16) by (17)

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

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

$$\therefore \boxed{\alpha = -\beta\cot\beta a} \quad \text{------ (20)}$$

unless $B=0$ and $C-D=0$ i.e $C=D$.

There exist two types of admissible solutions.

(1) When $B=0$ and $C=D$, then from eqn. (15) we get

$$2De^{-\alpha a} = 2A\cos\beta a$$

$$\therefore \boxed{D = Ae^{\alpha a}\cos\beta a} \quad \text{---- (21)}$$

(2) When $A=0$, and $C=-D$

$\therefore$ from eqn. (17)

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

$$\therefore \boxed{D = B e^{\alpha a}\sin\beta a} \quad \text{-----(22)}$$

Hence we get two set of eqns.

$$\boxed{\begin{aligned} \alpha &= \beta\tan\beta a \\ C &= D \\ B &= 0 \\ D &= A e^{\alpha a}\cos\beta a \end{aligned}} \quad \text{---(23)} \qquad \text{and,} \qquad \boxed{\begin{aligned} \alpha &= -\beta\cot\beta a \\ C &= -D \\ A &= 0 \\ D &= B e^{\alpha a}\sin\beta a \end{aligned}} \quad \text{---(24)}$$

(b) <u>The energy Eigenvalues :-</u>
<u>(Discrete spectrum)</u>

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

We have $-\alpha^2 = \dfrac{2mE}{\hbar^2}$ and $\beta^2 = \dfrac{2m(E+V_0)}{\hbar^2}$

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

$$\therefore \quad = \frac{2mV_0}{\hbar^2}$$

Multiplying by a^2 on both the sides we get

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

$$\therefore (\alpha^2+\beta^2)a^2 = V_0/\hbar^2/2ma^2 = \frac{V_0}{\Delta} \quad \text{-----(25)}$$

where $\Delta = \dfrac{\hbar^2}{2ma^2}$ is a natural unit of energy.

In eqn. (25) $\dfrac{V_0}{\Delta}$ is a measure of the strength of the potential.

since α and β are positive. Hence

$\alpha/\beta = \tan\beta a$ must be positive and hence values of βa lying in the intervals

$$2r\frac{\pi}{2} \leq \beta a \leq (2r+1)\frac{\pi}{2} \quad \text{------} (26)$$

$$(r = 0, 1, 2, \ldots)$$

are admissible.

Now substituting $\alpha = \beta \tan\beta a$ in eq^n. (25) we get,

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

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

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

$$\therefore \quad \sec^2\beta a = \frac{V_0}{\beta^2 a^2 \Delta} \quad \text{-----} (27)$$

$$\underline{\underline{\text{or}}} \quad \boxed{|\cos\beta a| = \left(\frac{\Delta}{V_0}\right)^{1/2} \beta a} \quad \text{---} (28)$$

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

Similarly, for the second type of solution of the wave equation, given by eq^n. (24), substitute $\alpha = -\beta\cot\beta a$ in eq^n. (25) we get

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

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

$$\therefore \quad \mathrm{cosec}^2\beta a = \frac{V_0}{\beta^2 a^2 \Delta} \quad \text{--------} (29)$$

or

$$\boxed{|\sin \beta a| = \left(\frac{\Delta}{V_0}\right)^{1/2} \beta a} \quad ------(30)$$

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

$$(2r-1)\frac{\pi}{2} \leq \beta a \leq 2r\frac{\pi}{2} \quad ------(31)$$

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

Eq^{ns}. (28) and (30) 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 $(\Delta/V_0)^{1/2} \beta a$ with the curves for $|\cos \beta a|$ and $|\sin \beta a|$ are shown as solid lines and dashed lines respectively in fig (a). The parts to be ignored are indicated by dotted lines.

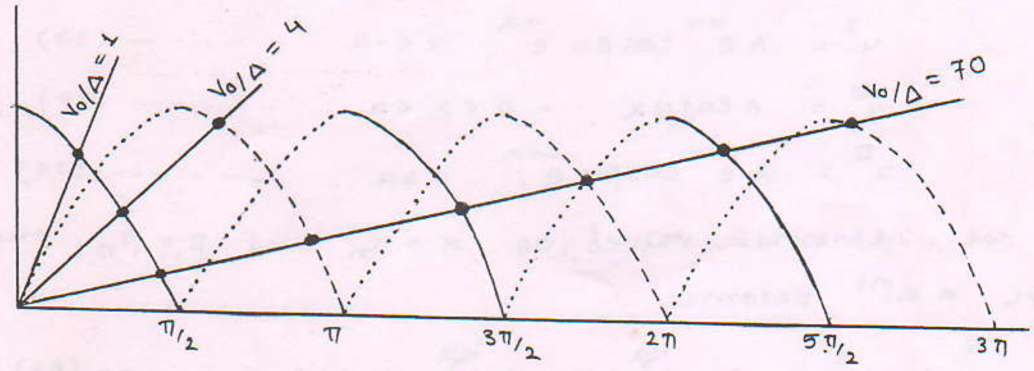


Fig: (a)

If the intersections occur at $\beta = \beta_n$ $(n = 0, 1, 2 \ldots)$ the corresponding allowed values of the energy are obtained from eq^n. (3).

$$\therefore \quad E_n = \frac{\hbar^2}{2m}\beta_n^2 - V_0 = \left[(\beta_n a)^2 \frac{\Delta}{V_0} - 1\right] V_0 \quad ----(32)$$

From fig (a), if $\left(\frac{\Delta}{V_0}\right)^{1/2} \beta a \to 1$ in the interval $\frac{1}{2}\pi N \le \beta a < \frac{1}{2}\pi(N+1)$, then there are $(N+1)$ intersections. In other words, the number of discrete energy level is $(N+1)$ if

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

i.e

$$N \le \frac{2}{\pi}\left(\frac{V_0}{\Delta}\right)^{1/2} < (N+1) \quad \text{-----} (33)$$

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

(C) The energy eigenfunctions; Parity :-

We have the eigen functions

$$u^{I} = C e^{\alpha x}, \quad x < -a \quad \text{---------} (34)$$

$$u^{II} = A\cos\beta x + B\sin\beta x, \quad -a < x < a \quad \text{----} (35)$$

$$u^{III} = D e^{-\alpha x}, \quad x > a \quad \text{-----} (36)$$

using eq^{ns}. (23) we get

$$u^{I} = A e^{\alpha a} \cos\beta a \, e^{\alpha x}, \quad x < -a \quad \text{------} (37)$$

$$u^{II} = A\cos\beta x, \quad -a < x < a \quad \text{------} (38)$$

$$u^{III} = A e^{\alpha a} \cos\beta a \, e^{-\alpha x}, \quad x > a \quad \text{-------} (39)$$

If we represents values of $\alpha = \alpha_n$ and $\beta = \beta_n$ then above eq^{ns} becomes

$$u_n^{I} = A_n e^{\alpha_n a} \cos\beta_n a \, e^{\alpha_n x}, \quad x < -a \quad \text{----} (40)$$

$$u_n^{II} = A_n \cos\beta_n x, \quad -a < x < a \quad \text{----} (41)$$

$$u_n^{III} = A_n e^{\alpha_n a} \cos\beta_n a \, e^{-\alpha_n x}, \quad x > a \quad \text{-----} (42)$$

$$(n = 0, 2 \ldots)$$

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

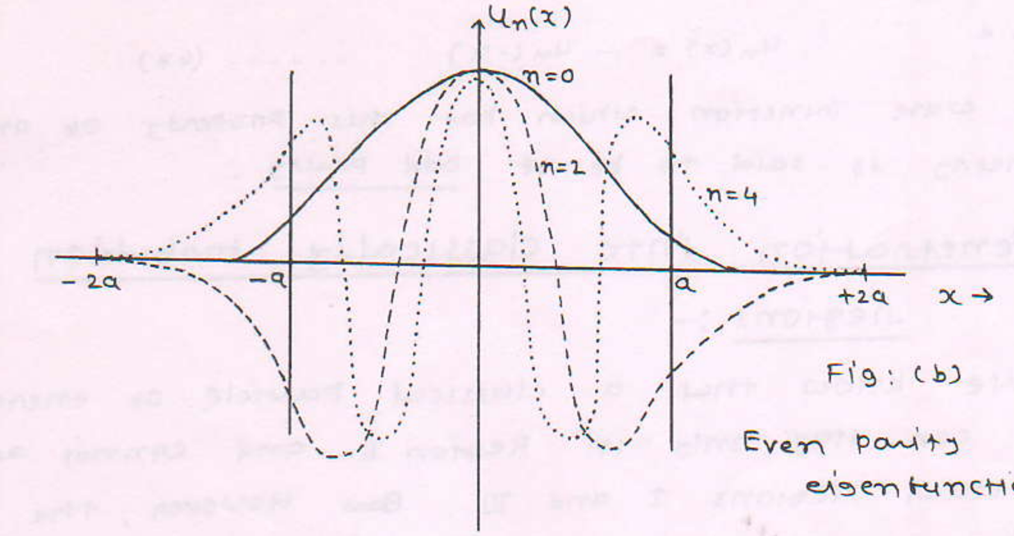


Fig: (b) Even parity eigen functions

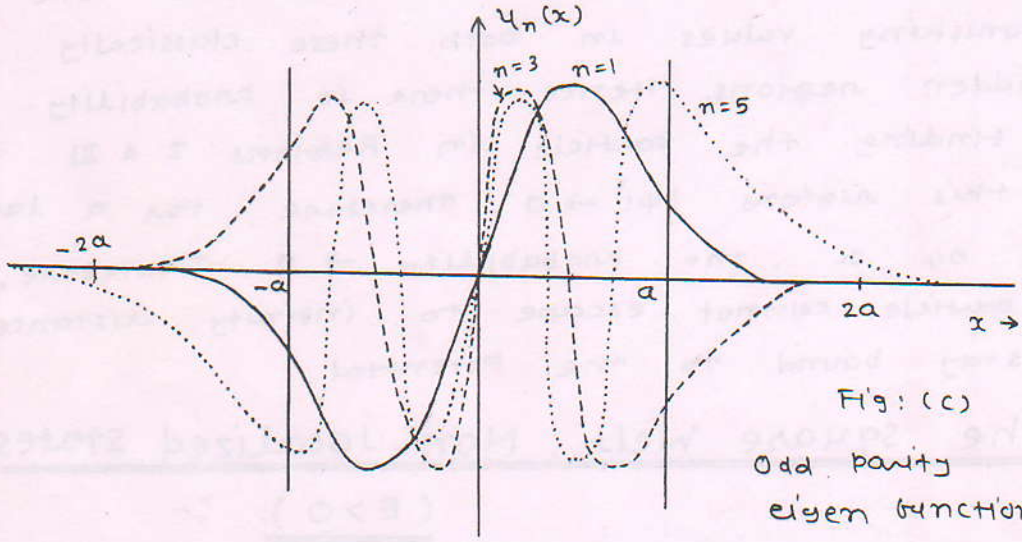


Fig: (c) Odd parity eigen functions.

$$u_n(x) = u_n(-x) \quad \text{------} \quad (43)$$

Any wave function which has this symmetry property is said to be of <u>even parity</u>.

The eigenfunction corresponding to $n = 1, 3 \ldots$ are characterized by eqn. (24). We have

$$u_n^{I} = -(B_n e^{\alpha_n a} \sin \beta_n a) e^{\alpha_n x}, \quad x < a \quad \text{----} \quad (44)$$

$$u_n^{II} = B \sin \beta_n x, \quad -a < x < a \quad \text{------} \quad (45)$$

$$u_n^{III} = (B e^{\alpha_n a} \sin \beta_n a) e^{-\alpha_n x}, \quad x > a \quad \text{------} \quad (46)$$

These functions are illustrated in Fig. (c). They are ~~sym~~ antisymmetric with respect to the origin i.e. $$u_n(x) = -u_n(-x) \quad \text{------ (47)}$$

Any wave function which has this property or anti-symmetry 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 enter Regions I and III. ~~But~~ However, the quantum mechanical wave functions $u(x)$ have nonvanishing values in both these classically forbidden regions. Hence there is probability of finding the particle in Regions I & III. In this regions $|\psi|^2 \rightarrow 0$, therefore, 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,

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dx^2} = Eu \quad \text{for } x<-a \text{ and } x>a \quad \text{--- (1)}$$
(Region : I & III)

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dx^2} - V_0 u = Eu \quad \text{for } -a<x<a \quad \text{---- (2)}$$
(Region : II)

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

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

Hence eqns. (1) and (2) becomes

$$\frac{d^2u}{dx^2} + k^2u = 0 \quad , \begin{cases} x < -a \\ x > a \end{cases} \quad \text{------} (3)$$

$$\frac{d^2u}{dx^2} + \beta^2 u = 0 \quad -a < x < a \quad \text{------} (4)$$

The solⁿ of eqⁿˢ. (3) and (4) are

$$u^{I} = C_+ e^{ikx} + C_- e^{-ikx} , \quad x < -a \quad \text{----} (5)$$

$$u^{III} = D_+ e^{ikx} + D_- e^{-ikx} , \quad x > a \quad \text{----} (6)$$

and, $$u^{II} = A_+ e^{i\beta x} + A_- e^{-i\beta x} , \quad -a < x < a \quad \text{----} (7)$$

→ Physical interpretation :-

In eqⁿ (5) 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 $D_- e^{-ikx}$ nerepresents the wave travel towards R.H.S and L.H.S from $x = a$ to $x = \infty$ respectively. same we can interpreted eqⁿ. (7) between the limit $x = -a$ 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 can not stay in the region. Therefore the boundary conditions

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

are not satisfied. A particle with the wave functions (5), (6) & (7) is not localized. It is not ~~confied~~ 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 sol^n and its first derivatives must be continuous at $x = -a$ and $x = +a$. Here there is not any restriction on k or β. Hence any energy $E > 0$ is an eigenvalue. When $E > 0$, the continuity conditions give 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 eigenvalues form a continuous (not a discrete) set. Hence the energy spectrum for $E > 0$ is a continuum.

The probability of reflection is given by

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

This expression is shown graphically in fig (a).

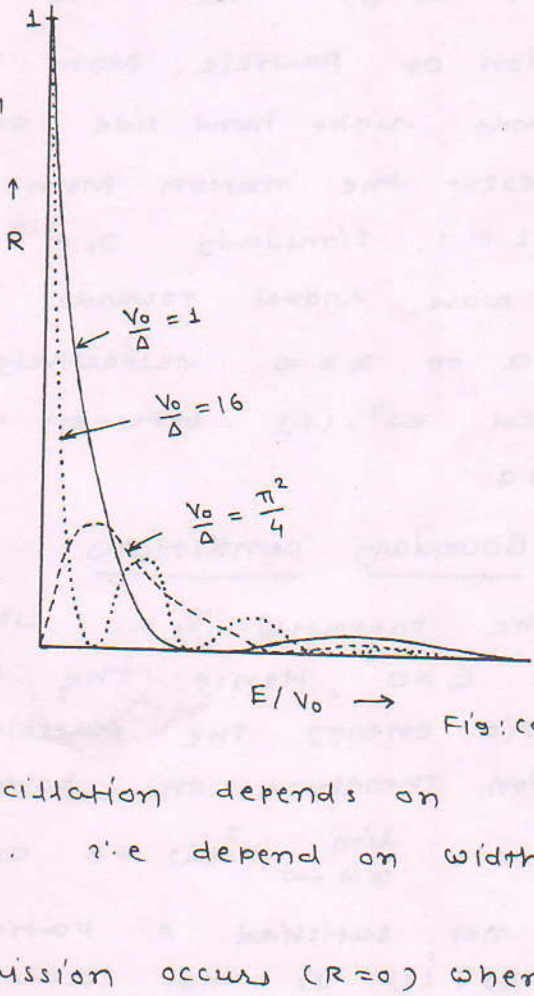


Fig: (a)

→ For very low energies ($E \to 0$), the reflection is almost total. As (E/V_0) increases, R oscillates bet^n zero and $[1 + 4E(E+V_0)/V_0^2]^{-1}$. This bound depends only on (E/V_0), 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 $\{2\sqrt{(E+V_0)/\Delta}\} = \sin 2\beta a = 0$.

* Square Potential Barrier OR

(a) Quantum Mechanical Tunnelling :-

Let us consider a potential barrier as shown in fig (a). 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.

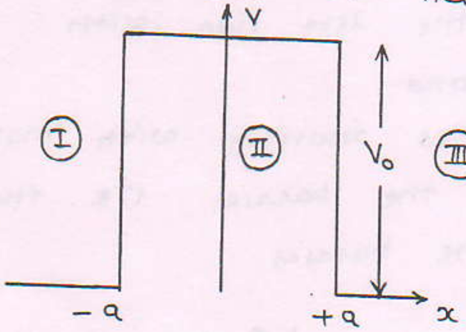


Fig: (a)

The potential of the square well barrier is given by

$$V_0 = \begin{cases} 0, & x < a \\ V_0, & -a < x < a \\ 0, & x > a \end{cases} \quad \text{---(1)}$$

The schrodinger equations for region I and III becomes

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

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

$$\therefore \frac{d^2u}{dx^2} + \alpha^2 u = 0 \quad \text{--------(2)}$$

where $\alpha^2 = \frac{2mE}{\hbar^2}$.

The schrodinger eq^n in region II is given by

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dx^2} + V_0 u = Eu$$

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

$$\therefore \frac{d^2u}{dx^2} - \beta^2 u = 0 \quad \text{--------(3)}$$

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

The solutions of eqns (2) are

$$u^{I} = A_+ e^{i\alpha x} + A_- e^{-i\alpha x} \quad (x < -a) \quad ---- (4)$$

and, $$u^{III} = C_+ e^{i\alpha x} + C_- e^{-i\alpha x} \quad (x > a) \quad ---- (5)$$

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

In region III the particles can not moving to the left $\therefore$ $C_- = 0$

$$\therefore u^{III} = C_+ e^{i\alpha x} \quad ------ (6)$$

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

$\therefore$ The amplitude for tunnelling $= \frac{C_+}{A_+}$

Tunnelling probability $= \left| \frac{C_+}{A_+} \right|^2$ ---- (7)

Now, the continuity conditions are

$$u^{I} = u^{II}$$

and $\frac{du^{I}}{dx} = \frac{du^{II}}{dx}$ at $x = -a$.

The sol^n of eq^n (3) in region II is

$$u^{II} = B_+ e^{\beta x} + B_- e^{-\beta x} \quad ------ (8)$$

$\therefore$ Using the continuity condition we have

$$\boxed{A_+ e^{-i\alpha a} + A_- e^{i\alpha a} = B_+ e^{-\beta a} + B_- e^{\beta a}} \quad ----- (9)$$

and,

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

$$\therefore \boxed{i\alpha A_+ e^{-i\alpha a} - i\alpha A_- e^{i\alpha a} = \beta B_+ e^{-\beta a} - \beta B_- e^{\beta a}} \quad --- (10)$$

Similarly at $x = a$

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

$$\therefore \boxed{B_+ e^{\beta a} + B_- e^{-\beta a} = C_+ e^{i\alpha a}} \quad ------- (11)$$

and,

$$\boxed{\beta B_+ e^{\beta a} - \beta B_- e^{-\beta a} = i\alpha C_+ e^{i\alpha a}} \quad ------ (12)$$

Dividing eq^n (12) by (11)

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

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

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

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

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

$$\therefore \boxed{B_- = B_+ \frac{\beta - i\alpha}{\beta + i\alpha} e^{2\beta a}} \quad ------- (13)$$

Now, dividing eq^n (10) by (9), 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 value of B_- from eqn (13), we get

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

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

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

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

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

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

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

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

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

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

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

$$\therefore \boxed{\frac{A_-}{A_+} = \frac{-i(\alpha^2+\beta^2)\, e^{-2i\alpha a}\sinh(2\beta a)}{-i(\alpha^2-\beta^2)\sinh(2\beta a) + 2\alpha\beta\cosh(2\beta a)}} \quad \text{--- (14)}$$

Now,

$$\frac{C_+}{A_+} = \frac{C_+}{B_+}\cdot\frac{B_+}{A_+} \quad \text{------- (15)}$$

But eqn. (11) is

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

$$\therefore B_+ e^{\beta a} + B_+ \frac{(\beta - i\alpha)}{(\beta + i\alpha)} e^{-2\beta a}\cdot e^{\beta a} = C_+ e^{i\alpha a} \quad (\text{using eqn } (13))$$

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

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

$$\therefore \boxed{\frac{C_+}{B_+} = \frac{e^{\beta a}(2\beta)\, e^{-i\alpha a}}{(\beta + i\alpha)}} \quad \text{---- (16)}$$

||ly we can obtain

$$\boxed{\frac{B_+}{A_+} = \frac{\left\{\alpha\, e^{-\beta a}\, e^{-i\alpha a}(\beta + i\alpha)\right\}}{\left\{-i(\alpha^2-\beta^2)\sinh(2\beta a) + 2\alpha\beta\cosh(2\beta a)\right\}}} \quad \text{--- (17)}$$

Using eqns. (16) & (17) in (15) we get

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

$$= \frac{2\alpha\beta\, e^{-2i\alpha a}}{\left\{-i(\alpha^2-\beta^2)\sinh(2\beta a) + 2\alpha\beta\cosh(2\beta a)\right.} \quad \text{---- (18)}$$

But $T = \left| \frac{C_+}{A_+} \right|^2$ is the transmission probability

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

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

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

$$\therefore T = \left[1 + \frac{(\alpha^2+\beta^2)^2\sinh^2(2\beta a)}{4\alpha^2\beta^2} \right]^{-1} \quad \text{------ (19)}$$

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

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

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

$$= \frac{(\alpha^2+\beta^2)^2\sinh^2(2\beta a)}{(\alpha^2+\beta^2)^2\sinh^2(2\beta a) + 4\alpha^2\beta^2} \quad \text{------ (20)}$$

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

$$= 1$$

$$\therefore R + T = 1 \quad \text{------ (21)}$$

From eqⁿ. (19)

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

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

Case: 1 If $2\sqrt{(V_0 - E)/\Delta} = y >> 1$

$$\therefore T = \left[1 + \frac{V_0^2}{4(V_0 - E)E} \cdot \sinh^2 y \right]^{-1} \quad \text{------ (22)}$$

But $y >> 1$

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

$$\therefore \sinh^2 y = \frac{1}{4} e^{2y}$$

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

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

$$\therefore \boxed{T = \frac{16(V_0 - E)E}{V_0^2} \exp\left\{-4\sqrt{(V_0 - E)/\Delta}\right\}} \quad \text{------ (23)}$$

Hence, if $V_0 >> E$, $T << 1$.

i.e transmission probability decreases exponentialy.

Case: 2 If $y << 1$

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

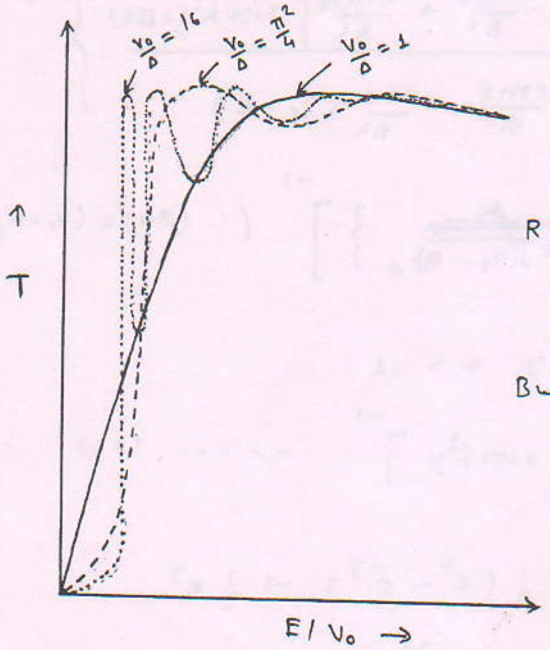
$$= y$$

Hence eqⁿ. (22) becomes

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

$$\therefore T = \left[1 + \frac{V_0^2}{\Delta E} \right]^{-1} \quad \text{------ (24)}$$

The graph of transmission probability is given below.



* Probability of reflection:

For $E > V_0$

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

But in case of $E < V_0$

$$\beta = i\beta'$$

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

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

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

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

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

substituting the values of α and β we get

$$R = \left[1 + \frac{4E(E - V_0)}{V_0^2 \sin^2\left[2\sqrt{(E - V_0)/\Delta}\right]} \right]^{-1} \quad --- (25)$$

* **The schrodinger equation and the Probability Interpretation for an N - particle system :-**

A system of N particles is represented by the position and momentum variables $\vec{x}_1, \vec{x}_2, \dots \vec{x}_N$ and $\vec{p}_1, \vec{p}_2 \dots \vec{p}_N$. Its energy is given by

$$E = H(\vec{x}_1, \vec{x}_2, \dots \vec{x}_N, \vec{p}_1, \vec{p}_2, \dots \vec{p}_N, t) \quad \text{--- (1)}$$

The operators are $\quad E \rightarrow i\hbar \frac{\partial}{\partial t}, \; \vec{p}_i \rightarrow -i\hbar \vec{\nabla}_i \quad$ ---- (2)

$(i = 1, 2 \dots N)$.

where $\vec{\nabla}_i = \left(\frac{\partial}{\partial x_i}, \frac{\partial}{\partial y_i}, \frac{\partial}{\partial z_i} \right)$.

These operators have to act on the wave function ψ.

The 3N coordinates of the N particles can be taken as the coordinates of a single point in a 3N - dimensional space. Such a space is called the configuration space.

The wave equation for N-particle system can be written as

$$i\hbar \frac{\partial \psi(\vec{x}_1, \vec{x}_2 \dots \vec{x}_N, t)}{\partial t} = H(\vec{x}_1, \vec{x}_2, \dots \vec{x}_n, -i\hbar\vec{\nabla}_1, -i\hbar\vec{\nabla}_2 \dots -i\hbar\vec{\nabla}_N)\, \psi(\vec{x}_1, \vec{x}_2, \dots \vec{x}_N, t) \quad \text{--- (3)}$$

This is the general form of the schrodinger equation.

* **The Fundamental Postulates of Wave Mechanics**

(a) Representation of states

Postulate : 1 "The state of a quantum mechanical system is described or represented by a wave function $\psi(\vec{x}, t)$."

Postulate : 2 - The superposition principle :

"If ψ_1 and ψ_2 are wave functions for any two states of a given system then corresponding to every linear combination $(c_1\psi_1 + c_2\psi_2)$ of the two functions there exists a state of the system."

This is a fundamental principal of quantum mechanics to which there is no correspondence in classical mechanics. It is the possibility of superposition which makes interference phenomena possible.

→ The scalar product of ϕ and ψ is defined as

$$(\phi, \psi) = \int \phi^*(\vec{x})\, \psi(\vec{x})\, d\tau$$

It follows that $(\phi, \psi) = (\psi, \phi)^*$

$$(\phi, c\psi) = c(\phi, \psi), \quad (c\phi, \psi) = c^*(\phi, \psi)$$

The norm of $\psi = (\psi, \psi) \geq 0$.

(b) Representation of dynamical variables;

Expectation values, observables :-

Postulates : 3 Each dynamical variable $A(\vec{x}, \vec{p})$ is represented in quantum mechanics by a linear operator $A_{op} = A(\vec{x}_{op}, \vec{P}_{op}) \equiv A(\vec{x}, -i\hbar\vec{\nabla})$.

The operators acts on the wave functions of the system. The effect of an operator A on a wave function ψ is to convert into another wave function denoted by $A\psi$.

Linearity of the operator means that a linear combination of two wave functions ψ_1 and ψ_2 is converted into the same linear combination of $A\psi_1$ and $A\psi_2$.

$$A(c_1\psi_1 + c_2\psi_2) = c_1(A\psi_1) + c_2(A\psi_2) \quad \text{— (1)}$$

→ The dynamical variables in quantum mechanics do not commute i.e $AB \neq BA$.

The difference $AB - BA$ is called the commutator of A and B. In notation $[A, B] = AB - BA$ — (2)

→ Commutation relations of position and momentum is deduce as follows:

For one dimension

$$(xp - px)\psi = \left[x(-i\hbar\vec{\nabla}) - (-i\hbar\vec{\nabla})x \right]\psi$$

$$= -i\hbar \left[x \frac{\partial}{\partial x}\psi - \frac{\partial}{\partial x}(x\psi) \right]$$

$$= -i\hbar \left[\cancel{x \frac{\partial \psi}{\partial x}} - \frac{\partial x}{\partial x}\psi - \cancel{x \frac{\partial \psi}{\partial x}} \right]$$

$$= i\hbar\psi$$

$$\therefore \quad [x, p] = i\hbar \qquad \text{------ (3)}$$

For three dimensions

$$(x_i p_j - p_j x_i)\psi = \left[x_i\left(-i\hbar\frac{\partial}{\partial x_j}\right)\psi - \left(-i\hbar\frac{\partial}{\partial x_j}\right)x_i\psi \right]$$

$$= \left[-i\hbar\, x_i \frac{\partial \psi}{\partial x_j} + i\hbar \frac{\partial}{\partial x_j}(x_i\psi) \right]$$

$$= -i\hbar \left[\cancel{x_i \frac{\partial \psi}{\partial x_j}} - \frac{\partial x_i}{\partial x_j}\psi - \cancel{x_i \frac{\partial \psi}{\partial x_j}} \right]$$

$$= i\hbar\, \delta_{ij}\psi$$

$$\therefore \quad [x_i, p_j] = i\hbar\, \delta_{ij} \qquad \text{—— (4)}$$

where $\frac{\partial x_i}{\partial x_j} = \delta_{ij}$ is called kronecker delta function

$$\delta_{ij} = 1 \quad \text{if} \quad i = j$$
$$= 0 \quad \text{if} \quad i \neq j$$

Also $[x_i, x_j] = 0$, $[p_i, p_j] = 0$ —— (5)

We can write

$$[x, p_x] = [y, p_y] = [z, p_z] = i\hbar \qquad \text{—— (6)}$$

The basic commutation relations and the identities are

$$[AB, C] = A[B, C] + [A, C]B \qquad \text{—— (7)}$$

$$[A, BC] = [A, B]C + B[A, C] \qquad \text{—— (8)}$$

where A, B & C are arbitrary operators.

Regions : I & III, $\dfrac{d^2\psi}{dx^2} + \dfrac{2mE}{\hbar^2}\psi = 0$ --- (4)

Region : II $\dfrac{d^2\psi}{dx^2} + \dfrac{2m}{\hbar^2}V_0\psi + \dfrac{2mE}{\hbar^2}\psi = 0$

$$\therefore \frac{d^2\psi}{dx^2} + \frac{2m(E+V_0)}{\hbar^2}\psi = 0 \qquad \text{--- (5)}$$

Eq$^{ns.}$ (4) & (5) can be written as

$$\frac{d^2\psi}{dx^2} - \alpha^2\psi = 0, \quad \text{for } |x| > a \qquad \text{--- (6)}$$

(Region : I & III)

and $\dfrac{d^2\psi}{dx^2} + \beta^2\psi = 0$, for $|x| < a$ --- (7)

(Region : II)