unit II.

2. Applications of schroedinger Equation.

The time independent schroedinger equation.

$$H\varphi(x) = E\varphi(x)$$

is eigen value equation,

$$H = \frac{p^2}{2m} + V(x)$$

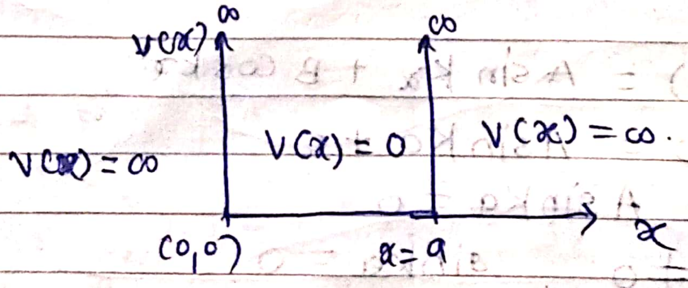
$$H = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x).$$

The solutions of this schroedinger equation give a set of energy eigen values, which may form a discreate set of energy values.
This set of energy eigen values are referred to as energy levels or energy spectrum.

* Particle in a Rigid box in one dimension. (ie. in infinitely deep potential well)

Let us consider a particle of mass (m) in an infinitely deep potential well; characterised by the potential $V(x)$ as,

$$V(x) = 0 \quad \text{for} \quad 0 < x < a$$
$$= \infty \quad \text{for} \quad x < 0 \text{ and } x > a.$$



* 1 D infinitely deep potential well.

consider time independent schroedinger equ
may be written

$$\frac{d^2 \varphi(x)}{dx^2} + k^2 \varphi(x) = 0 \quad \text{—— (1)}$$

where, $k^2 = \frac{2mE}{\hbar^2}$ —— (2)

general solution of equation (I)

$$\varphi(x) = A . \sin kx + B \cos kx$$

From boundary conditions,

ie. $x = 0$ $\varphi(x) = 0$

$$\varphi(x) = A \sin k(0) + B \cos k(0)$$

$$0 = 0 + B$$

$$\therefore \boxed{B = 0}$$

Therefore, constant $B = 0$

$$\varphi(x) = A \sin kx$$

again, put boundary conditions.

ie. $x = a$ $\varphi(x) = 0$.

$$\therefore \varphi(x) = A \sin kx + B \cos kx$$

$$\therefore 0 = A \sin ka + 0$$

$$\therefore A \sin ka = 0$$

but, $A \neq 0$, $\sin ka = 0$

$$\therefore ka = n\pi$$

$$\therefore k = \frac{n\pi}{a} \quad \text{where, } n = 1, 2, 3 \ldots$$

$n = 0$ is not possible. $\therefore \boxed{k^2 = \frac{n^2\pi^2}{a^2}}$

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From equation (2) $K^2 = \frac{2mE}{\hbar^2}$

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

$$\therefore \boxed{E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}} \quad \text{——— (3)}$$

Hence, it shoulde be noted that For $n=1$ ie. ground state.

$\therefore$ put $n=1$, then $\boxed{E_1 = \frac{\pi^2\hbar^2}{2ma^2}}$ ie. $E_1 \neq 0$

This is known as zero point energy.
and $n = 2, 3, 4, 5 \dots$ are excited states.

$$E_n \propto n^2 \quad \text{or} \quad E_n = E_1 n^2 \quad \text{——— (4)}$$

To determine A normalisation constant;
we use normalisation condition.

$$\int_0^a \varphi_n^* \varphi_n \, dx = 1$$

$$\therefore \int_0^a A \sin kx \cdot A \sin kx \, dx = 1$$

$$\therefore \int_0^a A^2 \sin^2 kx \, dx = 1$$

$K = \frac{n\pi}{a}$

$$\therefore A^2 \int_0^a \sin^2 kx \, dx = 1$$

$\sin 2 \frac{n\pi}{a} \cdot a$

$$\therefore A^2 \int_0^a \left(\frac{1 - \cos 2kx}{2} \right) dx = 1$$

$$= \frac{A^2}{2} \int_0^a 1 \, dx - \int_0^a \cos 2kx \, dx = 1$$

$$= \frac{A^2}{2} [x]_0^a - \left[\frac{\sin 2kx}{2}\right]_0^a = 1$$

$$A^2 = \frac{2}{a} - \sin 2 \times \frac{n\pi}{a} \times a$$

$$A = \sqrt{\frac{2}{a}} - 0$$

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

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin kx$$

$$\boxed{\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)}$$

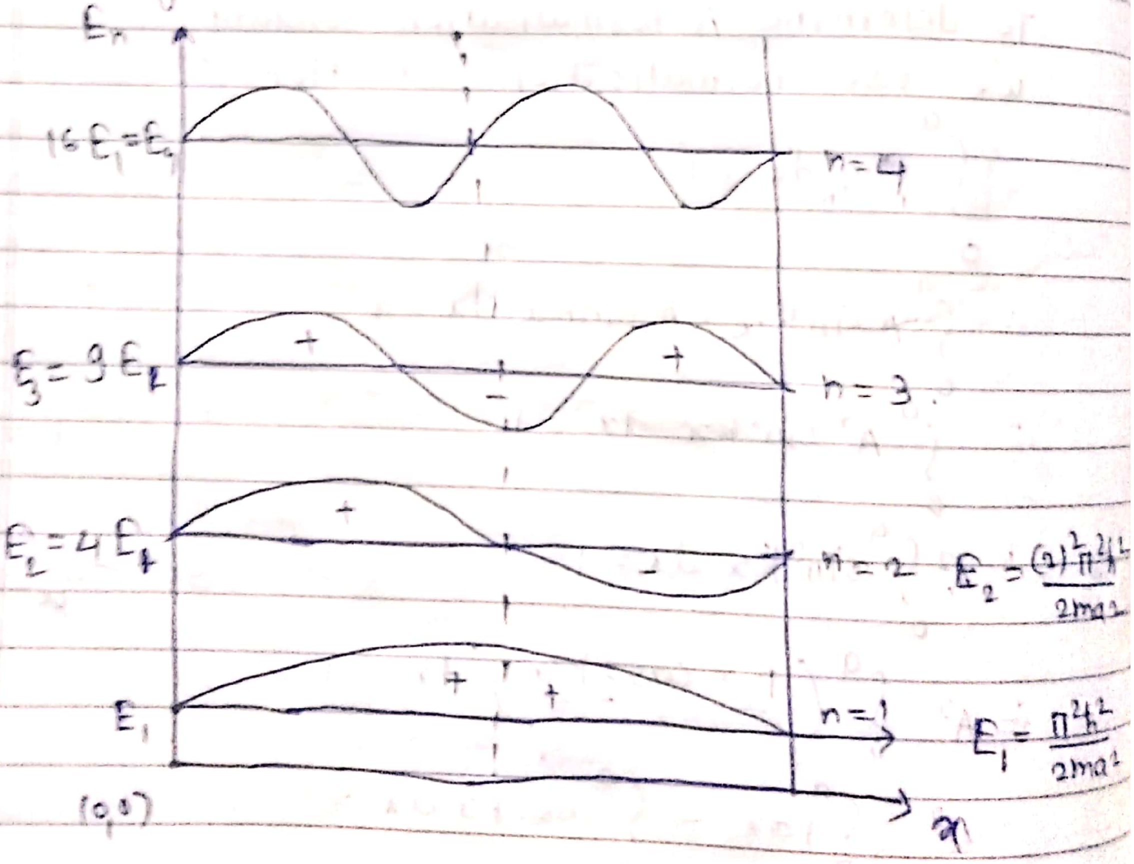
$\psi_n(x)$ are the eigen functions for $n = 1, 2, 3 \ldots$

* Energy levels and eigen functions for $n = 1, 2, 3 \ldots$

wave functions are either symmetric or antisymmetric and energy levels are discrete.

symmetric for $(n = 1, 3, 5)$

antisymmetric for $(n = 2, 4, 6)$.



2,3 - - .

=1,2,3 . . .

crete

* momentum Eigen values :-

From eqn ② we have,

$$K^2 = \frac{2mE}{\hbar^2} = \frac{2m}{\hbar^2} \cdot \frac{p^2}{2m} = \frac{p^2}{\hbar^2}$$

$$\therefore \boxed{K = \frac{P}{\hbar}}$$

$$\therefore K = \frac{n\pi}{a} = \frac{P}{\hbar}$$

$$\therefore \boxed{\frac{\pi\hbar}{a} \cdot n = P} \quad \text{--- (6)}$$

where, $n = 1, 2, 3 \dots$ is the quantum number.

Thus momentum eigen values are also discrete.

* step potential (Reflection and Transmission coefficients)

consider a particle of mass (m) moving from left in the X - Positive direction, which is incident on a step potential ...

Case (a) :- Let us first,

consider that the particle energy $E > V_0$
Time independent schroedinger equation,

$$\frac{d^2\psi(x)}{dx^2} + K^2 \psi(x) = 0, \quad \text{for } x < 0 \quad \text{—— (1)}$$

where, $K^2 = \frac{2mE}{\hbar^2}$

and $$\frac{d^2\psi(x)}{dx^2} + K_1^2 \psi(x) = 0, \quad \text{for } x > 0 \quad \text{—— (2)}$$

where, $K_1^2 = \frac{2m}{\hbar^2}(E - V_0)$

The solutions for these diff. equations are,

$$\psi(x) = A.e^{ikx} + B.e^{-ikx}, \quad \text{for } x < 0 \quad \text{—— (3)}$$

and $$\psi(x) = C.e^{ik_1x} + D.e^{-ik_1x}, \quad \text{for, } x > 0 \quad \text{—— (4)}$$

As the wave function $\psi(x)$ and $\frac{d\psi}{dx}$ are continuous at $x = 0$
from eqn (3) and (4) we obtain,

At $\psi(x=0)$ $$A + B = C + 0 \quad \text{—— (5)}$$

and for $\left.\frac{d\psi}{dx}\right|_{x=0}$ $$ik(A - B) = ik_1C$$

$$\therefore (A - B) = \frac{k_1}{k} C \quad \text{—— (6)}$$

solving eqn (5) and (6)
by adding eqn (5) and (6)

$$A + B = C$$

$$+ \quad A - B = \frac{k_1}{k} C$$

$$2A + 0 = C\left(1 + \frac{k_1}{k}\right)$$

$$\therefore 2A = C\left(\frac{k + k_1}{k}\right)$$

$$\boxed{C = \left(\frac{2k}{k+k_1}\right) A} \quad \text{——} \; (7)$$

subtracting eq^n (6) from eq^n (5), we get,

$$A + B = C$$

$$- \quad A - B = \frac{k_1}{k} C$$

$$2B = C\left(1 - \frac{k_1}{k}\right)$$

$$\therefore 2B = C\left[\frac{k - k_1}{k}\right]$$

$$\therefore B = \left(\frac{k - k_1}{2k}\right) \cdot C$$

put value of C in eq^n (7).

$$\therefore B = \left(\frac{k - k_1}{2k}\right) \cdot \left(\frac{2k}{k + k_1}\right) \cdot A$$

$$\boxed{B = \frac{k - k_1}{k + k_1} \cdot A} \quad \text{——} \; (8)$$

$$\therefore A = \left(\frac{k + k_1}{k - k_1}\right) \cdot B$$

In general, the current density is given by,

$$\vec{J} = \text{Real part of } \left[\varphi^* \frac{\hbar}{im} \frac{\partial \varphi}{\partial x} \right] \cdot \hat{x}.$$

incident wave, $\varphi_i = A \cdot e^{ikx}$

current density of incident wave,

$$J_i = A^* e^{-ikx} \cdot \frac{\hbar}{2m} \cdot A\, ik\, e^{ikx}.$$

$$\therefore J_i = |A|^2 \cdot \frac{\hbar k}{m}$$

$$\boxed{J_i = \frac{\hbar k}{m} \cdot |A|^2}$$

simillarly, due to reflected wave,

$$\varphi_r = B \cdot e^{-ikx}.$$

$$\therefore J_r = \frac{\hbar k}{m} \cdot |B|^2$$

due to transmitted wave, $\varphi_t = c \cdot e^{-ik_1 x}$.

$$J_t = \frac{\hbar k_1}{m} |c|^2$$

$\therefore$ Reflection coefficient.

$$R = \frac{J_r}{J_i} = \frac{|B|^2}{|A|^2} = \frac{\left(\frac{k-k_1}{k+k_1}\right)^2 A^2}{|A|^2}$$

$$\boxed{R = \frac{(k-k_1)^2}{(k+k_1)^2}}$$

$\therefore$ T = Transmission coefficient.

$$\therefore T = \frac{J_t}{J_i} = \frac{\frac{\hbar k_1}{m}\cdot |C|^2}{\frac{\hbar k}{m}\cdot |A|^2} = \frac{k_1 |C|^2}{k |A|^2}$$

$$= \frac{k_1 \left(\frac{2k}{k+k_1}\right)^2 \cdot A^2}{k |A|^2}$$

$$= \frac{k_1 \frac{4k^2}{(k+k_1)^2}}{k}$$

$$\boxed{T = \frac{4kk_1}{(k+k_1)^2}} \quad \text{——} \quad (10).$$

It can be noted that,

$$R+T = \frac{(k-k_1)^2}{(k+k_1)^2} + \frac{4kk_1}{(k+k_1)^2}$$

$$= \frac{k^2 - 2kk_1 + k_1^2 + 4kk_1}{(k+k_1)^2}$$

$$= \frac{k^2 + 2kk_1 + k_1^2}{(k+k_1)^2}$$

$$= \cancel{\frac{(k+k_1)^2}{(k+k_1)^2}}$$

$$\therefore \boxed{R+T = 1}$$

Case b>

Now, let us consider particle with energy $E < V_0$

At $x < 0$,
Schroedinger eqn.

$$\frac{d^2\psi}{dx^2} + K^2\psi = 0 \quad , \quad K^2 = \frac{2mE}{\hbar^2}$$

$\therefore$ Solution is, $\psi(x) = A \cdot e^{iKx} + B \cdot e^{-iKx}$ —— (11)

and at $x > 0$

$$\frac{d^2\psi}{dx^2} - K_2^2\psi = 0$$

where, $K_2^2 = \frac{2m}{\hbar^2}(V_0 - E)$

Solution can be,

$$\psi(x) = C \cdot e^{-K_2 x} + D \cdot e^{K_2 x}.$$

we have, $D = 0$ as $e^{K_2 x}$ increases indefinitely with x

$\therefore$ $\psi(x) = C \cdot e^{-K_2 x}$ —— (12)

$\therefore$ Requirement of continuity of ψ and $\frac{d\psi}{dx}$ at $x=0$

$$A + B = C \quad \text{—— (13)}$$

and $\frac{\partial\psi}{\partial x} = iKA - iKB = -K_2 C$

$$\therefore A - B = \frac{-K_2 \cdot C}{iK} = \frac{iK_2 C}{K} \quad \text{—— (14)}$$

add eqⁿ (13) and (14)

$$A+B=C$$
$$+\quad A-B=\frac{ik_2C}{k}$$

$$2A = C\left[1+\frac{ik_2}{k}\right]$$

$$2A = C\left[\frac{k+ik_2}{k}\right]$$

$$\boxed{C = \frac{2k}{k+ik_2}\cdot A} \quad \text{--- (15)}$$

by subtracting eqⁿ (13) and (14)

$$A+B=C$$
$$-\quad A-B=\frac{ik_2C}{k}$$

$$2B = C\left[1-\frac{ik_2}{k}\right]$$

$$2B = C\left[\frac{k-ik_2}{k}\right]$$

$$B = C\cdot\left[\frac{k-ik_2}{2k}\right]$$

put value of C.

$$B = \frac{\cancel{2k}}{k+ik_2}\times\frac{k-ik_2}{\cancel{2k}}\cdot A$$

$$B = \frac{k-ik_2}{k+ik_2}\cdot A$$

$$\therefore \frac{B}{A} = \frac{k-ik_2}{k+ik_2} = \frac{\cancel{k}\left(1-\frac{ik_2}{k}\right)}{\cancel{k}\left(1+\frac{ik_2}{k}\right)}$$

Now, put, $\frac{k_2}{k} = \tan\vartheta$

$$\frac{B}{A} = \frac{(1 - i\tan\vartheta)}{(1 + i\tan\vartheta)} = \frac{\left(1 - i\frac{\sin\vartheta}{\cos\vartheta}\right)}{\left(1 + i\frac{\sin\vartheta}{\cos\vartheta}\right)} = \frac{\frac{\cos\vartheta - i\sin\vartheta}{\cos\vartheta}}{\frac{\cos\vartheta + i\sin\vartheta}{\cos\vartheta}}$$

$$\frac{B}{A} = \frac{\cos\vartheta - i\sin\vartheta}{\cos\vartheta + i\sin\vartheta}$$

$$\frac{B}{A} = \frac{e^{-i\vartheta}}{e^{i\vartheta}} = e^{-2i\vartheta} \quad \text{--- (16)}$$

$\therefore$ Reflection coefficient,

$$R = \frac{|B|^2}{|A|^2} = \left|\frac{B}{A}\right|^2 = e^{-2i\vartheta} \cdot e^{2i\vartheta} = 1 \quad \text{--- (17)}$$

$\psi(x)$ is real and transmitted current density $J_t = 0$. and hence,

Transmission coefficient $T = 0$. --- (18)

$$\therefore R + T = 1 + 0 = 1.$$

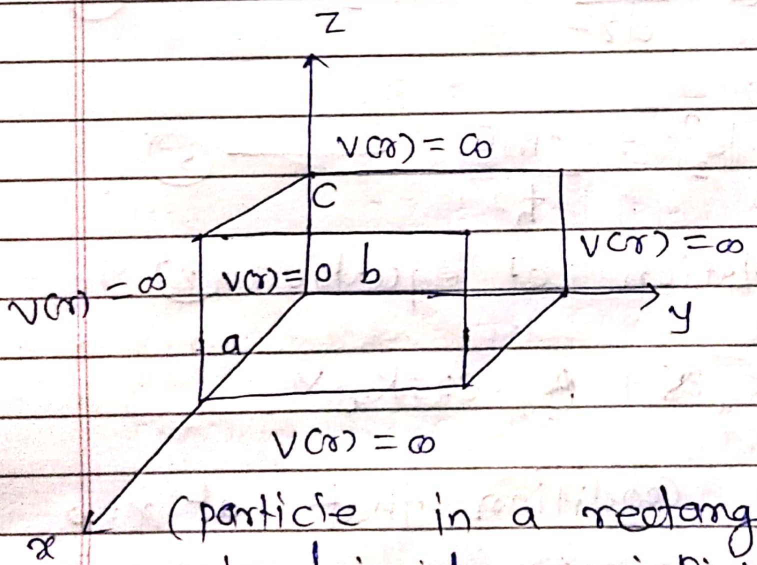
* Particle in a Three-dimensional Rigid-Box.

Let us consider a particle of mass (m), in a rectangular box, of side length a, b, c and placed in an infinitely deep potential well. The free electrons in metals and even valence electrons in atoms which are very loosely bound to the atoms as free electrons in a box. etc.

The nature of potential is,

$$V(r) = V(x,y,z) = 0, \quad \text{For } 0<x<a,\ 0<y<b \text{ and } 0<z<c \text{ ie. } V(r)=0 \text{ inside box,}$$

$$= \infty \quad \text{in the space outside the box.}$$



(particle in a rectangular box placed inside an infinitely deep potential well)

The time independent schroedinger's equation is,

$$\nabla^2\psi(r) + \frac{2mE}{\hbar^2}\psi(r) = 0$$

for $0<x<a$
$0<y<b$
$0<z<c$

Solution of Schrodinger's equation is

$$\psi(r) = X(x) \cdot Y(y) \cdot Z(z)$$

Substitute for $\psi(r)$ in above diff. equation ~~and~~ and divide throughout by $\psi(r)$ to give

$$\therefore \frac{1}{X}\frac{d^2X}{dx^2} + \frac{1}{Y}\cdot\frac{d^2Y}{dy^2} + \frac{1}{Z}\frac{d^2Z}{dz^2} = -\frac{2mE}{\hbar^2} \quad \text{--- (1)}$$

on LHS of equation (1) each term should be independently equal to some constant

ie.
$$\frac{1}{X}\frac{d^2X}{dx^2} = -K_x^2 \quad \text{--- (2)}$$

$$\frac{1}{Y}\frac{d^2Y}{dy^2} = -K_y^2 \quad \text{--- (3)}$$

and
$$\frac{1}{Z}\frac{d^2Z}{dz^2} = -K_z^2 \quad \text{--- (4)}$$

$$\therefore K_x^2 + K_y^2 + K_z^2 = \frac{2mE}{\hbar^2} \quad \text{--- (5)}$$

The general solution of equation (2) is,

$$X(x) = A_x \sin K_x x + B_x \cdot \cos K_x \cdot X$$

Now, the boundary condition that at $x=0$, $X(x)=0$

we must have, $B_x = 0$.

$$\therefore X(x) = A_x \cdot \sin K_x X \quad \text{--- (6)}$$

Again, imposing the boundary condition, at $X = a$, $X(x) = 0$

$(\because \psi = 0)$ $\quad \therefore A_x \sin K_x a = 0$

Since, $A_x \neq 0$ we, should have $\sin k_x a = 0$.

$$\therefore k_x a = n_x \pi$$

or,

$$k_x = \frac{n_x \pi}{a} \text{ etc } \quad \text{--- (7)}.$$

similarly, $k_y = \frac{n_y \pi}{b}$

$$k_z = \frac{n_z \pi}{c}$$

where, $n_x = 1, 2, 3 \ldots$ $n_y = 1, 2, 3 \ldots$ & $n_z = 1, 2, 3 \ldots$

(n_x, n_y, n_z) are quantum number's

From equation, $k_x^2 + k_y^2 + k_z^2 = \frac{2mE}{\hbar^2}$

we get,

$$\left(\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2}\right) \cdot \pi^2 = \frac{2mE}{\hbar^2}.$$

$$\therefore \boxed{E = \frac{\pi^2 \hbar^2}{2m}\left(\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2}\right)} \quad \text{--- (8)}.$$

For the cube of side length $L = a = b = c$.

$$\therefore \boxed{E = \frac{\pi^2 \hbar^2}{2mL^2}\left(n_x^2 + n_y^2 + n_z^2\right)} \quad \text{--- (9)}.$$

$\therefore$ The corresponding energy level is 3-fold degenerate etc.

$$\therefore \psi(r) = A_x A_y A_z \cdot \sin\left(\frac{\pi n_x}{a} \cdot x\right) \cdot \sin\left(\frac{\pi n_y}{b} \cdot y\right) \cdot \sin\left(\frac{\pi n_z}{c} \cdot z\right)$$

from normalisation condition,

$$\int \psi^*(r)\, \psi(r)\, dr = 1$$

$$\therefore \int_0^a X^*(x)\,X(x)\,dx = \int_0^a A_x^2 \cdot \sin^2 k_x \cdot x\,dx = 1$$

$$= A_x^2 \cdot \frac{a}{2}$$

$$\therefore A_x = \sqrt{\frac{2}{a}}.$$

Similarly $A_y = \sqrt{\frac{2}{b}}$ and $A_z = \sqrt{\frac{2}{c}}$.

$$\therefore \psi(r) = \sqrt{\frac{8}{abc}} \cdot \sin\left(\frac{\pi n_x \cdot x}{a}\right) \cdot \sin\left(\frac{\pi n_y \cdot y}{b}\right) \cdot \sin\left(\frac{\pi n_z z}{c}\right)$$

and $p^2 = \frac{\pi^2 \hbar^2}{L^2}\left(n_x^2 + n_y^2 + n_z^2\right)^{1/2}$.

for Cube of side length $L = a = b = c$.

* Density of energy states :-

Energy density $g(E)$ is an important physical quantity in solid state physics. The number of energy states lying between E to $E + dE$ is $g(E)\,dE$.

$\therefore$ Total number of energy states upto energy E is,

$$N(E) = \int_0^E g(E) \cdot dE.$$

$$\therefore g(E) = \frac{dN(E)}{dE} \quad \text{--- (1)}$$

But, $n_x^2 + n_y^2 + n_z^2 = \frac{2mEL^2}{\pi^2 \hbar^2} \equiv R^2$ --- (2).

$\therefore$ Total number of states in a sphere of Radius R is obtained

$$\therefore N(E) = \cancel{2} \times \frac{1}{8_4} \times \frac{4\pi R^3}{3}$$

$$\therefore N(E) = \frac{\pi}{3}\left(\frac{2mEL^2}{\pi^2\hbar^2}\right)^{3/2} \quad \text{from } (2)$$

$$\therefore N(E) = \frac{(2m)^{3/2} L^3}{3\pi^2\hbar^3} E^{3/2}.$$

$$\therefore \frac{dN(E)}{dE} = \frac{(2m)^{3/2} L^3}{2\pi^2 \cdot \hbar^3} \cdot E^{1/2}.$$

$$\therefore g(E) = \frac{(2m)^{3/2} L^3}{2\pi^2\hbar^3} E^{1/2} \quad \text{From } (1) \quad \text{———— } (3)$$

where, L^3 represents the volume of the Box. energy density $g(p)$ can be obtained by

$$\therefore E = \frac{p^2}{2m}.$$

The number of states in the momentum from $0 \rightarrow p$ is given by,

$$N(p) = \int_0^p g(p) \cdot dp.$$

$$\therefore g(p) = \frac{dN(p)}{dp} \quad \text{————} \quad (4)$$

from equation (2). we have,

$$n_x^2 + n_y^2 + n_z^2 = \frac{2mEL^2}{\pi^2\hbar^2} = \frac{L^2p^2}{\pi^2\hbar^2} = R_p^2$$

$\therefore$ In the momentum space $N(p)$ is the volume of the sphere of Radius R_p in the positive octant as n_x, n_y & n_z are positive

$$\therefore N(p) = 2 \times \frac{1}{8} \cdot \frac{4}{3} \cdot \pi R_p^3$$

$$= \frac{\pi}{3} \left(\frac{L^2 p^2}{\pi^2 \hbar^2} \right)^{3/2}$$

$$= \frac{\cancel{\pi}}{3} \times \frac{L^3 p^3}{\pi^{\cancel{3}2} \hbar^3}$$

$$= \frac{L^3 p^3}{3\pi^2 \hbar^3}$$

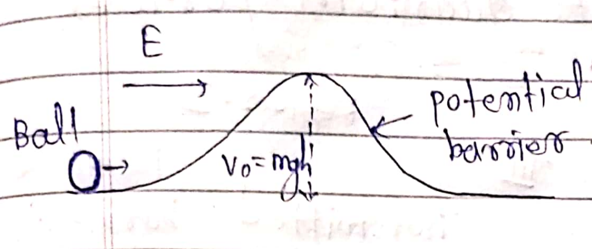
$$\therefore \frac{dN(p)}{dp} = \frac{L^3 p^2}{\pi^2 \hbar^3}.$$

$$\therefore g(p) = \frac{L^3 p^2}{\pi^2 \hbar^3} = \frac{V p^2}{\pi^2 \hbar^3} \quad \text{—— (5)}$$

or $$g(p) = \frac{8\pi V p^2}{h^3} \qquad \because \left[\hbar = \frac{h}{2\pi} \right]$$

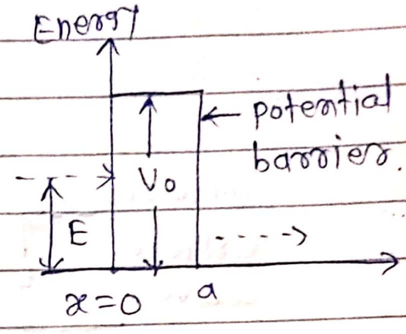
* Potential Barrier (Tunnelling Effect)

a) Classical situation



ⓐ.

Quantum mechanical situation.



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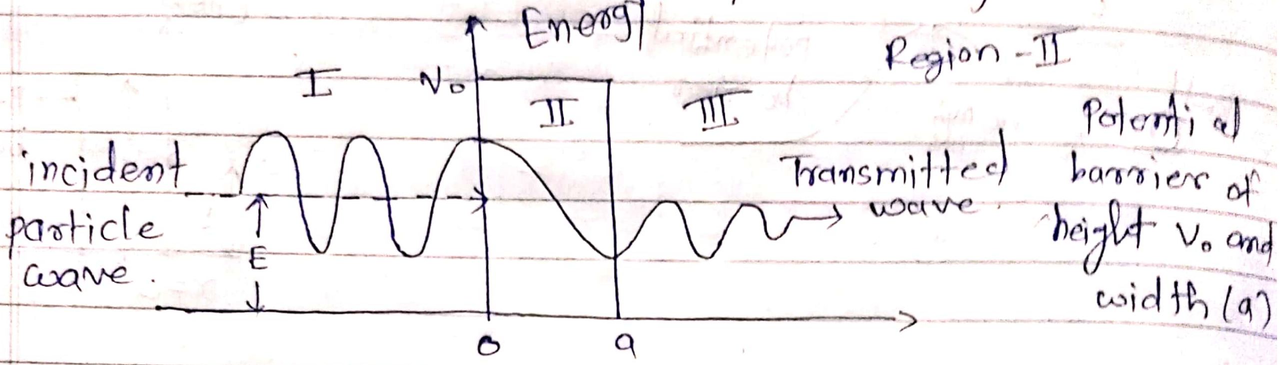
* If the kinetic energy of the particle is greater than the gravitational potential barrier ($E > V_0$) then the ball climbs the hill and reaches the other side. But if ($E < V_0$) then ball can't reach the hill-top and consequently can't reach the other side of hill.
If at all the ball has to reach the other side of hill, then there must be a tunnel in the hill at a potential height which is less than kinetic energy of the ball.
Thus the hill acts as a potential barrier.
But in quantum mechanics, we deal with microscopic particles called quantum particles like electron, proton, α-particle etc.
if $E > V_0$ then particle can be on the other side of the barrier. But if $E < V_0$ then there is certain probability that the particle can pass through the barrier and reach other side.

phenomenon of crossing the barrier without reaching the top of the barrier is called quantum tunnelling.
Quantum tunnelling is possible because of the wave nature of quantum particles.



Quantum tunnelling through potential barrier.

Then by solving the schroedinger equations in region I, II and III, it can be seen that there is certain probability that the particle wave reaches the region (III)
ie. the other side of barrier but with decreased energy (or amplitude)
while passing through