Quantum Mechanics

The photoelectric effect :-

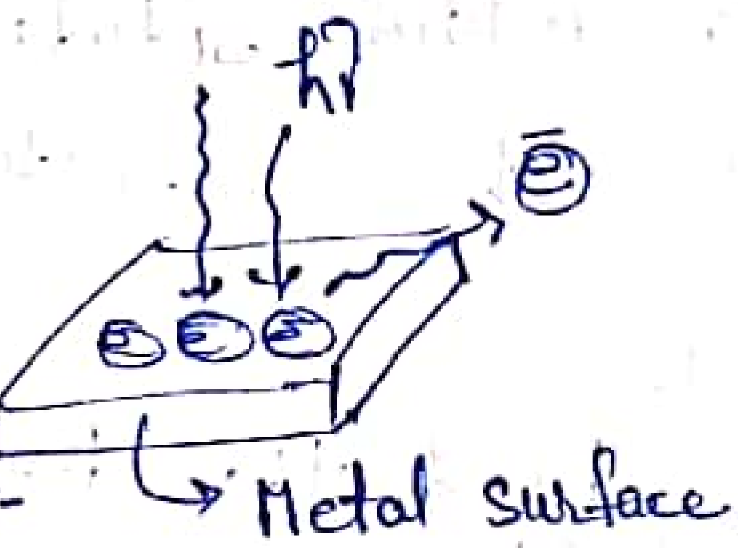
When a metallic surface is exposed to the light of suitable frequency or wave length, electrons are ejected from the surface. This effect is called photoelectric effect and electrons ejected out of the metal surface called photoelectrons.

It may be noted that the phenomenon is observed only if the frequency (or wavelength) of incident light radiation is more than a certain value for the metal. This frequency is called threshold frequency and the corresponding wave length is called threshold wavelength.

Frequency of light (EM wave) > Threshold frequency

wave length of " " < threshold wave length

Photo electric effect proposed that ∴ light has a dual character with both particle and wave ~~prop.~~ properties.



Louis De Broglie did in 1924, He proposed that moving objects have wave as well as particle characteristic.

de-Broglie hypothesis :

Whenever a particle is in motion, waves are associated with it. These wave are called matter waves or deBroglie waves.

For finding the expression of matter waves, consider the Einstein's theory of relativity. According to this theory, the momentum p and energy E of a particle of rest mass m_0 are related as

$$E = \sqrt{p^2c^2 + m_0^2c^4}$$

For a photon of light rest mass is zero

$$m_0 = 0$$

$$E = pc \quad \text{--- (1)}$$

If ν is the frequency of light radiation

$$E = h\nu = \frac{hc}{\lambda} \quad \text{--- (2)}$$

$h \rightarrow$ Planck's Const

$\lambda \rightarrow$ wavelength

$c \rightarrow$ speed of light

Eq^n (1) & (2)

$$\frac{hc}{\lambda} = pc \Rightarrow \boxed{\lambda = \frac{h}{p}}$$

Photon wave length

$$\lambda = \frac{h}{p} \quad \text{--- (3)}$$

De-Broglie suggested that eqn.-(3)
is a completely general one that applies to materials particles as well as to photons, The momentum of particle of mass m and velocity v is $p = \gamma m v$ and de-Broglie wave length

$$\lambda = \frac{h}{p} = \frac{h}{\gamma m v}$$

$\gamma \rightarrow$ is the relativistic factor

$$\gamma = \frac{1}{\sqrt{1 - v^2/c^2}}$$

As in case of EM wave, the wave and particle aspects of moving bodies can never be observed at the same time.
In a certain situation a moving body resembles a wave and in others it ~~some~~ resembles a particle.

example 1-
Find the de-Broglie wavelength of (a) a 46gm golf ball with a velocity of 30m/s and (b) $\bar{e}$ with a velocity of 10^7 m/s.

Solution $\rightarrow$ (a) $v \ll c$ we have take $\gamma = 1$

$$\lambda = \frac{h}{mv} = \frac{6.63 \times 10^{-34}\ J.s}{46 \times 10^{-3}\ kg \times 30\ m/s} = 4.8 \times 10^{-34}\ m$$

The wavelength of the golf ball is so small compared with its dimension that we would not expect to find any wave aspects in its behavior.

(b) Again $v \ll c$, $\gamma = 1$ $\quad m = 9.1 \times 10^{-31}$ kg

$$\lambda = \frac{h}{mv} = \frac{6.63 \times 10^{-34}\ (J.s)}{9.1 \times 10^{-31}\ kg \times 10^{7}\ m/s} = 7.3 \times 10^{-11}\ m$$
$$= 0.73 \times 10^{-10} = 0.73\ \mathring{A}$$

The dimension of atoms, are comparable with this figure - the radius of the hydrogen atom, for instance is 5.3×10^{-11} m. It is ~~not~~ therefore not surprising that the wave character of moving electrons is the key to understanding atomic structure and behavior.

The de-Broglie wave length associated with a moving particle travelling with a uniform velocity is given by

$$\lambda = \lambda_{} = \frac{h}{p} \quad \text{--- (3.1)}$$

De-Broglie wavelength in terms of energy of the particle

If E is the kinetic Energy of the particle, then

$$E = \frac{1}{2} m v^2 = \frac{m^2 v^2}{2m} = \frac{p^2}{2m}$$

$$p^2 = 2mE \Rightarrow \boxed{p = \sqrt{2mE}} \quad \text{--- (3.2)}$$

From equation (3.2) & (3.1)

$$\boxed{\lambda = \frac{h}{\sqrt{2mE}}} \quad \text{--- (3.3)}$$

De-Broglie wavelength of the electron, If an electron is accelerated under a potential of V volt. It acquired a kinetic energy E (eV)

the wavelength

$$\lambda = \frac{h}{\sqrt{2m\,eV}}$$

$$E = e.V$$

$$m = 9.1 \times 10^{-31}\ kg$$

$$e = 1.6 \times 10^{-19}\ C$$

$$h = 6.62 \times 10^{-34}\ J.s$$

$$\lambda = \frac{6.62 \times 10^{-34}\ J.s}{\sqrt{2 \times 9.1 \times 10^{-31}\ kg \cdot 1.6 \times 10^{-19}\ C \cdot V}} =$$

$$\lambda = \frac{12.27 \times 10^{-10}}{\sqrt{V}}\ m$$

$$\boxed{\lambda = \frac{12.27}{\sqrt{V}}\ \mathring{A}} \quad \text{--- (3.4)}$$

Equation 3.4 is used to find the wavelength associated with the electrons when accelerated under a potential 'V'.

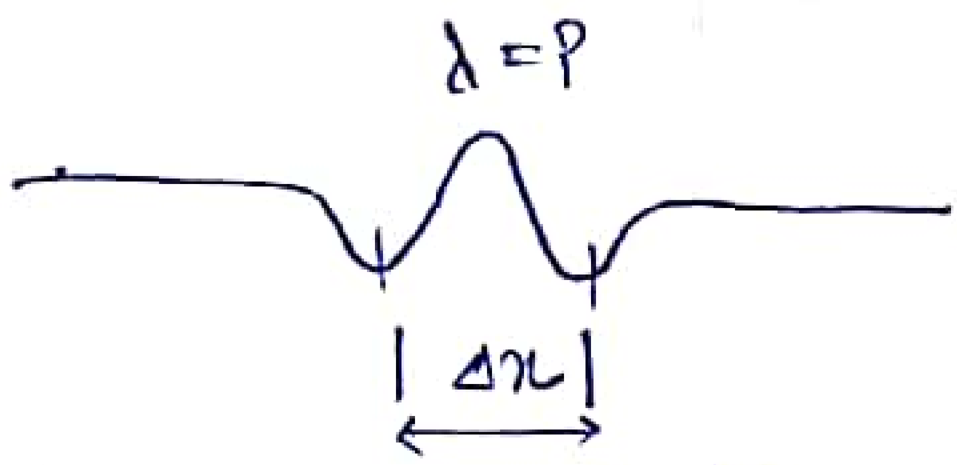
Heisenberg Uncertainty Principle :-

"The uncertainty principle says that we cannot measure the position (x) and momentum (p) of a particle with absolute precision."

Heisenberg's uncertainty principle states that in any simultaneous determination of the position and momentum of a particle, the product of the uncertainties is equal to or greater than Planck's constant or $h/4\pi$

For Microscopic $\quad \Delta x\,\Delta p \geq h/4\pi \Rightarrow \Delta x \cdot \Delta p \geq \frac{\hbar}{2}$ $\left[\begin{array}{l} \Delta x \cdot \Delta p \geq \hbar \\ \Delta x \cdot \Delta p \geq h \\ \Delta x \cdot \Delta p \geq \hbar/2 \end{array}\right]$

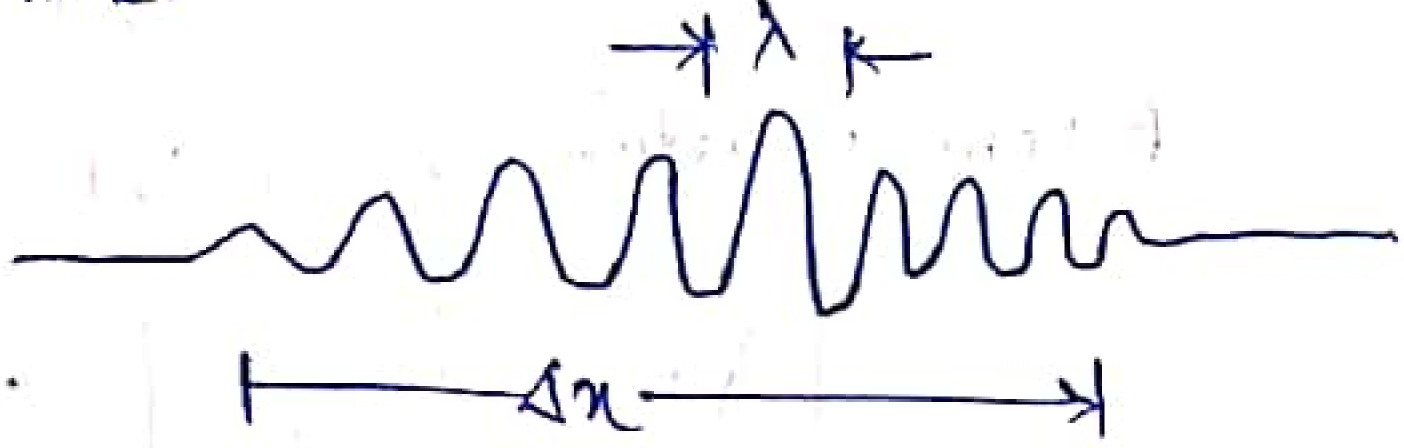
It is impossible to know both exact position and exact momentum of an object at the same time.



Δx - Small
Δp large

Figure 4.(a)

A narrow de Broglie wave group. The position of the particle can be precisely determined, but the wavelength (momentum) cannot be established because there are not enough wave to measure accurately



Δx large
Δp Small

Figure 4(b)

A wide wave group. Now the wave length can be precisely determined but not the position of the particle

Different form of Heisenberg Uncertainty principle:

1. Angular momentum and angular displacement uncertainty principle

A particle is moving in circular path, then at a smaller angular displacement (i.e. θ) the angular momentum is L, then the uncertainty in angular momentum ΔL and uncertainty in angular displacement Δθ

$$\boxed{\Delta L \cdot \Delta\theta \geq \hbar/2}$$

Time Energy Uncertainty Principle!

If an observation is carried out on a system at a point x within a time Δt and used to determine the energy of the system at that point x, then uncertainty ΔE in energy is such that

$$\boxed{\Delta t \cdot \Delta E \geq \frac{\hbar}{2}}$$

This relation we can find from position & momentum uncertainty principle

$$\Delta x \cdot \Delta p \geq \hbar/2 \quad \text{— (5.1)}$$

As we know

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

$$\Delta E = \frac{2p \cdot \Delta p}{2m} = \frac{p}{m} \Delta p$$

$$\Delta E = v \, \Delta p \quad \text{— (5.2)}$$

Now uncertainty in the time

$$\frac{\Delta x}{v} = \Delta t \quad \text{— 5}$$

$$\frac{\Delta x}{\Delta t} = v \quad \text{— (5.3)}$$

Multiplying eq^n (5.2) with eq^n (5.3)

$$\Delta E = \frac{\Delta x}{\Delta t} \Delta p$$

$$\Delta E \cdot \Delta t = \Delta x \cdot \Delta p$$

From uncertainty principle $\Delta x \cdot \Delta p \geq \hbar/2$

$$\boxed{\Delta E \cdot \Delta t \geq \hbar/2}$$

$$\boxed{\Delta t \cdot \Delta E \geq \hbar/2}$$

Applications of Heisenberg Uncertainty principle

1. Non existance of electron in Nucleus :→

We know that Radius of the nucleus of any atom $\sim 10^{-14}$ m, So that if an electron is confined within the nucleus, the uncertainty in the position

$$\Delta x = 2 \cdot 10^{-14} \text{ m.}$$

$$\Delta x = 2r = 2\times10^{-14} \text{ m}$$

$$\Delta x . \Delta p = \hbar = \frac{h}{2\pi}$$

$$\Delta p = \frac{6.624\times10^{-34}}{2\times3.14\times2\times10^{-14}} =$$

$$= 5.724 \times 10^{-21} \text{ kg m/s}$$

p = at least magnitude of Δp

Kinetic energy of $\bar{e}$ of mass m is given by

$$E = \frac{p^2}{2m} = \frac{[5.724 \times10^{-21}]^2}{2\times9.1\times10^{-31}\times 1.6\times10^{-19}}$$

$$= 195.5 \times 10^{0} \text{ eV}$$

$$\boxed{E = 95.5 \text{ MeV}}$$

It means that if electrons exist inside the nucleus, their kinetic energy must be of the order 95.5 MeV.. But experimental observations reveals that no electron in the atom can possess energy greater than 4 MeV. Therefore, electrons does not exist in the nucleus.

2. Minimum Energy of a particle in a box.

Consider a particle inside in a one-D box of length a. The particle moves inside the box and can be anywhere at a given instant.

Therefore Uncertainty in its position is

$$\Delta x = a$$

Using Uncertainty principle

$$\Delta x . \Delta p \geq \hbar/2$$

$$\Delta x \, \Delta p = \frac{h}{4\pi} \Rightarrow \Delta p = \frac{\hbar}{2\Delta x}$$

$$\Delta p = \frac{h}{4\pi a}$$

minimum value of momentum of particle is

$$p = \Delta p = \frac{h}{4\pi a}$$

Energy

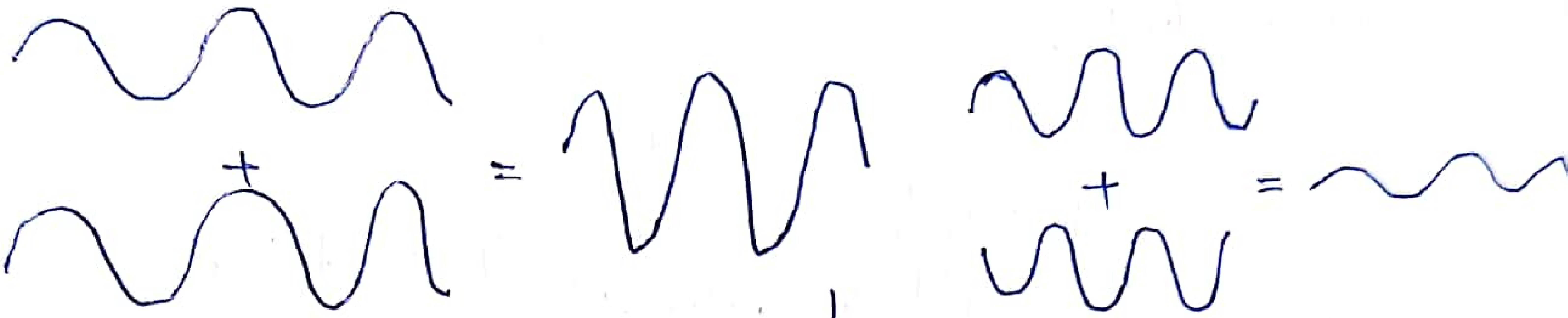
$$E = \frac{p^2}{2m} = \left(\frac{h}{4\pi a}\right)^2 \frac{1}{2m}$$

$$E = \frac{h^2}{4\times4\pi^2 a^2 \, 2m}$$

$$E = \frac{h^2}{4\times8\pi^2 m a^2} = \frac{h^2}{32\pi^2 m a^2}$$

This equation gives the minimum value of energy possessed by particle in the box. This is called Zero point energy. Expression shows that a particle does not have a zero energy in the free state.

Interfere: When two or more trains of light waves meet in a region, they interfere to produce a new wave there whose instantaneous amplitude is the sum of those of the original waves.



In Constructive Interference, Superposed waves in phase reinforce each other.

In destructive interference, waves out of phase partially or completely cancel each other.

Constructive interference refers to the reinforcement of waves with the same phase to produce a greater amplitude, and destructive interference refers to the partial or complete cancellation of wave whose phases differ.

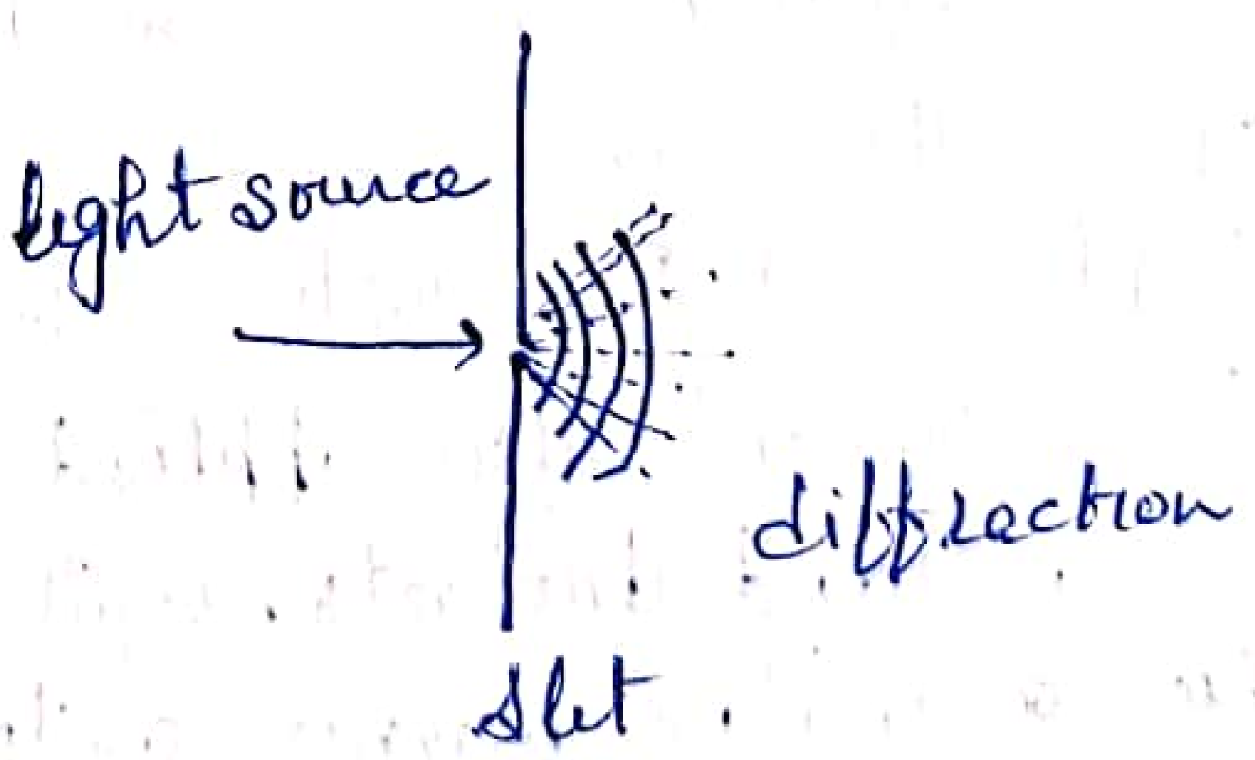
Diffraction: → Light bending around an object

Diffraction is slight bending of light as it passes around the edge of an object. The amount of bending depends on the relative size of the wavelength of light to the size of opening. If the opening size is much larger than the light wavelength the bending will be ~~un~~unnoticeable. However, if the two are closer in size or equal, the amount of bending is considerable.

Slit opening ~ light wavelength

~~light wavelength~~

~ nm



In the atomsphere, diffracted light is actually bend around atomsphere particles- most commonly, the atomsphere particles are tiny water droplets found in clouds. Diffracted light can produce fringes of light, dark or colored bands. An optical effect that results from diffraction of light is the silver lining sometimes found around the edges of clouds.

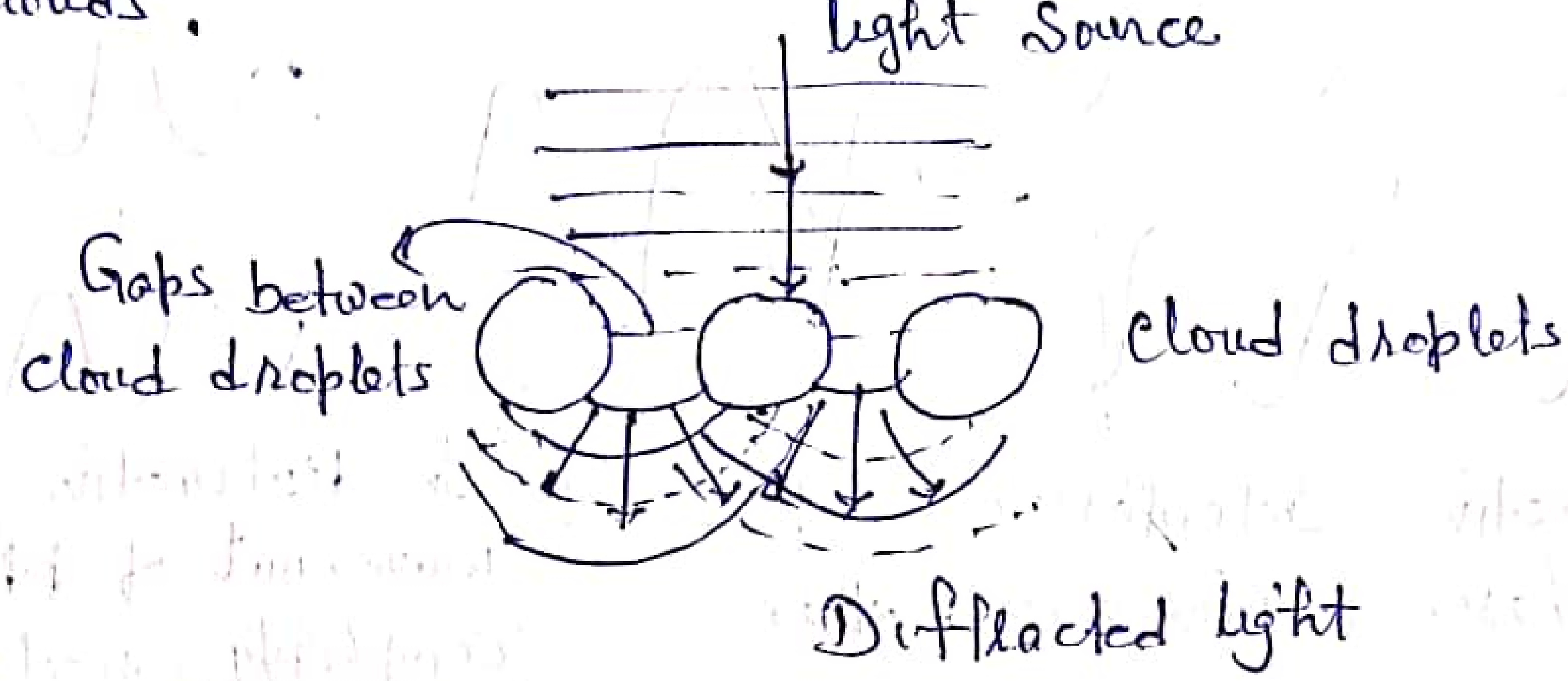
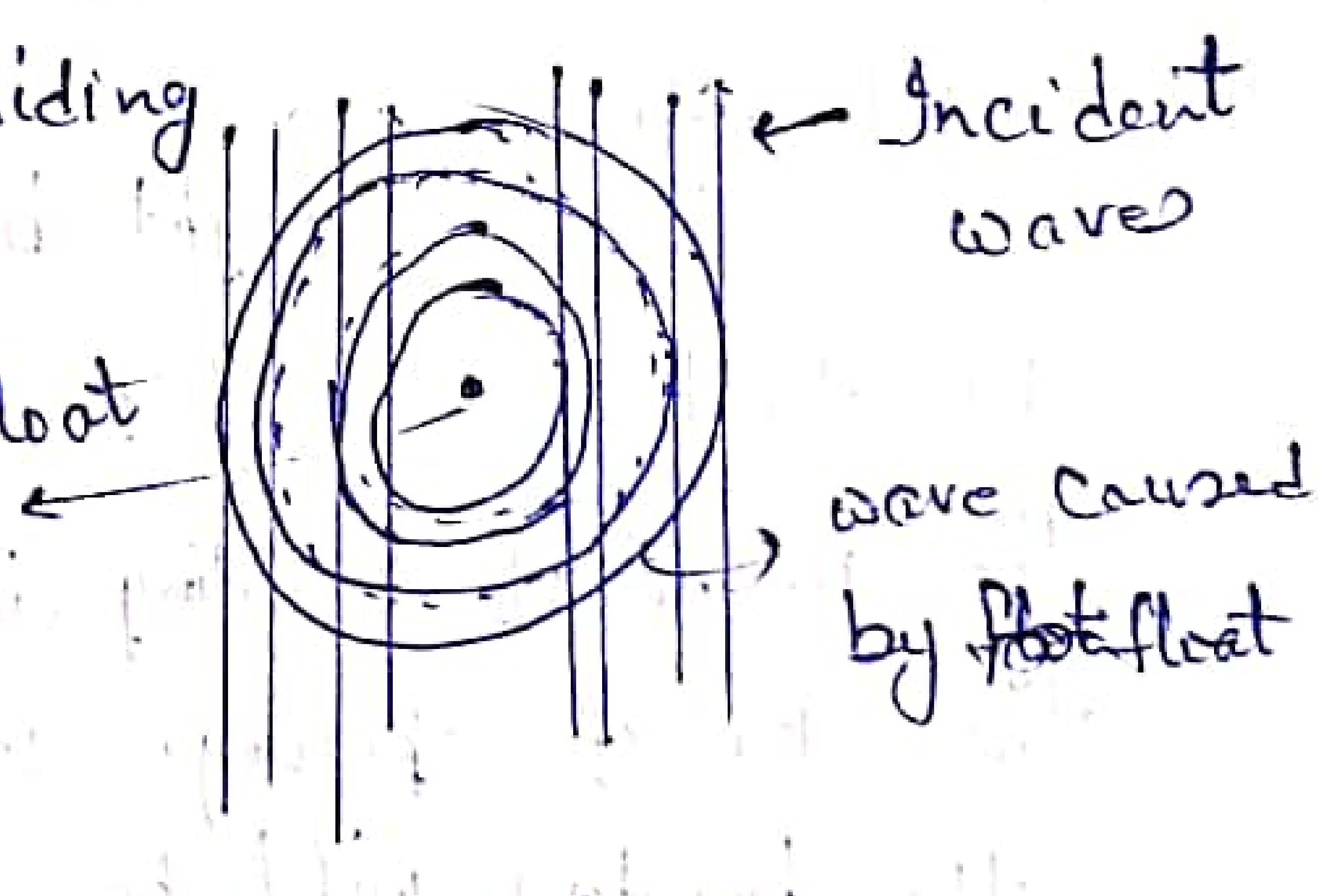


Figure shows how light is bent around small droplets in the cloud.

optical effects resulting from diffraction are produced through interface of light waves. To visualize this, imagine light waves as water waves. If water waves were incident upon a float residing on the water surface, the float would bounce up and down in responce to the incident waves, producing waves of its own. As these waves spread outward in all directions from the float, they interact with other water waves.



If the crest of two waves combine, an amplified wave is produced (constructive interference), However, if a crest of one wave and trough of another wave combine, they cancel each other out to produce no vertical displacement (destructive Interference).

This concept also applied to light waves, when sun light (or moon light) encounters a cloud droplets, light waves are Altered and interact with one another a similar manner as the water wave described above. If there is constructive interference, (the crest of two light wave combing), the light will appear brighter. If there is destructive interference (the through of one light meeting the crest of another), the light will appear darker or disappear entirely.

Wave function :- ψ

The quantity with which quantum mechanics is concerned is the wave function ψ of a body. Remember ψ itself has no physical significance, the square of its magnitude $|\psi|^2$ evaluated at a particular place at a particular time.

$|\psi|^2 \rightarrow$ Probability of finding the body (Particle) there at that time

$$\boxed{|\psi|^2 = P}$$

The linear momentum, angular momentum and energy of the particle are other quantities that can be established from ψ.

Wave functions are usually complex with both real and imaginary part. The probability, however must be positive real quantity.

Wave function

$$\psi = A + iB$$

A and B are real function.

Complex conjugate ψ^* of ψ is

Complex Conjugate

$$\psi^* = A - iB$$

$$|\psi|^2 = \psi^*\psi = (A - iB)(A + iB) = A^2 - i^2B^2$$

$$= A^2 + B^2$$

Hence $|\psi|^2 = \psi^*\psi$ is always a positive real quantity.

Normalization :-

The probability of finding the particle in a volume element $dx\,dy\,dz$ is given by $|\psi|^2 dx\,dy\,dz$. As we known the particle must be somewhere in space, hence total probability a finding the particle in all space is unity. This condition of unit probability in whole space is called normalization

$$\boxed{\int_{-\infty}^{\infty} |\psi|^2 dV = 1}, \Rightarrow \boxed{\int_{-\infty}^{\infty} \psi^*\psi\, dx\,dy\,dz = 1} \Rightarrow \boxed{\int_{-\infty}^{\infty} P\,dV = 1}$$

A wave function which satisfies the above equation is said to be normalized wave function

Well behaved Wave functions.

1. ψ must be normalized
2. ψ must be finite.
3. ψ must be Single valued function. Because the particle cannot be at two places at a given time
4. ψ must be Continuous in all Space, Since particle can be any where in space
5. $\frac{\partial\psi}{\partial x}, \frac{\partial\psi}{\partial y}, \frac{\partial\psi}{\partial z}$ must be Continuous and Single valued everywhere
6. ψ must vanish, where potential energy is infinite.

Wave Equation: Schrodinger's equation, which is the fundamental equation of QM in the same sense that the second law of motion is the fundamental equation of Newtonian mechanics, is a wave equation in the variable ψ.

We know the wave equation

$$\frac{\partial^2 y}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2 y}{\partial t^2} \quad \longleftarrow \quad (10.1)$$

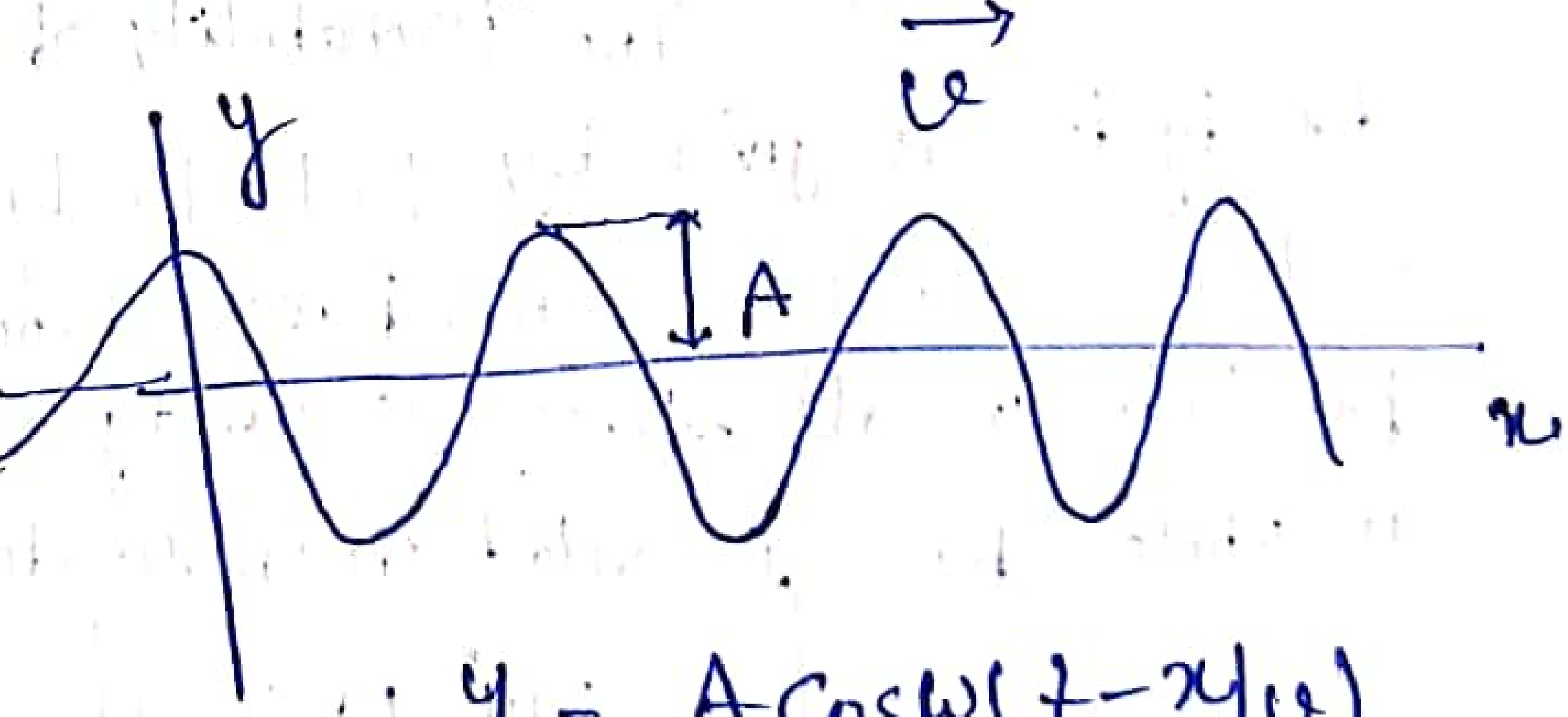
~~This~~ which governs, a wave whose variable quantity is y that propagates in the x-direction with the speed v.

In the case of ~~st~~ wave in stretched string, y is the displacement of the string from the x ~~axis~~ axis.

In case of sound wave, y is the pressure difference

In case of light wave, y is either the electric or the magnetic field magnitude

Let us consider the wave equivalent of a 'free particle' which is particle that is not under the influence of any forces and therefore flow a straight path at constant speed.



$$y = A\cos\omega(t - x/v)$$

Waves in the xy plane travelling in the $+x$ direction along a stretched string lying on the x axis.

Wave is described the general solution of eq^n (10.1) for und damped (that is constant amplitude A), monochromatic (constant angular freq.) harmonic waves in +ve x direction,

$$y = A e^{-i\omega(t - x/v)} \quad — (11.1)$$

$y \Rightarrow$ is complex quantity

But $\quad e^{-i\theta} = \cos\theta - i\sin\theta$

Now eq^n (11.1) become

$$y = A\cos\omega(t - x/v) - iA\sin(\omega(t - x/v)) \quad — (11.2)$$

Only the real part of eq^n (11.2) has significance in the case of waves in stretched string. ~~y → displace-~~

$y \rightarrow$ Represents the displacement of the string from its normal position

Imaginary part of eq^n (11.2) is discarded as irrelevant.

example:-

Verify that $y = Ae^{-i\omega(t - x/v)}$ is a solution of wave eq^n.

Solution:

The partial derivative of y with respect to x ($t \rightarrow$ treated as constant)

$$\frac{\partial y}{\partial x} = \left(A\left(-\frac{i\omega}{v}(-1)\right) e^{-i\omega(t - x/v)}\right)$$

$$\frac{\partial y}{\partial x} = \frac{i\omega}{v} y$$

Second partial derivative

$$\frac{\partial^2 y}{\partial x^2} = \left(\frac{i\omega}{v}\right)^2 y$$

$$\frac{\partial^2 y}{\partial x^2} = -\frac{\omega^2}{v^2} y \quad — (11.3)$$

Now partial derivative of y with respect to t ($x \rightarrow$ treated as constant)

$$\frac{\partial y}{\partial t} = (A)(-i\omega)\left(e^{-i\omega(t - x/v)}\right)$$

$$\partial y/\partial t = (-i\omega)\, y$$

As second derivative

$$\frac{\partial^2 y}{\partial t^2} = (-i\omega)^2 y \Rightarrow \frac{\partial^2 y}{\partial t^2} = -\omega^2 y \quad — (11.4)$$

eq^n (11.3) & (11.4)

$$\boxed{\frac{\partial^2 y}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2 y}{\partial t^2}}$$

Hence $y = Ae^{-i\omega(t - x/v)}$ is sol^n of wave equation

Schrodinger's Equation: Time dependent form

We assume that ψ for a particle moving freely in the $+x$ direction is specified by

$$\psi = A\, e^{-i\omega(t - x/v)} \quad \text{--- (12.1)}$$

Angular frequency $\omega = 2\pi\nu$

$$\nu = \frac{v}{\lambda} \Rightarrow v = \lambda \cdot \nu$$

frequency $\nu = v/\lambda$

$$\psi = A\, e^{-i2\pi\left[\nu t - \frac{x\nu}{\lambda\cdot\nu}\right]}$$

$$\psi = A\, e^{-2\pi i\left[\nu t - x/\lambda\right]} \quad \text{--- (12.2)}$$

As we known $E = h\nu$

$$= 2\pi \frac{h}{2\pi}\nu = 2\pi\hbar\nu$$

$$\lambda = \frac{h}{p}$$

$$\frac{1}{\lambda} = \frac{p}{h} = \frac{p}{2\pi\hbar}$$

put the values of ν & λ in eq^n (12.2)

we have

$$\psi = A\, e^{-2\pi i\left[\frac{E}{2\pi\hbar}t - \frac{xp}{2\pi\hbar}\right]}$$

$$\boxed{\psi = A\, e^{-i/\hbar\,[Et - px]}} \quad \text{--- (12.3)}$$

eq^n (12.3) described the wave equivalent of an unrestricted particle of total energy 'E' and momentum 'p' moving in $+x$ direction

We do the differentiating Eq (12.3) for ψ twice w.r.to x

$$\frac{\partial\psi}{\partial x} = A(-i/\hbar)(-p)\, e^{(-i/\hbar)[Et - px]}$$

$$\frac{\partial\psi}{\partial x} = (+ip/\hbar)\,\psi$$

$$\frac{\partial^2\psi}{\partial x^2} = \left(\frac{ip}{\hbar}\right)^2\psi \Rightarrow \frac{\partial^2\psi}{\partial x^2} = -\frac{p^2}{\hbar^2}\psi$$

$$p^2\psi = -\hbar^2\frac{\partial^2\psi}{\partial x^2} \quad \text{--- (12.4)}$$

Differentiating eq^n (12.3) one with to t

$$\frac{\partial\psi}{\partial t} = \left(\frac{-i}{\hbar}E\right)\psi$$

$$\boxed{E\psi = -\frac{\hbar}{i}\frac{\partial\psi}{\partial t}} \quad \text{--- (12.5)}$$

At speeds small compared with that of light, the total energy E of a particle is the sum of its kinetic energy ($p^2/2m$) and its potential energy $U(x,t)$

$U \rightarrow$ is in general a function of postion & time

$$E = \frac{p^2}{2m} + U(x,t) \quad \text{--- (13.1)}$$

Multiplying both sides of eqn (13.1) by the wave function ψ

$$E\psi = \frac{p^2\psi}{2m} + U\psi \quad \text{--- (13.2)}$$

Now we have substitute for $E\psi = (-\hbar/i)\frac{\partial\psi}{\partial t}$ and $p^2\psi = -\hbar^2\frac{\partial^2\psi}{\partial x^2}$ from Eqn (12.4) & (12.5) in eqn (13.2)

we get

$$-\frac{\hbar}{i}\frac{\partial\psi}{\partial t} = \frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + U\psi.$$

Time dependent Schrodinger eqn.

$$\boxed{i\hbar\frac{\partial\psi}{\partial t} = \frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + U(\psi)} \quad \text{--- (13.1)}$$

In 3-D the time dependent Schrodinger eqn

$$\boxed{i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\left[\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2}\right] + U\psi}$$

where the particle's potential energy U is some function x, y, z & t

Once U is known, Schrodingers may be solved for the wave function ψ of the particle, from which its probablity density $|\psi|^2$ may be determined for a specified x, y, z, t.

Time Independent Schrodinger Equation OR Steady State

In many cases, the potential energy of particle does not depend upon time explicitely; that forces that act on it, and hence U, vary with the position of the particle only. ~~when~~

In such cases, Schrodinger time dependent equation is simplefied by eliminating all references of time (t). The equation thus obtained is called Intime dependent Schrodinger equation.

For a particle moveing along x-axis, wave function in term of total energy E & momentum p giving by

$$\psi = A e^{-(i/\hbar)[Et - px]}$$

$$= A e^{-\frac{iEt}{\hbar}} \cdot e^{\frac{ipx}{\hbar}}$$

$$= \underline{A e^{\frac{ipx}{\hbar}}} \cdot e^{-(iE/\hbar)t}$$

$$\psi = \phi(x)\, e^{-(iE/\hbar)t} \quad \text{—— (14.1)}$$

Here $\phi(x) = A e^{ipx/\hbar}$ position dependent function

Partically differentiale eq^n (14.1) 2 times w.r.to x we get

$$\frac{\partial \psi}{\partial x} = e^{(-iE/\hbar)t} \cdot \frac{\partial \phi(x)}{\partial x}$$

$$\frac{\partial^2 \psi}{\partial x^2} = e^{(-iE/\hbar)t} \frac{\partial^2 \phi(x)}{\partial x^2} \quad \text{—— (14.2)}$$

Now taking partically derivation of eq^n (14.1) w.r.to t

$$\frac{\partial \psi}{\partial t} = \left(-\frac{iE}{\hbar}\right) e^{(-iE/\hbar)t} \cdot \phi(x) \quad \text{—— (14.3)}$$

Value

Value of eq^n (14.2) and (14.3) putting in ~~eq~~ time dependent S/e wave equation

~~We~~ Time dependent Schrodinger wave equation

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + U(x) \psi$$

$$i\hbar\left[\left(-\frac{iE}{\hbar}\right) \cdot e^{-i(E/\hbar)t} \phi(x)\right] = -\frac{\hbar^2}{2m} e^{-i(E/\hbar)t} \frac{\partial^2 \phi(x)}{\partial x^2}$$
$$+ U \cdot \phi(x)\, e^{-i(E/\hbar)t}$$

$$E\,\phi(x) = \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \phi(x) + U \phi(x)$$

$$\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \phi(x) + (E - U)\phi(x) = 0$$

So we insert $\psi(x)$

$$\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x) + (E-U)\,\psi(x) = 0$$

$$\boxed{\frac{\partial^2}{\partial x^2} \psi(x) + \frac{2m}{\hbar^2}(E - U)\,\psi(x) = 0}$$

Time independent wave equation in 1-D,

3D

$$\boxed{\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} + \frac{2m}{\hbar^2}(E-U)\psi = 0}$$

Schrodinger' steady state wave equation in 3-D.

Postulates of Quantum Mechanism :-

Postulates Cant be drive, It can be verifeded only.

Postulates -1

The state of any physical system is given by a state Vector $\psi(x,t)$ in Hilbert space. Thus $\psi(x,t)$ Contains all the information we need. Any Superpostion of state Vectors is a state Vector.

Physical system state $\xrightarrow{\text{Represent by}}$ (Vector) $|\psi(x,t)\rangle$

$$\psi'(x,t) = a\,\psi_1(x,t) + b\,\psi_2(x,t)$$

Postulates 2.

To every observables or dynamical variable there ~~Corrspone~~ Corresponding a linear Hermitian (Real eigen values) operator whose eigen function forms a complete basis.

observable or dynamical variable :- Position, momentum, Angular momentum, Kinetic energy potential energy,

We want to measure those" quantity known as dynamical Variable

$$\hat{p} = -i\hbar \frac{\partial}{\partial x}\psi(x,t)$$

example

$$y = e^{\gamma x} \Rightarrow \frac{dy}{dx} = \gamma\, e^{\gamma x}$$

operator $\rightarrow \frac{d}{dx}$; $\gamma \downarrow$ eigen Value

Postulate 3 :-

The measurement of an observable $\hat{A}$ may be represented by the action of $\hat{A}$ on state vector $\psi(x,t)$ which results $a\psi$ where a is called eigen value of $\hat{A}$

$$\hat{A}\psi = a\psi$$

In such case, the wave function ψ is said to be eigen function of $\hat{A}$ and 'a' is called the eigen value of $\hat{A}$ for that wave function.

Postulate 4.

The time evolution of the state vector $\psi(x,t)$ is governs by the time dependent schrodinger equation

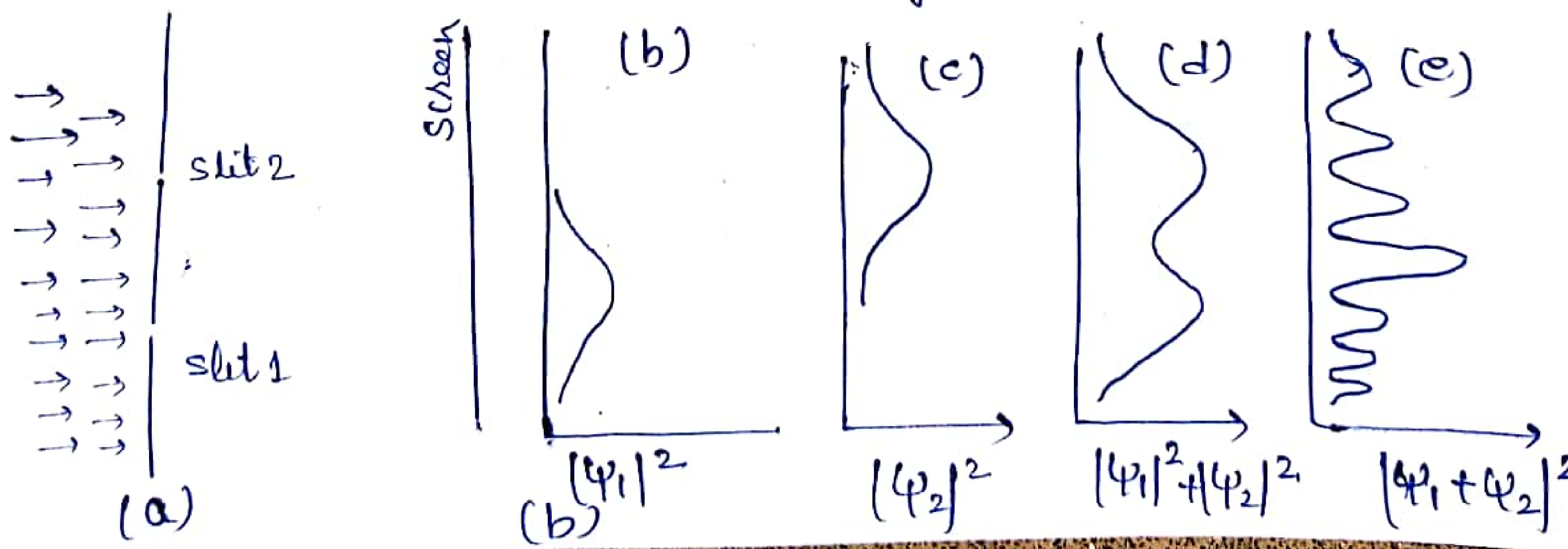
$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi = i\hbar\frac{\partial\psi}{\partial t}$$

Linearity & Superpostion :-

" wave function add, not probabilities"

$$\psi = a_1\psi_1 + a_2\psi_2 \qquad a_1 \; \& \; a_2 \text{ are Constant}$$

Wave obey the superposition principle. We conclude that interference effects can occur for wave functions just as they can for light, sound, water and electromagnetic waves.



Let us apply superpostion principle to the diffraction of an electron beam.

(b) Slit $\underline{\underline{1}}$ is open

Probability density $P_1 = |\psi_1|^2 = \psi_1^* \psi_1$

(c) Slit $\underline{\underline{2}}$ is open, Probability density

$$P_2 = |\psi_2|^2 = \psi_2^* \psi_2$$

(d) We might suppose opening both slits

Probability density

$$P_1 + P_2 = |\psi_1|^2 + |\psi_2|^2$$

That is not correct. In Quantum Mechanics wave function add, not probabilities

(e) The diffraction pattern of (e) arises from the superposition ψ of wave function ψ_1 & ψ_2 of the electrons that have passed through slits 1 & ~~slit~~ 2

$$\psi = \psi_1 + \psi_2$$

The probabilityes density at the screen is

$$P = |\psi|^2 = |\psi_1 + \psi_2|^2 = (\psi_1^* + \psi_2^*)(\psi_1 + \psi_2)$$

$$= \psi_1^* \psi_1 + \psi_2^* \psi_2 + \psi_1^* \psi_2 + \psi_2^* \psi_1$$

$$= P_1 + P_2 + \underline{\psi_1^* \psi_2 + \psi_2^* \psi_1}$$

The two terms at the right of this equation represent the difference between (d) & (e) which are responsible for the oscillation of the electron intensity at the screen.

Expectation Values

" How to extract information from a wave function"

With in restrictions imposed by the uncertainity principle, the wave funtion $\psi(x,y,z,t)$ a solution of the schrodinger wave equation, Conveys all the information ~~of~~ about the particle. But this information is in the form of probability. therefore We can't talk of exactness, but can speak about average or what we call the expection value

$$\langle x \rangle = \frac{N_1 x_1 + N_2 x_2 + \cdots}{N_1 + N_2 + \cdots} = \frac{\sum N_i x_i}{\sum N_i}$$

If ~~N_1~~ $\rightarrow$ N total number of students in class,

$N_1 x_1 \rightarrow N_1$ student have got x_1 rupees.

In Q.M. the exact position of the particles can not found, we always talks about the probability of finding the particles. There fore If P_1 is the probability of occurrance of N_1 particles at the position x_1
P_2 is the probability " " N_2 " " x_2

The average position of a particle would be

$$\langle x \rangle = \frac{x_1 P_1 + x_2 P_2 + x_3 P_3 + \cdots}{P_1 + P_2 + P_3 + \cdots} = \frac{\sum x_i P_i}{\sum P_i}$$

The particle be found in an interval dx at x_i

then $P_i = |\psi_i|^2 dx$

where ψ_i = Particle wave function evaluated at $x = x_i$

$$\langle x \rangle = \frac{\int_{-\infty}^{\infty} x |\psi|^2 dx}{\int_{-\infty}^{\infty} |\psi|^2 dx}$$

Probability

If ψ is normalized wave function, denominator equal to

$$\int_{-\infty}^{\infty} |\psi|^2 dx = 1$$

Expection Value for position

$$\langle x \rangle = \int_{-\infty}^{\infty} x |\psi|^2 dx = \int_{-\infty}^{\infty} \psi^* x \psi \, dx$$

example:-

$\psi = ax$ between $x=0$ to $x=1$

$\psi = 0$ elsewhere

(i) Find the probability of particle can be found between $x = 0.45$ and $x = 0.55$

(ii) Find the expection value of particle postion

(i) Probability is

$$\int_{x_1}^{x_2} |\psi|^2 dx = \int_{0.45}^{0.55} a^2 x^2 dx = a^2 \left[\frac{x^3}{3}\right]_{0.45}^{0.55}$$

$$= \frac{a^2}{3}\left[0.55^3 - 0.45^3\right] = 0.0251 a^2$$

(ii) Expectation value

$$\langle x \rangle = \int_0^1 x |\psi|^2 dx = \int_0^1 x \, a^2 x^2 dx = a^2 \left[\frac{x^4}{4}\right]_0^1$$

$$= a^2/4$$

Expectation value of momentum and energy:-

(i) momentum operator

$$\hat{p} = -i\hbar \, \partial/\partial x$$

$$\langle p \rangle = \int_{-\infty}^{\infty} \psi^* \hat{p} \psi \, dx = \int_{-\infty}^{\infty} \psi^* \left(-i\hbar \frac{\partial}{\partial x}\right) \psi \, dx$$

$$\boxed{\langle p \rangle = -i\hbar \int_{-\infty}^{\infty} \psi^* \frac{\partial}{\partial x} \psi \, dx}$$

Energy operator $\hat{E} = i\hbar \frac{\partial}{\partial t}$

$$\langle E \rangle = \int_{-\infty}^{\infty} \psi^* \hat{E} \psi \, dx = \int_{-\infty}^{\infty} \psi^* \left(i\hbar \frac{\partial}{\partial t}\right) \psi \, dx$$

$$\boxed{\langle E \rangle = i\hbar \int_{-\infty}^{\infty} \psi^* \frac{\partial}{\partial t} \psi \, dx}$$

Knowing the variation of ψ with t, can find expetn of E

OPERATORS

Another way to find expectation Values.

An operator tells us what operation to carry out on the quantity that follows it.

$$y = e^{3x} \Rightarrow$$

$$\frac{dy}{dx} = \frac{d}{dx} e^{3x}$$

$$\frac{dy}{dx} = 3e^{3x}$$

operator $\rightarrow \frac{d}{dx}$

Energy operator :-

The wave function $\psi(x,t)$ may generally be written as ψ, wave function in the form Energy E & momentum (p) represented as

$$\psi = A e^{(-i/\hbar)[Et - px]} \quad (21.1)$$

w.r.t. to t, we get

$$\frac{\partial \psi}{\partial t} = E(-i/\hbar) A e^{(-i/\hbar)[Et-px]}$$

$$\frac{\partial \psi}{\partial t} = \left(-\frac{i}{\hbar} E\right) \cdot \psi$$

$$E\psi = -\frac{\hbar}{i} \frac{\partial \psi}{\partial t}$$

$$\boxed{E\psi = i\hbar \frac{\partial}{\partial t} \psi} \quad — 21.2$$

Eq (21.2) shows that the operator $i\hbar \frac{\partial}{\partial t}$ operates upon ψ to produce $E\psi$. This is called energy operator

$$\boxed{\hat{E} = i\hbar \frac{\partial}{\partial t}}$$

Momentum Operator

Partial differentiation of equation (21.1) with respect to x

$$\psi = A e^{(-i/\hbar)(Et - px)}$$

$$\frac{\partial \psi}{\partial x} = (+i/\hbar) p A e^{(-i/\hbar)[Et - px]}$$

$$\frac{\partial \psi}{\partial x} = \frac{+i}{\hbar} p \psi$$

$$\boxed{p\psi = -i\hbar \frac{\partial \psi}{\partial x}}$$

Therefore, the operator $-i\hbar \frac{\partial \psi}{\partial x}$ operates upon ψ to give us momentum multiplied by wave function ψ. This is called Linear momentum operator

$$\boxed{\hat{p} = -i\hbar \frac{\partial}{\partial x}}$$

Kinetic energy operator

Kinetic energy in term of momentum

$$T = \frac{p^2}{2m} =$$

Kinetic energy operator

$$\hat{T} = \frac{(\hat{p})^2}{2m} = \frac{1}{2m}\left[-i\hbar \frac{\partial}{\partial x}\right]^2 = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$$

$$\boxed{\hat{T} = -\frac{\hbar^2}{2m} \partial^2/\partial x^2}$$

4. Hamiltonian operator

Time Independent Schrodinger's wave equation in 3-D.

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2}{\partial z^2}\psi + \frac{2m}{\hbar^2}(E-V)\psi = 0$$

We can write

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

$$(E-V)\psi = -\frac{\hbar^2}{2m}\nabla^2\psi$$

$$E\psi - V\psi = -\frac{\hbar^2}{2m}\nabla^2\psi$$

$$E\psi = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi$$

$$E\psi = \left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\psi$$

OR

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\psi = E\psi$$

clearly the operator $-\frac{\hbar^2}{2m}\nabla^2 + V$ operates upon ψ to give $E\psi$.

This is the total energy operator and is called the Hamiltonian operator $\hat{H}$.

$$\boxed{\hat{H}\psi = E\psi}$$

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V$$

In case of one dimension

$$\boxed{\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V}$$

$V \to$ Potential energy

$V \to V(x)$

5. Angular Momentum operator

If $\vec{r}$ is the position vector and $\vec{p}$ is the linear momentum of the particle

$$\vec{r} = x\hat{i} + y\hat{j} + z\hat{k}$$

and $$\vec{p} = p_x\hat{i} + p_y\hat{j} + p_z\hat{k}$$

If $\vec{L}$ is the angular momentum of particle then

$$\vec{L} = \vec{r} \times \vec{p}$$

$$L_x\hat{i} + L_y\hat{j} + L_z\hat{k} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix}$$

$$= (yp_z - zp_y)\hat{i} + (zp_x - xp_z)\hat{j} + (xp_y - yp_x)\hat{k}$$

Comparing the co-efficient of $\hat{i}, \hat{j}, \hat{k}$

$$L_x = yp_z - zp_y$$

$$L_y = zp_x - xp_z$$

$$L_z = xp_y - yp_x$$

Now the operator $p_x = -i\hbar\frac{\partial}{\partial x}$

$$p_y = -i\hbar\,\partial/\partial y$$

$$p_z = -i\hbar\,\partial/\partial z$$

Therefore angular momentum operator $\hat{L}_x, \hat{L}_y, \hat{L}_z$ can be written as

$$\boxed{\begin{aligned} \hat{L}_x &= -i\hbar\left[y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right] \\ \hat{L}_y &= -i\hbar\left[z\frac{\partial}{\partial x} - x\,\partial/\partial z\right] \\ \hat{L}_z &= -i\hbar\left[x\,\partial/\partial y - y\,\partial/\partial x\right] \end{aligned}}$$

Table 1 Operators Associated with Various observable quantities

Quantity		Operator
Position, x	$\hat{x}$	x
Linear Momentum	$\hat{p}$	$\frac{\hbar}{i}\frac{\partial}{\partial x}$
Potential Energy	V	$V(x)$
Kinetic Energy	$\hat{K.E}$	$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$
Total Energy	$\hat{E}$	$i\hbar\, \partial/\partial t$
(Total Energy) Hamiltonian	$\hat{H}$	$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$

- **Commutators** :→

If we can measure two observables at the same time. If the commutator of two observable is zero

If $\hat{A}$ & $\hat{B}$

$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$

$[\hat{A}, \hat{B}] = 0$ Commutators

$[\hat{A}, \hat{B}] \neq 0$ Anti Commutators

We Cannot measure at same time
non-Commutator

Heisenberg Uncertainty Principle.

We can not know the value of position and momentum at same time.

$$[\hat{x}, \hat{p}]\psi = [\hat{x}\hat{p} - \hat{p}\hat{x}]\psi$$

$$= x\hat{p}\psi - \hat{p}\hat{x}\psi$$

$$= x\frac{\hbar}{i}\frac{\partial \psi}{\partial x} - \frac{\hbar}{i}\frac{\partial}{\partial x}(x.\psi)$$

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

$$[\hat{x}, \hat{p}] = i\hbar \Rightarrow [\hat{x}, \hat{p}] \neq 0$$

$$[\hat{p}, \hat{x}]\psi = [\hat{p}\hat{x} - \hat{x}\hat{p}]\psi$$

$$= \frac{\hbar}{i}\frac{\partial}{\partial x}(x\psi) - x\frac{\hbar}{i}\frac{\partial}{\partial x}\psi$$

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

$$[\hat{p}, \hat{x}]\psi = \frac{\hbar}{i}\psi$$

$$\boxed{[\hat{p}, \hat{x}] = \frac{\hbar}{i}}$$

p, x do not Commutate to each other

Example

Compute the Commutator

(i) $[E, t]$

(ii) $[E, x]$

(iii) $[p, x]$

(iv) $[L_x, L_y]$

(I) $[E, t]$

$$[\hat{E}, \hat{t}]\psi = [\hat{E}\hat{t} - \hat{t}\hat{E}]\psi$$

$$= i\hbar\frac{\partial}{\partial t}(t\psi) - t\, i\hbar\frac{\partial}{\partial t}\psi$$

$$= i\hbar\left[\psi + t\frac{\partial\psi}{\partial t} - t\frac{\partial\psi}{\partial t}\right]$$

$$[\hat{E}, \hat{t}]\psi = i\hbar\psi$$

$$\boxed{[\hat{E}, \hat{t}] = i\hbar}$$

(ii) $[\hat{E}, \hat{x}]\psi = \hat{E}\hat{x}\psi - \hat{x}\hat{E}\psi$

$$= i\hbar\frac{\partial}{\partial t}(x\psi) - x\, i\hbar\frac{\partial}{\partial t}\psi$$

$$= i\hbar\left[0 + x\frac{\partial\psi}{\partial t} - x\frac{\partial\psi}{\partial t}\right]$$

$$= 0$$

E, x Commutate to each other

(iii)

(iv) $[\hat{L}_x, \hat{L}_y]\psi = [L_x L_y - L_y L_x]\psi$

$$L_x = -i\hbar\left[y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right] = -i\hbar[$$

$$L_y = -i\hbar\left[z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right]$$

$$[L_x, L_y] = [y p_z - z p_y,\ z p_x - x p_z]$$

$$= [y p_z, z p_x] - [y p_z, x p_z] - [z p_y, z p_x] + [z p_y, x p_z]$$

Solve on next page

Some useful Rules for commutation

$$[\hat{A}, \hat{B}] + [\hat{B}, \hat{A}] = 0$$

$$[\hat{A}, \hat{A}] = 0$$

$$[\hat{A}, \hat{B} + \hat{C}] = [\hat{A}, \hat{B}] + [A, \hat{C}]$$

$$[\hat{A} + \hat{B}, \hat{C}] = [\hat{A}, \hat{C}] + [\hat{B}, \hat{C}]$$

$$[\hat{A}, \hat{B}\hat{C}] = [\hat{A}, \hat{B}]\hat{C} + \hat{B}[\hat{A}, \hat{C}]$$

$$[\hat{A}\hat{B}, \hat{C}] = [\hat{A}, \hat{C}]\hat{B} + \hat{A}[\hat{B}, \hat{C}]$$

$$\begin{vmatrix} \hat{i} & \hat{j} & k \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix}$$

$$[\hat{L}_x, \hat{L}_y] = [L_x L_y - L_y L_x]$$

$$= (-i\hbar)^2 \left[\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)\cdot\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right) - \left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)\cdot\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)\right]$$

$$= -\hbar^2 \Big[y\frac{\partial}{\partial z}\left(z\frac{\partial}{\partial x}\right) - y\frac{\partial}{\partial z}\left(x\frac{\partial}{\partial z}\right) - z\frac{\partial}{\partial y}\left(z\frac{\partial}{\partial x}\right) + z\frac{\partial}{\partial y}\left(x\frac{\partial}{\partial z}\right)$$

$$- z\frac{\partial}{\partial x}\left(y\frac{\partial}{\partial z}\right) + z\frac{\partial}{\partial x}\left(z\frac{\partial}{\partial y}\right) + x\frac{\partial}{\partial z}\left(y\frac{\partial}{\partial z}\right) - x\frac{\partial}{\partial z}\left(z\frac{\partial}{\partial y}\right)\Big]$$

$$= -\hbar^2 \Big[y\frac{\partial}{\partial x} + \cancel{yz\frac{\partial^2}{\partial z\partial x}} - \cancel{yx\frac{\partial^2}{\partial z^2}} - \cancel{z^2\frac{\partial^2}{\partial y\partial x}} + \cancel{zx\frac{\partial^2}{\partial y\partial z}}$$

$$- \cancel{zy\frac{\partial^2}{\partial x\partial z}} + \cancel{z^2\frac{\partial^2}{\partial x\partial y}} + \cancel{xy\frac{\partial^2}{\partial z^2}} - x\frac{\partial}{\partial y} - \cancel{xz\frac{\partial^2}{\partial z\partial y}}\Big]$$

$$= -\hbar^2\left[y\frac{\partial}{\partial x} - x\frac{\partial}{\partial y}\right] = +\hbar^2\left[x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right]$$

$$= \hbar^2 \frac{L_z}{-i\hbar} = -\frac{\hbar}{i} L_z$$

$$[\hat{L}_x, \hat{L}_y] = i\hbar \hat{L}_z$$

$$[L_y, \hat{L}_z] = i\hbar \hat{L}_x$$

$$[L_z, L_x] = i\hbar \hat{L}_y$$

$[L_x, x] = [\hat{L}_x \hat{x} - \hat{x} L_x]$

$[\hat{L}_x, \hat{x}]\psi = (-i\hbar)\left[\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)x - x\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)\right]\psi$

$= -i\hbar\left[y\frac{\partial}{\partial z}(x\psi) - z\frac{\partial}{\partial y}(x\psi) - xy\frac{\partial\psi}{\partial z} + xz\frac{\partial\psi}{\partial y}\right]$

$= -i\hbar\left[yx\frac{\partial\psi}{\partial z} - zx\frac{\partial\psi}{\partial y} - xy\frac{\partial\psi}{\partial z} + xz\frac{\partial\psi}{\partial y}\right]$

$[\hat{L}_x, \hat{x}]\psi = -i\hbar\,[0]\psi$

$\boxed{[L_x, \hat{x}] = 0}$

Find the values of

$[L_x, \hat{y}] = [L_y, \hat{z}] = ?$

$[L^2, \hat{x}] = [\hat{L}\hat{L}, \hat{x}]$

$= [\hat{L}, \hat{x}]\hat{L} + \hat{L}[L, \hat{x}]$

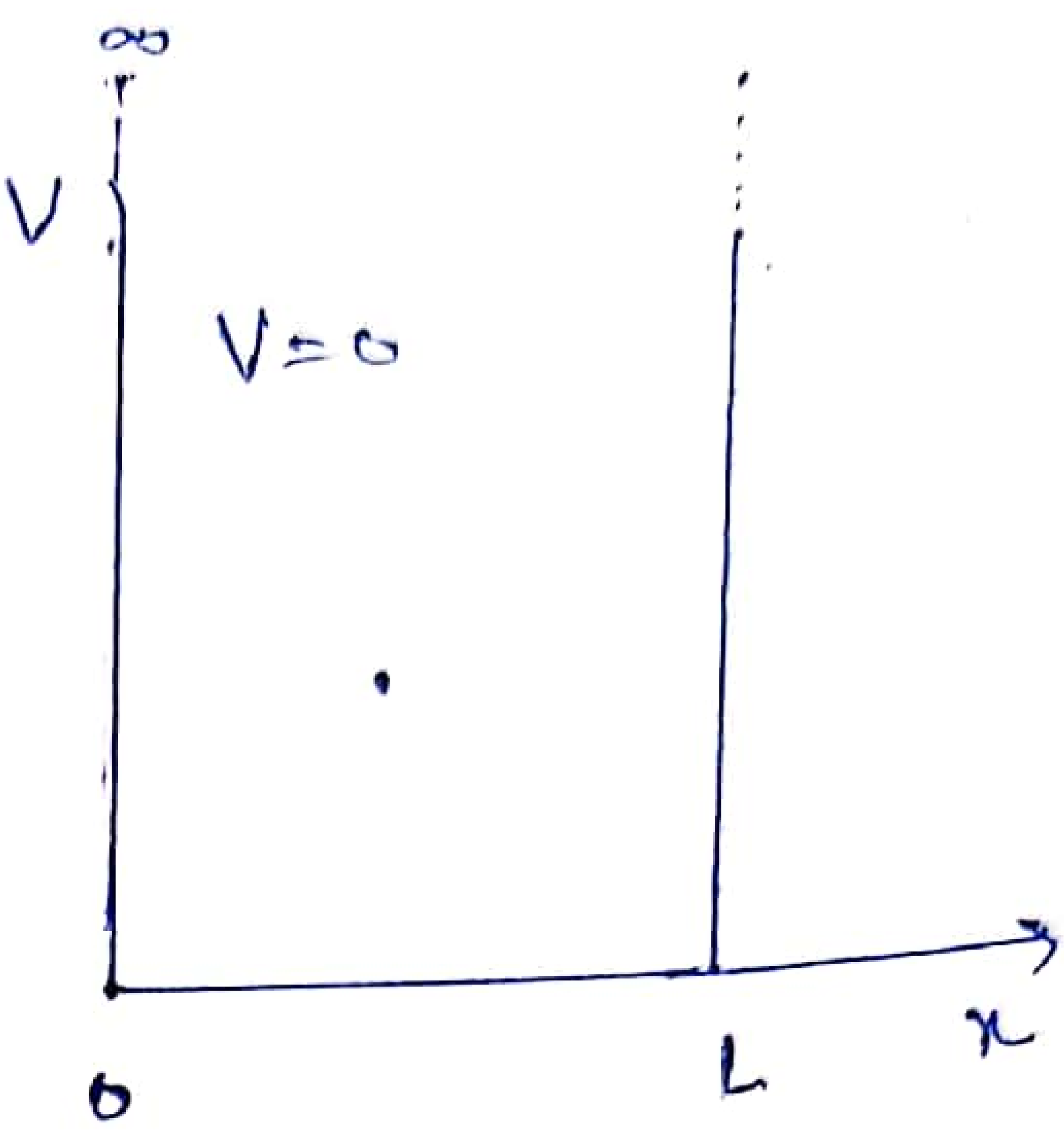
$= 0\,\hat{L} + \hat{L}[0]$

$= 0$

Particle in a One dimensional Box

OR

Particle in infinitely hard walls



Suppose that there is a particle of mass 'm' which is free to move in a one dimensional box having infinite hard walls.

Particle motion is restricted to travelling along the x-axis between $x=0$ and $x=L$ by infinitely hard walls. A particle does not lose energy when it collides with such walls, so that its total energy stays constant.

A square potential well with infinitely high barrier at each end corresponds to a box with infinitely hard walls.

The Potential energy (V) of the Particle is infinite on both sides of the box. While V is constant - say zero (0) for convenience - on the inside. Because particle cannot have an infinite amount of energy, it cannot exist outside the box and so its

$$\psi \text{ is } 0 \text{ for } x \leq 0 \text{ and } x \geq L$$

our task is to find what ψ is within the box between $x=0$ to $x=L$

$$V = \begin{cases} 0 & \text{for } 0 < x < L \\ \infty & \text{for } x=0 \text{ and } x=L \end{cases}$$

One dimension time independent Schrodinger wave equation

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E-V)\psi = 0 \quad \text{--- (27.1)}$$

Inside the box

$$V = 0$$

put $V=0$ in eqn (27.1)

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}E\psi = 0 \quad \text{— (28.1)}$$

This eqn is of the form

$$\frac{d^2\psi}{dx^2} + \omega^2 x = 0$$ and solution

$$\psi = A\sin\omega x + B\cos\omega x$$

Solution of equation (28.1) will be of the form

$$\psi = A\sin\sqrt{\frac{2mE}{\hbar^2}}x + B\cos\sqrt{\frac{2mE}{\hbar^2}}x \quad \text{— (28.2)}$$

Applying the boundary conditions

i.e. at $x=0$, $\psi=0$

$$0 = A\times 0 + B.$$

$$\boxed{B=0}$$

put $B=0$ in eqn (28.2), Now equation

$$\psi = A\sin\sqrt{\frac{2mE}{\hbar^2}}x \quad \text{— (28.3)}$$

Boundary condition

at $x=L$, $\psi=0$

$$0 = A\sin\sqrt{\frac{2mE}{\hbar^2}}L$$

$$A\sin\sqrt{\frac{2mE}{\hbar^2}}L = 0$$

$A \neq 0$ | So $\sin\sqrt{\frac{2mE}{\hbar^2}}L = 0$

$$\sqrt{\frac{2mE_n}{\hbar^2}}L = n\pi \qquad n=1,2,3,4$$

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

Energy level of system

$$\boxed{E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}} \quad \text{—(29.1)}$$

$$n = 1, 2, 3, \ldots$$

Eqn (29.1) shows the energy level of particle is quantized and have only discrete values. those values of energy is called eigen values.

Eigen function:-

We have the value of E_n in eqn (28.3)

$$\psi_n = A\sin\sqrt{\frac{2m}{\hbar^2}\cdot\frac{n^2\pi^2\hbar^2}{2mL^2}}\,x$$

$$\boxed{\psi_n = A\sin\frac{n\pi}{L}x} \quad (29.2)$$

where ψ_n is the eigen function for energy eigen value E_n.

Normalization of wave function

As the particle certainly within the box, we have the normalization condition

$$\int_0^L \psi^*\psi\,dx = 1$$

$$\int_0^L A\sin\frac{n\pi}{L}x \cdot A\sin\frac{n\pi}{L}x\,dx = 1$$

$$A^2\int_0^L \sin^2\frac{n\pi}{L}\cdot x\,dx = 1$$

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

$$\frac{A^2}{2}\left[(x)_0^L - \frac{L}{2n\pi}\left[\sin\frac{2n\pi}{L}\cdot x\right]_0^L\right] = 1$$

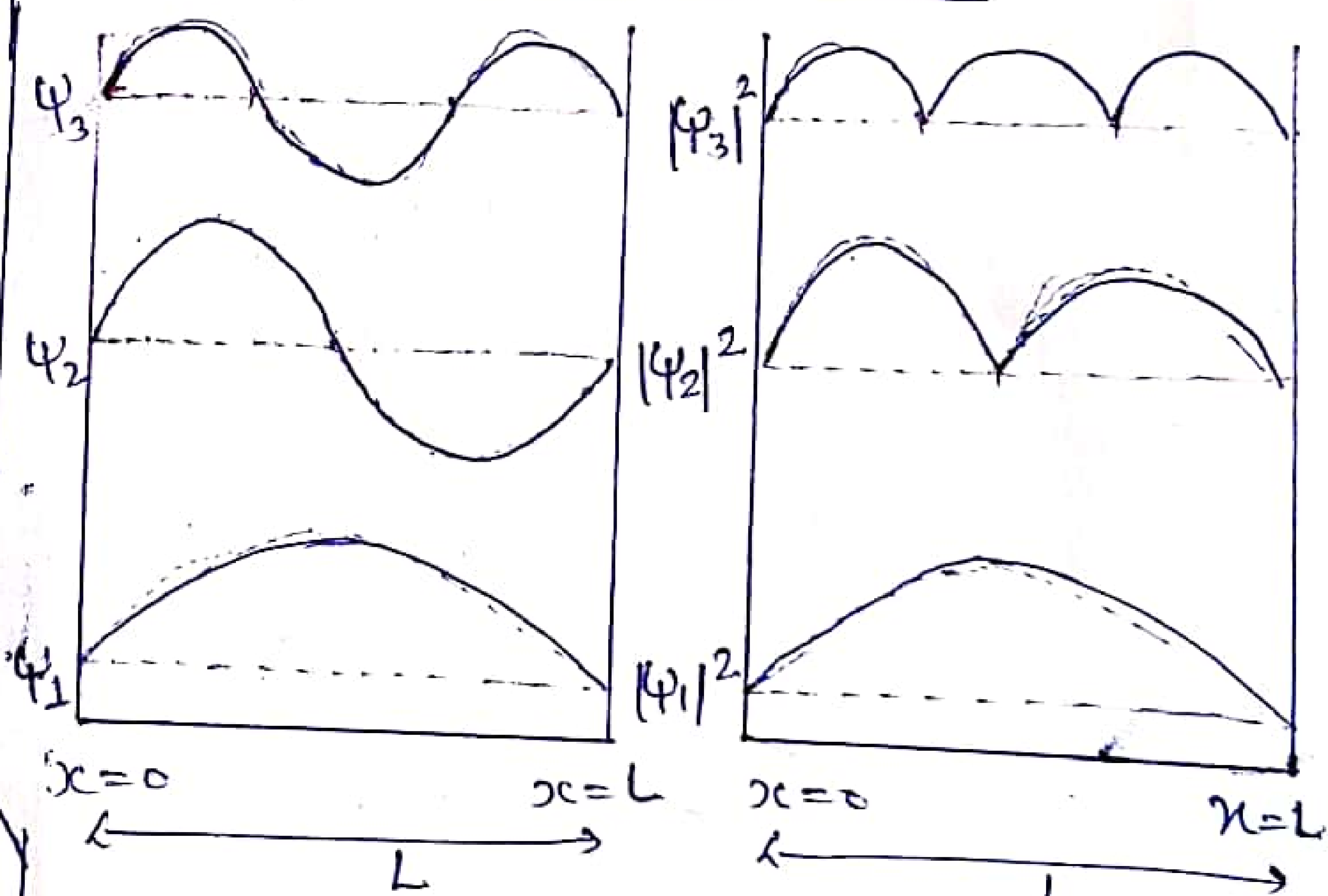
$$\frac{A^2}{2}\left[L - 0 - 0 - 0\right] = 1$$

$$A^2 = 2/L$$

$$\boxed{A = \sqrt{\frac{2}{L}}} \quad (29.3)$$

Eqn (29.2) become

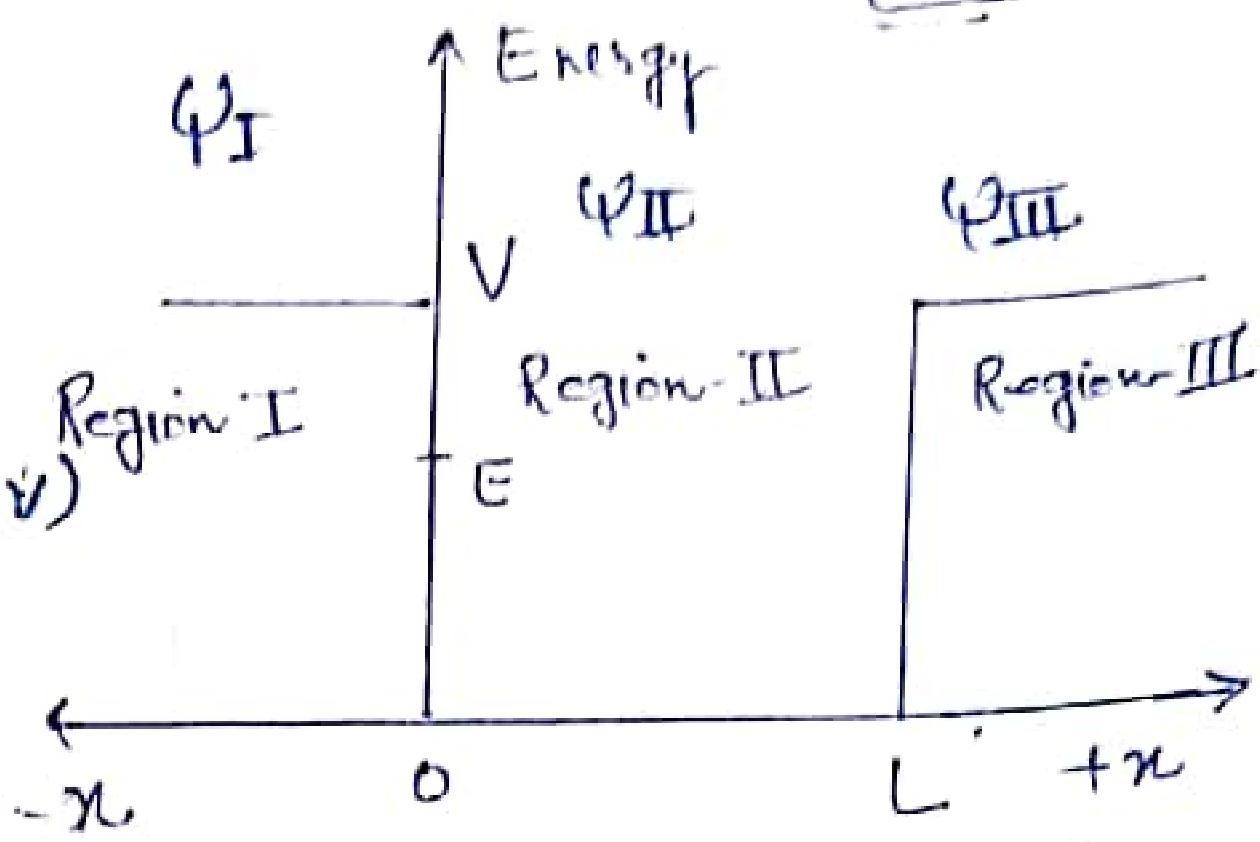
$$\boxed{\psi_n = \sqrt{\frac{2}{L}}\sin\frac{n\pi}{L}\cdot x}$$



wave functions and probability densities of a particle confined to a box with rigid walls

Finite Potential Well

A potential well with square corners that is 'V' high and L wide and contains a particle whose energy E is less than V. (E<V)
According the Quantum Mechanics, the particles also bounces back and forth, but now it has a certain probability of penetrating into regions I and III eventhough E<V.



A square potential well with finite Barriers. The energy E of the trapped particle is less than the height of V of the barriers.

In

$$V = \begin{cases} 0 & 0<x<L \\ & \end{cases}$$

In region I & III Schroodinger steady state equation

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

$$\frac{d^2\psi}{dx^2} - \frac{2m}{\hbar^2}(V-E)\psi = 0 \quad (30.1)$$

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

Here $a = \sqrt{\frac{2m}{\hbar^2}(V-E)}$

Solution of eq^n (30.1) for Region I & III

$$\psi_I = C e^{ax} + D e^{-ax} \quad (30.2)$$

$$\psi_{III} = F e^{ax} + G e^{-ax} \quad (30.2)$$

Both ψ_I & ψ_{III} must be finite everywhere

Since $e^{-ax} \to \infty$ as $x \to -\infty$ for Region-I

Co-efficient of D must be zero, Bcause wave function must be finite

Region-III

$e^{+ax} \to \infty$ as $x \to \infty$

~~F~~ F must be zero

Hence the wave function

$$\psi_I = C e^{ax} \quad (30.4)$$

$$\psi_{III} = G e^{-ax} \quad (30.5)$$

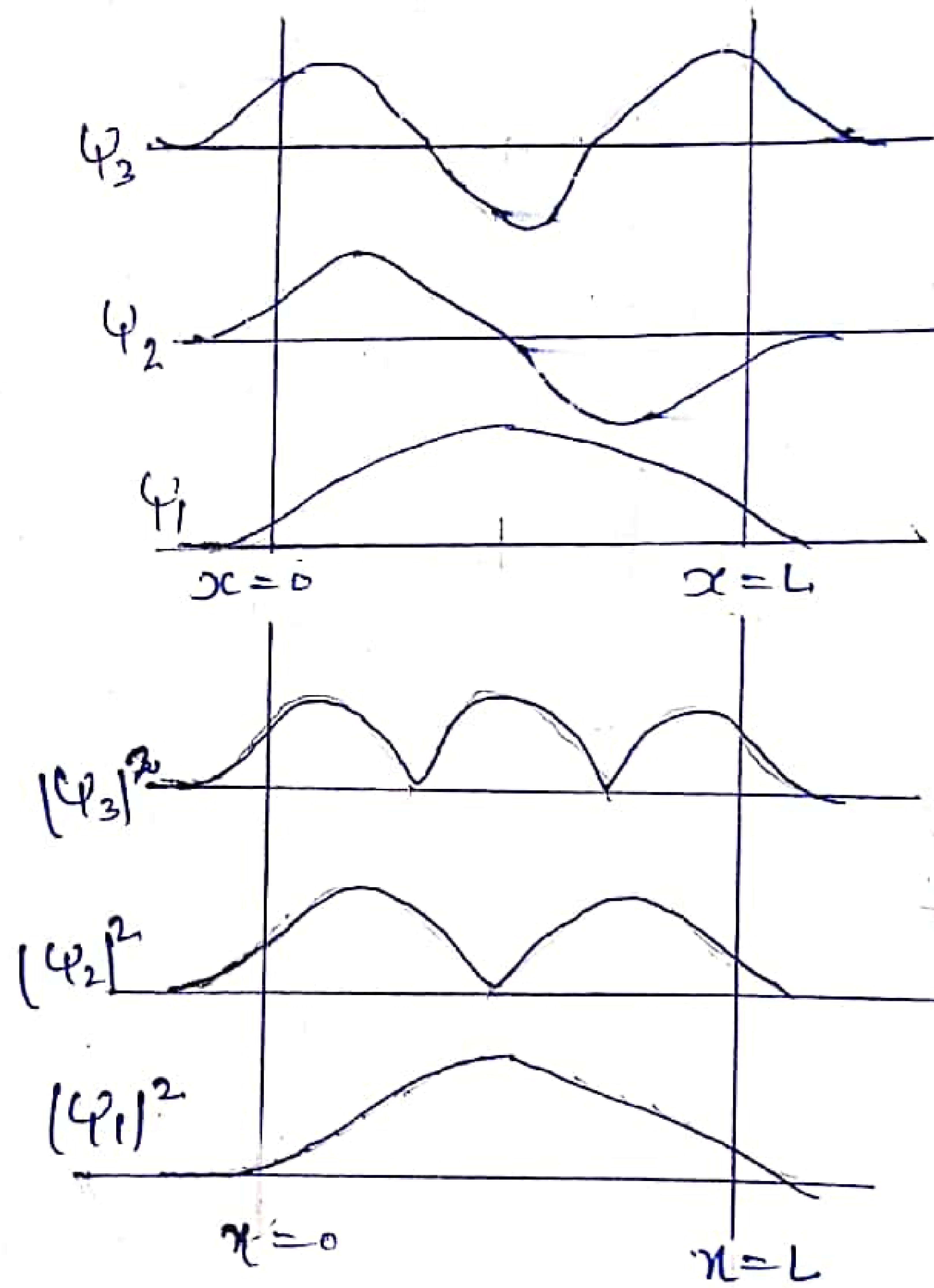
These wave functions decrease ~~exp~~ expontially inside the barrier at the sides of the well.

Within the well Schrodinger wave equation

$$\psi_{II} = A \sin \sqrt{\frac{2mE}{\hbar^2}}\, x + B \cos \sqrt{\frac{2mE}{\hbar^2}}\, x \quad \text{--- (31.1)}$$

For the Solution, both ψ and $\frac{d\psi}{dx}$ must be Continuous at $x=0$ and $x=L$; the wave functions inside and outside each side of the well must not only have the same where they join but also the same slopes, so they match up perfectly.

When these boundary conditions are taken into account, the result is that matching only occurs for certain specific values E_n of the particle energy.



Wave functions and probability densities of a particle in a finite potential well. The particle has a certain probability of being found outside the well.

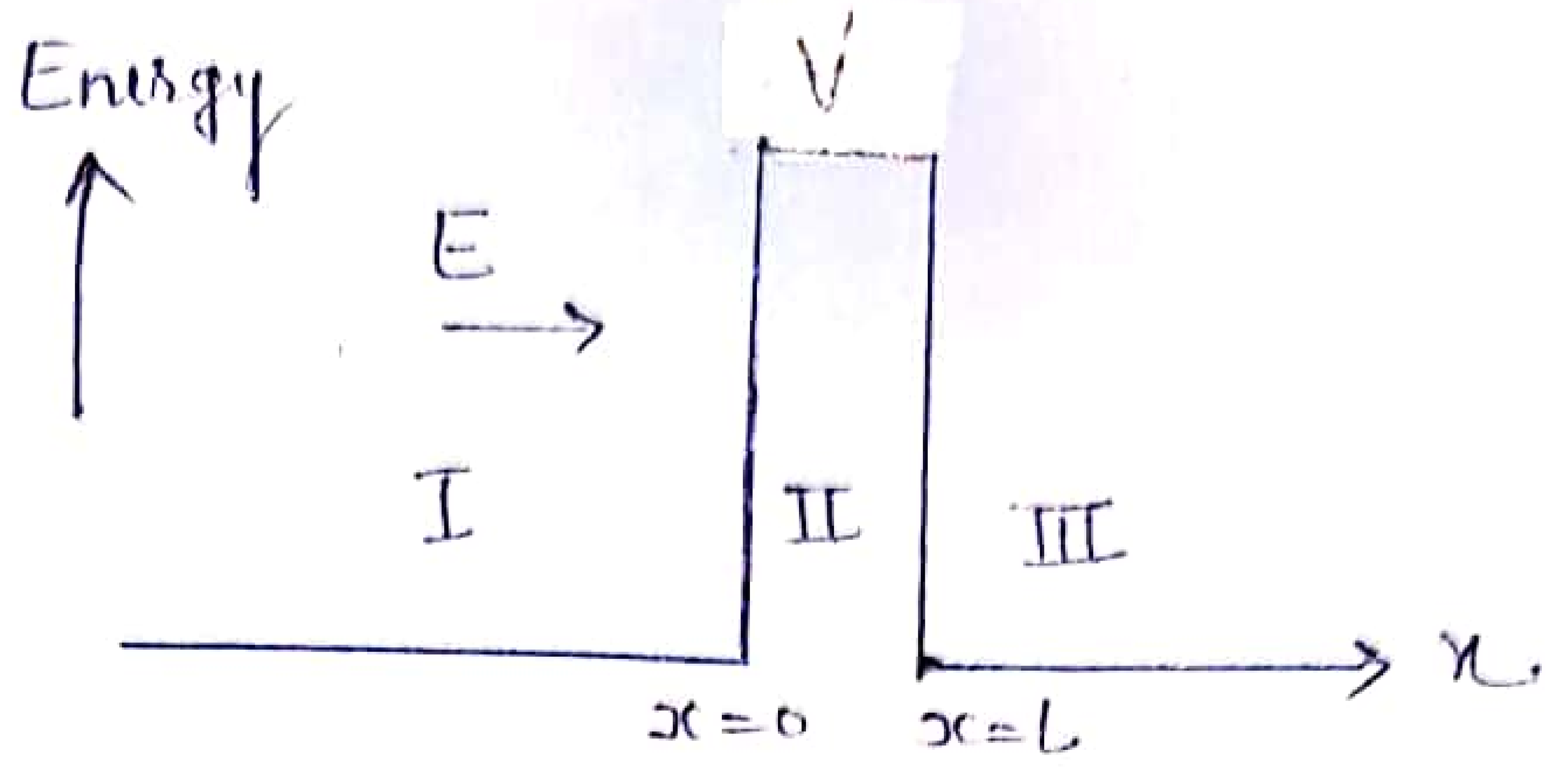
Potential Barrier

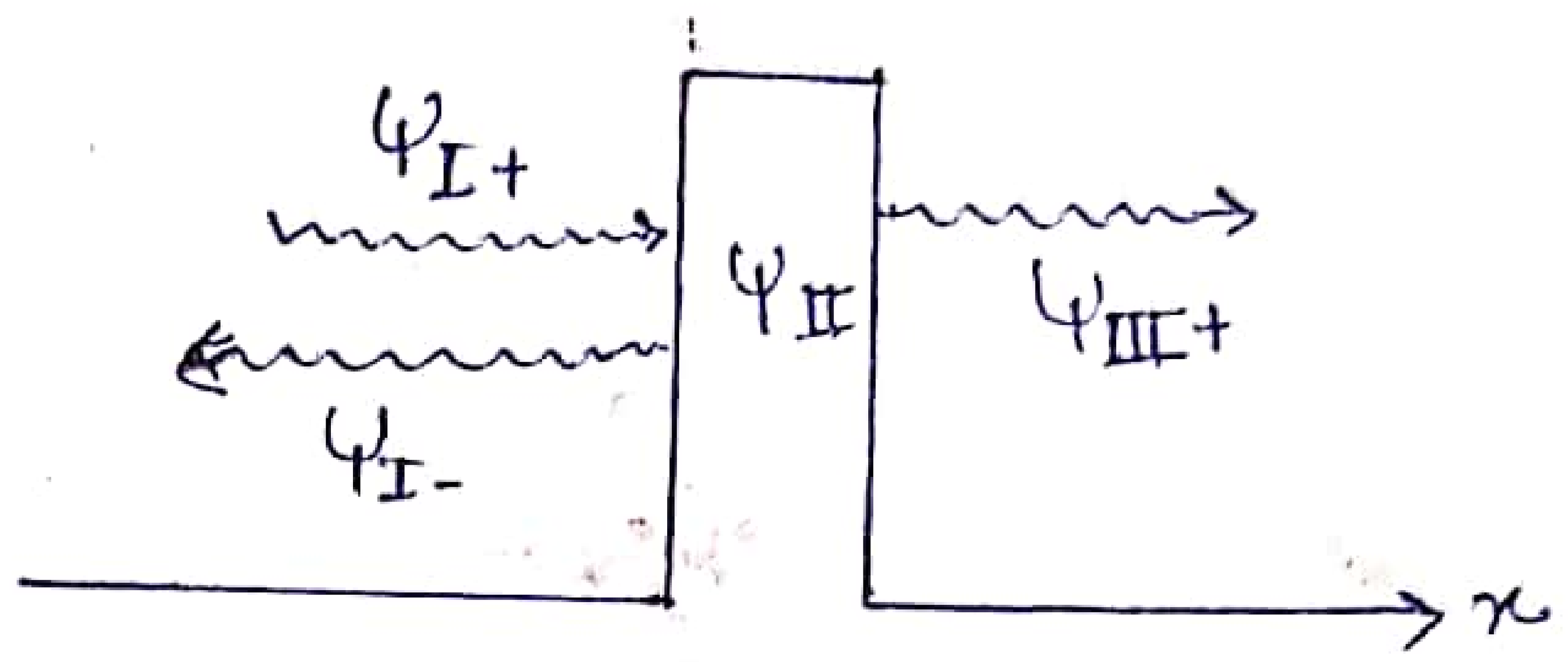
Tunnel Effect

A particle of mass m and energy E that strikes a potential Barrier of height V, again E < V, But here Barrier finite width. The partical have a certain probability of passing through the barrier and emerging on the other side.

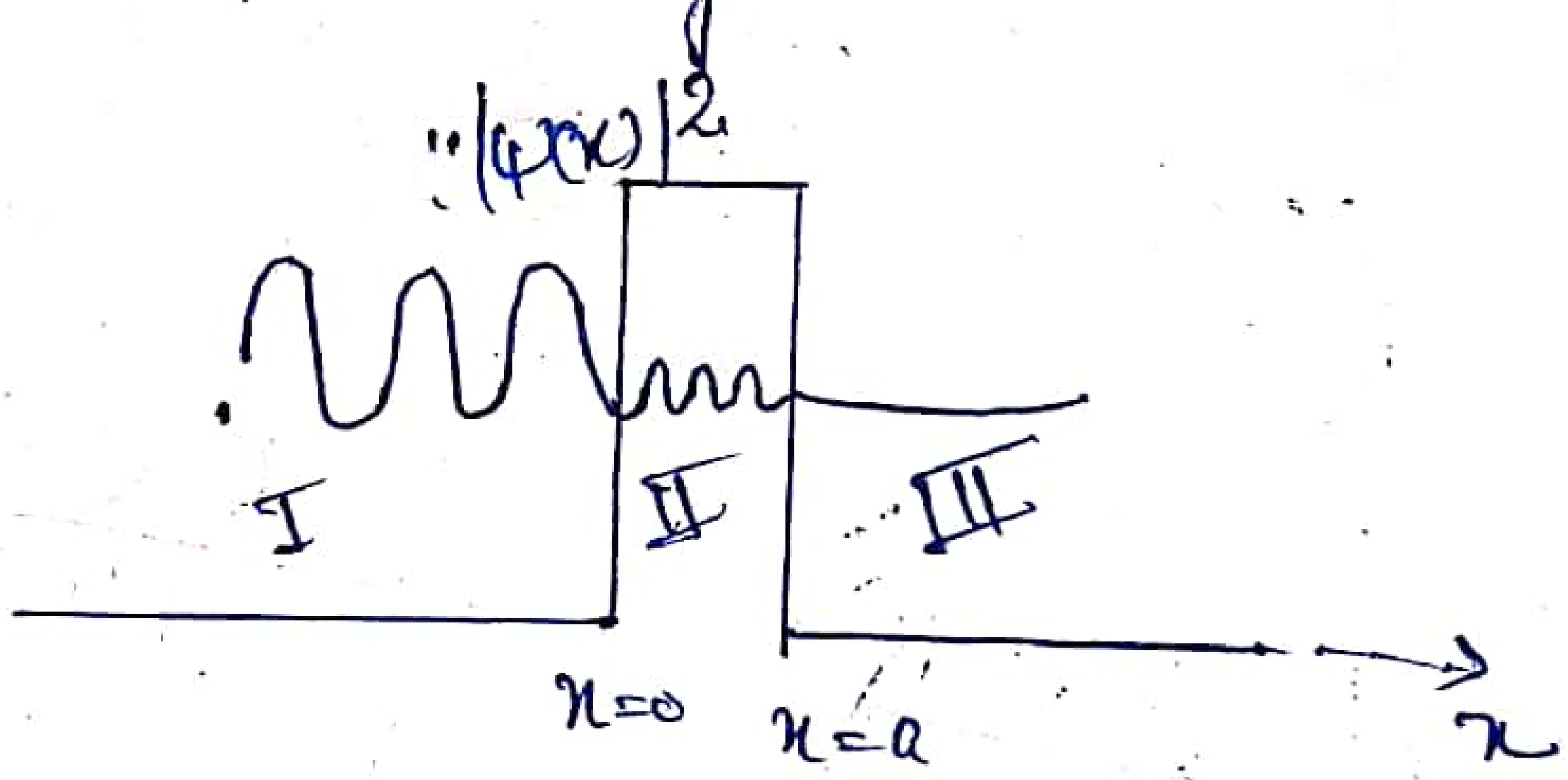
The particle lacks the energy to go ~~ve~~ over the top of the barrier but it can still tunnel through it.

Higher the barrier and wider it is, less chance to the particle can get through.





When a particle of energy E < V approaches a potential barrier, according to classical mechanics the particle must be reflected. In Quantum mechanics the de Broglie waves that corresponds to the particle are partly reflected and partly transmitted, which means that the particle has a finite chance to panetrating the barrier.



Let us consider a beam of identical particles all of which have the kinetic energy E. The beam is incident from the left on a potential Barrier of height 'V' and width 'L' as shown in figure. On both sides of the barrier V=0 No force act on the particles.

The wave function ψ_{I+} represents the incoming particles moving to the right and ψ_{I-} represents the reflected particles moving to the left.; ψ_{III} represents the transmitted particles moving to the right. The wave function ψ_{II} represents the particles insides the barrier, Some of which end up in region III while the others return to the region I.

The Transmission probability T for a particle to pass through the barrier is equal to the fraction of incident beam that gets through the barrier.

Approximate transmission Probability

$$T = e^{-2K_2L}$$

where $K_2 = \sqrt{\dfrac{2m(V-E)}{\hbar^2}}$ $\quad L \rightarrow$ width of the barrier

example :→ Electrons with energies of 1.0eV and 2.0eV are incident on a barrier 10.0eV high and 0.50nm wide. (a) Find their respective transmission probabilities (b) How are these affected if the barrier is doubled in width

Solution :→

For ~~1.0eV~~ 1.0eV electrons

$$K_2 = \sqrt{\frac{2m(V-E)}{\hbar^2}}$$

$$= \sqrt{\frac{2\times 9.1\times 10^{-31}\,kg\cdot(10-1)\times 1.6\times 10^{-19}}{(1.054\times 10^{-34})^2}}$$

$$K_2 = 1.6\times 10^{10}\ m^{-1}$$

$$T = e^{-2K_2L} \qquad L = 0.50nm$$

$$T_1 = e^{-2\times 1.6\times 10^{10}\times .50\times 10^{-9}}$$

$$= e^{-16} = 1.1\times 10^{-7}$$

One 1.0eV electron out of 8.9 million (1/1.1×10⁻⁷) can tunnel through the 10-eV barrier on average

For 2.0eV electrons we have calculated in the similar manner we found

$$T_2 = 2.4 \times 10^{-7}$$

These electrons are over twice as likely to tunnel through the barrier

(b) If the barrier is doubled in width . 1.0nm Then Transmission probability

For 1.0eV electron

$$K_2 = \sqrt{\frac{2m(U-E)}{\hbar^2}} = \sqrt{\frac{2 \times 9.1 \times 10^{-31}(10-1)}{\hbar^2}}$$

$$K_2 = 1.6 \times 10^{10}\ m^{-1}$$

Here $L = 1.0nm$

$$2K_2L = 2 \times 1.6 \times 10^{10} \times 1 \times 10^{-9} = 2 \times 16 = 32$$

Transmission probability

$$T_1' = e^{-32} = 1.3 \times 10^{-14}$$

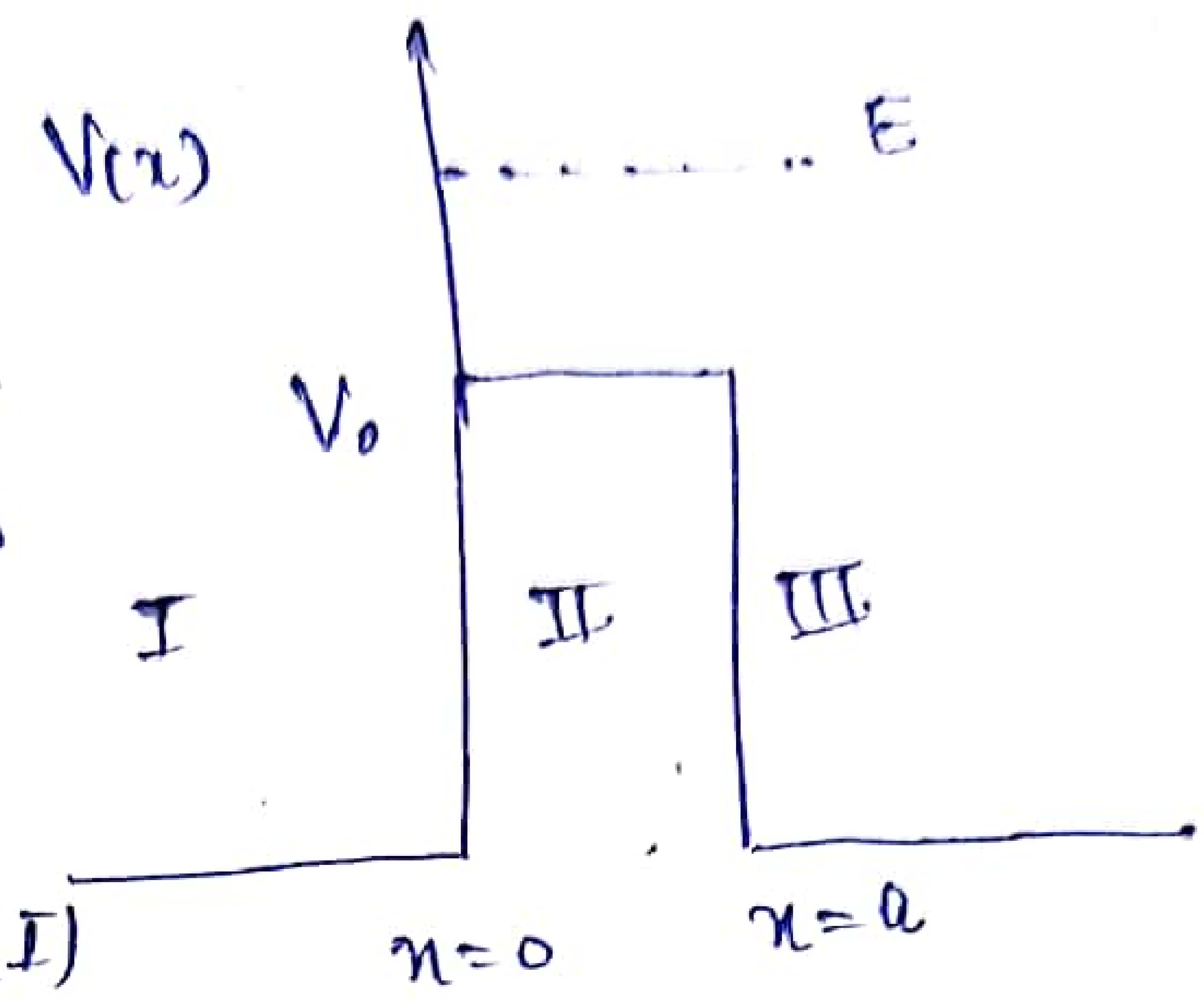
One 1.0eV electrons out of 7.69×10^{13} can tunnel through 10eV the (1.0nm) barrier on average

For 2.0eV electrons

$$T_2' = 5.1 \times 10^{-14}$$

Same as One 2.0 eV electrons out of 1.9×10^{13} can tunnel through the 10.0eV 1.0nm barrier on average.

The Potential Barrier :→



Consider a beam of particles of mass m that are moving along the +ve x axis they encountered a potential barrier expressed as

$$V(x) = \begin{cases} 0 & x < 0 \ (I) \\ V_0 & 0 < x < a \ (II) \\ 0 & x > a \ (III) \end{cases}$$

Case - When $E > V_0$

classically, the particles that approaches the barrier from left at constant momentum $p_1 = \sqrt{2mE}$, as they entered the region $0 < x < a$ they will slow down to the momentum $p_2 = \sqrt{2m(E - V_0)}$. In the region $(x > a)$ they will accelerated to with a momentum $p_3 = \sqrt{2mE}$

Quantum Mechanically the behaviour can be found by Schrodinger time independent wave equation for all the three region

For Region - I $\quad x < 0$

$$\frac{d^2\psi_1}{dx^2} + \frac{2m}{\hbar^2} E\psi_1 = 0 \qquad V(x) = 0$$

(35.1)

$$\frac{d^2\psi_1}{dx^2} + k_1^2 \psi_1 = 0$$

$\psi_1 \to$ Eigen function in Region I

$$k_1 = \sqrt{\frac{2mE}{\hbar^2}}$$

Region - II

$0 < x < a$

$$\frac{d^2\psi_2}{dx^2} + \frac{2m}{\hbar^2}(E - V_0)\psi_2 = 0$$

$$\frac{d^2\psi_2}{dx^2} + K_2^2\psi_2 = 0 \quad \text{(36.1)}$$

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

For Region III

$x > a$

$$\frac{d^2\psi_3}{dx^2} + \frac{2m}{\hbar^2}E\psi_3 = 0$$

$$\frac{d^3\psi_3}{dx^2} + k_1^2\psi_3 = 0 \quad \text{(36.2)}$$

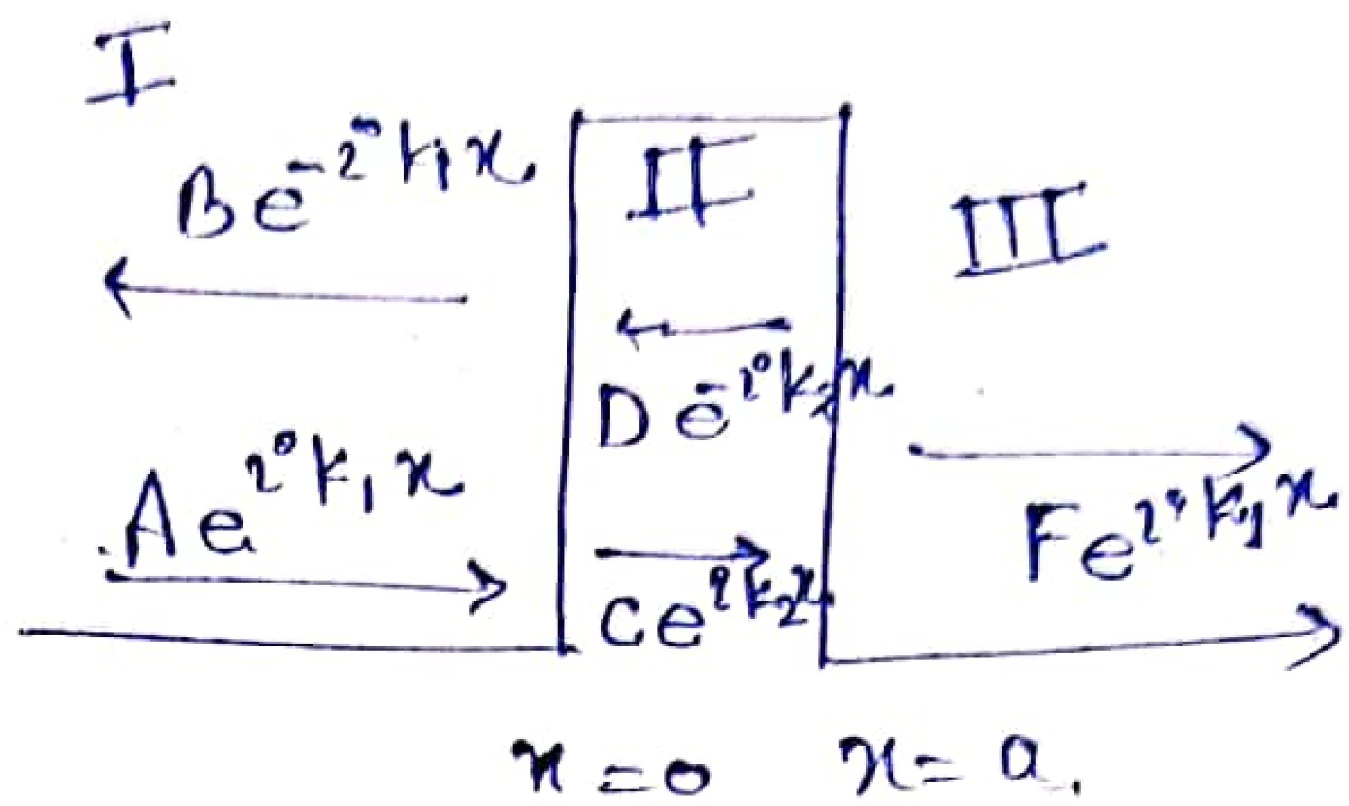
where $k_1 = \sqrt{\frac{2mE}{\hbar^2}}$

Solving eqⁿ (35.1), (36.1) & (36.2) we get

$$\psi_1(x) = A e^{ik_1x} + B e^{-ik_1x} \quad \text{(36.3)}$$

$$\psi_2(x) = C e^{ik_2x} + D e^{-ik_2x} \quad \text{(36.4)}$$

$$\psi_3(x) = F.e^{ik_1x} \quad \text{(36.5)}$$



No. of particles incident on the barrier are proportional to A

No of particles reflected back from the barrier are proportional to B

The constant B, C, D & F can be obtain in term of A from the boundary conditions

At boundary $\boxed{x=0}$

$$\psi_1(0) = \psi_2(0)$$

$$A + B = C + D \quad \text{(36.6)}$$

$$\left.\frac{d\psi_1}{dx}\right|_{x=0} = \left.\frac{d\psi_2}{dx}\right|_{x=0}$$

$$ik_1A - ik_1B = Cik_2 + (-ik_2)D$$

$$A - B = \frac{k_2}{k_1}(C - D) \quad \text{(36.7)}$$

At boundary $x = L$

$$\psi_2|_{x=L} = \psi_3|_{x=L}$$

At boundary $x = a$

$$\psi_2(a) = \psi_3(a) \Rightarrow C e^{ik_2 a} + D e^{-ik_2 a} = F e^{ik_1 a} \quad \cdots (37.1)$$

and

$$\left.\frac{d\psi_2}{dx}\right|_{x=a} = \left.\frac{d\psi_3}{dx}\right|_{x=a}$$

$$ik_2 C e^{ik_2 a} - ik_2 D e^{-ik_2 a} = i k_1 F e^{ik_1 a} \quad (37.2)$$

Solving for F

$$F = 4k_1 k_2 A e^{-ik_1 a}\left[4k_1 k_2 \cos k_2 a - 2i(k_1^2 + k_2^2)\sin k_2 a\right]^{-1}$$

The Transmission Co-efficient

$$T = \frac{k_1 |F|^2}{k_1 |A|^2} = \frac{|F|^2}{|A|^2}$$

$$= \left[1 + \frac{1}{4}\left(\frac{k_1^2 - k_2^2}{k_1 k_2}\right)^2 \sin^2 k_2 a\right]^{-1}$$

We put $k_1 = \sqrt{\frac{2mE}{\hbar^2}}$ $\quad k_2 = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$

$$T = \left[\left[1 + \frac{V_0^2}{4E(E-V_0)}\left\{\sin^2 a\sqrt{\frac{2mV_0}{\hbar^2}}\sqrt{\frac{E}{V_0} - 1}\right\}\right]\right]^{-1}$$

Let us denote $\lambda = a\sqrt{\frac{2mV_0}{\hbar^2}}$ & $\epsilon = \frac{E}{V_0}$

$$T = \left[1 + \frac{1}{4\epsilon(\epsilon - 1)}\sin^2(\lambda\sqrt{\epsilon - 1})\right]^{-1}$$

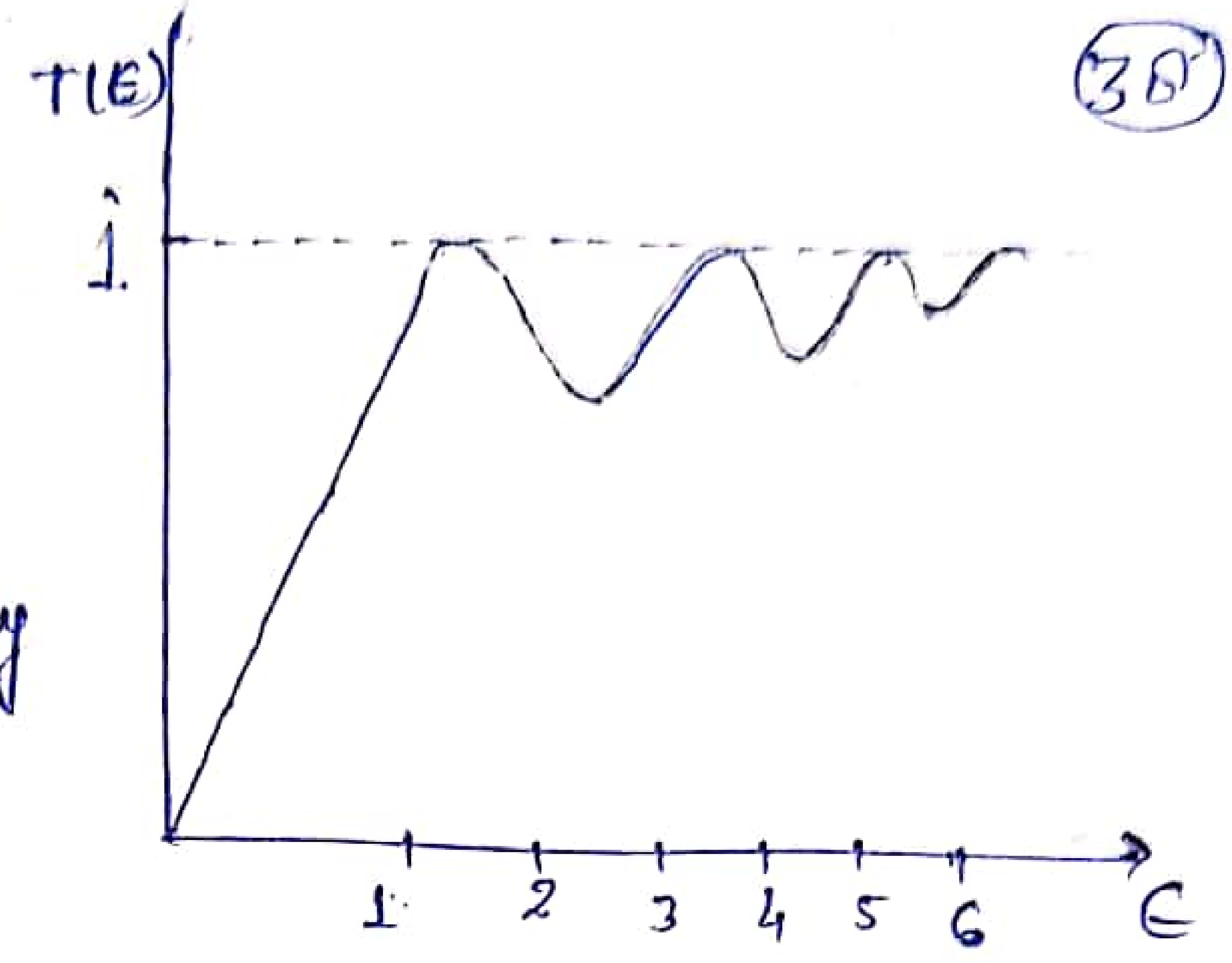
Reflaction Co-efficient

$$R = \frac{k_1 |B|^2}{k_1 |A|^2} = \left[1 + \frac{4\epsilon(\epsilon - 1)}{\sin^2(\lambda\sqrt{\epsilon - 1})}\right]^{-1}$$

$\epsilon = E/V_0$

If $E \gg V_0$ hence $\epsilon \gg 1$

T will becomes asymptotically equal to unity



$T \simeq 1$

$R \simeq 0$

So at very high energy and weak potential Barrier the particle would not feel the effect of Barrier. We observed total transmission

$T = 1$

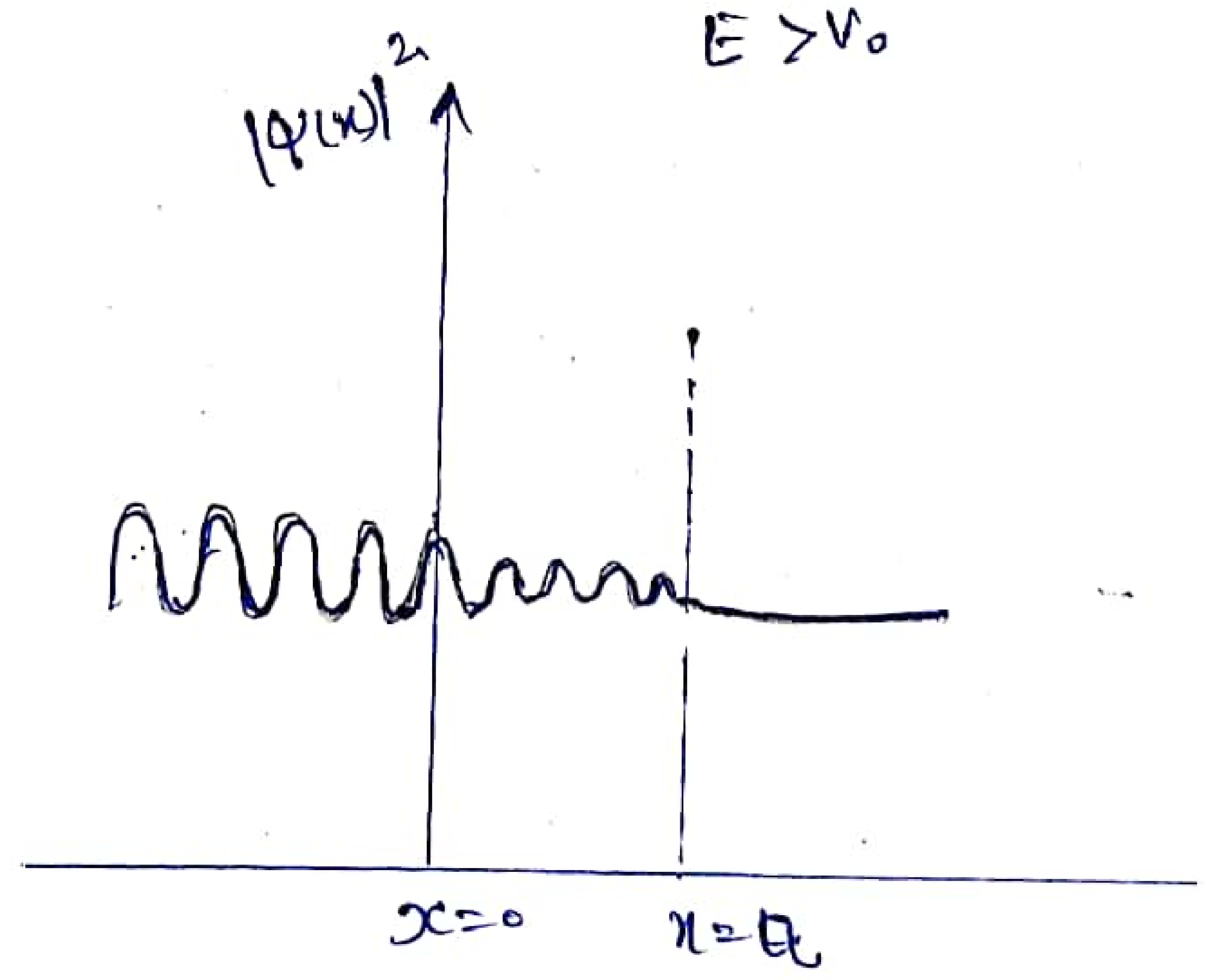
If $\sin \lambda \sqrt{(\epsilon - 1)} = 0$

$\lambda \sqrt{\epsilon - 1} = n\pi$

$n = 0, 1, 2, 3$

Periodicity occurs in the graph.

$E > V_0$

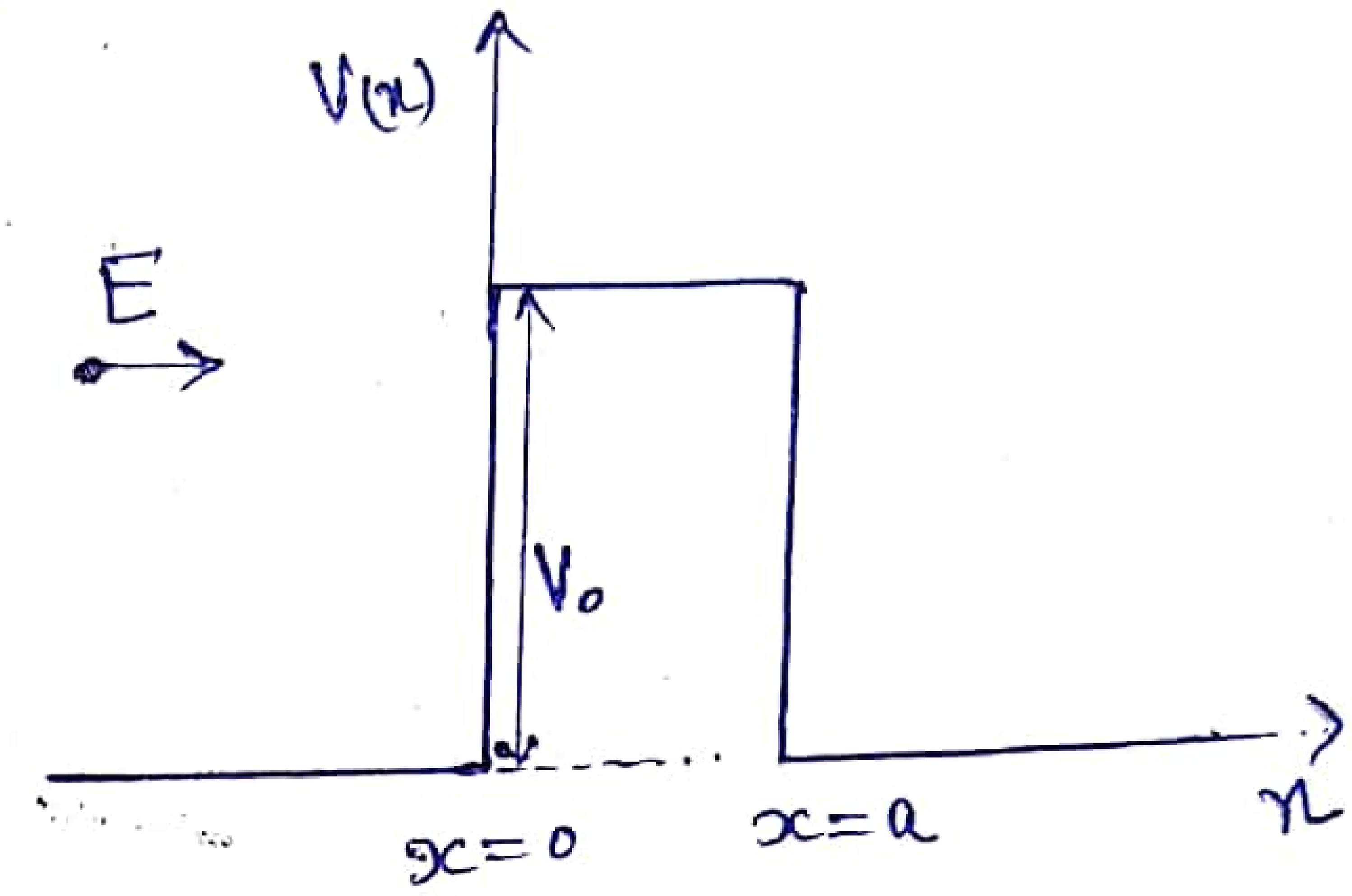


The potential Barrier Case $(E < V_0)$

Quantum Tunneling

According to classical mechanics if $E < V_0$ then there will always be total reflection of all the particles.

Quantum mechanically this is true if $V_0 = \infty$



Case $E < V_0$

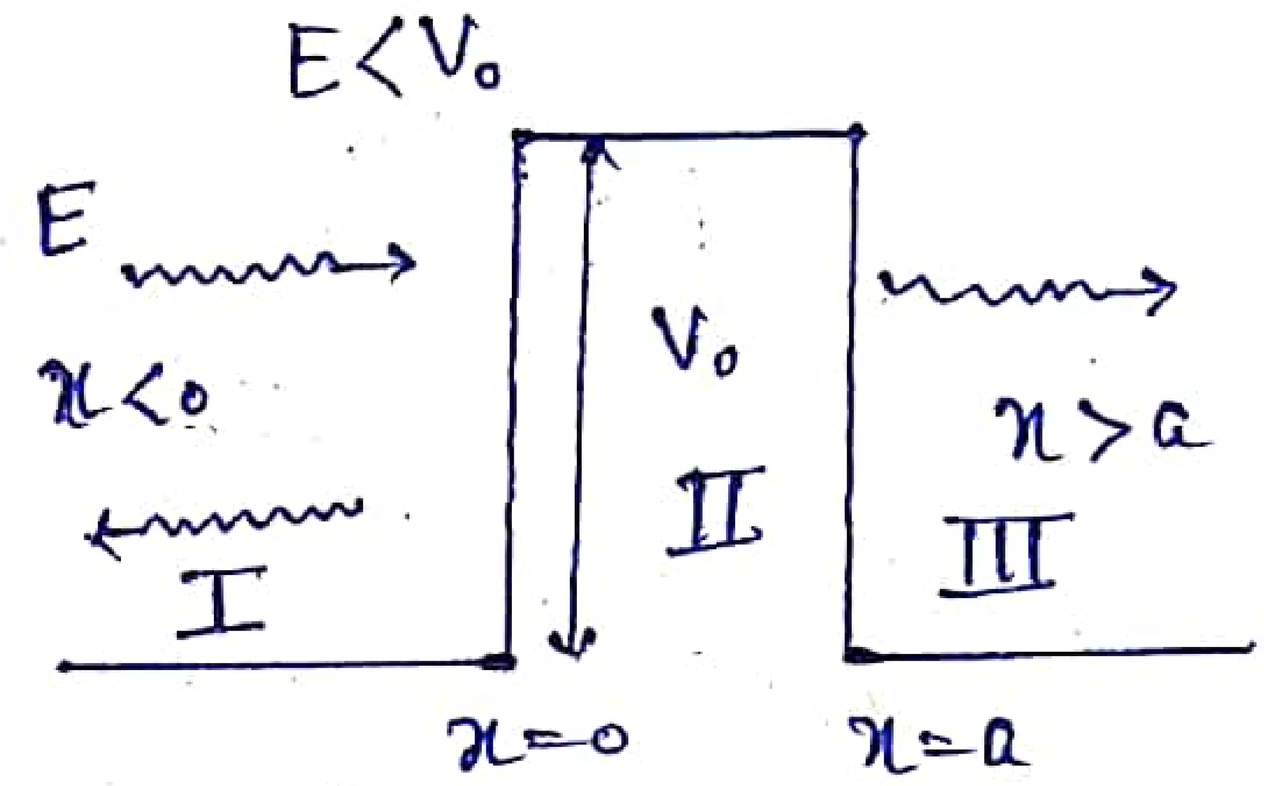
Schrodinger time Independent equation

Region-I

$x < 0$ $$\frac{d^2\psi_1}{dx^2} + \frac{2m}{\hbar^2}E\psi_1 = 0$$

$$\frac{d^2\psi_1}{dx^2} + K_1^2\psi_1 = 0$$

$$K_1 = \sqrt{\frac{2mE}{\hbar^2}}$$



$$\psi = Ae^{+ik_1x} + Be^{-ik_1x} \quad \text{--- (39.1)}$$

Region -II

$$\frac{d^2\psi_2}{dx^2} + \frac{2m}{\hbar^2}(E - V_0)\psi_2 = 0$$

$\boxed{K = \frac{2\pi}{\lambda}}$

Where $K_2' = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$

$$\frac{d^2\psi_2}{dx^2} + K_2'^2\psi_2 = 0$$

Where $\boxed{K_2 = -i K_2'}$

$= \sqrt{-\text{Ve term}}$

$\because E < V_0$

$$\psi_2 = Ce^{-k_2x} + De^{k_2x}$$

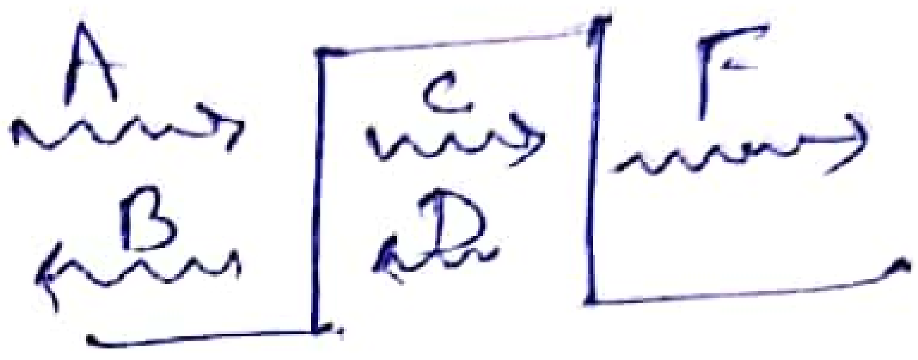
The Solution of Schrodingers equation in II region contains real exponentials contrary to region I & III.

$$K_2' = \sqrt{\frac{2m(E-V_0)}{\hbar^2}} = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}\sqrt{-1} = ik_2$$

$$K_2' = ik_2 \Rightarrow \boxed{K_2 = -iK_2'}$$

For Region III

$$\frac{d^2\psi_3}{dx^2} + \frac{2mE}{\hbar^2}\psi_3 = 0$$



$$\psi_3 = F e^{ik_1 x} + \underset{\substack{\Downarrow \\ 0}}{G} e^{-ik_1 x}$$

$$= F e^{ik_1 x} \quad \text{— (40.1)}$$

A is arbitrary constant. B, C, D and F depends on barrier. hight, E, Barrier width.

Reflection Coefficient

$$R = \frac{k_1 |B|^2}{k_1 |A|^2} \quad \text{— (40.2)}$$

$p = \frac{h}{\lambda}$ $\boxed{p \propto k}$

$k = 2\pi/\lambda$

Transmission Co-efficient

$$T = \frac{k_1 |F|^2}{k_1 |A|^2} \quad \text{— (40.3)}$$

We will determine B, C, D & F in term of A by applying the boundary conditions.

ψ and $\frac{d\psi}{dx}$ must be continuous at boundary

$x = 0$

$$\psi_1(0) = \psi_2(0)$$

$$\boxed{A + B = C + D} \quad \text{— (40.4)}$$

$$\left.\frac{d\psi_1}{dx}\right|_{x=0} = \left.\frac{d\psi_2}{dx}\right|_{x=0}$$

$$ik_1(A - B) = k_2(-C + D)$$

$$\boxed{A - B = \frac{k_2}{ik_1}(-C + D)} \quad \text{— (40.5)}$$

at $x = a$.

$$\psi_2(L) = \psi_3(L) \qquad \left.\frac{d\psi_2}{dx}\right|_{x=L} = \left.\frac{d\psi_3}{dx}\right|_{L}$$

$$\boxed{Ce^{-k_2 L} + De^{k_2 L} = Fe^{ik_1 L}} \quad \text{— (40.6)}$$

$$\boxed{-k_2 C e^{-k_2 L} + k_2 D e^{k_2 L} = ik_1 F e^{ik_1 L}}$$

(40.7)

By Solving B, C, D & F in terms of A then

$$R = \frac{T}{4\epsilon(1-\epsilon)} \sinh^2(\lambda\sqrt{1-\epsilon})$$

$$T = \left[1 + \frac{1}{4\epsilon(\epsilon-1)} \sinh^2(\lambda\sqrt{1-\epsilon})\right]^{-1}$$

Here $\lambda = a\sqrt{\frac{2mV_0}{\hbar^2}}$ and $\epsilon = \frac{E}{V_0}$

This shows that transmission coefficient is not zero but has a finite value

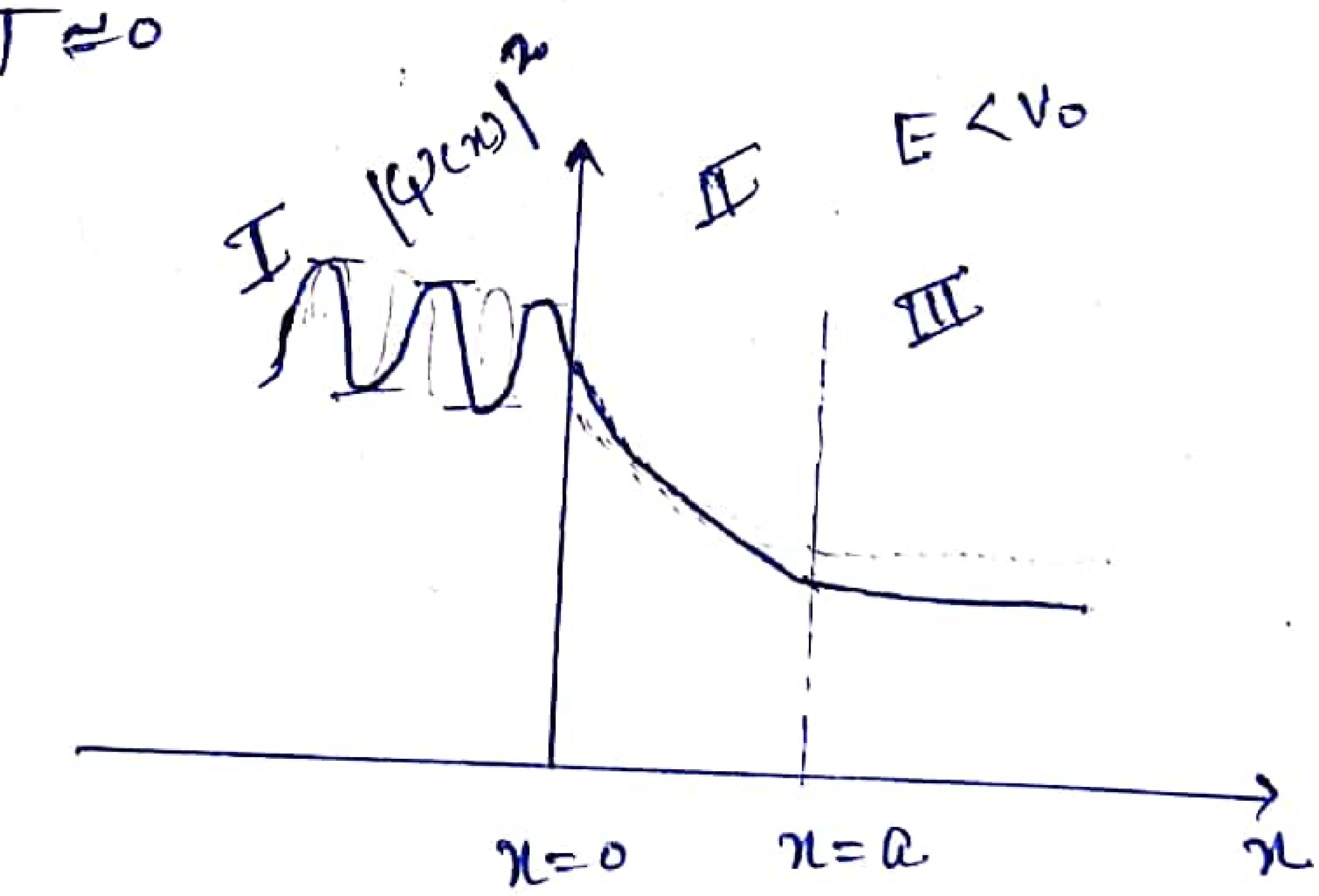
T is vanishingly small in classical limit because in that limit that $\lambda = \frac{2mV_0a^2}{\hbar^2}$

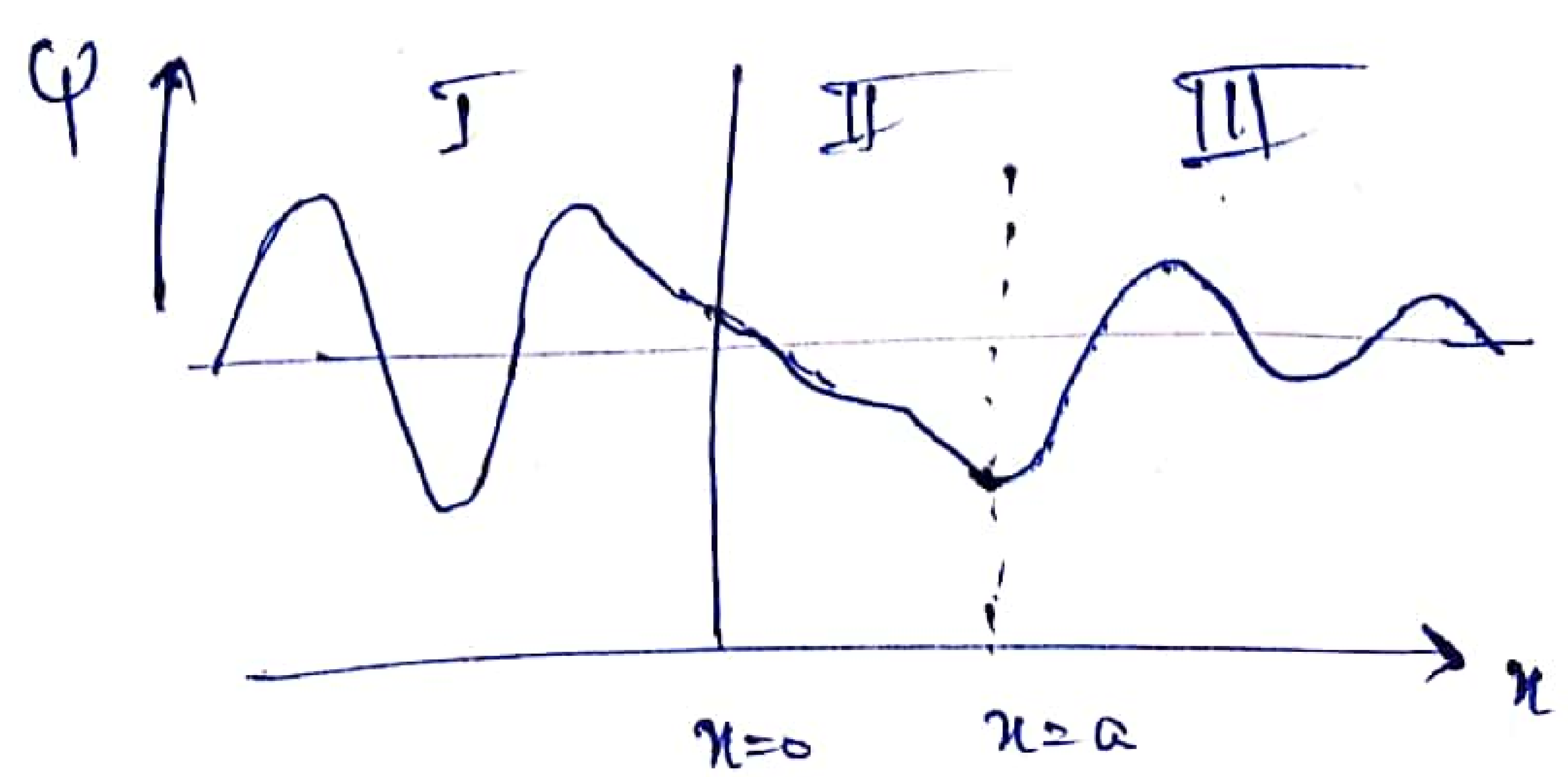
For classical Dust, $m = 10^{-5}$ kg

e $m \approx 10^{-31}$ kg

In classical λ extremely large

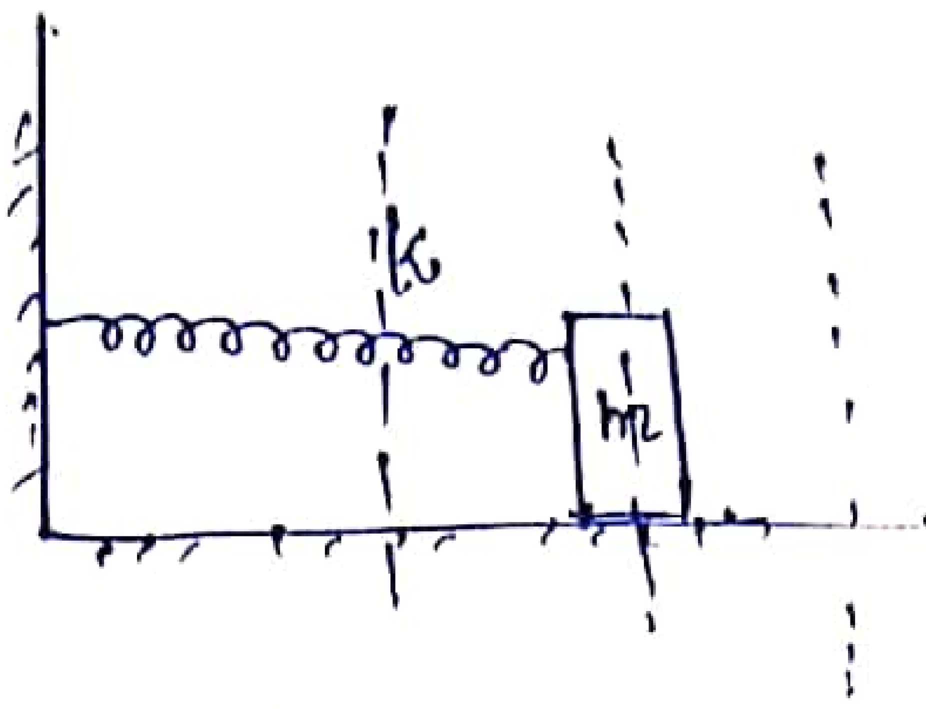
$R \simeq 1$, $T \neq 0$

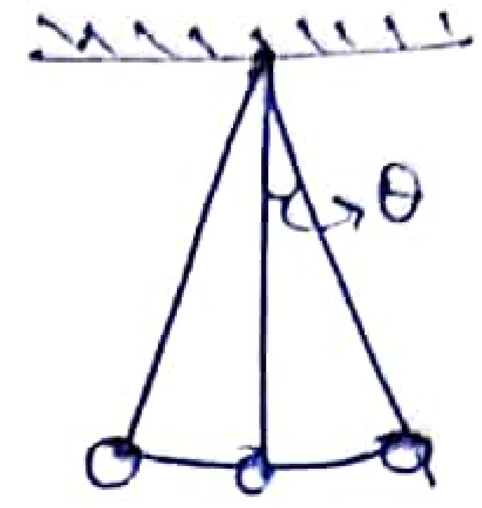


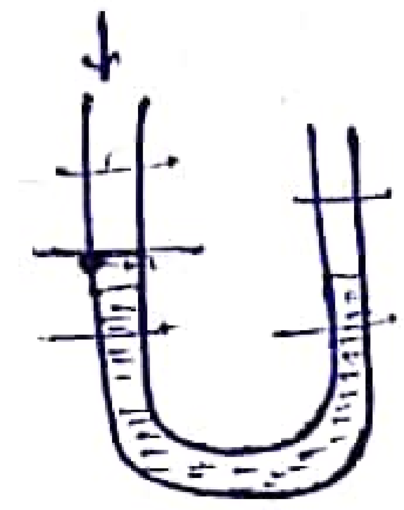


Harmonic Oscillator :-

In harmonic motion there is a point about which the system oscillates. There is a force which brings the mass again and again at a point where the force is zero. The force is known as restoring force and the point is called equilibrium point or mean position.







According the Hooke's law

$$F(x) = -kx$$

$$m\frac{d^2x}{dt^2} = -kx$$

$$m\frac{d^2x}{dt^2} + kx = 0$$

$$\boxed{\frac{d^2x}{dt^2} + \frac{k}{m}x = 0} \Rightarrow \boxed{\frac{d^2x}{dt^2} + \omega^2 x = 0}$$

This is Simple Harmonic Motion

Solution of this eqn $\qquad \omega = \sqrt{\frac{k}{m}}$

$$x(t) = A\cos(\omega t + \phi)$$

Where Angular frequency $\omega = \frac{2\pi}{T} = 2\pi\nu$

$$\omega^2 = k/m \Rightarrow \boxed{k = 4\pi^2\nu^2 m}$$

$\phi \rightarrow$ Phase difference

$\nu \rightarrow$ frequency of oscillation

Periodic motion $\rightarrow$ Repeat itself

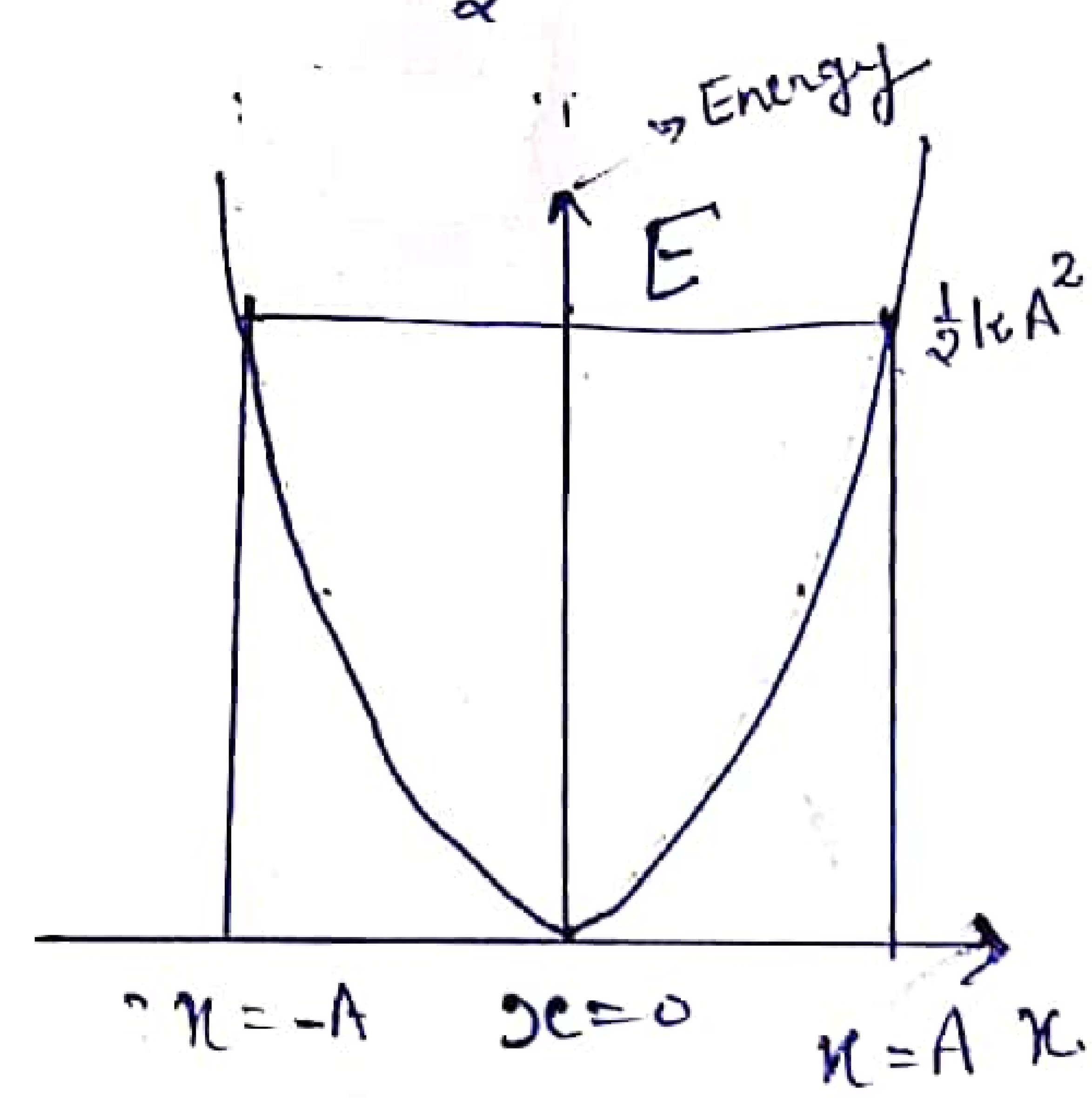
Potential energy of S.H.M.

$$V = \text{work done}$$

$$= -\int_0^x F \cdot dx$$

$$= +\int_0^x kx\,dx$$

$$= +\frac{1}{2}kx^2$$



* The Probability of finding a mass is
  $P_{max} \rightarrow$ extreme position
  $P_{min} \rightarrow$ at mean position
  $P = 0$ for $x > A$, $x < -A$

* The allowed energy of S.H. Oscillator forms a Continuous Spectrum. Energy have any value. $\boxed{E = \frac{1}{2}kA^2}$
* Lowest possible energy is zero.
* Particle can oscillate only within the classical limit A to $-A$.

$$F = -kx$$

$$m\frac{d^2x}{dt^2} = -kx$$

$$\frac{d^2x}{dt^2} + \frac{k}{m}x = 0$$

$$\boxed{\frac{d^2x}{dt^2} + \omega^2 x = 0} \quad \text{--- (43.1)}$$

Here
$$\omega = \sqrt{\frac{k}{m}}$$

Angular frequency
$$\omega = \frac{2\pi}{T} = 2\pi\nu$$

Solution of eq^n (43.1)

$$\boxed{x = A\cos(\omega t + \phi)}$$

And Potential Energy

$$V = \frac{1}{2}kx^2$$

$$V = \frac{1}{2}m\omega^2 x^2 \quad \text{--- (43.2)}$$

$$V = 2\pi^2 m \nu^2 x^2 \quad \text{--- (43.3)}$$

Quantum Mechanically Harmonic problem is solved by Schrodinger time independent eq^n

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

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}\left[E - 2\pi^2\nu^2 m x^2\right]\psi = 0 \quad \text{--- (43.4)}$$

put $a = \frac{2mE}{\hbar^2}$ or $b = \frac{2\pi\nu m}{\hbar}$

$$b^2 = \frac{4\pi^2\nu^2 m^2}{\hbar^2}$$

Eq^n (43.4) become

$$\frac{d^2\psi}{dx^2} + (a - b^2x^2)\psi = 0 \quad \text{--- (43.5)}$$

To solve equation (43.5) it is convenient to substitute

$\sqrt{b}\,x = q$ a dimensionless cont

$$q = \sqrt{b}\,x$$

$$dq = \sqrt{b}\,dx \Rightarrow \frac{dq}{dx} = \sqrt{b}$$

$$\frac{d\psi}{dx} = \frac{d\psi}{dq}\cdot\frac{dq}{dx} = \sqrt{b}\cdot\frac{d\psi}{dq}$$

$$\frac{d\psi}{dx} = \sqrt{b}\,\frac{d\psi}{dq}$$

$$\frac{d^2\psi}{dx^2} = \sqrt{b}\cdot\sqrt{b}\,\frac{d^2\psi}{dq^2}$$

$$\frac{d^2\psi}{dx^2} = b\,\frac{d^2\psi}{dq^2}$$

Substitute in eq^n (43.5)

$$b\frac{d^2\psi}{dq^2} + \left(a - \frac{b^2q^2}{b}\right)\psi = 0$$

$$\frac{d^2\psi}{dq^2} + \left(\frac{a}{b} - q^2\right)\psi = 0 \quad \text{--- (43.6)}$$

$$\frac{d^2\psi}{dq^2} + \left(\frac{a}{b} - q^2\right)\psi = 0 \quad \text{--- (43.6)}$$

To get a acceptable solution of eqn (43.6) we first try to get an asymptotic solution i.e. where $q \gg a/b$

, so a/b can be neglected

$$\frac{d^2\psi}{dq^2} - q^2\psi = 0$$

Solution of this equation

$$\psi = e^{+q^2/2} \quad \text{and} \quad \psi = e^{-q^2/2}$$

$\psi = e^{q^2/2}$ is not a acceptable solution

As the probability of finding a particle is somewhere along x-axis is given by $|\psi|^2$. Therefore it must decrease continuously to zero as $x \to -\infty$ and $x \to +\infty$. But the solution $\psi = e^{q^2/2}$ increase rapidly with increasing q. Hence $e^{q^2/2}$ is not acceptable soln.

$\psi = e^{-q^2/2}$ is only acceptable solution

$$\psi = A\, e^{-q^2/2} H(q)$$

$A \to$ Constant

$H(q)$ H $\to$ Hermite polynomial.

Energy level :- $$\frac{d^2H(q)}{dq^2} - 2q\frac{dH(q)}{dq} + [a/b - 1]H(q) = 0$$

only those solutions of this equation are acceptable for which

$$\frac{a}{b} = 2n+1 \Rightarrow \frac{2mE/\hbar^2}{2\pi\nu m/\hbar} = (2n+1)$$

$$E_n = (2n+1)\hbar\nu\pi = (n+1/2)h\nu$$

$$\boxed{E_n = [n + 1/2]h\nu} \qquad n = 0, 1, 2, 3$$

The energy of a harmonic oscillator is thus quantized in steps of $h\nu$

when $n = 0$

$$E_0 = (0+\tfrac{1}{2})h\nu = \tfrac{1}{2}h\nu$$

Zero point Energy

$$\boxed{E_0 = \tfrac{1}{2}h\nu}$$

Which is the lowest value of energy of the oscillator can have. This value is called zero-point energy because a harmonic oscillator in equilibrium with its ~~surronding~~ surrounding would approach an energy $E = E_0$ and not $E = 0$ as the temperature approaches 0K

General wave function

General wave function of harmonic oscillator is given by

$$\psi_n = A\, e^{-q^2/2} H_n(q)$$

$A \rightarrow$ Constant

$H_n(q) \rightarrow$ Hermite polynomial

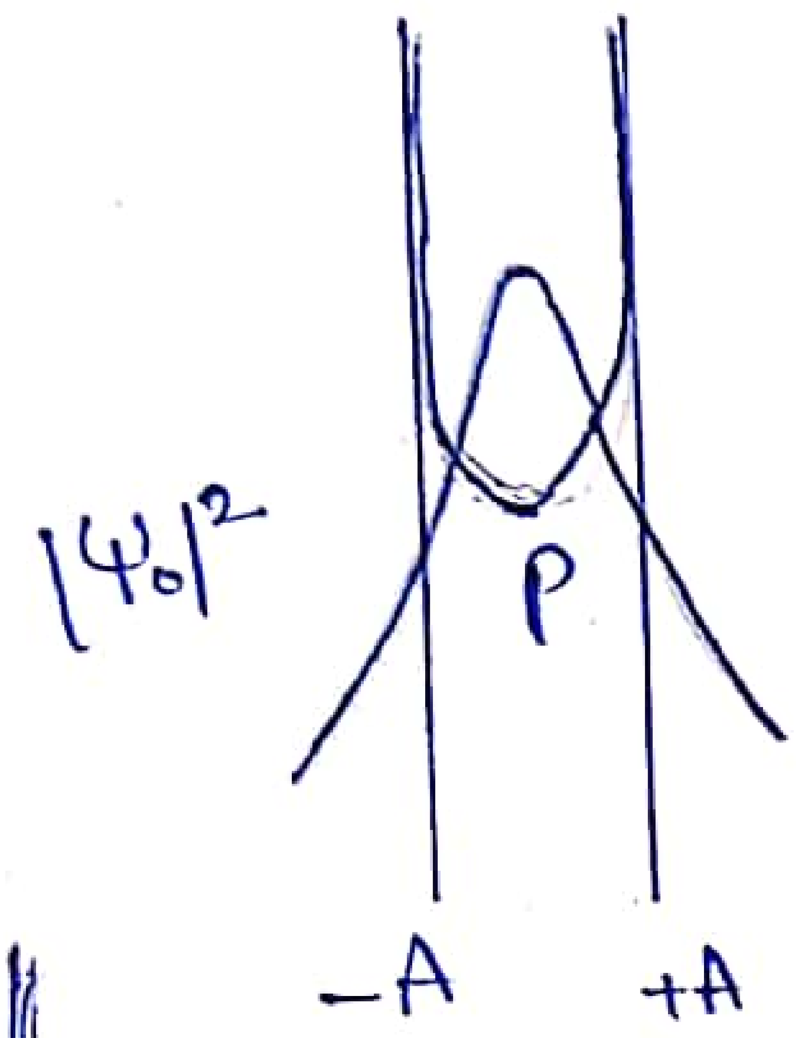
Applying the Normalization Condition on ψ_n then we get the value of A.

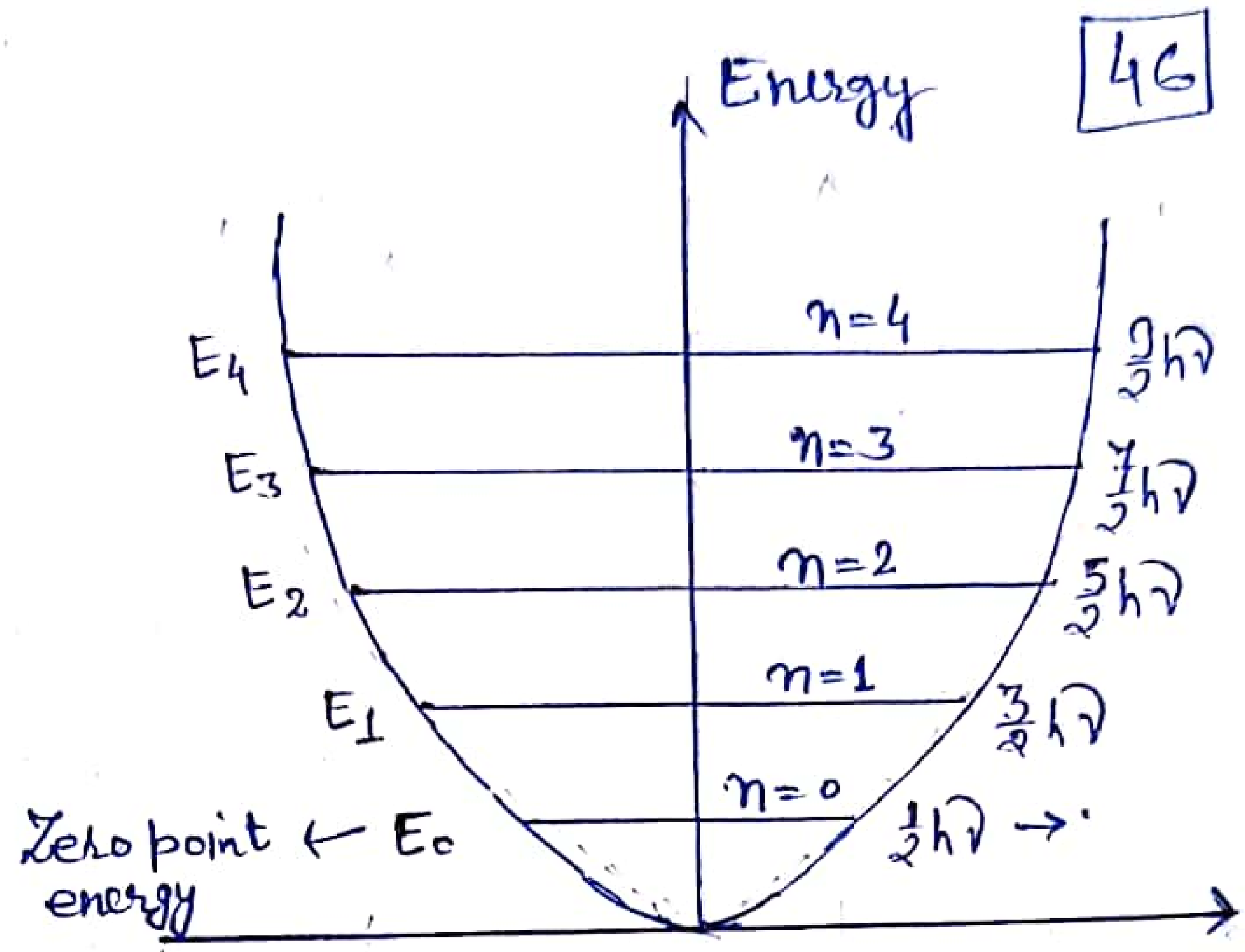
Wave function

$$\boxed{\psi_n = \left(\frac{2m\nu}{\hbar}\right)^{1/4} (2^n n!)^{-1/2} H_n(q)\cdot e^{-q^2/2}}$$

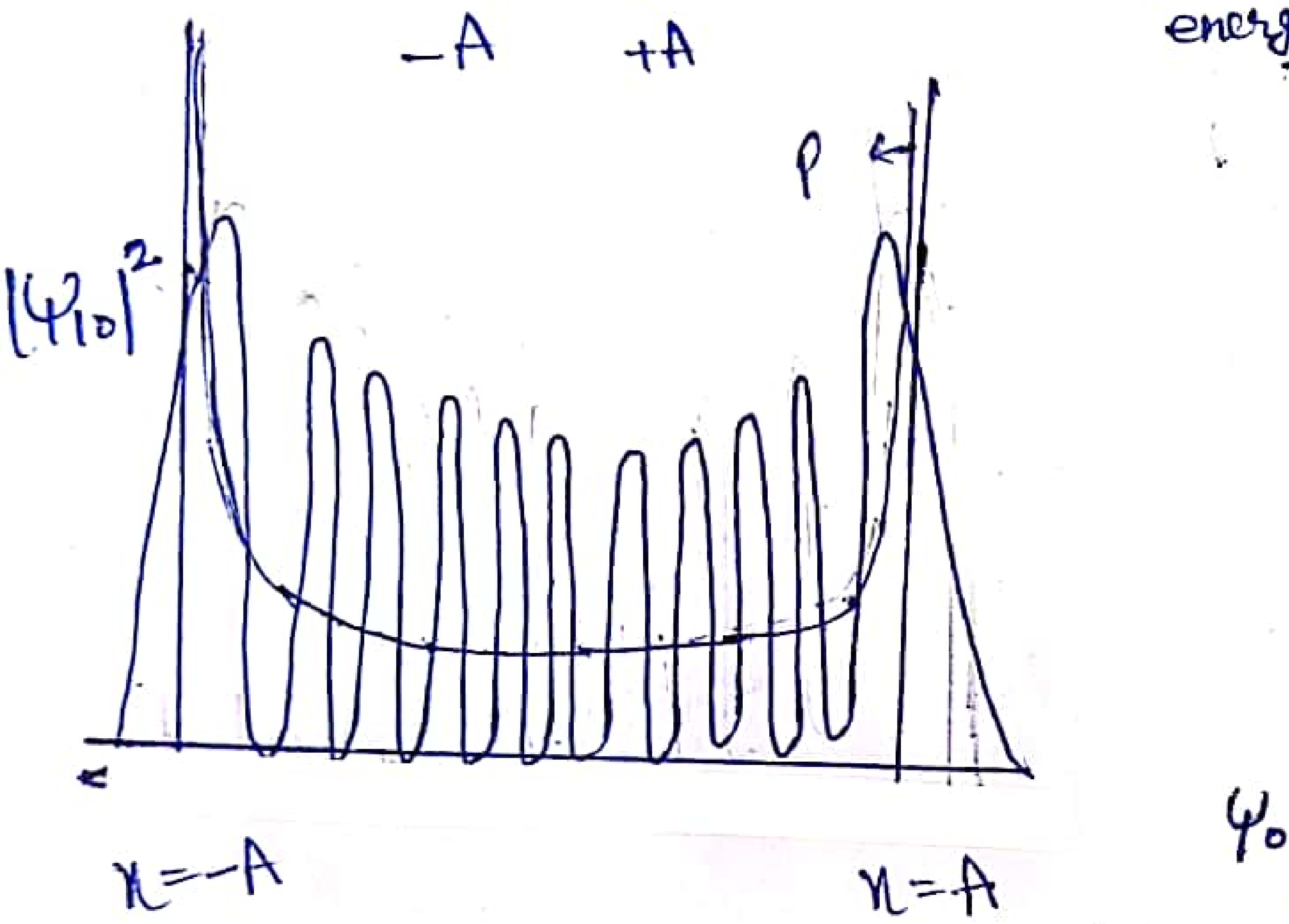
The first ~~8~~ Five Hermite polynomial are listed in table

n	$H_n(q)$	E_n
0	1	$\frac{1}{2}h\nu$
1	$2q$	$\frac{3}{2}h\nu$
2	$4q^2 - 2$	$5/2\, h\nu$
3	$8q^3 - 12q$	$\frac{7}{2}h\nu$
4	$16y^4 - 48y^2 + 12$	$\frac{9}{2}h\nu$
5		

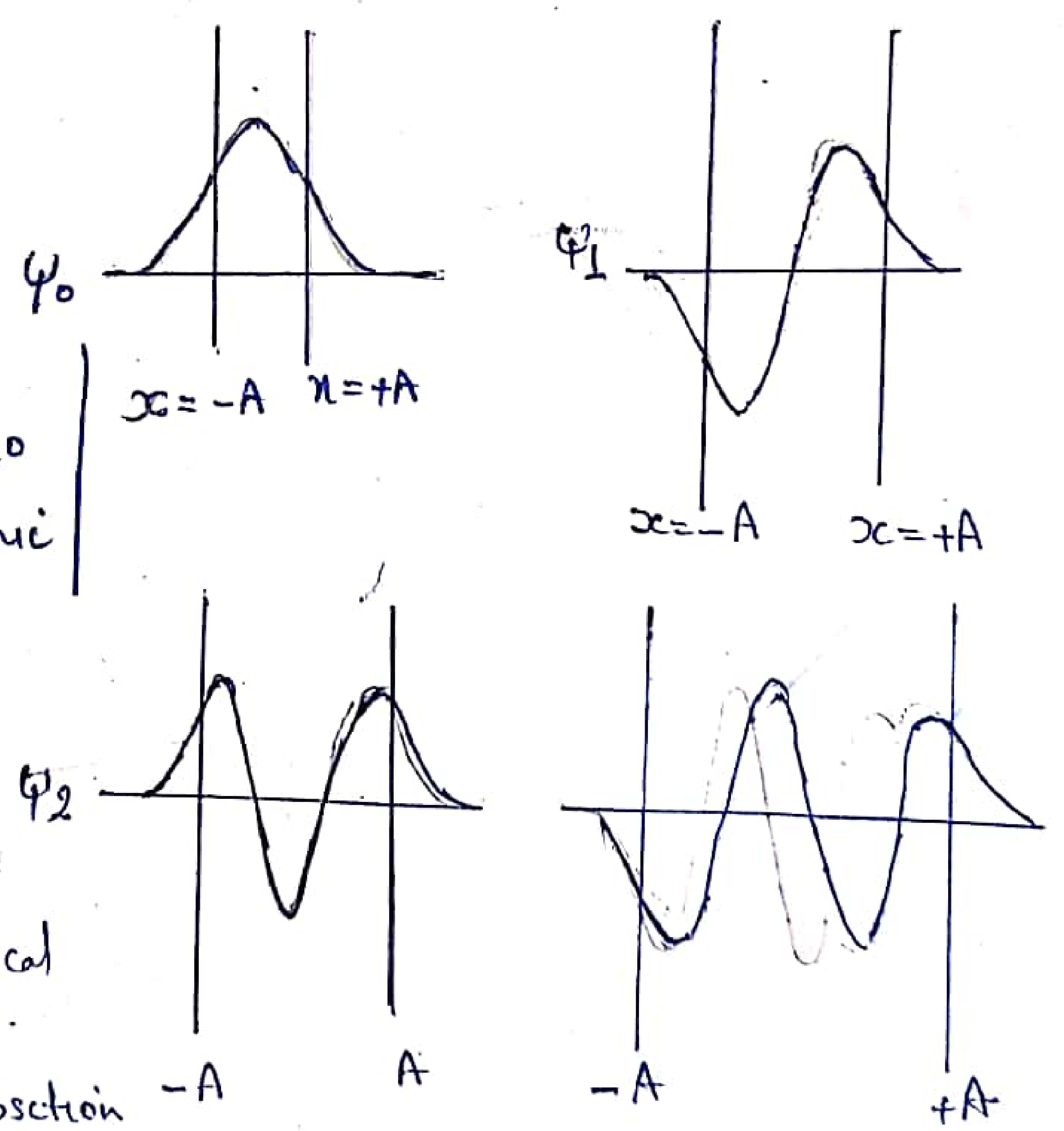




Energy level of harmonic oscillator are equally spaced.



Probability densities for $n=0$ and $n=10$ states of a quantum Mechanical Harmonic Oscillator. The probability densities for classical Harmonic oscillator with the same energies are shown by in 'P'.



Probabilities densities ~~of~~ for the classical oscillator (P). The probability of P of finding the particle at a given position is maximum at the endpoint of its motion. minimum ~~at~~ near the equilibrium position $x=0$, where it move rapidly.

The first four Harmonic oscillator wave functions. The vertical lines shows that limits $-A$ and $+A$ between which a classical oscillator with the same energy would vibrate.

Exactly the opposite behaviour occur when a Q.M H.O. in its lowest energy level state at $n=0$. The Probability density $|\psi_0|^2$ has its maximum value at $x=0$ and drops off on either side of this position. However this disagreement becomes less and less marked with increasing n.