

Unit-1 Quantum Mechanics.

Quantum Mechanics:- (Microscopic)

" Science dealing with the behaviour of Matter & light on atomic & subatomic scale."

It attempts to describe the Properties of Molecules atoms and their constituents (Electron, Protons, Neutrons and other subatomic Particle).

Classical Mechanics:-

Branch of Physics deals with the motion of object smaller as well as large objects.

OR Classical Mechanics deals with the motion of bodies under the influence of force.

Classical Mechanics

- I) Deals with Macroscopic objects
- II) Based on Newton's Law of Motion.
- III) In classical mechanics Behaviour of Particle can be completely known.
- IV) classical mechanics deals with certainties

Quantum Mechanics

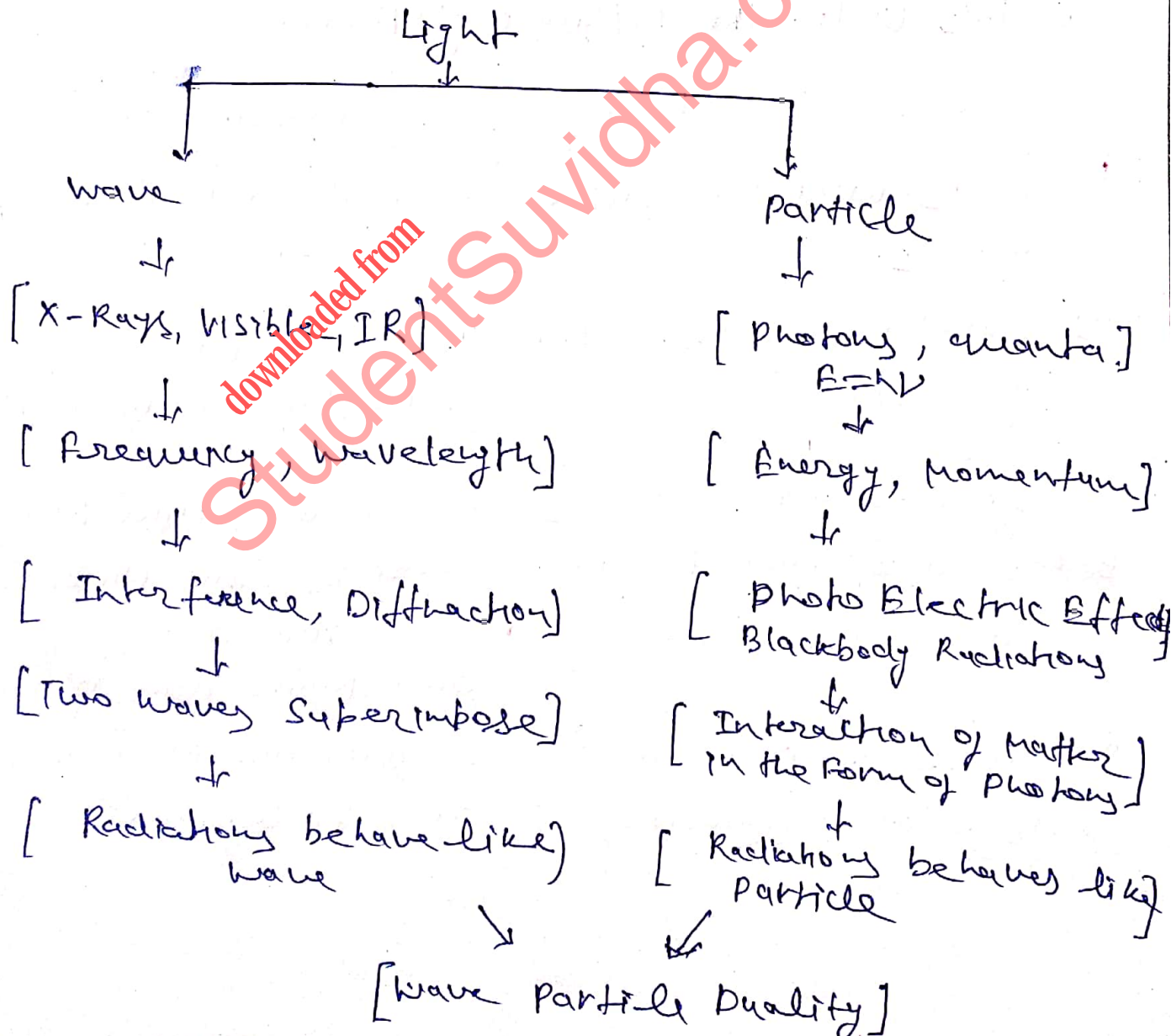
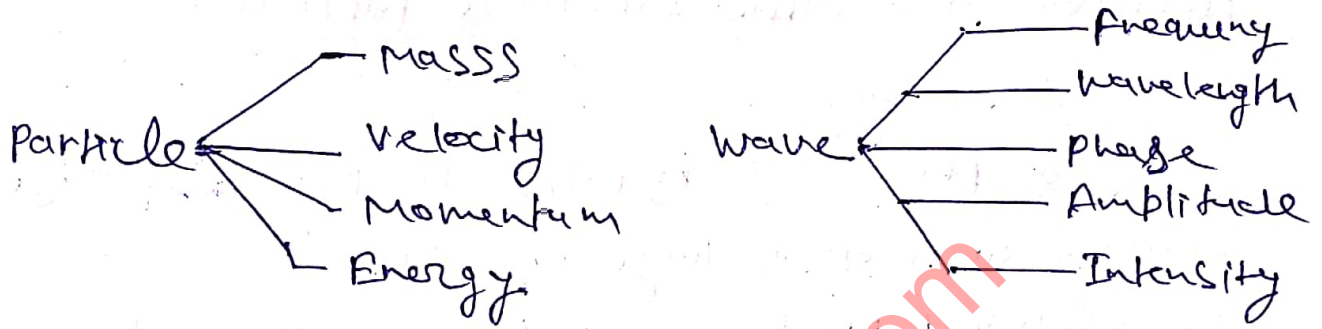
- I) Deals with Microscopic objects
- II) Based on Schrodinger wave Equation.
- III) In Quantum Mechanics there is some Uncertainty in determination of position and momentum of Particle.
- IV) Quantum Mechanics deals with probabilities.

Wave Particle Duality :-

"Wave Particle Duality Describe the properties of both photons and subatomic particles to exhibit the properties of both waves & particles"

OR

"It is the concept of Quantum mechanics that every particle or entity may be described as a particle or wave"



De Broglie Hypothesis - (4)

Light wave can act as a wave sometimes and as a Particle at other times this is known as de Broglie Hypothesis.

Matter Waves :-

According to de Broglie Hypothesis any moving particle is associated with a wave. The wave associated with a particle known as de Broglie waves or matter waves.

The wavelength, λ of matter waves associated with a particle moving with velocity v is inversely proportional to the magnitude of momentum of particle. Thus

$$\lambda = \frac{h}{mv} = \frac{h}{p} \quad (p = mv)$$

The relation $\lambda = \frac{h}{mv}$ is known as de-Broglie Equation and wavelength λ is called de-Broglie wavelength.

De-Broglie wavelength associated with an accelerated charge particle :-

If a charge particle, say an electron is accelerated by a potential difference of V volts, then its kinetic energy is given by $K.E = eV$

$$\frac{1}{2} mv^2 = eV$$

$$v = \sqrt{\frac{2eV}{m}}$$

Then electron wavelength is given by - (5)

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

$$\lambda = \frac{h}{\sqrt{2emv}}$$

De Broglie wavelength Expressed in term of Kinetic Energy:-

If a particle has K.E, Kinetic Energy

$$K.E = \frac{1}{2} mv^2$$

$$= \frac{1}{2} mv^2 \times \frac{m}{m}$$

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

$$p = \sqrt{2m(K.E)}$$

(Substituting value of h/mv) $\lambda = \frac{h}{p} = \frac{h}{\sqrt{2m(K.E)}} = \frac{12.28}{\sqrt{V}} \text{ \AA}$

De Broglie wavelength associated with a particle in thermal Equilibrium:-

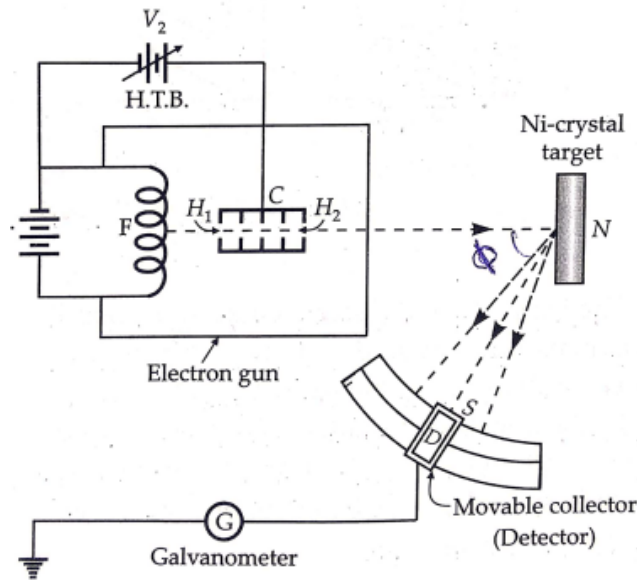
For a particle in thermal Equilibrium at temperature T , then their Kinetic Energy is given by -

$$K.E = \frac{3}{2} kT$$

$$\lambda = \frac{h}{\sqrt{2m(K.E)}} = \frac{h}{\sqrt{3m kT}}$$

Davisson & Germer Experiment:-

(Experiment to show the Existence of Matter waves)
 Davisson & Germer shows that electron beam can undergo diffraction when passed through an atomic crystal. It confirms the wave nature of electron and De-Broglie wave length.



- * In Experimental Arrangement of Davisson & Germer
- The Electron beam is generated from a hot Tungsten filament F. The filament is connected to Variable voltage source (V).
- The electron emerges through an opening and falls normally on the surface of Nickel crystal.
- The intensity of scattered electron can be measured by detector D in different direction. The detector can be moved in different directions.

Note:-

$$\theta + 50^\circ + \theta = 180^\circ$$

$$2\theta = 130^\circ$$

$$\theta = 65^\circ$$

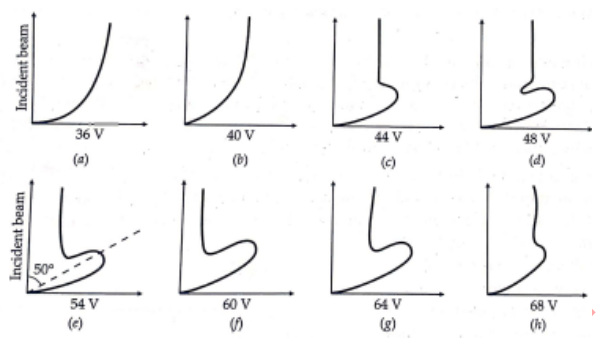


~~Answers~~

* First of all accelerating voltage V is given a low value and detector on the circular scale moved to various position and value of current was measured.

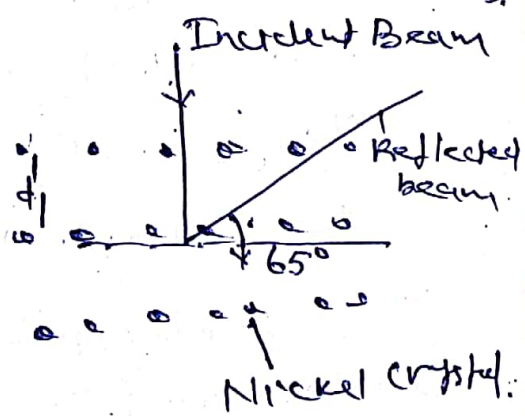
* The current (which measures the intensity of diffracted beam) is plotted against angle ϕ .

(ϕ is the angle between Incident beam on the crystal and the beam entering in the detector).



* It is seen that bump begins to appear in the curve for 44-volt electron. With increasing potential (V) the bump becomes most prominent (Maximum Intense) for 54 volt at $\phi = 50^\circ$.

* As Nickel is made up of crystal using Bragg's law of Diffraction wave length (λ) can be calculated



$$\lambda = 2d \sin \theta$$

$$\lambda = 2 \times 0.91 \text{ \AA} \times \sin 65^\circ$$

$$\lambda = 1.65 \text{ \AA} \quad \text{--- (1)}$$

($d = 0.91 \text{ \AA}$, d is the interlayer spacing).

The wavelength of electron can also be calculated from accelerating potential V using de-Broglie equation.

$$\lambda = \frac{h}{\sqrt{2meV}}$$

Note:-

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

$$p = mv$$

$$p^2 = m^2 v^2 = m \times m v^2$$

$$= m \times 2E \quad (K.E = \frac{1}{2}mv^2)$$

$$\Rightarrow p^2 = 2mE$$

$$E = \frac{p^2}{2m} \Rightarrow p = \sqrt{2mE}$$

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mE}}$$

Hence $\lambda = \frac{h}{\sqrt{2meV}} = \frac{6.6 \times 10^{-34}}{\sqrt{2 \times 9.1 \times 10^{-31} \times 54 \times 1.6 \times 10^{-19}}}$

Substituting
 $h = 6.6 \times 10^{-34}$
 $m = 9.1 \times 10^{-31}$
 $e = 1.6 \times 10^{-19}$

Note $E = 54 eV$
 $= 54 \times 1.6 \times 10^{-19} J$

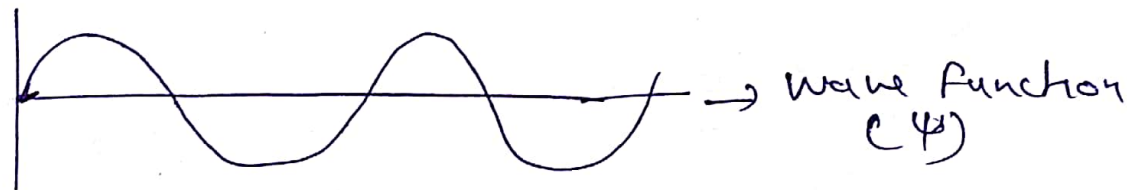
$$\lambda = 1.66 \text{ \AA} \quad \text{--- (2)}$$

It is seen that the values obtained experimentally using Bragg's equation and de-Broglie equation agreed well. Therefore Davisson - Germer conclude that electrons exhibit diffraction properties.

Wave Function:- Function describing the probability of each possible observation such as position & momentum.

Represented by $(\psi) - \Psi(x, t)$

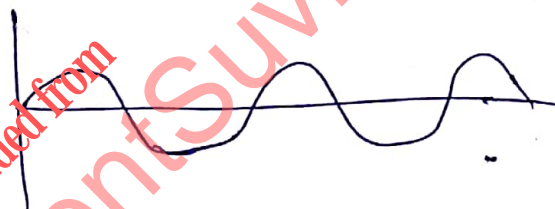
$\psi(x, t)$
Position time



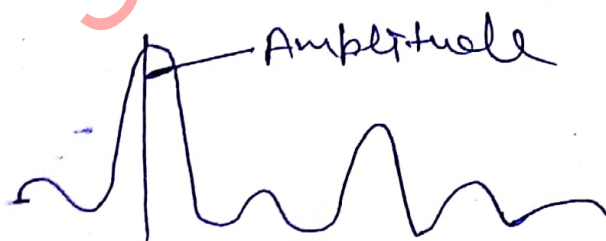
Note- A wave is associated with a particle.

Characteristics:-

(I) If a wave has higher energy it rotates with high frequency.



(II) Maximum Amplitude of a wave has maximum probability of finding the particle. (ψ^2)

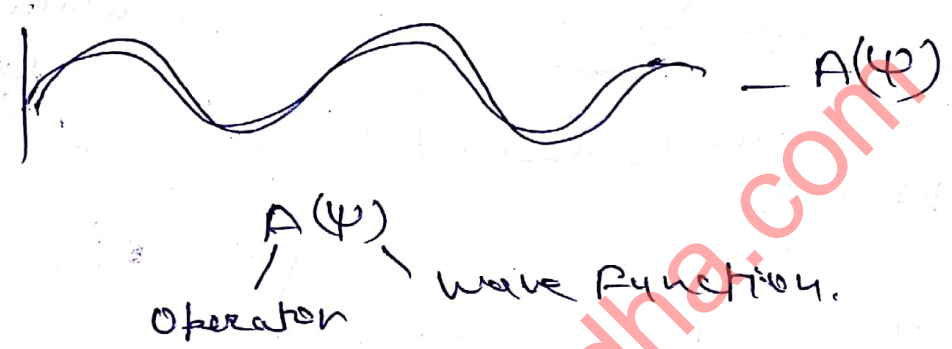
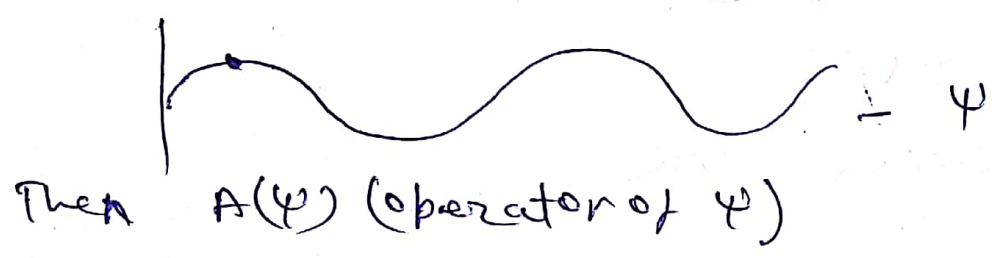


(III) Momentum of a wave is inversely proportional to wavelength.

$$p \propto \frac{1}{\lambda} \quad (p - \text{Momentum})$$

Operator: An operator is a mathematical operation on the wave function that produce another wave function.

Suppose ψ be any wave function



E.g - Hamiltonian operator (H)

Hamiltonian operator (H) represent total Energy of a system

$$H = T + V$$

Hamiltonian
Kinetic Energy
Potential Energy

Normalization of a wave function:

Normalization, when the probability of finding a particle is 1 then the function is said to be Normalized

$$\int \psi^* \psi dx = 1$$

Suppose ~~if~~ a function is not normalized

(1)

$$\int \psi^* \psi dx = N \quad (N \neq 1)$$

Then

$$\frac{1}{N} \int \psi^* \psi dx = 1$$

$$\boxed{\int \frac{\psi^*}{\sqrt{N}} \frac{\psi}{\sqrt{N}} dx = 1}$$

↓
Normalized

→ means Probability of finding Particle is 1

($\psi^* \psi$ - represent Probability of finding Particle)
(Probability density)

25 Normalize the wave function

$\psi(x) = 0$ outside the box of size l

$\psi(x) = A \sin kx$ $0 < x < l$

where $k = \frac{\pi}{l}$

Hint: $\int_{-\infty}^{+\infty} |\psi|^2 dx = 1,$

Here $\psi(x) = A \sin kx = A \sin \frac{\pi x}{l} = \int_0^l A^2 \sin^2 \frac{\pi x}{l} dx = 1$

From above expression, $A = \sqrt{\frac{2}{l}}$

Then $\psi_n = \sqrt{\frac{2}{l}} \sin \frac{\pi x}{l}$

[GGSIPU, May 2012 (4 marks)]

Wave Function & Probability Interpretation:- (12)

Micro particles exhibit wave properties, quantity ψ represent a de broglie wave, This quantity (ψ) is called Wave Function.

ψ describe wave as a function of position & time. It is an observable quantity.

ψ is a complex valued function.

We can only know the probable value in a measurement. The probability cannot be negative.

Probability Interpretation of wave function:-

$|\psi|^2$ (Square of magnitude of wave function) represent the probability of finding particle in that region.

Probability of finding the particle ~~at~~ is proportional to $|\psi(x,y,z)|^2 dx dy dz$ at time t .

$$P \propto |\psi(x,y,z)|^2 dv$$

$|\psi|^2$ is called probability density

ψ is probability amplitude.

Physical Interpretation of Wave Function ψ :

A satisfactory interpretation of wave function ψ associated with a moving particle was given by Born in 1926.

He postulated that square of magnitude of wave function $|\psi|^2$ at a particular point is proportional to probability of finding the particle at that point.

Also
$$\int_{-\infty}^{\infty} |\psi|^2 d\tau = 1.$$

A wave function that obey this equation said to be normalized. Beside being normalized ψ must fulfill the following requirement.

i) ψ must be finite everywhere.

If ψ is ~~not~~ infinite it would have infinite probability of finding the particle at that point. This would violate the uncertainty principle. Hence ψ must be finite.

ii) ψ must be single valued.

If ψ has ~~a~~ more than one value at any point, it would have more than one value of probability of finding the particle at that point. Hence it must be single valued.

iii) ψ must be continuous and have continuous first derivative everywhere.

$d^2\psi/dx^2$ must be finite everywhere. This possible is so only if $d\psi/dx$ has no discontinuity. Further $d\psi/dx$ as a continuous function implies that ψ too continuous across boundary.

Heisenberg's Uncertainty Principle:-

(18)

This Principle was discovered by Heisenberg in 1927. It states that we can measure either position or momentum of a particle with any desired degree of accuracy (within limit of experimental equipment). OR

It is impossible to measure both, position and momentum simultaneously with accuracy.

$$\Delta x \cdot \Delta p_x \geq \frac{h}{4\pi}$$

$\Delta x \rightarrow$ Uncertainty in position.

$\Delta p \rightarrow$ Uncertainty in momentum.

Physical Significance!

- I) Uncertainty Principle Explain why it is possible for Radiation and matter to have dual (wave-particle) character.
- II) It also make it clear that we can predict only the probable behaviour of quantum mechanical system not the exact behaviour.
- III) It helps in understanding many phenomenon like absence of electron within nuclei, natural broadening of spectral lines etc.

Energy Momentum Uncertainty!

The uncertainty relation for simultaneous measurement of Energy E & time t expressed as.

$$\Delta E \cdot \Delta t \geq \frac{\hbar}{2} \quad \left(\hbar = \frac{h}{2\pi} \right)$$

Derivation let us consider a microparticle moving with velocity v , Its kinetic Energy will be -

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

$$\Delta E = \Delta \left(\frac{1}{2} m v^2 \right) \\ = m v \Delta v = v \Delta p$$

$$\left(v^2 \frac{\Delta x}{\Delta t} \right)$$

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

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

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

$$\Delta x \cdot \Delta p \geq \frac{\hbar}{2}$$

Example 1.5 Find the smallest possible uncertainty in position of the electron moving with velocity 3×10^7 m/s (Given $h = 6.63 \times 10^{-34}$ Js, $m_0 = 9.1 \times 10^{-31}$ kg) [GGSIPU, May 2007 (2.5 marks)]

Solution. Given $v = 3 \times 10^7$ m/s

Let Δx_{\min} be the minimum uncertainty in position of the electron and Δp the maximum uncertainty in the momentum of the electron.

Thus we have,
$$\Delta x_{\min} \cdot \Delta p_{\max} = \frac{h}{2\pi} \quad \dots(i)$$

or

$$\Delta p_{\max} = p = mv$$

$$\Delta p_{\max} = \frac{m_0 v}{\sqrt{1 - \frac{v^2}{c^2}}} \quad \dots(ii)$$

$$\Delta x_{\min} = \frac{h \sqrt{1 - \frac{v^2}{c^2}}}{2\pi m_0 v} = \frac{6.63 \times 10^{-34} \sqrt{1 - \left(\frac{3 \times 10^7}{3 \times 10^8}\right)^2}}{2 \times 3.14 \times 9.1 \times 10^{-31} \times 3 \times 10^7} \text{ m}$$

$$= 0.03867 \times 0.9949 \times 10^{-10} \text{ m} = 3.8 \times 10^{-12} \text{ m}$$

Example 1.7 Show that the uncertainty in the location of the particle is equal to de-Broglie wavelength the uncertainty in its velocity is equal to its velocity. [GGSIPU, April 2014 (2 marks)]

Solution. Given $\Delta x = \lambda$,

Since we know that the uncertainty principle

$$\Delta x \Delta p_x = h \quad \text{or} \quad \lambda \Delta p_x = h$$

or
$$\Delta p_x = \frac{h}{\lambda} \quad \text{or} \quad \Delta p_x = p$$

or
$$m \Delta v_x = m v_x \quad \text{or} \quad \Delta v_x = v_x$$

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p

- 1.23 A typical atomic nucleus is about 5 Fermi in radius. Use the uncertainty principle to place a lower limit on the energy an electron must have if it is part of nucleus. [GGSIPU, Feb. 2012 (2 marks)]

Hint : We know that 1 Fermi = 10^{-15} m

The uncertainty principle in electron's position is

$$\Delta x = 5 \times 10^{-15} \text{ m}$$

$$\Delta p \geq \frac{\hbar}{\Delta x} = \frac{6.626 \times 10^{-34} \text{ Js}}{2\pi \times 5 \times 10^{-15} \text{ m}} = 2.11 \times 10^{-20} \text{ kg m/s}$$

The momentum would also be of the same order if this is the uncertainty in it. This suggests that the kinetic energy of electron is far greater than its rest energy and it can be written as

KE = pc , so that

$$pc \geq (2.11 \times 10^{-20} \text{ kg m/s}) \times (3 \times 10^8 \text{ m/s}) \geq 6.33 \times 10^{-12} \text{ J} \geq 39 \text{ MeV}$$

Thus, the kinetic energy of an electron must exceed 39 MeV, for it to be a nucleus constituent. Experiments indicate that the electrons in an atom have only a fraction of this energy. Thus, we can conclude that the electrons are present in the nucleus.

- 1.24 An electron has a speed of $2 \times 10^4 \text{ ms}^{-1}$ within the accuracy 0.01%. Calculate the uncertainty in the position of the electron. [GGSIPU, May 2017 (2.5 marks)]

Hint : $\Delta x \Delta p_x = \Delta x (m \Delta v_x) = \frac{h}{n\pi}$

$$\Rightarrow \Delta x = \frac{h}{n\pi m \Delta v_x} = \frac{6.63 \times 10^{-34}}{4\pi \times 9.1 \times 10^{-31} \times (2 \times 10^4 \times 0.0001)} = 29 \mu\text{m}$$

1.2 Calculate the de-Broglie wavelength of (i) a 46 g golf ball moving with velocity 30 m/s and (ii) an electron moving with velocity 10^7 m/s. Which one is measurable? [GGSIU, May 2010 (2.5 marks)]

Hint: $\lambda = \frac{h}{mv}$

(i) For golf ball: $\lambda = \frac{6.63 \times 10^{-34}}{46 \times 10^{-3} \times 30} = 4.8 \times 10^{-34}$ m [Not measurable]

(ii) For electron: $\lambda = \frac{6.63 \times 10^{-34}}{9.1 \times 10^{-31} \times 10^7} = 72$ nm [measurable].

1.5 A ball of mass 10^{-3} kg moves with a velocity of 10^{-2} ms⁻¹. What is the de-Broglie wavelength of the ball?

Hint: $\lambda = \frac{h}{p} = \frac{h}{mv} = \frac{6.626 \times 10^{-34} \text{ Js}}{10^{-3} \text{ kg} \times 10^{-2} \text{ ms}^{-1}} = 6.626 \times 10^{-29}$ m

1.6 An electron and a proton have the same de Broglie wavelength. Prove that the energy of electron is greater. [GGSIU, April 2015 (2 marks)]

Hint: $\lambda = \frac{h}{p} = \frac{h}{mv} = \frac{h}{\sqrt{2mE}}$ then $\lambda_e = \lambda_p \Rightarrow \frac{h}{\sqrt{2m_e E_e}} = \frac{h}{\sqrt{2m_p E_p}}$

$m_e E_e = m_p E_p \Rightarrow E_e = \frac{m_p E_p}{m_e}$ since $m_e < m_p$, so $E_e > E_p$

1.7 An electron and a proton are moving with same velocity. Find the ratio of their (i) de Broglie wavelength, (ii) phase velocity and (iii) group velocity. [GGSIU, May 2015 (6 marks)]

Hint: (i) $\frac{\lambda_e}{\lambda_p} = \frac{h}{m_e v_e} \times \frac{m_p v_p}{h} = \frac{m_p}{m_e}$

(ii) $\frac{v_{se}}{v_{sp}} = \frac{v_e}{v_p} = 1$ and (iii) $v_p v_g = c^2$ so $\frac{v_{pe}}{v_{pp}} = \frac{v_e}{v_p} = 1$

1.8 Calculate the de Broglie wavelength of basket ball of mass 1 kg, moving at a speed of 10 ms⁻¹. Discuss the reason, why we cannot observe its wave nature. [GGSIU, May 2015 (4.5 marks)]

Hint: $\lambda = \frac{h}{mv} = \frac{6.63 \times 10^{-34}}{1 \times 10} = 6.63 \times 10^{-36}$ m which is not measurable.

1.13 Determine the de-Broglie wavelength of an electron having kinetic energy 2.0 eV

[Given : mass of electron = 9.1×10^{-31} kg, $h = 6.63 \times 10^{-34}$ J.s]

[GGSIU, Feb. 2010 (2 marks)]

Hint: $\lambda = \frac{hc}{\sqrt{K(K + 2m_0c^2)}}$

$$= \frac{6.63 \times 10^{-34} \times 3 \times 10^8}{[2.0 \times 1.6 \times 10^{-19} (2.0 \times 1.6 \times 10^{-19} + 2 \times 9.1 \times 10^{-31} \times (3 \times 10^8)^2)]^{1/2}}$$

1.16 Find the phase and group velocities of an electron whose de-Broglie wavelength is 1.2 \AA .

[GGSIPU, Feb. 2012 (5 marks)]

Hint : $m_0 c^2 = 511 \text{ keV}$, $m_0 = 9.1 \times 10^{-31} \text{ kg}$

$$\frac{p^2}{2m} = \frac{h^2}{2m\lambda^2} \Rightarrow \frac{1}{2}mv^2 = \frac{h^2}{2m\lambda^2}$$

$$\Rightarrow v = \frac{h}{m\lambda} = 6.07 \times 10^6 \text{ m/s}$$

$$v = v_g = 6.07 \times 10^6 \text{ m/s}$$

But $v_p v_g = c^2$

$$\Rightarrow v_p = \frac{c^2}{v_g} = \frac{(3 \times 10^8)^2}{6.07 \times 10^6} = 1.48 \times 10^{10} \text{ m/s.}$$

1.17 Calculate the de-Broglie wavelength of 40 keV electrons used in certain electron microscope.

[GGSIPU, May 2011 (2.5 marks)]

Hint : $E = 40 \text{ keV} = 4.0 \times 10^3 \times 1.6 \times 10^{-16} \text{ J} = 6.4 \times 10^{-15} \text{ J}$

$$E = \frac{1}{2}mv^2 \quad \text{or} \quad v = \sqrt{2E/m}$$

$$\text{de-Broglie wavelength, } \lambda = \frac{h}{mv} = \frac{h}{\sqrt{2mE}} = 6.15 \times 10^{-15} \text{ m}$$

1.18 Calculate the de-Broglie wavelength of an electron accelerated through a potential difference 100 V.

[GGSIPU, April 2011 (2 marks)]

$$\text{Hint : } \lambda = \frac{h}{mv} = \frac{h}{\sqrt{2mE}} = \frac{1.228 \times 10^{-10}}{\sqrt{V}} = 1.228 \times 10^{-10} \text{ m} = 1.228 \text{ \AA}$$

1.19 A nuclear particle is confined to a nucleus of diameter $5 \times 10^{-14} \text{ m}$. Calculate the minimum uncertainty in the momentum of the nucleon. Also calculate the minimum kinetic energy of the nucleon.

[GGSIPU, Feb. 2009 (2 marks)]

Hint : The diameter of nucleus $(\Delta x) = 5 \times 10^{-14} \text{ m}$

$$\therefore \Delta p \Delta x = \hbar$$

$$\Rightarrow \Delta p = \frac{\hbar}{\Delta x} = \frac{1.05 \times 10^{-34}}{5 \times 10^{-14}} \text{ kg m s}^{-1} = 2.1 \times 10^{-21} \text{ kg m s}^{-1}$$

$$\text{and the minimum K.E. of the nucleon} = \frac{p^2}{2m_0} = \frac{2.1 \times 10^{-21}}{2 \times m_0} \text{ here } m_0 = \text{mass of nucleon.}$$

Group velocity & Phase velocity:-

Phase velocity:- Velocity of individual wave forming wave packet is called phase velocity.

According to de Broglie Hypothesis



If a particle is in motion a wave is associated with it. called matter wave

wavelength of wave $\lambda = \frac{h}{mv}$ (1)

(where v is the velocity of particle)

h - Planck's constant

m - mass of the particle)

We have to calculate the velocity of wave

velocity of wave u

$u = v\lambda$ (2) (v - frequency)

Note

$E = hv \Rightarrow v = \frac{E}{h}$

But $E = mc^2$

$v = \frac{mc^2}{h}$ (3)

Note Extra

\Rightarrow using (1), (3) in (2)

$u = v\lambda = \frac{mc^2}{h} \times \frac{h}{mv} = \frac{c^2}{v} \Rightarrow u = \frac{c^2}{v}$ (4)

velocity of wave

A plane wave travelling along x-axis is given by -

$$\psi = A \sin(\omega t - kx)$$

$$u = v\lambda$$

$$\left(\begin{array}{l} \omega = 2\pi\nu \\ k = \frac{2\pi}{\lambda} \end{array} \right)$$

(where ω is Angular velocity
 k - Propagation constant)

Now $\psi = A \sin(\omega t - kx)$ $u = \frac{2\pi}{2\pi} v\lambda$

$$= \frac{\omega}{2\pi} \lambda = \frac{\omega}{k}$$

$$u = \frac{\omega}{k}$$

$$\boxed{v_p = \frac{\omega}{k}} \text{ --- phase velocity.}$$

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Group Velocity:-

~~Group velocity~~ is The velocity of wave packet formed by the individual waves is called group velocity.

Superposition of wave is called wave packet or wave group.



Let us consider a wave group which consist of two component of equal amplitude a , but slightly different angular frequencies ω_1, ω_2 and propagation constant k_1, k_2 . Displacement is given by.

$$y_1 = a \sin(\omega_1 t - k_1 x)$$

$$y_2 = a \sin(\omega_2 t - k_2 x)$$

Then Superposition gives -

$$y = y_1 + y_2$$

$$= a [\sin(\omega_1 t - k_1 x) + \sin(\omega_2 t - k_2 x)]$$

Using $\left(\begin{matrix} \sin A + \sin B = 2 \sin \frac{A+B}{2} \cos \frac{A-B}{2} \end{matrix} \right)$ we get -

$$y = 2a \sin \left(\frac{(\omega_1 t - k_1 x) + (\omega_2 t - k_2 x)}{2} \right)$$

$$\cos \left(\frac{\omega_1 t - k_1 x - \omega_2 t + k_2 x}{2} \right)$$

$$= 2a \sin \left(\frac{(\omega_1 + \omega_2)t}{2} - \frac{(k_1 + k_2)x}{2} \right)$$

$$\cos \left(\frac{(\omega_1 - \omega_2)t}{2} - \frac{(k_1 - k_2)x}{2} \right)$$

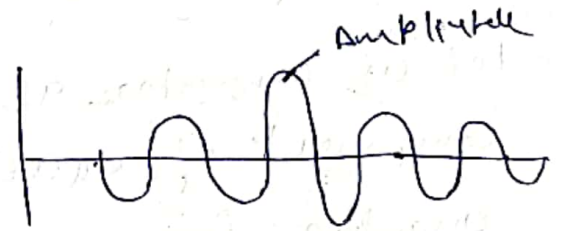
(16)

$$y = 2a \cos \left(\frac{(\omega_1 - \omega_2)t}{2} - \frac{(k_1 - k_2)x}{2} \right) \sin \left[\frac{(\omega_1 + \omega_2)t}{2} - \frac{(k_1 + k_2)x}{2} \right]$$

Amplitude Angle

Note ($\varphi = A \sin(\omega t - kx)$)

For group velocity we use Amplitude velocity



where Amplitude A

$$A = 2a \cos \left(\frac{(\omega_1 - \omega_2)t}{2} - \frac{(k_1 - k_2)x}{2} \right)$$

∴ Group velocity $V_g = \frac{\omega_1 - \omega_2}{k_1 - k_2}$

$$V_g = \frac{\Delta \omega}{\Delta k} \leftarrow \text{Group velocity}$$

Relation between group velocity & Phase velocity!

We have $V_p = \frac{\omega}{k} \Rightarrow \omega = (kV_p)$

$$V_g = \frac{d\omega}{dk} = \frac{d(kV_p)}{dk} = V_p + k \frac{dV_p}{dk}$$

(Using $k = \frac{2\pi}{\lambda}$)

$$V_g = V_p + \frac{2\pi}{\lambda} \frac{dV_p}{d(\frac{2\pi}{\lambda})}$$

$$v_g = v_p + \frac{1}{\lambda} \frac{dv_p}{d\left(\frac{1}{\lambda}\right)}$$

(17)

But $d\left(\frac{1}{\lambda}\right) = -\frac{1}{\lambda^2} d\lambda$, therefore

$$v_g = v_p - \lambda \frac{dv_p}{d\lambda}$$

1.20 An electron has a de Broglie wavelength 2 pm. Find its kinetic energy, phase velocity and group velocity of its de Broglie wave. Rest mass energy of electron is 511 keV.

[GGSIPU, Feb. 2017 (3 marks)]

Hint: $m_0 c^2 = 511 \text{ keV} \Rightarrow m_0 = 9.1 \times 10^{-31} \text{ kg}$

$$\text{K.E.} = \frac{p^2}{2m} = \frac{h^2}{2m\lambda^2} = \frac{1}{2} m v_g^2 \Rightarrow v_g = ? \Rightarrow v_p v_g = c^2 = ?$$

1.1 Find the phase velocity and group velocity of the de-Broglie wave of an electron whose speed is $0.9c$.

[GGSIPU, Feb. 2009 (2 marks), May 2009 (2.5 marks); May 2019 (2.5 marks)]

Hint: $v_p v_g = c^2$ and $v_g = 0.9c$. Then $v_p = 3.33 \times 10^8 \text{ m/s}$.

Expectation values:- (Average value)

The average value of a large number of measurement of physical quantity is represented by large Expectation value of a function $f(r)$.

$$\langle f(r) \rangle = \text{Average } f(r) = \overline{f(r)}$$

$$\langle f(r) \rangle = \int \psi^*(r,t), f(r) \psi(r,t) d\tau$$

Average value of position vector -

$$\langle \vec{r} \rangle = \int \psi^*(\vec{r},t) \vec{r} \psi(\vec{r},t) d\tau$$

Average value of momentum.

①

(Expectation)

$$\langle P \rangle = \int \psi^* P \psi d\tau$$

$$\hat{P} = -i\hbar \nabla$$

$$\langle P \rangle = \int \psi^* (-i\hbar \nabla \psi) d\tau$$

Expectation value of potential Energy V can be written as -

②

$$\langle V \rangle = \int \psi^*(r,t) V(r) \psi(r,t) d\tau$$

③

Eqnⁿ ①, ②, ③ are valid for Normalized wave function. If wave function are not Normalized then average value function can be written as -

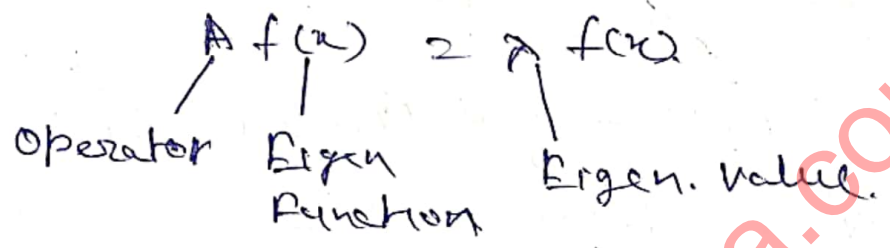
$$\langle f(r) \rangle = \frac{\int \psi^* f(r) \psi d\tau}{\int \psi^* \psi d\tau}$$

Eigen Values & Eigen Function

If there is some function $f(x)$ which when operated on operator A gives the Equation

$$\boxed{\hat{A}f(x) = \lambda f(x)}$$

λ is constant and various possible value of λ are called eigen values of the operator and these functions are called Eigen Function.



Note
 Eigen values for matrices
 $|A - \lambda I| = 0$

Suppose ψ be any wave function



where A is operator.

(Note: An operator is a mathematical operation on wave function that produce another wave function)

Thus "Eigen value Equation is that Equation in which operator operates on a function give the function multiplied by some constant"

$$\boxed{A f(x) = \lambda f(x)}$$

Example 2.2 A particle limited to the x -axis has the wave function $\psi = ax$ between $x = 0$ and $x = 1$, $\psi = 0$ elsewhere. Find (a) the probability that particle can found between $x = 0.45$ and $x = 0.55$. (b) The expectation value $\langle x \rangle$ of the particle's position. [GGSIPU, May 2014 (3 marks), Feb. 2008, April 2007, Feb. 2012 (2 marks)]

Solution. (a) The probability is

$$\int_{x_1}^{x_2} |\psi|^2 dx = a^2 \int_{0.45}^{0.55} x^2 dx = a^2 \left[\frac{x^3}{3} \right]_{0.45}^{0.55} = 0.0251 a^2$$

(b) The expectation value of the particle's position is

$$\langle x \rangle = \int_0^1 x |\psi|^2 dx = a^2 \int_0^1 x^3 dx = a^2 \left[\frac{x^4}{4} \right]_0^1 = \frac{a^2}{4}$$

2.13 The eigenfunctions for a particle in a 1-D box are given by $\psi(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}$. Find the expectation values of (i) position and (ii) momentum in the n th quantum state.

[GGSIPU, May 2016 (4 marks)]

Hint: (i) $\langle x \rangle = \int_{-\infty}^{\infty} \psi_n^* x \psi_n dx = \frac{2}{a} \int_0^a x \sin^2 \frac{n\pi x}{a} dx$

Integrating by parts, we get: $\langle x \rangle = \frac{a}{2}$.

This result is as expected; the probability density $\psi^* \psi$ is symmetric about $\langle x \rangle = \frac{a}{2}$, indicating that the particle spends as much time to the left of the center as to the right.

(ii)
$$\langle p_x \rangle = \int_{-\infty}^{\infty} \psi_n^* \left(i\hbar \frac{d}{dx} \right) \psi_n dx = \frac{2i\hbar}{a} \int_0^a \sin \frac{d}{dx} \left(\sin \frac{n\pi x}{a} \right) dx$$

$$= -\frac{2i\hbar}{a} \frac{n\pi}{a} \int_0^a \sin \frac{n\pi x}{a} \cos \frac{n\pi x}{a} dx = -\frac{i\hbar n\pi}{a^2} \int_0^a \sin \frac{2n\pi x}{a} dx$$

Solving the integral, we get $\langle p_x \rangle = 0$.

Again the result is expected. The particle moves back and forth, spending half its time moving towards the left and half its time moving towards the right. Thus, the average momentum must be zero.

Schrodinger Time dependent Equation in one dimension

Schrodinger presented the wave Equation describing the properties of electron in the form of equation called Schrodinger wave Equation to calculate the probabilities of electron at different places around nucleus in the atom OR.

It is a differential Equation for de-Broglie waves associated with particle and describing motion of particle.

$$i\hbar \frac{d\psi}{dt} = -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V\psi$$

m - Mass of electron

V - Potential Energy with reference to nucleus

ψ - wave function.

Derivation:- Equation of a particle moving freely in positive x direction is.

$$\psi = A e^{-i(\omega t - kx)} \quad \text{--- (1)}$$

Note

$\omega = 2\pi\nu$, $E = h\nu$	$k = \frac{2\pi}{\lambda}$, $\lambda = \frac{h}{p}$
$\omega = \frac{2\pi E}{h}$, $\nu = E/h$	

$$\boxed{k = \frac{2\pi p}{h}}$$

where A - Amplitude, k - Propagation constant
 ω - Constant Angular Frequency.

Now substituting value of ω & k in Equation (1)

$$\psi = A e^{-i(\omega t - kx)}$$

$$\psi = A e^{-i\left(\frac{2\pi E t}{h} - \frac{2\pi p x}{h}\right)}$$

$$\psi = A e^{-i \left(\frac{2\pi}{h} (Et - Px) \right)}$$

Using $\hbar = \frac{h}{2\pi}$ here \hbar is modified form of Planck's constant.

$$\Rightarrow \psi = A e^{-\frac{i}{\hbar} (Et - Px)}$$

$$= A e^{\frac{i}{\hbar} (Px - Et)} \quad \text{--- (2)}$$

Now Differentiating (2) wrt x

$$\frac{d\psi}{dx} = A e^{\frac{i}{\hbar} (Px - Et)} \frac{d}{dx} \left(\frac{i}{\hbar} (Px - Et) \right)$$

Note using $\left(\frac{d}{dx} e^y = e^y \frac{dy}{dx} \right)$

$$= \psi \frac{iP}{\hbar} \quad \text{from (2)}$$

$$\Rightarrow P\psi = \frac{\hbar}{i} \frac{d\psi}{dx} \quad \text{--- (3)}$$

Now Differentiating wrt t

$$\frac{d\psi}{dt} = A \left(-\frac{iE}{\hbar} \right) e^{\frac{i}{\hbar} (Px - Et)}$$

$$= -\frac{E}{\hbar} \psi \quad \text{from (2)}$$

$$\Rightarrow E\psi = -\hbar \frac{d\psi}{dt} = \hbar i \frac{d\psi}{dt} \quad \text{--- (4)}$$

Now Total Energy

$E = \text{Kinetic Energy} + \text{Potential Energy}$

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

$$\boxed{E = \frac{p^2}{2m} + V}$$

$$E(\psi) = \frac{p^2}{2m} (\psi) + V(\psi) \quad \text{--- (5)}$$

Now substituting value of (3) (4) in (5)

we get
$$i\hbar \frac{d\psi}{dt} = \left(\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} \right) + V(\psi).$$

$$\Rightarrow \boxed{i\hbar \frac{d\psi}{dt} = \left(-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V(\psi) \right)} \quad \text{--- (6)}$$

Time dependent Schrodinger wave Equation.

Time independent ~~Schrodinger~~ Schrodinger Equation

We have Equation of a Particle moving freely in positive x direction.

$$\psi = A e^{-i(\omega t - kx)}$$

(Using $\omega = \frac{2\pi E}{h}$ & $k = \frac{2\pi P}{h}$)

$$\psi(x,t) = A e^{-i \frac{2\pi}{h} (Et - Px)}$$

$$= A e^{i \frac{2\pi}{h} (Px - Et)}$$

$$= A \left(e^{\frac{2\pi i Px}{h}} \right) \left(e^{-\frac{2\pi i Et}{h}} \right)$$

Again we have. --- (1)

$$\psi = A e^{-i(\omega t - kx)}$$

For time independent $t=0$

$$\psi(x) = A e^{-i(-kx)}$$

$$= A e^{-i \left(-\frac{2\pi P}{h} x \right)}$$

$$\psi(x) = A e^{\frac{2\pi i Px}{h}}$$

--- (2)

Substituting (2) in (1) we get.

$$\Psi(x,t) = \Psi(x) e^{-2\pi iEt/h} \quad \text{--- (A)}$$

Differentiating wrt t

$$\frac{d\Psi}{dt} = \Psi(x) e^{-\frac{2\pi iEt}{h}} \left(-\frac{2\pi iE}{h} \right) \quad \text{--- (B)}$$

Differentiating wrt x

$$\frac{d\Psi}{dx} = e^{-\frac{2\pi iEt}{h}} \frac{d\Psi}{dx}$$

$$\Rightarrow \frac{d^2\Psi}{dx^2} = e^{-\frac{2\pi iEt}{h}} \frac{d^2\Psi}{dx^2} \quad \text{--- (C)}$$

Substituting value of A, B, C in (5)

From (5) we have

$$-\frac{\hbar^2}{2m} \frac{d^2\Psi}{dx^2} + V\Psi = \frac{i\hbar}{2\pi} \frac{d\Psi}{dt}$$

$$\Rightarrow -\frac{\hbar^2}{2\pi^2 m} \frac{d^2\Psi}{dx^2} + V\Psi = \frac{i\hbar}{2\pi} \frac{d\Psi}{dt}$$

$$\Rightarrow -\frac{\hbar^2}{8\pi^2 m} \left(e^{-\frac{2\pi iEt}{h}} \frac{d^2\Psi}{dx^2} \right) + V \left(\Psi(x) e^{-\frac{2\pi iEt}{h}} \right)$$

$$= \frac{i\hbar}{2\pi} \Psi(x) e^{-\frac{2\pi iEt}{h}} \left(-\frac{2\pi iE}{h} \right)$$

$$\Rightarrow \frac{e^{-\frac{2\pi iEt}{h}}}{h} \left(-\frac{\hbar^2}{8\pi^2 m} \frac{d^2\Psi}{dx^2} + V\Psi \right) = \frac{e^{-\frac{2\pi iEt}{h}}}{h} E\Psi$$

$$\Rightarrow \boxed{\frac{d^2\Psi}{dx^2} + \frac{8\pi^2 m}{\hbar^2} (E-V)\Psi = 0}$$

↓
Time independent Schrodinger Eqn

The Free Particle!

The particle is said to be a free particle when it is moving in space without being subjected to any external force in any region of space and its potential energy is constant ($V = \text{constant}$).

Then time-independent Schrodinger wave Equation for free particle is given as -

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2m}{h^2}(E - V)\psi = 0$$

$$V=0$$

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2m}{h^2}E\psi = 0$$

Note

$\text{Kinetic Energy} = \frac{1}{2}mv^2$ $= \frac{1}{2} \frac{m}{m} mv^2$ $E = \frac{p^2}{2m}$ $p = \sqrt{2mE}$	$\text{propagation constant}$ $k = \frac{2\pi}{\lambda}$ $= \frac{2\pi p}{h}$ $k = \frac{2\pi \sqrt{2mE}}{h}$ <p>on squaring</p> $k^2 = \frac{8\pi^2mE}{h^2}$
--	---

Hence $\frac{d^2\psi}{dx^2} + k^2\psi = 0$

where $k^2 = \frac{8\pi^2mE}{h^2}$ (1)

a) Wave Function \rightarrow General solution of Equation (1)

is given by

$$\psi(x) = Ae^{ikx} + Be^{-ikx}$$

b) Energy \rightarrow Energy of particle is given by -

$$\text{we have } k^2 = \frac{8\pi^2mE}{h^2}$$

(Using $h = \frac{h}{2\pi}$)

$$E = \frac{h^2 k^2}{8\pi^2 m} = \frac{h^2 k^2}{2m}$$

c) Momentum! $\psi = A e^{-i(\omega t - kx)}$

$$\left(\begin{array}{l} \omega = 2\pi\nu \\ \quad = \frac{2\pi E}{h} \end{array} \quad \begin{array}{l} k = \frac{2\pi}{\lambda} \\ \quad = \frac{2\pi p}{h} \end{array} \right)$$

$$\psi = A e^{-i \left(\frac{2\pi}{h} (Et - px) \right)}$$

using
 $\left(\hbar = \frac{h}{2\pi} \right)$

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

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

$$\frac{d\psi}{dx} = A \frac{i p}{\hbar} e^{\frac{i}{\hbar} (px - Et)}$$

$$= \frac{i p}{\hbar} \psi$$

$$\Rightarrow \boxed{p\psi = \hbar \frac{d\psi}{dx}}$$

d) Position of particle's Probability of finding the particle is given by -

$$P dx = \psi^*(x,t) \psi(x,t)$$

The Probability density P for the position of particle with definite value of momentum is constant over x -axis.

Particle in a Rigid one Dimensional box (Infinite Square well potential):

Let us consider a particle restricted to move along x-axis between $(x=0$ and $x=L)$.

Suppose potential Energy V of the particle is zero inside the box, but rises to infinity outside.

that is $V=0$ for $(0 \leq x \leq L)$ - inside box
 $V=\infty$ for $(x < 0 + x > L)$ - outside the box

In such case the particle is said to be moving in an infinitely deep square well potential

Schrodinger Equation for the particle within box is -

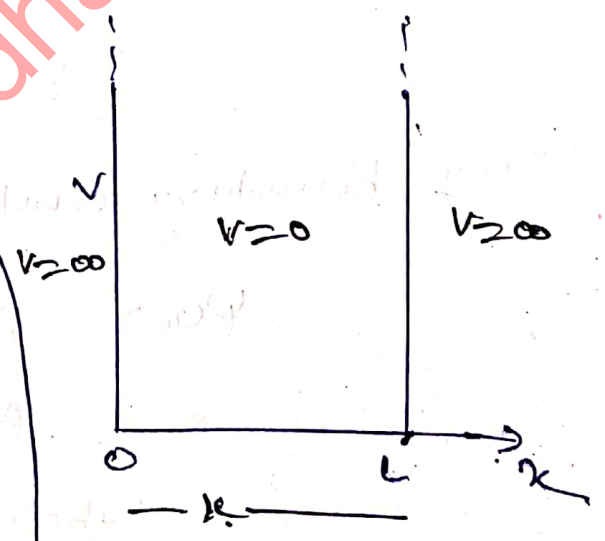
$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2mE}{h^2} \psi = 0 \quad \text{--- (1)}$$

$V=0$ (inside the box)

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2m(E-V)}{h^2} \psi = 0$$

Substitute $V=0$

$$\Rightarrow \frac{d^2\psi}{dx^2} + \frac{8\pi^2mE}{h^2} \psi = 0$$



Suppose $\frac{8\pi^2mE}{h^2} = k^2$ --- (2)

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \quad \text{--- (3)}$$

General Solution of differential Equation of the form -

$$\psi(x) = A \sin kx + B \cos kx \quad (4)$$

where the constant A & B are to be determined by boundary conditions. Therefore, the wavefunction ψ must be zero outside the box.

ψ must also be zero at the walls ($x=0, x=L$ at walls)

Using the boundary condition $\psi=0$ at $x=0$ in (4)

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

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

$$0 = 0 + B(1)$$

$$\boxed{B=0} \Rightarrow \boxed{\psi(x) = A \sin kx} \quad (5)$$

Using boundary condition $\psi(x)=0$ at $x=L$ in (4)

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

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

Substituting $B=0$

$$0 = A \sin kL + 0$$

$$A \sin kL = 0$$

$$\sin kL = 0$$

$$\sin kL = 0 \quad (n = 1, 2, 3, \dots)$$

$$\sin kL = \sin n\pi$$

$$kL = n\pi$$

$$\boxed{k = \frac{n\pi}{L}}$$

Substituting $k = \frac{n\pi}{L}$ in (5)

$$\psi(x) = A \sin\left(\frac{n\pi x}{L}\right) \quad (6)$$

Now for Energy we have

$$k^2 = \frac{8\pi^2 m E}{h^2} \quad (\text{by (2)})$$

$$E = \frac{k^2 h^2}{8\pi^2 m}$$

Substituting $k = \frac{n\pi}{L}$

$$E = \frac{n^2 h^2}{8mL^2} \quad (n = 1, 2, 3, \dots)$$

Thus we see that in a potential well the particle can not have an arbitrary energy but can have only certain energy values corresponding to $n = 1, 2, 3, \dots$ these are Eigen values of the particle in the well and correspond to energy level of the system.

$$E_n = \frac{n^2 h^2}{8mL^2}$$

Ground state Energy ($n=1$)

$$E_1 = \frac{h^2}{8mL^2}$$

First Excited State Energy ($n=2$)

$$E_2 = \frac{4h^2}{8mL^2}$$

We have calculated the values of Energy (24)

Now we will find the solution of wave function in Equation (6) and value of A

From (6) we have

$$\psi(x) = A \sin\left(\frac{n\pi x}{L}\right)$$

where A \rightarrow Normalization factor or Normalization constant

To find the value of A we will use Normalization condition.

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

Normalization condition

$$\Rightarrow \int_0^L \left(A \sin\left(\frac{n\pi x}{L}\right) \right) \left(A \sin\left(\frac{n\pi x}{L}\right) \right) dx = 1$$

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

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

$$\left(\begin{array}{l} \text{using } \cos 2\theta = 1 - 2\sin^2\theta \\ 2\sin^2\theta = 1 - \cos 2\theta \\ \sin^2\theta = \frac{1 - \cos 2\theta}{2} \end{array} \right)$$

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

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

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

$$A^2 = \frac{2}{L}$$

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

in (6) $\psi(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$ *

Solution of wave function

Plotting of wave function :-

First three Eigen function ψ_1, ψ_2, ψ_3 together with the Probability densities $|\psi_1|^2, |\psi_2|^2, |\psi_3|^2$ are shown in Figure

we have $\psi_n = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$

1) $n=1$ for ground state

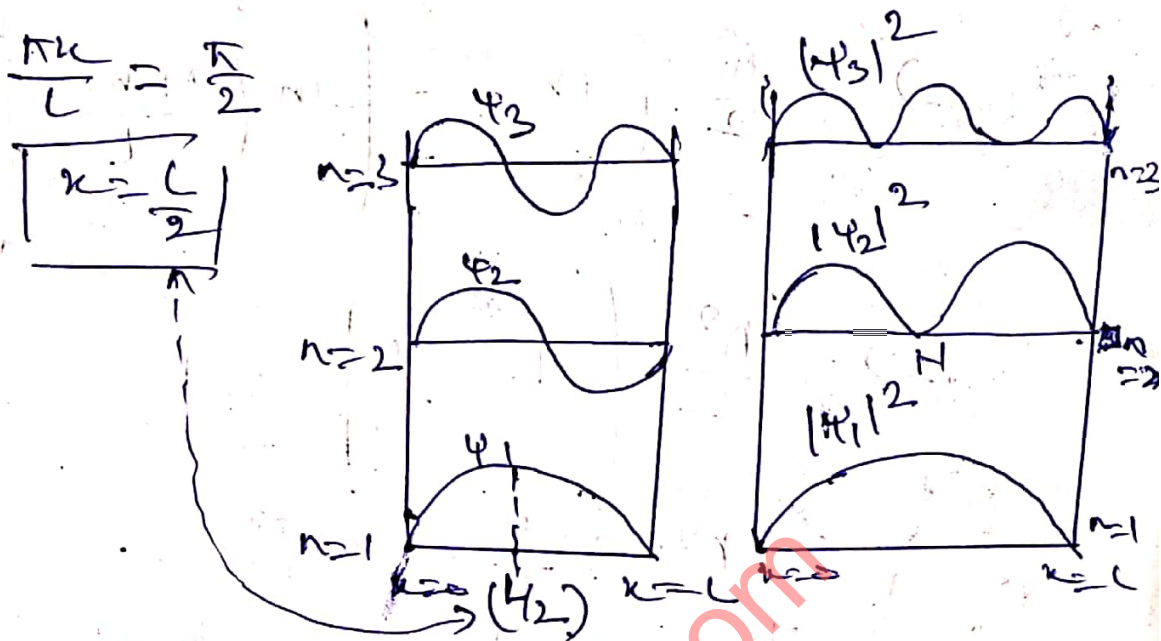
$$\psi_1 = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi x}{L}\right)$$

Maximum value of $\psi = \sin 90^\circ = \sin\left(\frac{\pi}{2}\right)$

$$\Rightarrow \sin\left(\frac{n\pi x}{L}\right) = \sin\left(\frac{\pi}{2}\right) = 1$$

$$\frac{n\pi x}{L} = \frac{\pi}{2}$$

$$\boxed{x = \frac{L}{2}}$$



ii)

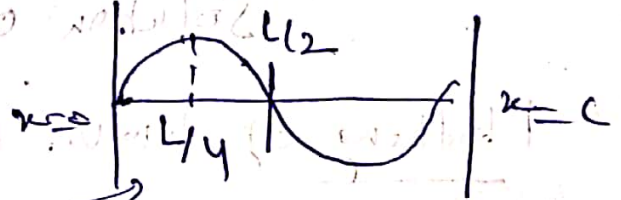
$n=2$

$$\psi_2 = \sqrt{\frac{2}{L}} \sin\left(\frac{2\pi x}{L}\right)$$

$$\sin\left(\frac{2\pi x}{L}\right) = \sin\frac{\pi}{2}$$

$$\frac{2\pi x}{L} = \frac{\pi}{2}$$

$$\boxed{x = \frac{L}{4}}$$



iii)

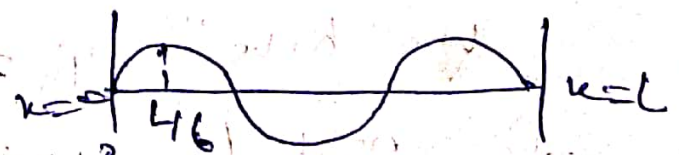
$n=3$

$$\psi_3 = \sqrt{\frac{2}{L}} \sin\left(\frac{3\pi x}{L}\right)$$

$$\sin\left(\frac{3\pi x}{L}\right) = \sin\frac{\pi}{2}$$

$$\frac{3\pi x}{L} = \frac{\pi}{2}$$

$$\boxed{x = \frac{L}{6}}$$



- 2.9 Consider a particle confined in one-dimensional box of width l . Find the probability that the particle is found between $x = 0$ and $x = l/n$ when it is in n th state. [IGGSIPU, April 2015 (2 marks)]

Hint : $\psi_n(x) = \sqrt{\frac{2}{l}} \sin \frac{n\pi x}{l}$

$$p = \int_{x_1}^{x_2} |\psi_n(x)|^2 dx = \frac{2}{l} \int_{x_1}^{x_2} \sin^2 \frac{n\pi x}{l} dx$$

$$= \left[\frac{x}{l} - \frac{1}{2n\pi} \sin \frac{2n\pi x}{l} \right]_{x_1=0}^{x_2=l/n} = \left[\frac{1}{n} - \frac{1}{2n\pi} \sin \frac{2n\pi l}{nl} \right] = \frac{1}{n}$$

- 2.10 An electron is constrained to move in a one dimensional box of length 0.1 nm. Find the first three energy eigen values and the corresponding de Broglie wavelengths. [IGGSIPU, May 2015 (4 marks)]

Hint : $E_n = \frac{n^2 h^2}{8ml^2} \Rightarrow E_n = \frac{n^2 \times (6.623 \times 10^{-34})^2}{8 \times (9.1 \times 10^{-31}) \times (0.1 \times 10^{-9})^2}$

$$E_n = \frac{n^2 \times (6.623 \times 10^{-34})^2}{8 \times (9.1 \times 10^{-31}) \times (0.1 \times 10^{-9})^2 \times (1.6 \times 10^{-19})} \text{ eV} = 37.5 n^2 \text{ eV}$$

Then $E_1 = 37.5 \text{ eV}$, $E_2 = 150 \text{ eV}$, $E_3 = 337.5 \text{ eV}$

For de Broglie wavelength $\lambda_n = \frac{h}{\sqrt{2mE_n}}$

- 2.11 Find the probability that a particle trapped in a box ' L ' wide can be found between $0.45L$ and $0.55L$ for the first excited state. [IGGSIPU, May 2015 (4 marks)]

Hint : $\psi_n = \sqrt{\frac{2}{l}} \sin \frac{n\pi x}{l}$; $P = \int_{x_1}^{x_2} |\psi_n(x)|^2 dx = \frac{2}{l} \int_{x_1}^{x_2} \sin^2 \frac{2n\pi x}{l} dx$

$$= \left[\frac{x}{l} - \frac{1}{2n\pi} \sin \frac{2n\pi x}{l} \right]_{x_1}^{x_2}$$

Now $x_1 = 0.45L$ and $x_2 = 0.55L$ and $n = 2$ for first excited state, on solving it we get $P = 9.8\%$.

- 2.12 The wave function for a particle in a 1-D box is given by $\psi(x) = \sqrt{\frac{2}{a}} \sin \frac{m\pi x}{a}$. Show that the wave function for two different states are orthonormal. [IGGSIPU, May 2016 (3 marks)]

Hint : For the eigenfunctions in the m th and n th states, $m \neq n$, to be orthogonal, we must have

$$\int_{-\infty}^{\infty} \psi_m^* \psi_n dx = 0$$

For the given wavefunction, $\psi_m(x) = \sqrt{\frac{2}{a}} \sin \frac{m\pi x}{a}$, then $\psi_n(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}$

$$\int_{-\infty}^{\infty} \psi_m^* \psi_n dx = \frac{2}{a} \int_0^a \sin \frac{m\pi x}{a} \sin \frac{n\pi x}{a} dx$$

Therefore $= \frac{2}{a} \left[\int_0^a \cos \frac{(m-n)\pi x}{a} dx - \int_0^a \cos \frac{(m+n)\pi x}{a} dx \right]$

2.8 An electron is in a box of 0.01 nm. Find its permitted energy.

[IGGSIPU, Feb. 2013, (2 marks) ; May 2008 (2.5 marks)]

Hint :

$$E_n = \frac{n^2 h^2}{8ml^2} = \frac{n^2 \times (6.626 \times 10^{-34})^2}{8 \times 9.1 \times 10^{-31} (0.01 \times 10^{-9})^2}$$

$$= 6 \times 10^{-16} n^2 \text{ J} = \frac{6 \times 10^{-16}}{1.6 \times 10^{-19}} \text{ eV} = \frac{60000}{16} n^2 \text{ eV}$$

For $n = 1, 2, 3, \dots$ the energy eigen value E_1, E_2, E_3, \dots

$$E_1 = 3750 \text{ eV}, E_2 = 15000 \text{ eV}, E_3 = 33750 \text{ eV}, \dots$$

2.13 The eigenfunctions for a particle in a 1-D box are given by $\psi(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}$. Find the expectation values of (i) position and (ii) momentum in the n th quantum state.

[IGGSIPU, May 2016 (4 marks)]

Hint : (i) $\langle x \rangle = \int_{-\infty}^{\infty} \psi_n^* x \psi_n dx = \frac{2}{a} \int_0^a x \sin^2 \frac{n\pi x}{a} dx$

Integrating by parts, we get : $\langle x \rangle = \frac{a}{2}$.

This result is as expected ; the probability density $\psi^* \psi$ is symmetric about $\langle x \rangle = \frac{a}{2}$, indicating that the particle spends as much time to the left of the center as to the right.

(ii)
$$\langle p_x \rangle = \int_{-\infty}^{\infty} \psi_n^* \left(i\hbar \frac{d}{dx} \right) \psi_n dx = \frac{2i\hbar}{a} \int_0^a \sin \frac{n\pi x}{a} \frac{d}{dx} \left(\sin \frac{n\pi x}{a} \right) dx$$

$$= -\frac{2i\hbar}{a} \frac{n\pi}{a} \int_0^a \sin \frac{n\pi x}{a} \cos \frac{n\pi x}{a} dx = -\frac{i\hbar n\pi}{a^2} \int_0^a \sin \frac{2n\pi x}{a} dx$$

Solving the integral, we get $\langle p_x \rangle = 0$.

Again the result is expected. The particle moves back and forth, spending half its time moving towards the left and half its time moving towards the right. Thus, the average momentum must be zero.

- 2.4 For an electron in a one-dimensional box of width 2 \AA , calculate the separation between the lowest two levels in eV. [GGSIPU, June 2013 (4.5 marks)]

Hint : $E_n = \frac{n^2 h^2}{8ml^2}$

$$\Rightarrow E_1 = \frac{1 \times (6.63 \times 10^{-34})^2}{8 \times 9.1 \times 10^{-31} \times (2 \times 10^{-10})^2} = 2.273 \times 10^{-19} \text{ J} = 1.42 \text{ eV}$$

- 2.17 An electron is confined to move between two rigid walls separate by $2 \times 10^{-9} \text{ m}$. Find the de Broglie wavelengths representing the first three allowed energy states of the electron. [GGSIPU, May 2017 (4 marks)]

Hint : $E_n = \frac{n^2 h^2}{8ml^2} \Rightarrow \frac{hc}{\lambda_n} = \frac{n^2 h^2}{8ml^2} \Rightarrow \lambda_n = \frac{c}{n^2 h} \times 8ml^2$

$$\lambda_1 = \frac{3 \times 10^8}{(6.62 \times 10^{-34})} \times 8 \times (9.1 \times 10^{-31}) \times (2 \times 10^{-9})^2 = 1.32 \times 10^{-5} \text{ m}$$

$$\lambda_2 = \frac{3 \times 10^8}{4 \times (6.62 \times 10^{-34})} \times 8 \times (9.1 \times 10^{-31}) \times (2 \times 10^{-9})^2 = 3.3 \times 10^{-6} \text{ m}$$

$$\lambda_3 = \frac{3 \times 10^8}{9 \times (6.62 \times 10^{-34})} \times 8 \times (9.1 \times 10^{-31}) \times (2 \times 10^{-9})^2 = 1.47 \times 10^{-6} \text{ m}$$

Problem 2.8 The wave function of a certain particle is $\psi = A \cos^2 x$ for $-\frac{\pi}{2} < x < \frac{\pi}{2}$

- (a) Find the value of A (b) Find the probability that the particle be found between $x=0$ and $x = \frac{\pi}{4}$.

[GGSIPU, Feb. 2012, (5 marks) reappear]

Solution. As $\psi = A \cos^2 x$ $-\frac{\pi}{2} < x < \frac{\pi}{2}$

(a) $\int_{-\pi/2}^{\pi/2} |\psi|^2 dx = 1$

$$\Rightarrow 2A^2 \int_0^{\pi/2} \cos^4 x dx = 1 \quad \text{or} \quad 2A^2 \frac{3\pi}{16} = 1$$

$$\frac{3\pi}{8} A^2 = 1 \quad \therefore \quad A = \sqrt{\frac{8}{3\pi}}$$

(b) $P = \int_0^{\pi/4} |\psi|^2 dx = A^2 \int_0^{\pi/4} \cos^4 x dx$ as $A = \sqrt{\frac{8}{3\pi}}$

$$P = \frac{8}{3\pi} \int_0^{\pi/4} \cos^4 x dx = 0.462$$

Schrodinger wave Equation for finite well:-

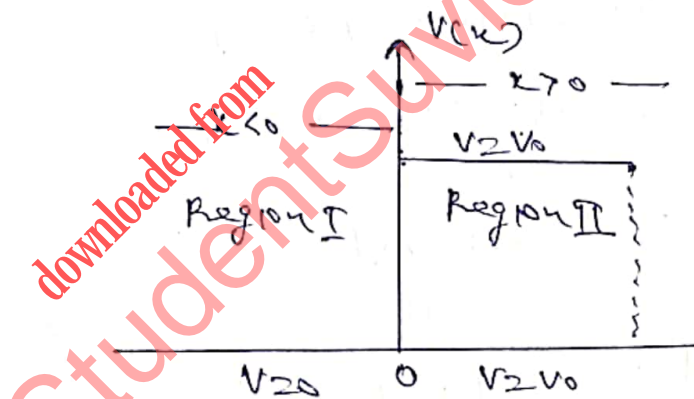
(Skip barrier / Potential barrier & tunnel Effect).

1) Step barrier / Potential barrier.

When a particle approaches a region in which entrance of particle is opposed by some force then that region is said to form a barrier for a particle.

Note:- Potential barrier is also a system used to identify incident, reflected & transmitted matter waves.

Let us consider a particle moving along x -axis from left to right and meeting a barrier of height V_0 . Let E be the total energy of particle and V be the value of constant potential.



We have two different regions supported by discontinuous change of potential -

Region I : $x < 0 \Rightarrow V = 0$

$x > 0 \Rightarrow V = V_0$

Behaviour of particle can be described in quantum mechanics as if energy of particle -

1) If $(E < V_0)$

Then there is a probability that the particle will be reflected back from the barrier



2) If $(E > V_0)$

Then there is a probability that it will penetrate through the barrier.



Such behaviour of particle is impossible from the classical viewpoint. It follows Schrodinger Wave Equation

a) Region I

Let us consider the region $x < 0$ time independent Schrodinger wave Equation is given by -

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2m}{h^2} (E - V) \psi = 0$$

($V=0$ in the region $x < 0$)

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2m}{h^2} E \psi = 0$$

$$\text{Let } k_1^2 = \frac{8\pi^2mE}{h^2}$$

$$\Rightarrow \frac{d^2\psi}{dx^2} + k_1^2 \psi = 0 \quad \text{--- (1)}$$

b) Region II

Schrodinger wave Equation is given by -

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2m}{h^2} (E - V_0) \psi = 0$$

$$\frac{d^2\psi}{dx^2} + k_2^2 \psi = 0$$


$$\text{where } k_2^2 = \frac{8\pi^2m}{h^2} (E - V_0) \quad \text{--- (2)}$$

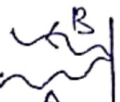
Solution of Differential Equation (1) & (2) are -


$$\psi_1 = A e^{ik_1 x} + B e^{-ik_1 x}$$

$$\psi_2 = C e^{ik_2 x} + D e^{-ik_2 x}$$

Where -

A - Amplitude of incident wave in Region I 

B - Amplitude of reflected wave in Region I 

C - Amplitude of wave penetrate the barrier in Region II 

D - No particle can flow to left hence $D=0$

Now In order to be a proper wave function ψ must be finite & continuous everywhere on x -axis.

It means at boundary ($x=0$) wave function inside & outside must have same values.

Hence ψ_1, ψ_2 & its derivatives must be continuous at the boundary ($x=0$)

Where $\psi_1 = \psi_2$ (at $x=0$)

$$\Rightarrow A e^{ik_1 x} + B e^{-ik_1 x} = C e^{ik_2 x}$$

Substituting $x=0$

$$\Rightarrow A + B = C \quad \text{--- (3)}$$

Also its derivatives must be continuous at $x=0$

$$\Rightarrow \frac{d\psi_1}{dx} = \frac{d\psi_2}{dx}$$

$$\frac{d(A e^{ik_1 x} + B e^{-ik_1 x})}{dx} = \frac{d(C e^{ik_2 x})}{dx}$$

$$\Rightarrow A i k_1 e^{ik_1 x} - B i k_1 e^{-ik_1 x} = C i e^{ik_2 x}$$

Now at $x=0$ we have

$$A i k_1 - B i k_1 = C i k_2$$

$$\Rightarrow (A-B) = \frac{k_2}{k_1} C \quad \text{--- (4)}$$

on solving (3) & (4) we get

$$2B = \left(1 - \frac{k_2}{k_1}\right) C$$

$$= \frac{k_1 - k_2}{k_1} \times \frac{2k_1}{k_1 + k_2} \times A$$

$$\Rightarrow \boxed{B = \left(\frac{k_1 + k_2}{k_1 - k_2}\right) A}$$

Note
For solving
Add (3) + (4)
& Subtract (3) - (4)

Also $2A = \left(1 + \frac{k_2}{k_1}\right) C$

$$\Rightarrow \boxed{A = \frac{k_1 + k_2}{2k_1} C}$$

Now substituting value of A in (3)

we get $\boxed{C = \frac{2k_1}{k_1 + k_2} A}$

Now case I For $E < V_0$

Probability density is given by

$$(J_x) = \frac{\hbar}{2im} \left(\psi_1^* \frac{d\psi_1}{dx} - \psi_1 \frac{d\psi_1^*}{dx} \right)$$

we have

$$\psi_1 = A e^{ik_1 x} + B e^{-ik_1 x}$$

$$\psi_1^* = A e^{-ik_1 x} + B e^{ik_1 x}$$

$$\Rightarrow (J_x) = \frac{\hbar}{2im} \left[(A e^{-ik_1 x} + B e^{ik_1 x}) \times \frac{d}{dx} (A e^{ik_1 x} + B e^{-ik_1 x}) \right. \\ \left. - [(A e^{ik_1 x} + B e^{-ik_1 x}) \times \frac{d}{dx} (A e^{-ik_1 x} + B e^{ik_1 x})] \right]$$

$$= \frac{\hbar}{2im} \left((Ae^{-ik_1x} + Be^{ik_1x}) \times (ik_1) (Ae^{ik_1x} - Be^{-ik_1x}) \right)$$

$$\rightarrow \left((Ae^{ik_1x} + Be^{-ik_1x}) \times (-ik_1) (Ae^{-ik_1x} - Be^{ik_1x}) \right)$$

$$= \frac{k_1 \hbar}{m} (A^2 - B^2)$$

Here A^2 represent magnitude of incident current
 B^2 - magnitude of Reflected current

Reflection coefficient = $\frac{\text{Magnitude of Reflected current}}{\text{Magnitude of incident current}}$

$$R = \frac{B^2}{A^2}$$

$$= \frac{\left(\frac{k_1 - k_2}{k_1 + k_2} \right)^2 A^2}{A^2} = \left(\frac{k_1 - k_2}{k_1 + k_2} \right)^2$$

Case - II Region II

$$\psi_2 = ce^{ik_2x} \quad \psi_2^* = ce^{-ik_2x}$$

$$J_x = \frac{\hbar}{2im} \left(\psi_2^* \frac{d\psi_2}{dx} - \psi_2 \frac{d\psi_2^*}{dx} \right)$$

$$= \frac{\hbar}{2im} \left(ce^{-k_2x} \frac{d}{dx} (ce^{+ik_2x}) - (ce^{+ik_2x}) \frac{d}{dx} (ce^{-ik_2x}) \right)$$

$$= \frac{\hbar}{2im} (cxc(ik_2) - cxc(ik_2))$$

$$\boxed{J = 0}$$

How

Transmittance coefficient =

Magnitude of Transmittance current

Magnitude of incident current

$$= \frac{C^2}{A^2}$$

$$= \frac{\left(\frac{2k_1}{k_1+k_2}\right)^2 A^2}{A^2} \times \frac{k_2}{k_1}$$

$$T = \frac{4k_1 k_2}{(k_1+k_2)^2}$$

Also according to definition $R+T=1$ can be verified.

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Tunneling Effect:

When a particle is able to cross the potential barrier even when ~~the~~ its energy is less than the barrier height ($E < V_0$), then this phenomenon is called Tunnel Effect."

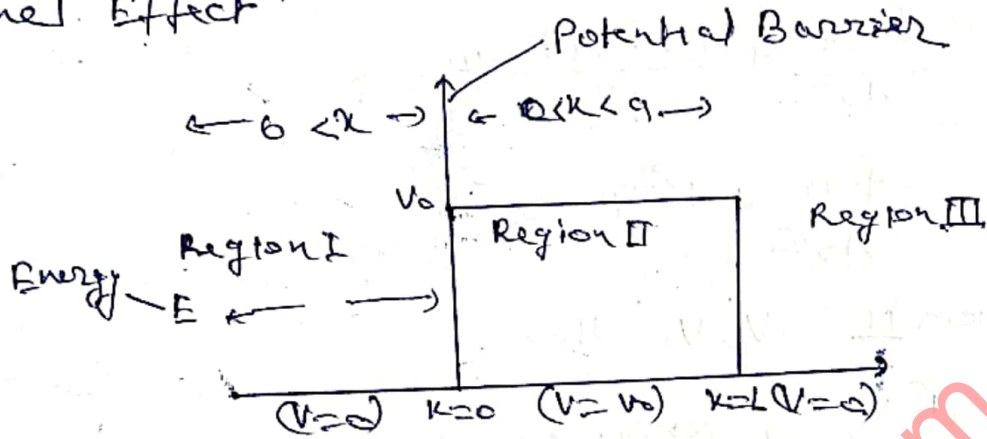


Figure represent a potential barrier of height V_0 & thickness L . Let us consider a particle moving along x -axis from left to right and moving a rectangular potential barrier of height V_0 and length L .

We have three different region separated by discontinuous change of potential energy.

- Potential energy is zero in the region I & III for $x < 0$ & $x > L$.
- potential energy is V_0 in the Region II.

If $E < V_0$ according to quantum mechanics, still there is a finite chance for the electron to leak the other side of barrier. Hence the electron is tunneled through the potential barrier. This phenomenon called Tunneling.

The Schrodinger wave Equation for a particle along X-AXIS is given by -

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2m}{h^2} (E-V)\psi = 0$$

In Region I $V=0$ then

$$\frac{d^2\psi_1}{dx^2} + \frac{8\pi^2mE}{h^2} \psi_1 = 0$$

$$\frac{d^2\psi_1}{dx^2} + \frac{k^2}{h^2} \psi_1 = 0 \quad \text{--- (1)}$$

$$\left(\begin{aligned} k^2 &= \frac{8\pi^2mE}{h^2} \\ k &= \sqrt{\frac{2mE}{h}} \end{aligned} \right.$$

In Region II $V=V_0$ then

$$\frac{d^2\psi_2}{dx^2} + \frac{8\pi^2m}{h^2} (E-V_0)\psi_2 = 0$$

$$\frac{d^2\psi_2}{dx^2} - \frac{8\pi^2m}{h^2} (V_0-E)\psi_2 = 0$$

$$\frac{d^2\psi_2}{dx^2} - \beta^2\psi_2 = 0 \quad \text{--- (2)}$$

$$\beta = \sqrt{\frac{8\pi^2m}{h^2} (V_0-E)} = \sqrt{\frac{2m(V_0-E)}{h}}$$

(Note: - In Region II wave is decaying exponentially so Negative value of E in (V_0-E) is used Hence solution of this Eqn (ψ_2) doesn't give i (total) term)

Region -III $V=0$ then

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

Solution of Equation (1), (2) & (3) will be

$$\psi_1 = Ae^{ikx} + Be^{-ikx}$$

$$\psi_2 = Ce^{\beta x} + De^{-\beta x}$$

$$\begin{aligned}\psi_3 &= Ge^{ikx} + He^{-ikx} \\ &= Ge^{ikx}\end{aligned}$$

H=0 because no wave travel back from infinity

Applying boundary conditions to particle

1) At $x=0$ $\psi_1 = \psi_2$

$$Ae^{ikx} + Be^{-ikx} = Ce^{\beta x} + De^{-\beta x}$$

At $x=0$

$$A+B = C+D \quad \text{--- (4)}$$

We also have -

$$\frac{d\psi_1}{dx} = \frac{d\psi_2}{dx}$$

$$ikAe^{ikx} - ikBe^{-ikx} = \beta Ce^{\beta x} - \beta De^{-\beta x}$$

at $x=0$ $ik(A-B) = \beta(C-D)$

$$A-B = \frac{\beta}{ik}(C-D) \quad \text{--- (5)}$$

From equation (4) & (5) we get

$$A = \frac{1}{2} \left[\left(1 + \frac{\beta}{ik}\right)C + \left(1 - \frac{\beta}{ik}\right)D \right] \quad \text{--- (6)}$$

$$B = \frac{1}{2} \left[\left(1 - \frac{\beta}{ik}\right)C + \left(1 + \frac{\beta}{ik}\right)D \right] \quad \text{--- (7)}$$

At $x=0$ we have

$$\psi_2 = \psi_3$$
$$C e^{\beta x} + D e^{-\beta x} = G e^{ikx}$$

At $x=a$

$$\Rightarrow C e^{\beta a} + D e^{-\beta a} = G e^{ika} \quad \text{--- (8)}$$

Also we have -

$$\frac{d\psi_2}{dx} = \frac{d\psi_3}{dx}$$

$$C \beta e^{\beta x} - D \beta e^{-\beta x} = G i k e^{ikx}$$

At $x=a$

$$C \beta e^{\beta a} - D \beta e^{-\beta a} = i k G e^{ika} \quad \text{--- (9)}$$

From eqn (8) and (9)

$$C = \frac{1}{2} \left(1 + \frac{ik}{\beta} \right) e^{-\beta a} G e^{ika}$$

$$D = \frac{1}{2} \left(1 - \frac{ik}{\beta} \right) e^{\beta a} G e^{ika}$$

Put the value of C + D in eqn (8)

From (8) we have -

$$A = \frac{1}{2} \left(\left(1 + \frac{\beta}{ik} \right) C + \left(1 - \frac{\beta}{ik} \right) D \right)$$

$$A = \frac{1}{4} \left(\left(1 + \frac{\beta}{ik} \right) \left(1 + \frac{ik}{\beta} \right) e^{-\beta a} G e^{ika} \right)$$

$$+ \frac{1}{4} \left(\left(1 - \frac{\beta}{ik} \right) \left(1 - \frac{ik}{\beta} \right) e^{\beta a} G e^{ika} \right)$$

$$A = \frac{G}{4} e^{ika} \left(\left(1 + \frac{ik}{\beta} + \frac{\beta}{ik} + \frac{\beta ik}{\beta ik} \right) e^{-\beta a} + \left(1 - \frac{ik}{\beta} - \frac{\beta}{ik} - \frac{ik \beta}{ik \beta} \right) e^{\beta a} \right)$$
$$= \frac{G}{4} e^{ika} \left(2 + \frac{ik}{\beta} + \frac{\beta}{ik} \right) e^{-\beta a} + \left(2 - \frac{ik}{\beta} - \frac{\beta}{ik} \right) e^{\beta a}$$

$$\begin{aligned}
 A &= \frac{4}{4} e^{ika} \left(2C e^{-\beta a} + e^{\beta a} \right) + \left(\frac{\beta}{ik} + \frac{ik}{\beta} \right) e^{-\beta a} - \left(\frac{\beta}{ik} + \frac{ik}{\beta} \right) e^{\beta a} \\
 &= \frac{4}{4} e^{ika} \left(2 \frac{(e^{-\beta a} + e^{\beta a})}{2} + \left(\frac{\beta}{ik} + \frac{ik}{\beta} \right) \cdot (e^{-\beta a} - e^{\beta a}) \right) \\
 &= \frac{4}{4} e^{ika} \left(2 \frac{(e^{-\beta a} + e^{\beta a})}{2} + 2 \left(\frac{\beta}{ik} + \frac{ik}{\beta} \right) \left(\frac{e^{\beta a} - e^{-\beta a}}{2} \right) \right) \\
 &= \left[\cosh \beta a + \frac{i}{2} \left(\frac{\beta}{k} - \frac{k}{\beta} \right) \sinh \beta a \right] 4e^{ika}
 \end{aligned}$$

$$\Rightarrow \frac{A}{4} = \left[\cosh \beta a + \frac{i}{2} \left(\frac{\beta}{k} - \frac{k}{\beta} \right) \sinh \beta a \right] e^{ika} \quad \text{--- (10)}$$

we have Transmittance coefficient (T)

$$(T) = \frac{\text{Magnitude of Transmitted wave}}{\text{Magnitude of Incident wave}} = \left(\frac{4^2}{A^2} \right)$$

From (10)

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

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

$$= 1 + \left[\frac{1}{4} \left(4 + \left(\frac{\beta}{k} - \frac{k}{\beta} \right)^2 \right) \sinh^2 \beta a \right] \quad \text{--- (11)}$$

we have $k = \frac{\sqrt{2mE}}{\hbar}$ & $\beta = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$

$$\Rightarrow \frac{\beta}{k} - \frac{k}{\beta} = \sqrt{\frac{V_0 - E}{E}} - \sqrt{\frac{E}{V_0 - E}} = \frac{V_0 - E - E}{\sqrt{E(V_0 - E)}} = \frac{V_0 - 2E}{\sqrt{E(V_0 - E)}}$$

$$\begin{aligned}
 \text{Now } \left(\frac{\beta}{k} - \frac{k}{\beta} \right)^2 + 4 &= \frac{(V_0 - 2E)^2}{E(V_0 - E)} + 4 = \frac{V_0^2 + 4E^2 - 4EV_0 + 4EV_0 - 4E^2}{E(V_0 - E)} \\
 &= \frac{V_0^2}{E(V_0 - E)}
 \end{aligned}$$

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

$$T = \frac{1}{1 + \frac{V_0^2}{4E(V_0 - E)}} \sinh^2 \beta a$$

Also $\sinh^2 \beta a = \left(\frac{e^{\beta a} - e^{-\beta a}}{2} \right)^2 = e^{\frac{2\beta a}{4}}$

$$2) \quad T = \frac{1}{1 + \frac{V_0^2}{4E(V_0 - E)}} \times e^{\frac{2\beta a}{4}}$$

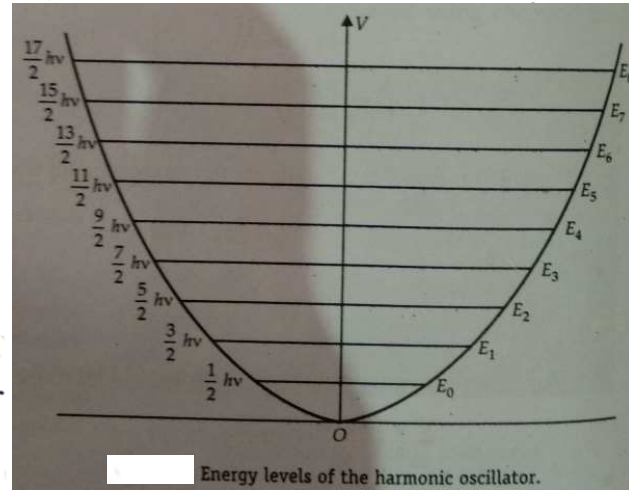
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Transmission coefficient

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Simple Harmonic oscillator & Zero Point Energy!

A simple harmonic oscillator is a particle performing one dimensional motion under restoring force F which is proportional to particle displacement x from equilibrium position.

The plot of V against x is a parabola and we may describe that the particle being a periodic potential well. If E be the total energy of particle. It oscillate back & forth from center.



Now force is proportional to particle displacement x from equilibrium position

$$F \propto -x$$

$$F = -kx$$

Potential Energy of harmonic oscillator is,

$$V(x) = -\int_0^x F(x) dx$$

$$= \int_0^x kx dx$$

$$V(x) = \frac{1}{2} kx^2$$

$$k = m\omega^2$$

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

Schrodinger wave Equation for particle motion is given by

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2m(E-V)}{h^2} \psi = 0$$

Substituting value of ①

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2m}{h^2} (E - 2\pi^2mv^2x^2) \psi = 0$$

$$\frac{d^2\psi}{dx^2} + \left(\frac{8\pi^2mE}{h^2} - \frac{16\pi^4m^2v^2x^2}{h^2} \right) \psi = 0$$

Let $\frac{8\pi^2mE}{h^2} = \alpha$ and $\frac{4\pi^2mv}{h} = \beta$

$$\beta^2 = \frac{16\pi^4m^2v^2}{h^2}$$

$$\Rightarrow \frac{d^2\psi}{dx^2} + (\alpha - \beta^2x^2)\psi = 0 \quad \text{--- (2)}$$

Let $y = \sqrt{\beta}x$

on sq. $y^2 = \beta x^2$

$$x^2 = \frac{y^2}{\beta}$$

$$\text{in (2)} \quad \frac{d^2\psi}{dx^2} + \left(\alpha - \beta^2 \times \frac{y^2}{\beta} \right) \psi = 0$$

$$\frac{d^2\psi}{dx^2} + (\alpha - \beta y^2) \psi = 0 \quad \text{--- (3)}$$

Now we have $y = \sqrt{\beta}x$

$$\frac{d\psi}{dx} = \frac{d\psi}{dy} \times \frac{dy}{dx} = \frac{d\psi}{dy} \times \sqrt{\beta}$$

$$\Rightarrow \frac{d^2\psi}{dx^2} = \beta \frac{d^2\psi}{dy^2}$$

Substituting in (3)

$$\Rightarrow \beta \frac{d^2\psi}{dy^2} + (\alpha - \beta y^2) \psi = 0$$

$$\frac{d^2\psi}{dy^2} + \left(\frac{\alpha}{\beta} - y^2 \right) \psi = 0 \quad \text{--- (4)}$$

The Solution of Equation (4)

will satisfy the condition $\frac{\alpha}{\beta} = (2n+1)$

$$\alpha = \frac{8\pi^2 m E}{h^2} \quad \beta = \frac{4\pi^2 m \nu}{h}$$

$$\frac{\frac{8\pi^2 m E}{h^2}}{\frac{4\pi^2 m \nu}{h}} = (2n+1)$$

$$\Rightarrow E = \frac{h\nu}{2} (2n+1)$$

$$E_n = h\nu \left(n + \frac{1}{2} \right)$$

The lowest value of Energy which oscillation can take for $n=0$ is

$$E_0 = \frac{1}{2} h\nu$$

- * This level is ground state. The Energy E_0 is called zero point Energy.
- * A very significant result that E_0 is never zero but has a lowest or minimum value.
- * A harmonic oscillator approaches this value as the temperature approaches 0K. This energy called zero point energy.
- * The existence of zero point Energy is a consequence of Uncertainty Principle. At ~~T=0K~~ T=0K position & momentum can be determined precisely.

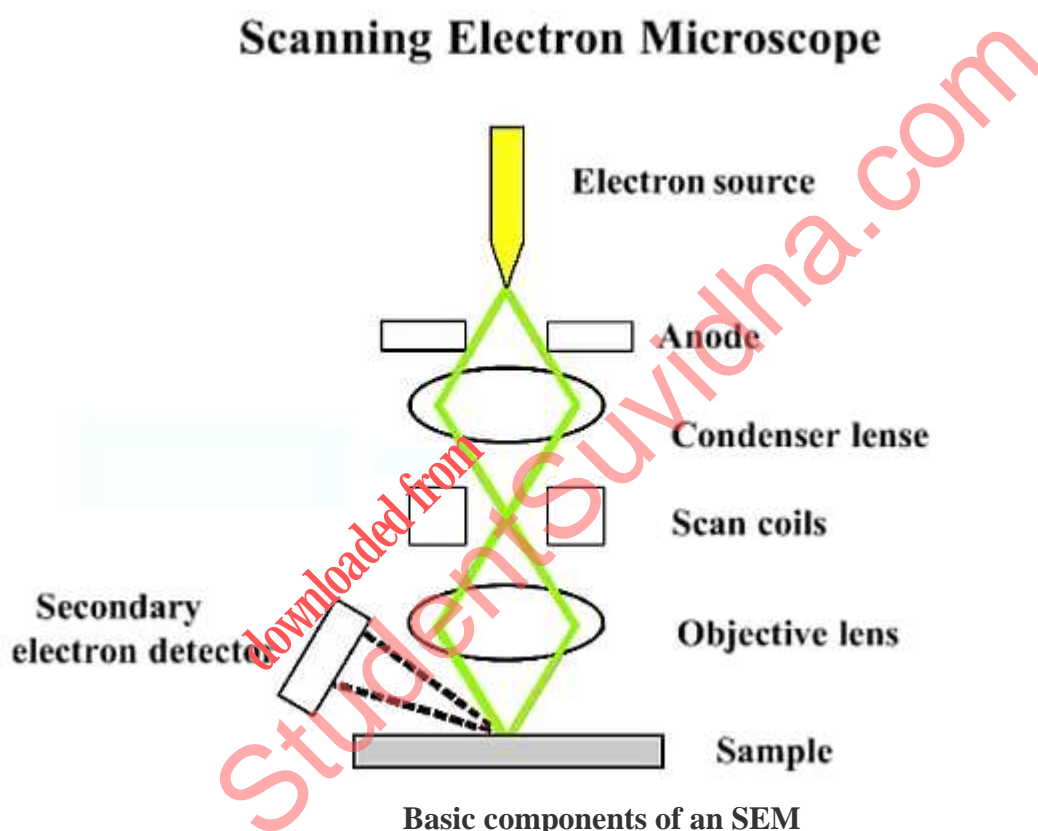
Scanning electron microscopes

Scanning electron microscopes (SEMs) have become powerful and versatile tools for material characterization, especially in recent years, as the size of materials used in various applications.

Electron microscopes use electrons for imaging in a similar way that light microscopes use visible light. SEMs use the electrons that are reflected or knocked off the near-surface region of a sample to create an image. Since the wavelength of electrons is much smaller than that of light, the resolution of SEMs is superior to that of a light microscope.

How SEMs work

In scanning electron microscopy, the electron beam scans the sample in a raster pattern. First, electrons are generated at the top of the column by the **electron source**.



Due to very narrow electron beam SEM Micrograph have large depth of field giving structure of sample.

The scan coil produces a magnetic field which deflect the electron beam in a controlled way. Varying voltage is applied to the coil of the cathode ray tube which produce pattern of light. When the electron beam hit the sample, it produces secondary electron.

The entire electron column needs to be under vacuum. Like all components of an electron microscope, the electron source is sealed inside a special chamber to preserve vacuum and protect it against contamination, vibrations, and noise.

Advantages: 1. Bulk/powder samples can be used

2. Provide much greater depth of view so it can produce image that can represent 3D structure of sample.