Module II - Quantum Mechanics

Mechanics is a branch of physics that deals with the motion of physical objects with respect to force and displacement.

Mechanics is classified into 3 :

1. Classical mechanics
2. Statistical mechanics
3. Quantum mechanics

Classical mechanics deals with large and macro sized particles so does statistical mechanics.

Quanta - tiny packet of energy.

→ **The laws of Quantum mechanics**

Within a few short years, scientists developed a consistent theory of the atom that explained its fundamental structure and its interactions. Crucial to the development of the theory was new evidence indicating that light and matter have both wave and particle characteristics at the atomic and subatomic levels.

* Introduction

Newtonian mehanics, Maxwell's Electromagnetic theory and thermodynamics constitute classical physics.

Some assumptions of classical physics are :

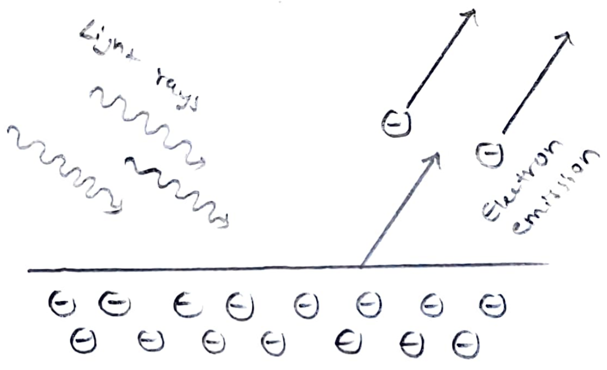
- Energy is continuous
- Position and momentum of a particle can be determined exactly.

- If a charge oscillates with a constant frequency, it produces an EM wave of same frequency ν.

* Photo electric Effect

[31 Oct]

- When light is incident on certain metallic surfaces, electrons are released. these are called photo electrons and the effect is called Photoelectric Effect.



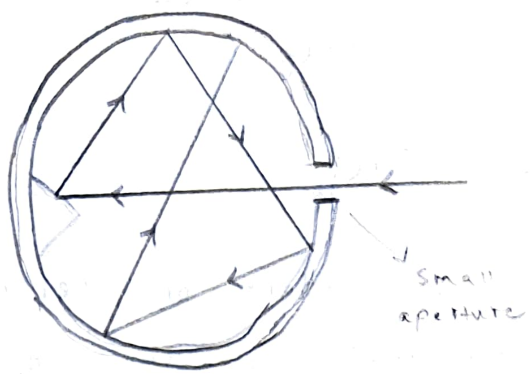
- The photoelectric effect was first observed by Heinrich Hertz in 1887 and was studied in detail by his student, Phillipp Lenard.

* Black Body Radiation

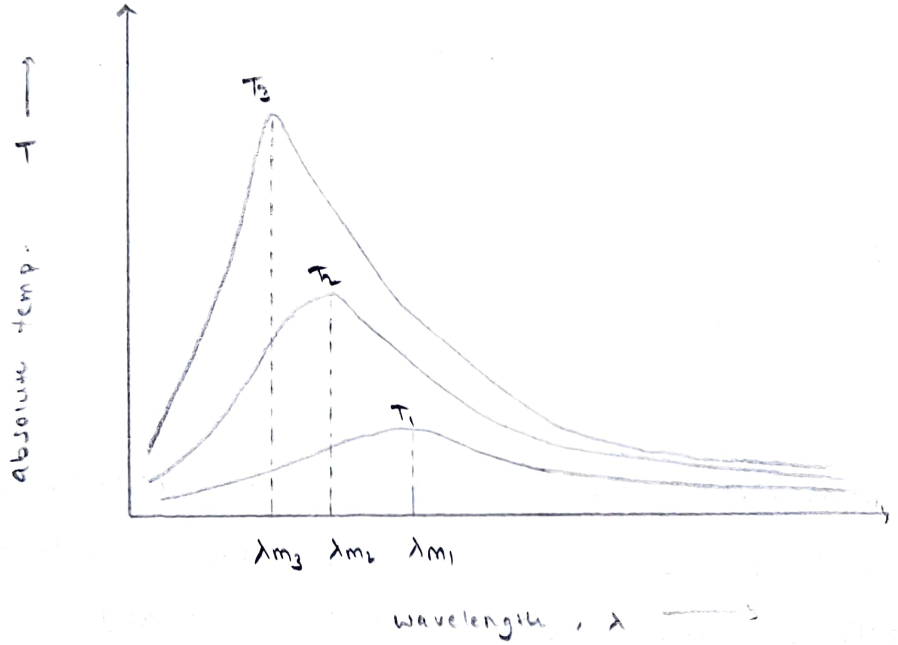
A body which absorbs all the radiations falling on it is a black body. When a black body is heated, it radiates energy and is called black body radiation.

A Practical realization of a black body is an iso-thermal cavity painted with lamp black inside it and contains a small aperture such that light enters the cavity through it.

iso-thermal cavity painted with lamp black inside



Graph relating wavelength and absolute temperature.



E_λ = Emissive power of a black body in the wavelength range λ and $\lambda + d\lambda$

T_1, T_2, T_3 = absolute temp of a black body.

$T_3 > T_2 > T_1$ $\quad$ $\lambda m_3 < \lambda m_2 < \lambda m_1$

→ Stefan - Boltzmann law :

According to Stefan - Boltzmann, the energy radiated is directly proportional to fourth power of the temperature of the body.

$$E \propto T^4$$

→ Wien's displacement law :

$\lambda_m T$ = constant $\quad E_m \propto T^5$

$E_\lambda d\lambda = c_1 \exp(-c_2/\lambda T)\, d\lambda$

→ Ray-Leigh Jean's law :

$$E_\lambda d\lambda = \frac{8\pi kT}{\lambda^4} d\lambda$$

* Planck's Quantum theory [INov]

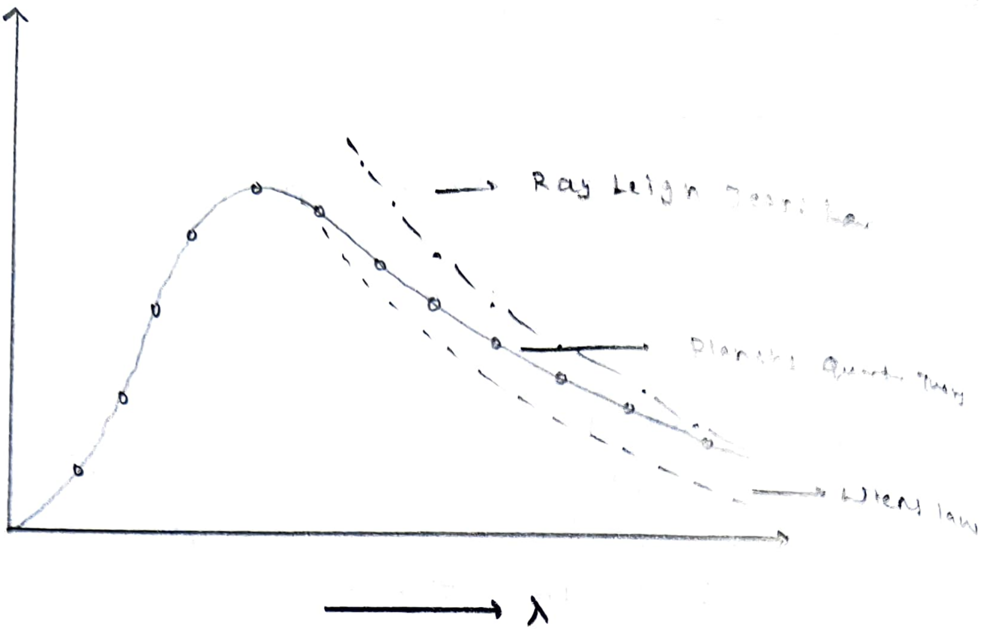
- The atomic oscillators in a body cannot have any arbitrary amount of energy, they could have only a discrete unit of energy given as

- Where h is planck's constant, n is quantum number, ν is frequency.

- The atomic oscillators cannot absorb or emit energy of any arbitrary amount. They absorb or emit energy in indivisible discrete units. The amount of radiant energy in each unit is called a quantum of energy, each quanta carries an energy.

$$\boxed{E_\lambda d\lambda = \frac{8\pi hc}{\lambda^5} \frac{1}{\exp\left(\frac{hc}{\lambda kT}\right) - 1} d\lambda}$$

At shorter wavelengths the Planck's quantum theory deduced to wein's law and at longer wavelengths, its deduced to Ray-Leigh-Jean's law.



* Einstein's explanation of photo-electric effect

Einstein assumed that light falling on the metallic surface to be a stream of photons, each photon having an energy of $h\nu$.

When electrons absorb the photon energy, part of it is sent in overcoming potential barrier and the remaining part of energy gives into its kinetic energy.

So, Energy of photon = Energy needed to liberate electron + kinetic energy of the electron.

$$h\nu = W + KE$$

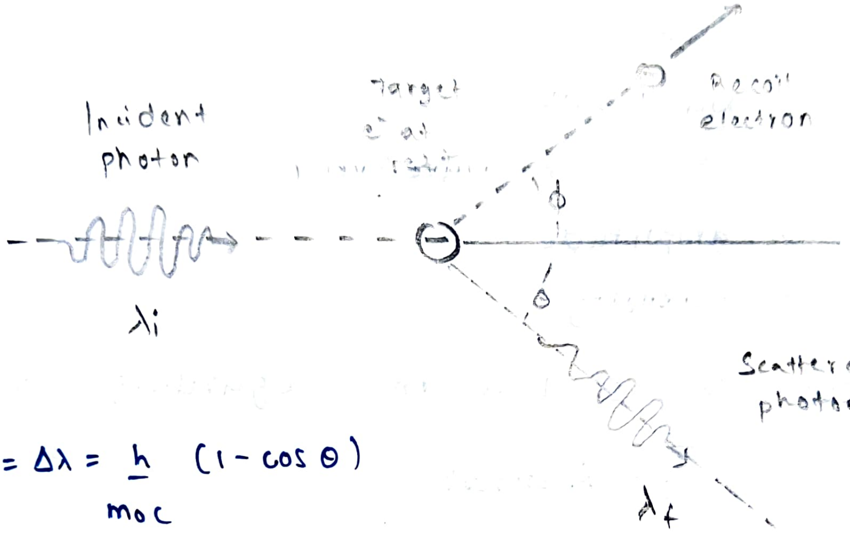
$$h\nu = h\nu_0 + KE$$

where $h\nu_0$ is called the work function.

where W is the minimum energy required to remove an electron from the surface of the material. It is called the work function of the surface.

* Compton effect

It is defined as scattering of a photon by a charged particle like an electron. It results in a decrease in energy of the photon called the compton effect. Part of the energy of the photon is transferred to the recoiling electron.



$$\lambda_f - \lambda_i = \Delta\lambda = \frac{h}{m_0 c}(1 - \cos\theta)$$

* Wave - Particle Duality

[2 Nov]

Particle : It has mass, it is located at some definite point, and it can move from one place to another, it gives energy when slowed down or stopped.

The particle is specified by the following :

- mass (m)
- velocity (v)
- momentum (p)
- Energy (E)

The motion of a particle can be explained by the eqn of ~~Ein~~ Newton's second Law.

i.e. $\boxed{F = ma}$

Wave: A wave is spread out over a relatively large region of space, it cannot be said to be located just here and there. Actually, a wave is nothing but rather a spread out of disturbance.

A wave is specified by its following features:

- frequency
- wavelength
- phase or wave velocity
- amplitude
- intensity

Generally, the displacement regarding wave is

$$\boxed{y = A \sin \omega t}$$

- The photoelectric effect and the compton effect established that light behaves as a flux of photons.
- On the other hand, the phenomena of interference, diffraction and polarization can be explained only when light is treated as a continuous wave.
- Neither of the modes can separately explain all the experimental facts.
- The particle nature and wave nature appear mutually exclusive.
- So, light exhibits both wave nature and particle nature i.e, called as wave-particle duality.

* **Debroglie's Hypothesis :**

In 1924, Louis Debrogile put a bold suggestion that the correspondence between wave and particle should not be confined only to EM radiation, but it should also be valid for material particle i.e., like radiation matter also has a dual (particle like & wave like) characteristics.

According to Debrogile, Nature loves symmetry, since energy or radiation exhibits wave - particle duality, matter must also possess this dual character.

A moving particle is associated with a wave which is know as Debroglie wave or matter wave.

The wavelength of debroglie wave is

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

Proof :

According to Planck's theory the energy E of a photon of frequency ν is given by

$$E = h\nu = \frac{hc}{\lambda} \quad \text{--- (1)} \qquad (\nu = \frac{c}{\lambda})$$

Where λ = wavelength, c = speed of light, h = planck's constant, ν = frequency.

If photon is treated as a particle, its energy as given by Einstein's mass-energy relation

$$E = mc^2 = Pc \quad \text{--- (2)} \qquad \text{Since } (P = mc)$$

from (1) and (2), $\frac{hc}{\lambda} = mc^2 \Rightarrow \lambda = \frac{h}{mc}$ or $\lambda = \frac{h}{P}$

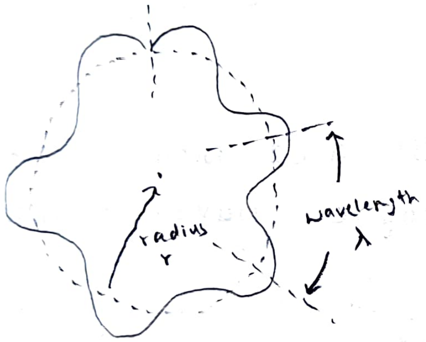
According to Bohr orbital angular momentum is given by,

$$mvr = \frac{nh}{2\pi}$$

where 'r' is radius of permitted circular orbit, 'n' is integer. From above equation and 'λ' we have

$$2\pi r = \frac{nh}{mv} = n\lambda \quad (\text{since } \lambda = h/mv)$$

($2\pi r$) is circumference of electronic orbit.
Thus, the permitted orbits correspond to integral multiples of Debrogile wavelength.



$$m_e v r = n\hbar \qquad n = 1, 2, 3 \ldots$$

$$\hbar = h/2\pi$$

an integer no. of wavelengths fits into the circular orbit

$\boxed{n\lambda = 2\pi r}$ where $\boxed{\lambda = h/p}$

λ – the deBroglie's wavelength

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* Matter wave properties

3 NOV

The wavelength of matter is $\lambda = h/mv$, so wavelength is inversely proportional to velocity. A group of waves each wave having wavelength given above, is associated with the particle. This group as a whole must travel with the particle velocity v. Hence group velocity of matter waves $= V_{gr} = V$.
Each wave of the group of matter waves travel with a velocity known as phase velocity of the wave.

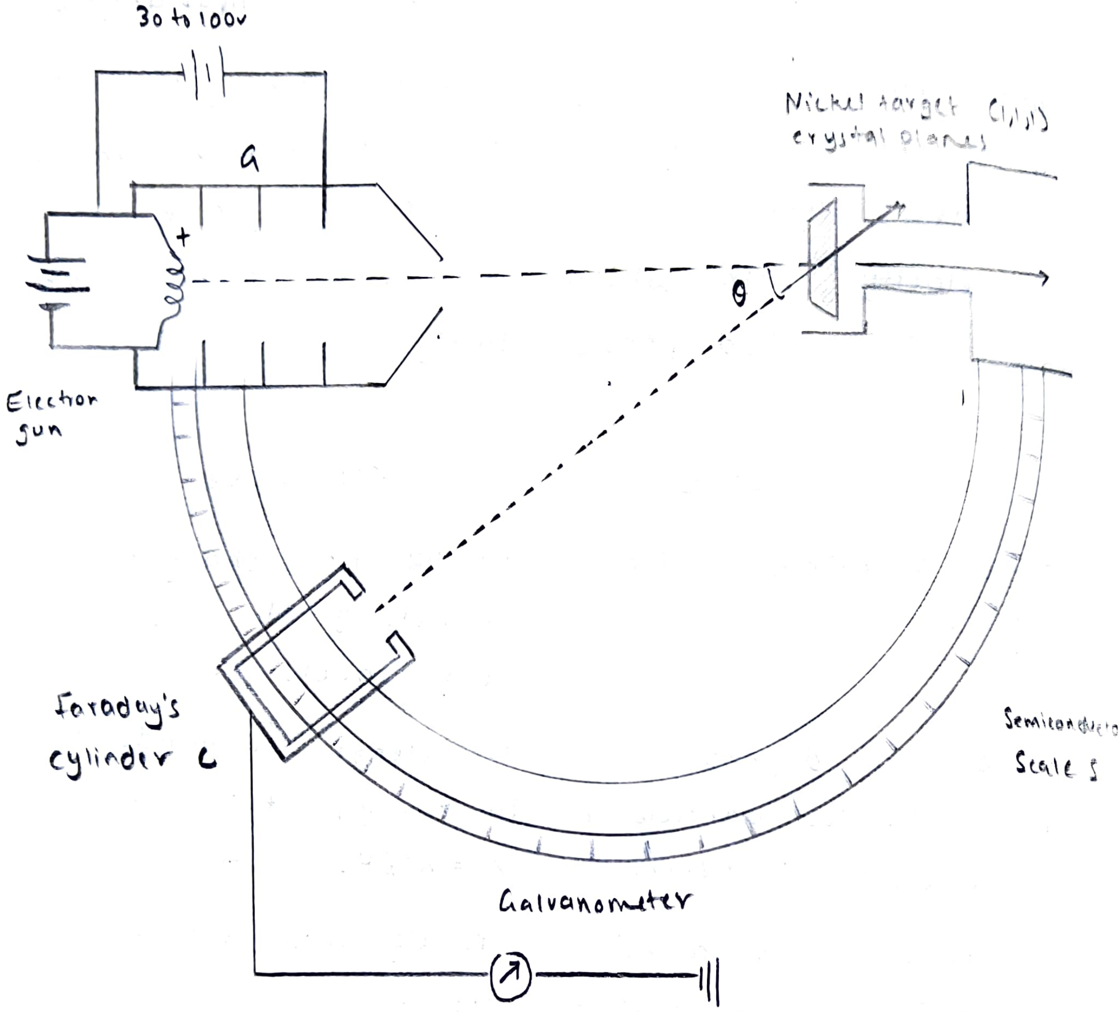
wavelength of electron : $\sqrt{\frac{150}{V}}$ A°

We have to remember that no single phenomena eitur matter or radiation exhibits both particle nature and wave nature simultaneously.

Waves can be in a group and such groups are called wave packets so tu velocity with which a wave packet travels is called group vel. Tu velocity with which tu phase of a wave travels is called phase velocity.

	Matter wave	EM wave
1.	It is associated with a particle.	Oscillating charged particle gives rise to EM waves.
2.	Wavelength depends on tu mass of tu particle and its velocity. $\lambda = h/mv$.	Wavelength depends on tu energy of tu photon. $\lambda = hc/E$.
3.	Can travel with a vel. greater than tu velocity of light.	Travels with velocity of light.
4.	Matter wave is not EM waves.	Electric field and magnetic field oscillate perpendicular to each other.
5.	Matter wave require medium for propagation.	Electromagnetic waves do not require medium i.e, tuy travel in vacuum also.

Initial atomic models proposed by scientists could only explain tu particle nature of electrons but failed to explain wave nature properties. CJ Davisson and L.H Germer in tu year 1927, carried out an experiment, popularly known as Davisson Germer's experiment to explain wave nature of electrons through electron diffraction.

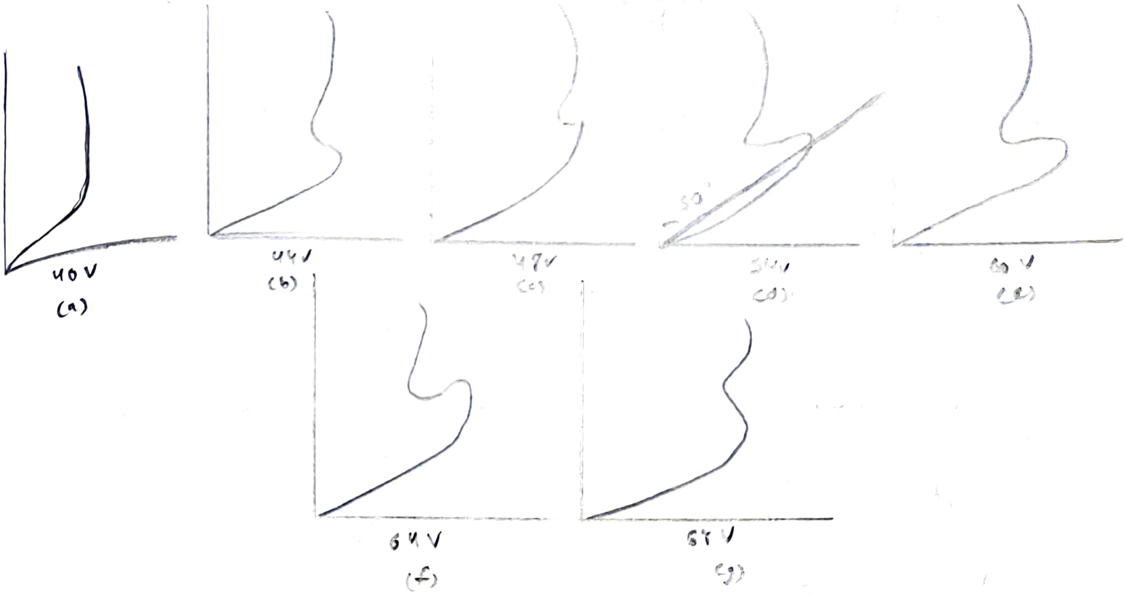


The electrons emitted from gun strikes the target, [7 Nov] which is rotated about an axis along the direction of the beam.

The speed of the electron can be measured by the voltage used for accelerating electrons.

The scattered beam is detected by the chamber D and its intensity is measured in different directions.

The plot of the electron beam intensity versus the angle φ between the incident and scattered beams show maxima and minima.



The wavelength value depending on V is given as

$$\lambda = \sqrt{\frac{150}{V}}\, A^\circ \Rightarrow \lambda = \sqrt{\frac{150}{54}}\, A^\circ = 1.67 A^\circ$$

Bragg's law equated to Davisson Germer Exp.

If θ is the correspondence angle of diffraction at the Bragg's plane then θ and ϕ are related as $\theta = \frac{180 - \phi}{2}$.

So if θ is diffraction angle, n is order of maxima then from Bragg's law : $2d\sin\theta = n\lambda$

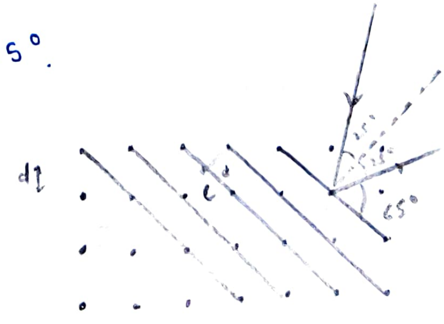
Davission & Germer observed that maximum diffraction occurs at $\phi = 50^\circ$ and $d = 0.91 A^\circ$

Now, $\phi = 50^\circ$, $\Rightarrow$ $\theta = \frac{180 - 50}{2} = 65^\circ$.

Therefore, $\lambda = 2d\sin\theta$ (for $n = 1$)

$= 2 \times 0.91 \times \sin 65^\circ$.

$= 1.65 \mathring{A}$



* Debrogile wavelength in terms of Energy

we know that kinetic energy, $KE = \frac{1}{2}mv^2$

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

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

$$m^2v^2 = 2Em$$

$$\sqrt{m^2v^2} = \sqrt{2Em}$$

$$mv = \sqrt{2Em}$$

$$p = \sqrt{2mE}$$

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

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

$$E = \frac{p^2}{2m} \quad (\text{since } p = mv)$$

$$p^2 = 2mE$$

$$p = \sqrt{2mE}$$

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mE}} \quad (\text{since } p = \sqrt{2mE})$$

For an electron with kinetic Energy 'E' accelerated by a Potential difference 'v'.

Then, $\lambda = \frac{h}{\sqrt{2mE}} = \frac{h}{\sqrt{2meV}}$

substituting for h, m and e. we get,

$$\lambda = \frac{6.625 \times 10^{-34}}{\sqrt{2 \times 9.11 \times 10^{-31} \times 1.602 \times 10^{-19} \times V}} = \frac{12.26}{\sqrt{V}} \text{ Å}$$

thus for V = 100 volts

$$\therefore \lambda = \frac{12.26}{\sqrt{100}} = 1.226 \text{ Å}$$

$h = 6.626 \times 10^{-34}$ Js or J / Hertz

$\hbar = \frac{h}{2\pi} = 1.0545 \times 10^{-34}$ Js or J / Hertz

* Schrodinger time independent wave equation

Schrodinger wave equation is a mathematical expression describing the energy and position of the electron in space and time, taking into account the matter wave nature of the electron inside an atom.

wave function $\psi = \psi_0 \sin(\omega t - kx)$ —— ①

where $\psi = \psi(x)$,

ψ_0 = amplitude,

$k = 2\pi/\lambda$,

$\omega = 2\pi\nu = 2\pi/T$

Now differentiating ① with respect to 'x' we get,

$$\frac{\partial \psi}{\partial x} = -k\psi_0 \cos(\omega t - kx)$$

differentiating again,

$$\frac{\partial^2 \psi}{\partial x^2} = -k^2 \psi_0 \sin(\omega t - kx)$$

$$\frac{\partial^2 \psi}{\partial x^2} = -k^2 \psi \quad \text{(from eqn ①)}$$

$$\frac{\partial^2 \psi}{\partial x^2} + k^2 \psi = 0 \quad \text{—— ②}$$

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{4\pi^2}{\lambda^2} \psi = 0 \quad \text{—— ③}$$

We know that Debrogile wavelength, $\lambda = h/mv$

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{4\pi^2 m^2 v^2}{h^2} \psi = 0 \quad \text{—— ④}$$

Now, we know that the total energy E of the particle is sum of its kinetic energy k and its potential energy V,

$E = K + V$ and $K = \frac{1}{2} mv^2$

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

$$E - V = \frac{1}{2}mv^2$$

$$2m(E-V) = m^2v^2 \quad \text{——— (5)}$$

from equations (4) and (5), we get.

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

The value of $h/2\pi$ is considered as $\hbar$

$\therefore \hbar = h/2\pi$

$$\boxed{\frac{\partial^2\psi}{\partial x^2} + \frac{2m(E-V)\psi}{\hbar^2} = 0} \quad \text{——— (6)}$$

This is schrodingers' time independent wave eqn in 1-D.

In 3 dimensions, it can be written as

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} + \frac{2m(E-V)\psi}{\hbar^2} = 0 \quad \text{——— (7)}$$

Time - dependent form of Schrodinger wave equation:

It is expressed as

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

where $\psi = \psi(\vec{r},t)$,

$\vec{r} = x\vec{i} + y\vec{j} + z\vec{k}$, $i = \sqrt{-1}$

(or)

$E\psi = \bar{H}\psi$ where $\bar{E} = i\hbar\frac{\partial}{\partial t}$ & $\bar{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r},t)$

$\bar{H}$ - Hamoltonion operater

$\bar{E}$ - Energy eign vector operator.

* Physical significance of ψ. [9 Nov]

The actual physical significance was not clear. Max Born's interpretation of 'ψ', given in 1926, is generally accepted at present.

As ψ is a complex function, $\psi^* \psi = |\psi|^2$ is a real value.

$|\psi|^2$ at a point is proportional to the probability of finding the particle at any given instant.

The probability ~~of~~ density at any point is represented by $|\psi|^2$, the probability P of finding the particle within any element of volume $dx\,dy\,dz$ is given by

$$P = \psi^* \psi \, dx\,dy\,dz$$

Since the total probability of finding the particle somewhere is unity, ψ is such a func. that satisfies the condition

$$\iiint |\psi|^2 \, dx\,dy\,dz = 1$$

ψ satisfying above equation is called a normalized function.

Besides this ψ is a single valued continuous func.

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* Characteristics of wave function

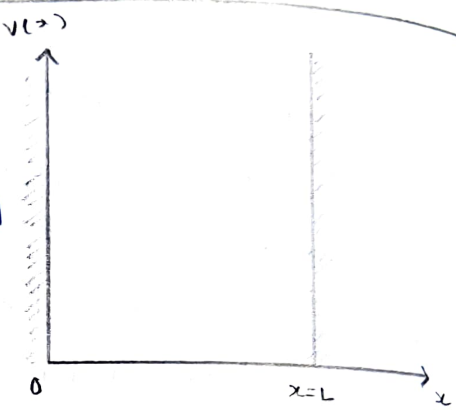
1. ψ function must be finite : The wave function should not tend to infinity. It must remain finite for all values of x, y, z.

2. ψ function must be single-valued : Any physical quantity can only have one value at a point. For this reason, the func related to physical quantity cannot have more than one value at that point.

3. ψ must be continuous : the wave function and its space derivatives should be continuous across any boundary.

Wave functions satisfying the above mathematical conditions are called well-behaved wave functions.

* Particle in a box



We consider a 1-D potential well of width 'L', Let the potential is $V=0$ inside the well and $V=\infty$ outside the well.

$$V(x) = 0 \;, \text{ for } 0 < x < L \quad \text{--- (1)}$$

$$V(x) = \infty \;, \text{ for } x > L$$

The time independent Schrodinger wave equation in 1-D case is given by

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

For the particle present inside the well $V=0$ and $\psi = \psi(x$

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2m(E)}{\hbar^2}\psi = 0 \quad \text{--- (3)}$$

Let the general solution of (3) is given as

$$\psi(x) = A\sin kx + B\cos kx \quad \text{--- (4)}$$

where A & B are constants are to be determined from the boundary conditions.

$$\psi(x) = 0 \quad \text{at} \quad x = 0$$

$$\psi(x) = 0 \quad \text{at} \quad x = L$$

So (4) simplifies to $\boxed{\psi(x) = A\sin\frac{n\pi}{L}x}$ --- (5)

differentiating twice we get,

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{n^2 \pi^2}{L^2}\psi = 0 \quad \text{—— (6)}$$

comparing (3) and (6) we get,

$$\frac{2mE}{\hbar^2} = \frac{n^2\pi^2}{L^2} \Rightarrow E = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

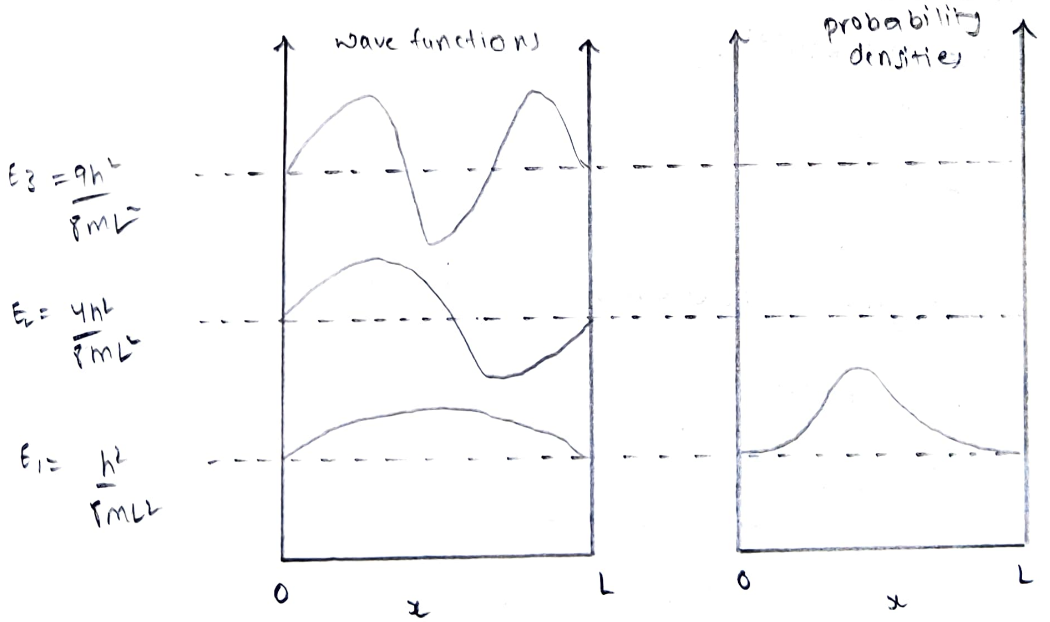
where n is called quantum number.

So the particle cannot possess any value of energy, it possesses only a discrete set of energy values.

Energy of n^{th} level is $\boxed{E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} = \frac{n^2h^2}{8mL^2}}$ —— (7)

In order to find value of A, we use normalization condition. i.e $\int_0^L \psi\cdot\psi \, dx = 1$ or $\int_0^L |\psi(x)|^2 dx = 1$

Then we get $A = \sqrt{2/L}$.



[10 Nov]

→ The quantum behavior in the box

• Energy quantization :

It is not possible for the particle to have any arbitrary definite energy. Instead only discrete definite energy levels are allowed.

- **Zero - point Energy :**

The lowest possible energy level of the particle, called the zero-point energy. is non-zero.

- **Spatial nodes :**

In contrast to classical mechanics the schrodinger equation predicts that for some energy levels there are nodes, implying positions at which the particle can never be found.