Unit – 1: Quantum Mechanics

Inadequacy of Classical Mechanics

Classical Picture: Till the late 19th century the universe appeared to be a simple and orderly place, consisting of **matter** and **electromagnetic radiation**.

- **Matter**, which consisted of particles that had mass and whose location and motion could be accurately described by Classical mechanics, which was based on Newton's three laws of motion (Law of Inertia, Law of Force & Action and Reaction Law) and gravitation which includes the concept of absolute mass, absolute space & absolute time.
- **EM radiation**, which was viewed as having no mass and whose exact position in space could not be fixed. Physicists could describe the properties of radiant energy using mathematical relationships known as Maxwell's equations (equations describing Electricity and Magnetism) developed by a Scottish physicist James Clerk Maxwell in 1873.

Thus, matter and energy were considered distinct and unrelated phenomena and the laws of physics described nature very well under most conditions.
When physicists started probing **very small sizes (electrons, protons etc.)**, and **high energy densities (speed comparable to light)**, there were discrepancies that could not be explained by classical physics.

Failures: The following phenomenon couldn't be explained by classical mechanics-

- Blackbody radiation: Classical physics predicted that hot objects would instantly radiate away all their heat into electromagnetic waves. This emission of energy is continuous as well. Wien and Rayleigh-Jeans came up with their explanations, but Wien's law failed to explain the longer wavelength and Rayleigh-Jean's law failed to explain short wavelengths. The calculation, which was based on Maxwell's equations and Statistical Mechanics, showed that the radiation rate went to infinity as the EM wavelength went to zero, ``The Ultraviolet Catastrophe''. Theory could not agree/match the experimental results.
- Photoelectric effect: *The photoelectric effect is the emission of electrons or other free carriers when light is shone onto a material. Electrons emitted in this manner can be called photo electrons.*
  According to the classical perspective of photoelectric effect, when light shines on a surface, it slowly transfers energy into the substance. This increases the kinetic energy of the particles until finally, they give off excited electrons. This process is called Thermionic Emission.
  To test the theories proposed by classical mechanics, Lenard conducted an experiment which showed that
  - Below a certain threshold frequency, no matter how intense the light was, there was *no* emission of electrons.
  - Above the threshold frequency, the current was directly *proportional* to the light intensity.
  - The current appeared almost *instantaneously* after the light was turned on
  - Higher frequency light increased the **kinetic energy** of the electrons,
  - Changing the light intensity had **no effect** on the kinetic energy.

  Classical ideas could not give appropriate explanation for the above experimental findings.
- Compton Effect: According to classical theory of scattering, the wavelength of X-ray would not be changing (Thomson scattering) after interaction with the electrons, however Compton did find a change in wavelength in experiment.
- Stability of Atom: After Rutherford found that the positive charge in atoms was concentrated in a very tiny nucleus, classical physics predicted that the atomic electrons orbiting the nucleus would radiate their energy away and finally fall into the nucleus following a spiral path. This clearly did not happen.
- Hydrogen Spectrum discreteness: According to classical mechanics, radiation spectra was continuous for all wavelengths from hydrogen atom, but experimentally it was observed that the spectrum consisted of discrete lines corresponding to Lymen series, Balmer series, Paschen series, Bracketseries, Pfund series.
- Waves and Particles: In diffraction experiments, light was shown to behave like a wave while in experiments like the Photoelectric effect, light behaved like a particle. More difficult diffraction experiments showed that electrons (as well as the other particles) also behaved like a wave, yet we can only detect an integer number of electrons (or photons).

Classical physics failed because it was wrong when probed at high energy and small distances. It still works very well for most macroscopic phenomena.

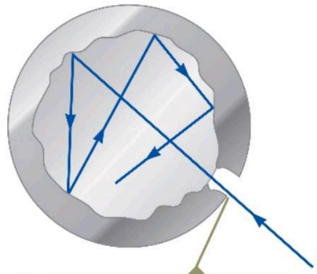
The problems with classical physics led to the development of **Quantum Mechanics (very small particles)** and **Special Relativity (very high speeds).**

Max Planck speculated that energy levels were quantized, and that accounted for what was seen. Quantum Mechanics incorporates a wave-particle duality and explains all of the above phenomena. In doing so, Quantum Mechanics changes our understanding of nature in fundamental ways.

Black Body

"An idealized physical body, which can absorb all the electromagnetic radiations when incident on it irrespective of its frequency or incident angle is known as a black body."

- ***A black body is a perfect absorber as well as a perfect emitter of radiation.***
- An object in thermal equilibrium with its surroundings radiates as much energy as it absorbs.
- It is impossible to realise a perfect/ideal black body in practice.
- A good approximation of a black body is a small hole leading to the inside of a hollow object blackened completely from inside (Kirchhoff's Black Body).
- The hole acts as a perfect absorber.
- The nature of the radiation leaving the cavity through the hole depends only on the temperature of the cavity.



The opening to a cavity inside a hollow object is a good approximation of a black body: the hole acts as a perfect absorber.

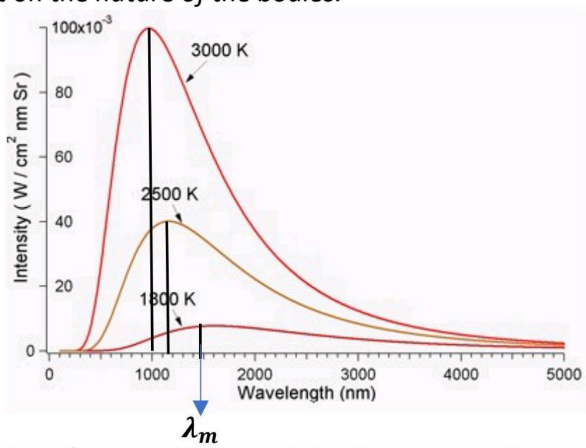
Black Body Radiation: A black body can start emitting electromagnetic radiations, once it is heated at high temperature.***The radiation emitted by a black body is called black body radiation.***

Characteristics of black body radiation spectra-

The distribution of energy of a black body radiation at different temperatures with its wavelength is as shown in the figure.

- A black body, according to its temperature, emits the radiations in a continuous spectrum. (*This is the main reason behind the different colours of stars, like red stars are mostly cooler, so they emit wavelengths equivalent to that of red colour.)*
- **Kirchhoff's Laws:-**There are two statements of this law -
  - *A black body not only absorbs all the radiation incident on it but is also a perfect radiator at higher temperatures.*
  - *The radiation emitted depends only on the temperature and not on the nature of the bodies.*

- The total power of the emitted radiation increases with increasing temperature.(This is according to **Stefan's law**).
- The energy distribution is not uniform. Peak of the radiated energy in the curveis obtained at a particular wavelength λ_m at a given temperature.
- Peak of the radiated energy in the curve shifts to shorter wavelengthsas the temperature increases. (This is according to **Wien'sDisplacement law**).
- A black body can emit radiation of all wavelengths lying in the region of ultraviolet, visible light and infrared.
- At room temperature, the wavelengths of the thermal radiation are mainly in the infrared region.



Stefan's law- *"The total radiant energy E_T of a black body is proportional to the 4th power of its absolute temperature T."*

i.e. $\boxed{E_T = \sigma T^4}$ where $\sigma = 5.67 \times 10^{-8} W/m^2K^4$).

The total energy radiated out is given as $\boxed{E_T = \int_{-\infty}^{\infty} U_{(\nu,T)} d\nu}$ where $U_{(\nu,T)}$= Emissive power of a black body for a radiation at frequency ν at temperature T.

Wien's Displacement Law:*"The wavelength of the peak radiation(**λ_m or λ_{peak}**) is inversely proportional to thetemperature (T) of the black body radiating it."*

i.e. $\boxed{\lambda_{peak} T = constant = 2.898 \times 10^{-3}\, mK\ (Wien's\ Const.)}$

Explanation of Black Body Radiation Spectra:

Wien's Distribution Law:

Wien derived a formula representing a relationship between the emissive energy in black body radiation spectra with the temperature and wavelength, using the principles of Classical Thermodynamics.

According to this the energy density of the emitted radiation $U_{(\lambda,T)}$for waves in a wavelength range $\lambda\ and\ \lambda + d\lambda$ is

$$\boxed{U_{(\lambda,T)} d\lambda = \frac{8\pi hc}{\lambda^5}\left[e^{\left(-hc/_{\lambda KT}\right)}\right] d\lambda}$$

**** This law holds good only for short wavelengths and fails at higher wavelengths at higher temperatures.***

Rayleigh-Jean's Law

Rayleigh and Jean derived a formula for the energy distribution in the black body radiation spectra by applying the principles of Statistical Physics and Electrodynamics.

This law This law represents the total energy density in the wavelength range $\lambda\ and\ \lambda + d\lambda$ as

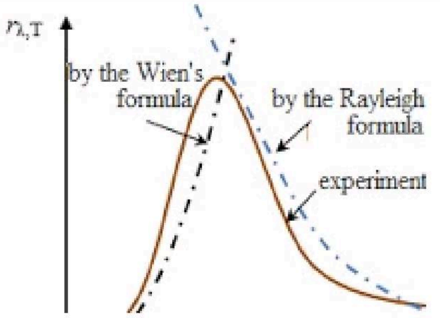
$$\boxed{U_{(\lambda,T)} d\lambda = \frac{8\pi}{\lambda^4}[KT] d\lambda}$$

**** This law holds good only for longer wavelengths and fails at shorter wavelengths.***

This is called "UV Catastrophe".

Failure of Classical Theory in case of Black Body Radiation.

- Classical physics predicted that hot objects would instantly radiate away all their heat into electromagnetic waves. This emission of energy is continuous as well.
- Wien and Rayleigh-Jeans came up with their explanations, but Wien's law failed to explain the longer wavelength and Rayleigh-Jean's law failed to explain short wavelengths.
- The calculation, which was based on Maxwell's equations and Statistical Mechanics, showed that the radiation rate went to infinity as the EM wavelength went to zero, ``The Ultraviolet Catastrophe''.
- Theory could not agree/match the experimental results.



Planck's Quantum Theory: In 1901, Wien's colleague, German physicist Max Planck, showed that the energies absorbed and emitted by blackbodies are 'quantised'. This means that only certain energies are allowed in transaction.
Max Planck developed a theory of blackbody radiation that leads to an equation for the intensity of the radiation.This equation was found to be in complete agreement with experimental observations.
Hence, Planck's quantum theory was validated as well.

Assumptions of Planck's quantum theory–

- The constituting atoms of a black body radiator behave like simple harmonic oscillators having a characteristic frequency of vibration.
- Matter radiatesor absorbs energy in discrete quantities discontinuously in the form of small packets or bundles.
- The smallest bundle or packet of energy is known as a "*quantum*".
- The energy of the *quantum* absorbed or emitted is directly proportional to the frequency of the radiation. So, energy of the radiation is expressed in terms of frequency as follows-

$$\boxed{\boldsymbol{E = h\nu}}$$

- A body or matter can radiate energy or absorb energy in whole number multiples of a quantum as -

$$\boxed{\boldsymbol{E = n(h\nu)}} \quad \textit{where n = 0, 1, 2, 3,4........}$$

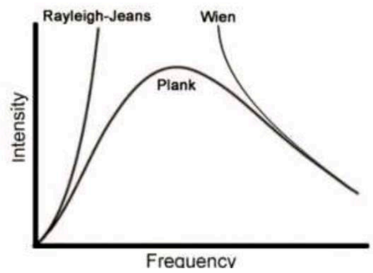
So, energy can be absorbed or radiated as hv, 2hv, 3hv, 4hv......etc. not in the form of 1.5hv, 2.5hv...etc.

Plank's Radiation Formula

On the basis of the assumptions of his proposed quantum theory Max Plank gave the following formula for the energy distribution in the black body radiation-

$$\boxed{\boldsymbol{U_{(\lambda,T)}}d\lambda = \frac{\boldsymbol{8\pi hc}}{\boldsymbol{\lambda^5}}\left[\frac{\mathbf{1}}{\boldsymbol{e^{\left(hc/_{\lambda kT}\right)}-1}}\right]d\lambda}$$

**** This formula was found to be in complete agreement with experimental observations.***



Derivation of Plank's Radiation Formula

Planck's radiation law is derived by assuming that each emitted radiation mode can be described by a quantized harmonic oscillator with energy $E_n = n(h\nu)$
Let N_o , $N_1, N_2, N_3, \ldots, N_n$ are the number of oscillators in different energy states given by $0, h\nu, 2h\nu, 3h\nu, \ldots\ldots, nh\nu$.
So the total number of all oscillators in all the states

$$N = N_o + N_1 + N_2 + N_3, \ldots. + N_n = N_o + N_o e^{\left(\frac{-h\nu}{kT}\right)} + N_o e^{\left(\frac{-2h\nu}{kT}\right)} + N_o e^{\left(\frac{-3h\nu}{kT}\right)} \,\ldots\ldots + N_o e^{\left(\frac{-nh\nu}{kT}\right)} \qquad \because N_n = N_o e^{\left(\frac{-nh\nu}{kT}\right)}$$

And the total energy of all the oscillators is

$$E = 0 + h\nu N_1 + 2h\nu N_2 + 3h\nu N_3 + \cdots .. + nh\nu N_n$$
$$E = 0 + h\nu N_o e^{\left(\frac{-h\nu}{kT}\right)} + 2h\nu N_o e^{\left(\frac{-2h\nu}{kT}\right)} + 3h\nu N_o e^{\left(\frac{-3h\nu}{kT}\right)} + \cdots .. + nh\nu N_o e^{\left(\frac{-nh\nu}{kT}\right)}$$

Therefore the average energy per oscillator is given as

$$\langle E \rangle = \frac{E}{N}$$

$$\langle E \rangle = \frac{0 + h\nu N_o e^{\left(\frac{-h\nu}{kT}\right)} + 2h\nu N_o e^{\left(\frac{-2h\nu}{kT}\right)} + 3h\nu N_o e^{\left(\frac{-3h\nu}{kT}\right)} + \cdots .. + nh\nu N_o e^{\left(\frac{-nh\nu}{kT}\right)}}{N_o + N_o e^{\left(\frac{-h\nu}{kT}\right)} + N_o e^{\left(\frac{-2h\nu}{kT}\right)} + N_o e^{\left(\frac{-3h\nu}{kT}\right)} \,\ldots\ldots + N_o e^{\left(\frac{-nh\nu}{kT}\right)}}$$

$$\langle E \rangle = \frac{\sum_{n=0}^{\infty} nh\nu \, e^{\left(\frac{-nh\nu}{kT}\right)}}{\sum_{n=0}^{\infty} e^{\left(\frac{-nh\nu}{kT}\right)}} = h\nu \frac{\sum_{n=0}^{\infty} nx^n}{\sum_{n=0}^{\infty} x^n} \qquad \textit{if we place } \; x = e^{\left(\frac{-h\nu}{kT}\right)}$$

Now using standard series solutions

$$\sum_{n=0}^{\infty} x^n = \frac{1}{1-x} \quad \text{and} \quad \sum_{n=0}^{\infty} nx^n = \frac{x}{(1-x)^2}$$

in the above we get

$$\langle E \rangle = h\nu \frac{\sum_{n=0}^{\infty} nx^n}{\sum_{n=0}^{\infty} x^n} = \frac{h\nu\left[\frac{x}{(1-x)^2}\right]}{\left[\frac{1}{1-x}\right]}$$

$$\langle E \rangle = \frac{h\nu\left[\frac{e^{\left(\frac{-h\nu}{kT}\right)}}{\left\{1-e^{\left(\frac{-h\nu}{kT}\right)}\right\}^2}\right]}{\left[\frac{1}{1-e^{\left(\frac{-h\nu}{kT}\right)}}\right]}$$

$$\langle E\rangle = h\nu\left[\frac{e^{\left(\frac{-h\nu}{kT}\right)}}{1-e^{\left(\frac{-h\nu}{kT}\right)}}\right] = \frac{h\nu}{\left[e^{\left(\frac{h\nu}{kT}\right)}-1\right]}$$

Now according to Rayleigh-Jeans law (in terms of frequency), the energy density in the frequency interval $\nu + d\nu$ is given as

$$U_\nu d\nu = \frac{8\pi\nu^2}{c^3}\langle E\rangle d\nu \;=\; \frac{8\pi\nu^2}{c^3}\times\frac{h\nu}{\left[e^{\left(\frac{h\nu}{kT}\right)}-1\right]}d\nu$$

$$\boldsymbol{U_\nu d\nu = \frac{8\pi h\nu^3}{c^3}\left[\frac{1}{e^{\left(\frac{h\nu}{kT}\right)}-1}\right]d\nu}$$

This is Plank's Radiation formula in terms of frequency.

*** Plank's Radiation formula in terms of wavelength**

We know that $\nu = \frac{c}{\lambda} \quad\Rightarrow\quad d\nu = -\left(\frac{c}{\lambda^2}\right)d\lambda$

Considering only the absolute value, $|d\nu| = \left(\frac{c}{\lambda^2}\right)d\lambda$

So, using above, Plank's radiation formula can be written as

$$U_\lambda d\lambda = \frac{8\pi hc^3}{\lambda^3c^3}\left[\frac{1}{e^{\left(\frac{hc}{\lambda kT}\right)}-1}\right]\left(\frac{c}{\lambda^2}\right)d\lambda$$

$$\boldsymbol{U_{(\lambda,T)}d\lambda = \frac{8\pi hc}{\lambda^5}\left[\frac{1}{e^{\left(hc/\lambda KT\right)}-1}\right]d\lambda}$$

This is Plank's Radiation formula in terms of wavelength

<u>Wien's Law from Plank's Formula</u>

Plank's formula is

$$\boldsymbol{U_{(\lambda,T)}d\lambda = \frac{8\pi hc}{\lambda^5}\left[\frac{1}{e^{\left(hc/\lambda KT\right)}-1}\right]d\lambda}$$

For shorter wavelengths

$$e^{\left(hc/\lambda KT\right)} >> 1$$

Hence ignoring 1 in the denominator, we get

$$\boldsymbol{U_{(\lambda,T)}d\lambda = \frac{8\pi hc}{\lambda^5}\left[\frac{1}{e^{\left(hc/\lambda KT\right)}}\right]d\lambda}$$

Or $\boldsymbol{U_{(\lambda,T)}d\lambda = \frac{8\pi hc}{\lambda^5}\left[e^{\left(-hc/\lambda KT\right)}\right]d\lambda}$

This is <u>Wien's Law</u>.

Hence, Plank's Law agrees with Wien's law for short wavelengths.

<u>Rayleigh-Jean Law from Plank's Formula</u>

Plank's formula is

$$\boldsymbol{U_{(\lambda,T)}(\quad \frac{8\pi hc}{\lambda^5}\left[\frac{1}{e^{\left(hc/\lambda KT\right)}-1}\right]d\lambda}$$

For longer wavelengths

$$\boldsymbol{e^{\left(hc/\lambda KT\right)} \cong 1 + \frac{hc}{\lambda KT} + \cdots}$$

On ignoring higher order terms, we get

$$\boldsymbol{U_{(\lambda,T)}d\lambda = \frac{8\pi hc}{\lambda^5}\left[\frac{1}{1+\frac{hc}{\lambda KT}-1}\right]d\lambda}$$

Or $\boldsymbol{U_{(\lambda,T)}d\lambda = \frac{8\pi}{\lambda^4}[KT]d\lambda}$

This is <u>Rayleigh-Jean Law</u>.

Hence, Plank's Law agrees with Rayleigh-Jean Lawfor longer wavelengths.

<u>Stefan's-Boltzmann law from Plank's Formula</u>

If energy density of the emanating em radiation in the frequency range ν *and* $\nu + d\nu$ from Plank's formula is

$$\boldsymbol{U_{(\nu)}d\nu = \frac{8\pi h}{c^3}\left[\frac{\nu^3}{e^{\left(h\nu/KT\right)}-1}\right]d\nu}$$

The total energy emanating, by Kirchhoff's law is

$$\boldsymbol{E_T = \int_0^\infty U_{(\nu,T)}d\nu}$$

$$\boldsymbol{= \frac{8\pi h}{c^3}\int_0^\infty\left[\frac{\nu^3}{e^{\left(h\nu/KT\right)}-1}\right]d\nu}\text{-----(1)}$$

Let $\frac{h\nu}{KT} = x \quad\Rightarrow\quad \nu = \frac{KT}{h}x$

If $\nu \longrightarrow 0, x \longrightarrow 0 \;\; and \;\; if \;\; \nu \longrightarrow \infty, x \longrightarrow \infty$

And $d\nu = \frac{KT}{h}\,dx$

Using the above substitutions to change eqn (1)

$$\boldsymbol{E_T = \frac{8\pi h}{c^3}\int_0^\infty\frac{(kT/h)^3x^3}{e^x-1}\times\frac{KT}{h}dx}$$

$$\boldsymbol{= \frac{8\pi h}{c^3}\left(\frac{KT}{h}\right)^4\int_0^\infty\frac{x^3}{e^x-1}dx}$$

$$\boldsymbol{= \frac{8\pi h}{c^3}\left(\frac{KT}{h}\right)^4\times\frac{\pi^4}{15}}$$

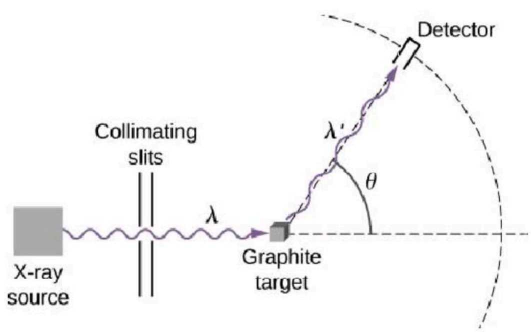
$$\boldsymbol{= \left[\frac{8\pi^5K^4}{15\,h^3c^3}\right]\times T^4}$$

$$\Rightarrow \quad \boxed{\boldsymbol{E \propto T^4}}$$

<u>This is Stefan's-Boltzmann Law.</u>

<u>Compton Effect</u>

- Compton Effect was discovered by Arthur Holly Compton in 1923 and for this discovery he was awarded by the Nobel Prize in Physics in 1927.
- According to classical theory of scattering, the wavelength of X-ray would not be changing (Thomson scattering) after interaction with the electrons, however Compton did find a change in wavelength in experiment. Then Compton Effect was explained on the basis of the quantum theory (particle "photon" model) of light.
- This Effect convinced remaining doubters of the existence of photons. It constitutes very strong evidence in support of the Quantum Theory of radiation.



Compton Effect

"When high energy photons (X-rays, γ-rays) are scattered by free charge particles (loosely bound outer shell electron in target material) resulting in increased wavelength of the scattered photons then this is called compton effect or compton scattering."

Amongs the scattered photon, two types of components are found –

ⓐ Unmodified Ratiation – These are those scattered photons which don't suffer any change in the wavelength after scattering.

ⓑ Modified Radiations – These are those scattered photons which get their wavelength increase after scattering.

The change in wavelength is given by

$$\boxed{\lambda' - \lambda = \frac{h}{m_o c}(1 - \cos\theta)}$$

where λ' = increased wavelength of the scattered photon

λ = wavelength of the incident photon

$h = 6.67 \times 10^{-34}$ Js (planck's constant)

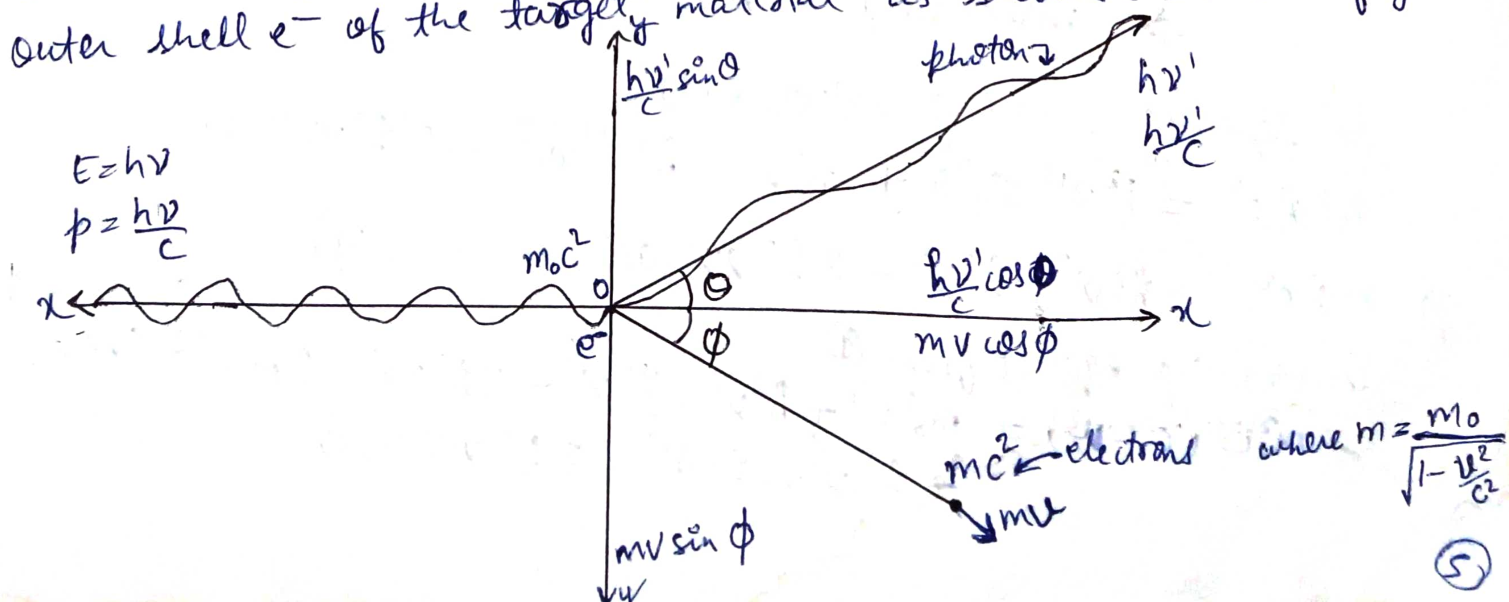
$c = 3 \times 10^{8}$ m/sec

m_o = Rest mass of e^-

θ = Angle of scattering.

Derivation:

Let us consider the collision of an X-ray photon with an outer shell e^- of the target material as shown in the figure.



Analysing before & after collision.

Before Collision	After Collision
Photon - Energy $= h\nu$	Photon - Energy $= h\nu'$
Momentum $= \frac{h\nu}{c}$	Momentum $= \frac{h\nu'}{c}$
Electron - Energy $= m_0 c^2$	Electron - Energy $= mc^2$
Momentum $= 0$	Momentum $= mv$
where, $m_0 = 9.1 \times 10^{-31}$ kgs	where, $\underset{\text{(Relativistic mass)}}{m} = \frac{m_0}{\sqrt{1 - \frac{v^2}{c^2}}}$

Now applying law of conservation of energy before & after collision.

$$h\nu + m_0 c^2 = h\nu' + mc^2$$

$$mc^2 = m_0 c^2 + h(\nu - \nu')$$

squaring both sides

$$m^2 c^4 = m_0^2 c^4 + h^2(\nu - \nu')^2 + 2 m_0 c^2 h(\nu - \nu') \quad \text{——— (1)}$$

Applying the law of conservation of momentum

Along x-axis -

$$\frac{h\nu}{c} + 0 = \frac{h\nu'}{c}\cos\theta + mv\cos\phi$$

$$\Rightarrow \quad mvc\cos\phi = h\nu - h\nu'\cos\theta \quad \text{——— (2)}$$

Applying

Along y-axis

$$0 + 0 = \frac{h\nu'}{c}\sin\theta - mv\sin\phi$$

$$\Rightarrow \quad mvc\sin\phi = h\nu'\sin\theta \quad \text{——— (3)}$$

squaring & adding eq's (2) & (3)

$$m^2 v^2 c^2 = h^2\nu'^2\sin^2\theta + h^2\nu^2 + h^2\nu'^2\cos^2\theta - 2h^2\nu\nu'\cos\theta$$

$$\Rightarrow \quad mv^2c^2 = h^2\nu'^2 + h^2\nu^2 - 2h^2\nu\nu'\cos\theta \quad \text{——— (4)}$$

Subtracting eq^n (4) from (1)

$$m^2c^2(c^2 - v^2) = m_0^2 c^4 + \cancel{h^2\nu^2} + \cancel{h^2\nu'^2} - 2h^2\nu\nu' + 2m_0c^2h(\nu - \nu')$$
$$- \cancel{h^2\nu^2} - \cancel{h^2\nu'^2} + 2h^2\nu'\nu\cos\theta$$

$$\Rightarrow \frac{m_0^2 c^4}{(c^2-v^2)}(c^2-v^2) = m_0^2 c^4 - 2h^2 \nu\nu'(1-\cos\theta) + 2 m_0 c^2 h(\nu-\nu').$$

$$\Rightarrow \cancel{2} m_0 c^2 \cancel{h}(\nu-\nu') = \cancel{2}\cancel{h^2}\nu\nu'(1-\cos\theta)$$

$$\frac{(\nu-\nu')}{\nu\nu'} = \frac{h(1-\cos\theta)}{m_0 c^2}$$

$$\frac{1}{\nu'} - \frac{1}{\nu} = \frac{h}{m_0 c^2}(1-\cos\theta)$$

$$\frac{c}{\nu'} - \frac{c}{\nu} = \frac{h}{m_0 c}(1-\cos\theta) \Rightarrow \boxed{\Delta\lambda = \lambda' - \lambda = \frac{h}{m_0 c}(1-\cos\theta)}$$

→ Oblique factor

* Compton shift depends on 'θ' only
↓ scattering angle

* when $\theta = 0$, $\Delta\lambda = \lambda' - \lambda = 0 \Rightarrow \boxed{\lambda' = \lambda}$

Unmodified Rad

* $\theta = \frac{\pi}{2}$, $\Delta\lambda = \frac{h}{m_0 c} = 0.024\,A^\circ$ → Compton wavelength

→ Modified radiation.

* $\theta = \pi$, $\Delta\lambda = \frac{2h}{m_0 c} = 0.048\,A^\circ$

Wien's Displacement Law from Planck's formula :

Planck's Radiatiation formula : $u_\lambda d\lambda = \frac{8\pi hc}{\lambda^5}\frac{d\lambda}{(e^{hc/\lambda KT}-1)}$

To find wavelength at which the emissitivity has its max, value put $\frac{du_\lambda}{d\lambda} = 0$

$$\therefore \frac{du_\lambda}{d\lambda} = 8\pi hc\left[-5\lambda^{-6}(e^{hc/\lambda KT}-1)^{-1} + \lambda^{-5}(-1)(e^{hc/\lambda KT}-1)^{-2} \times e^{hc/\lambda KT}\left(-\frac{hc}{\lambda^2 KT}\right)\right] = 0$$

or, $$\frac{-5}{\cancel{\lambda^6}(e^{hc/\lambda KT}-1)} + \frac{hc}{\lambda^2 KT}\left[\frac{e^{hc/\lambda KT}}{\cancel{\lambda^5}(e^{hc/\lambda KT}-1)^{\cancel{2}}}\right] = 0$$

or, $$5 = \frac{hc}{\lambda KT}\frac{e^{hc/\lambda KT}}{(e^{hc/\lambda KT}-1)} \qquad \left(\text{put } \frac{hc}{\lambda KT} = x\right)$$

$$5 = \frac{x\, e^{x}}{(e^{x}-1)} = \frac{x}{(1-e^{-x})} \Rightarrow \frac{x}{5} = 1-e^{-x} \text{ or } \frac{x}{5}+e^{-x} = 1$$

This eq^n has singh root given by $x = 4.965$ & ∴ x is constant

$$\frac{hc}{\lambda KT} = 4.965$$

wavelength for which emissibity is max is given by

$$\lambda_m T = \frac{hc}{4.965K} = b\,(\text{say})$$ This is wein's displacement Law.

PHOTON

*After Max Planck, German physicist **Albert Einstein** revisited the theory and proposed that quantization is a fundamental property of light and other electromagnetic radiation. He then explained photoelectric effect on the same basis.*
This led to the concept of "photons".

Definition: A quantum of light is known as a ***photon***.

The basic properties of photons:

- *They have zero mass and rest energy. They only exist as moving particles.*
- *They are elementary particles despite lacking rest mass.*
- *They have no electric charge.*
- *They are stable.*
- *They are spin-1 particles which makes them bosons.*
- *They carry energy and momentum which are dependent on the frequency.*
- *They can have interactions (collisions) with other particles such as electrons (e.g.Compton effect).*
- *They can be destroyed or created by many natural processes, for instance when radiation is absorbed or emitted.*
- *When in empty space, they travel at the speed of light.*

Duality of Light

- *Einstein extended Planck's concept of quantization to electromagnetic waves and explained Photoelectric effect.*
- *Then Compton and Debye extended Einstein's idea of photon momentum to explain scattering of x-rays from electrons, and called it the Compton effect.*

On the basis of above it was understood that a complete understanding of the observed behaviour of light can be attained only if light is supposed to possess Dual Nature,
i.e. ***Light (em waves) have wave nature as well as corpuscular or particle nature, both.***

de-Broglie Hypothesis

After Albert Einstein's photon theory became accepted, the question became whether this was true only for light that it has dual nature or whether material objects also exhibited wave-like behaviour.
In 1924 French physicist Louis de Broglie proposed that matter has dual characteristic just like radiation.

His Hypothesis was – ***"All moving particles (matter) possess a wave nature also."***

This hypothesis about the dual nature of matter was based on the following observations:-

(a) The whole universe is composed of matter and electromagnetic radiations. Since both are formsof energy so can be transformed into each other.

(b) The matter loves symmetry. As the radiation has dual nature, matter should also possess dualcharacter.

Matter Waves: These particles which exhibit wave nature according to de-Broglie's hypothesis are called the MATTER WAVES or de-Broglie's waves.

- *These waves are different from em waves because electrically neutral particles like neutrons exhibit wave nature.*
- *These waves are also different from mechanical waves because they can propagate through vacuum also.*

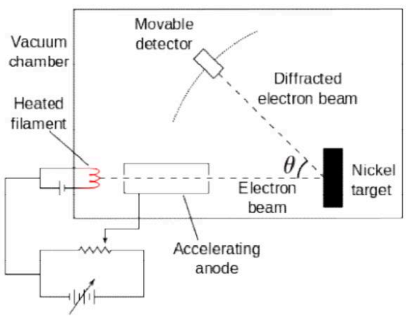
de-Broglie wavelength: de-Broglie's waves possess wave parameters. de Broglie derived the wavelength of a moving particle (matter wave) the wave nature of a particle as - $\boxed{\lambda = \frac{h}{p}}$ *where p = momentum of the particle, m = mass of the particle and v = velocity of the particle.*

This relation can also be applied to both microscopic and macroscopic matters.

Davisson- Germer Experiment: Experimental Confirmation of de-Broglie's Hypothesis

In 1927, physicists Clinton Davisson and Lester Germer, of Bell Labs, performed an experiment where they fired electrons at a crystalline nickel target with an objective to study the energies of the scattered electrons.

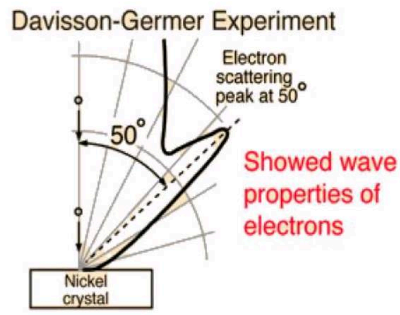
Same experiment was afterwards used to investigate the possibility of electron diffraction. The resulting diffraction pattern matched the predictions of the de Broglie hypothesis.



Experimental Set-up: The experimental setup is enclosed within a vacuum chamber to prevent the deflection and scattering of electrons by the medium.
The main parts of the experimental setup are:

- **Electron gun**: It is a Tungsten filament that emits electrons thermoionically when heated to a particular temperature.
- **Electrostatic particle accelerator**: Two oppositely charged plates, used to accelerate the electrons at a known potential.
- **Collimator**: A narrow cylindrical passage along the axis of the accelerator which renders a narrow & straight beam of electrons.

- **Target**: The target is a Nickel crystal. The electron beam is fired normally on the Nickel crystal. The crystal is placed such that it can be rotated about a fixed axis.
- **Detector**: A detector is used to capture the scattered electrons from the Ni crystal. The detector can be moved in a semicircular arc as shown in the figure.



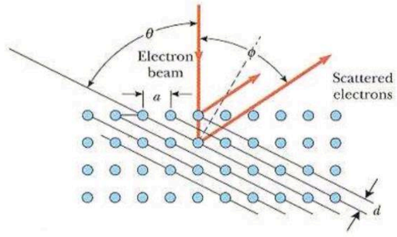
Working: Electrons were shot at the Ni target from the electron gun. The Ni target could be rotated about a fixed axis to observe angular dependence of the scattered electrons. These scattered electrons were detected at different scattering angles.

Observation: It was found that when the driving potential is 54V intensity of scattered electrons becomes significantly high at the scattering angle 50°.

Discussion: According to de-Broglie's hypothesis, the wavelength associated with the electrons accelerated through the potential difference V is given by

$$\lambda = \frac{h}{\sqrt{2m \times qV}} = \frac{h}{\sqrt{2m_e \times eV}} = \frac{6.6 \times 10^{-34}}{\sqrt{2 \times 9.1 \times 10^{-31} \times 1.6 \times 10^{-19} \times 54}} = 1.67A^o$$

Because for electron, $q = e = 1.6 \times 10^{-19}C$ & $m = m_e = 9.1 \times 10^{-31}Kg$



From X-ray analysis, it is known that Ni crystal acts as plane diffraction grating with inter planner spacing $\boldsymbol{d} = \mathbf{0.91}\boldsymbol{A^o}$. In this case we observe a maximum at $\boldsymbol{\theta = 50°}$. The corresponding angle of incidence relative to the family of Bragg planes (as shown in the figure) is $\boldsymbol{\theta = \frac{180-50}{2} = 65°}$. Bragg's equation for x-ray diffraction is

$$\boldsymbol{n\lambda = 2dsin\theta}$$

For n=1, $\lambda = 2dsin\theta = 2(0.91)sin65° = 1.65Å$

This is in good agreement with the wavelength computed from de-Broglie hypothesis.

Conclusion: This experiment establishes that electrons are found exhibiting diffraction. Hence, de-Broglie's hypothesis is confirmed.

de-Broglie wavelength: Derivation

Let us consider a photon whose energy is given as-

- According to Plank's theory $\boldsymbol{E = h\nu}$ ....(1)

  Where - ν= frequency

  & h = 6.6 ×10 $^{-34}$ J.s; Plank's const.
- *According to Einstein's relativity* $\boldsymbol{E = mc^2}$......(2)

Comparing eqn. (1) & (2), we ge

$$h\nu = mc^2$$

$$h\frac{c}{\lambda} = mc^2 \quad [\because c = \nu\lambda$$

$$\frac{h}{\lambda} = mc = p \quad \text{[p=momentum of photon}$$

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

This is the expression of *de-Broglie wavelength of a photon.*

On the same analogy, the ***de-Broglie wavelength*** **of a particle** of mass 'm' at velocity 'v' is given as

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

de-Broglie wavelength **of a particle in terms of its KE.**

Non-relativistic KE of a particle of mass 'm' at velocity 'v' is given as- $\mathrm{KE} = E_K = \frac{1}{2}mv^2$

$$E_K = \frac{1}{2}mv^2 = \frac{1}{2}mv^2 \times \frac{m}{m} = \frac{(mv)^2}{2m} = \frac{p^2}{2m}$$

Where p =mv, momentum of the particle

$$\Rightarrow \quad p = \sqrt{2m \times E_K}$$

We know that ***de-Broglie wavelength*** **of a particle** of mass 'm' at velocity 'v' is given as

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

$$\Rightarrow \quad \boxed{\lambda = \frac{h}{\sqrt{2m \times E_K}}}$$

de-Broglie wavelength **of a charged particle**

Let there be a charged particle carrying charge q and mass m moving with velocity v in a potential field V.

Then its KE is given as- $\mathrm{KE} = E_K = \frac{1}{2}mv^2 = qV$

$$E_K = \frac{(mv)^2}{2m} = \frac{p^2}{2m} = qV$$

Where p =mv, momentum of the particle

$$\Rightarrow \quad p = \sqrt{2m \times qV}$$

We know that ***de-Broglie wavelength*** **of a particle** of mass 'm' at velocity 'v' is given as $\lambda = \frac{h}{p}$

Or $\boxed{\boldsymbol{\lambda = \frac{h}{\sqrt{2m \times qV}}}}$

* ***If the charged particle be an electron***,

then $q = e = 1.6 \times 10^{-19}C$ & $m = m_e = 9.1 \times 10^{-31}Kg$

Above equation gives

$$\lambda_e = \frac{h}{\sqrt{2m_e \times eV}} = \frac{6.6 \times 10^{-34}}{\sqrt{2 \times 9.1 \times 10^{-31} \times 1.6 \times 10^{-19} V}} = \frac{12.28}{\sqrt{V}}A^o$$

de-Broglie wavelength **of a particle in thermal equilibrium**

Let there be a particle at temperature T Kelvin, with mass m moving with velocity v in a thermal equilibrium.

Then its KE is given as-

$$\mathrm{KE} = E_K = \frac{1}{2}m(v_{RMS})^2 = \frac{3}{2}KT$$

Where K = Boltzmann Cost.

$$E_K = \frac{(mv_{RMS})^2}{2m} = \frac{p^2}{2m} = \frac{3}{2}KT$$

Where p =mv_{RMS}, momentum of the particle

$$\Rightarrow \quad p = \sqrt{2m \times \frac{3}{2}KT} = \sqrt{3mKT}$$

We know that ***de-Broglie wavelength*** **of a particle** of mass 'm' at velocity 'v' is given as

$$\boxed{\lambda = \frac{h}{p} = \frac{h}{\sqrt{3mKT}}}$$

Wavelength of a particle : de-Broglie's wavelength :-

Let us consider the energy of a photon

$E = h\nu$ (Acc to Planck's Quantum Theory)

& $E = mc^2$ (Acc to Einstein's special theory)

$\Rightarrow$ $h\nu = mc^2$ $\Rightarrow$ $\frac{hc}{\lambda} = mc^2$ $\Rightarrow$ $\frac{h}{\lambda} = mc = p$ (momentum)

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

Similarly for a particle of mass 'm' at velocity 'v'

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

In terms of Kinetic Energy (K.E)

Non-relativistic K.E of a particle of mass 'm'

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

$\Rightarrow$ $p^2 = 2m \times (K.E)$

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

We know that de broglie's wavelength is

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

de-Broglie's wavelength of a charged particle :-

Let there be a particle of charge 'q' & mass 'm' at velocity 'v' in a potential difference 'V'. Then its K.E is given as

$KE = \frac{1}{2}mv^2 = qV$

$\Rightarrow$ $\frac{(mv)^2}{2m} = qV$ $\Rightarrow$ $\frac{p^2}{2m} = qV$ $\Rightarrow$ $\boxed{p = \sqrt{2mqV}}$

de-broglie's wavelength is

$$\boxed{\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mqV}}}$$ → use for charged particle

- if charge particle be an e^-

$q_e = 1.6 \times 10^{-19}$ C , $m_e = 9.1 \times 10^{-31}$ kg

$$\lambda = \frac{h}{\sqrt{2m_e q_e V}} = \frac{6.6 \times 10^{-34}}{\sqrt{2 \times 9.1 \times 10^{-31} \times 1.6 \times 10^{-19} \times V}} \Rightarrow \boxed{\lambda = \frac{12.28}{\sqrt{V}} \text{ Å}}$$

De-Broglie wavelength of a particle in thermal equilibrium

Let there be a particle at temperature 'T' Kelvin, with mass 'm' moving with velocity v in a thermal equilibrium.

Then it's K.E is given as :-

$$K.E = E_K = \frac{1}{2}m(v_{rms})^2 = \frac{3}{2}KT$$ where K = Boltzmann constant $K = 1.38 \times 10^{-23} J/K$

$$E_K = \frac{(m v_{rms})^2}{2m} = \frac{p^2}{2m} = \frac{3}{2}KT$$ where $p = m v_{rms}$, momentum of the particle.

$$\Rightarrow \quad p = \sqrt{2m \times \frac{3}{2}KT} = \sqrt{3mKT}$$

We known that de-broglie's wavelength of a particle of mass 'm' at velocity 'v' is given as

$$\lambda = \frac{h}{p} \Rightarrow \boxed{\lambda = \frac{h}{\sqrt{3mKT}}}$$

Q) Calculate the debroglie wavelength associated with a proton moving with a velocity equal to $(1/20)^{th}$ of velocity of light.

Soln Given : charge of proton

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

v_{p^+}, speed of proton $= \frac{1}{20}C = \frac{3 \times 10^8}{20} m/s$

m_{p^+}, mass of proton $= 1.67 \times 10^{-27} kg$

$$\Rightarrow \lambda = \frac{h}{mv} = \frac{6.6 \times 10^{-34} \times 20}{1.67 \times 10^{-27} \times 3 \times 10^8}$$

$$\boxed{\lambda = 2.634 \times 10^{-14} m}$$

Q) Calculate debroglie wavelength associated with a nitrogen atom at 3 atm & at 27°C.

Soln Given Temperature, T = 27°C

T in Kelvin = 27 + 273 K

= 300 K

$\because K = 1.38 \times 10^{-23} J/K$

m, mass of Nitrogen $= 4.65 \times 10^{-26} kg$

$$\lambda = \frac{h}{\sqrt{3mKT}}$$

$$= \frac{6.6 \times 10^{-34}}{\sqrt{3 \times 4.65 \times 10^{-26} \times 1.38 \times 10^{-23} \times 300}}$$

$$\boxed{\lambda = 2.754 \times 10^{-11} m}$$

Q) Find the de broglie wavelength of a neutron of energy 12.8 MeV (mass of neutron = 1.67×10^{-27} kg, $h = 6.63 \times 10^{-34}$ Js).

Soln Given:- $m = 1.67 \times 10^{-27}$ kg,

$h = 6.63 \times 10^{-34}$ Js

$E = 12.8$ MeV

$$\lambda = \frac{h}{\sqrt{2mE}} = \frac{6.63 \times 10^{-34}}{\sqrt{2 \times 1.67 \times 10^{-27} \times 12.8 \times 10^{6} \times 1.6 \times 10^{-19}}}$$

$$\boxed{\lambda = 8.02 \times 10^{-15}\ m}$$

Q) Calculate the de-broglie's wavelength of an α-particle accelerated through a P.D of 200V ($m_p = 1.67 \times 10^{-27}$ kg)

Soln Given:- $m_\alpha = 4 m_p = 4 \times 1.67 \times 10^{-27}$ kg

$q_\alpha = 2 q_e = 2 \times 1.6 \times 10^{-19}$ C

$V = 200$ V

$$\lambda = \frac{h}{\sqrt{2 m_\alpha q_\alpha V}} = \frac{h}{\sqrt{2 \times 4 m_p \times 2 q_e V}} = \frac{6.63 \times 10^{-34}}{\sqrt{16 \times 1.67 \times 10^{-27} \times 1.6 \times 10^{-19} \times 200}}$$

$$\lambda = \frac{6.63 \times 10^{-34}}{9.246 \times 10^{-23}}$$

$$= 0.713 \times 10^{-12}\ m$$

$$\boxed{\lambda = 0.00713\ A^\circ}$$

Wave Velocity

The velocity of advancement of a wave is called wave velocity is given as

$$\boxed{v_m = \nu\lambda}$$ where ν = frequency, λ = wavelength

Phase Velocity

It is the velocity with which the planes of constant phase (wavefronts) propagate through the medium.

It is given by $\boxed{v_p = \frac{\omega}{k}}$ where v_p = phase velocity

ω = angular frequency

k = propagation constant

Derivation:- Let there be a wave represented by

$$y = A\cos(\omega t - kx)$$

for the plane of constant phase $\Rightarrow$ $\{\omega t - kx = \text{constant}\}$

differentiating w.r.t 't' $\Rightarrow$ $\omega - k\frac{dx}{dt} = 0$

$$\frac{dx}{dt} = \frac{\omega}{k} \Rightarrow \boxed{v_p = \frac{\omega}{k}}$$

we know that

$$\omega = 2\pi\nu \quad \& \quad k = 2\pi/\lambda$$

$$v_p = \frac{\omega}{k} = \frac{2\pi\nu}{2\pi/\lambda} = \nu\lambda$$

$$\boxed{v_p = v_m}$$

Phase Velocity of a Particle Wave

Let us consider a particle of mass 'm' at velocity 'v' then its frequency, $\nu = \frac{mc^2}{h}$

& its wavelength, $\lambda = \frac{h}{mv}$

Then the phase velocity of the above particle is given by

$$v_p = \frac{\omega}{k} = \nu\lambda = \frac{\cancel{m}c^2}{\cancel{h}} \times \frac{\cancel{h}}{\cancel{m}v} \Rightarrow \boxed{v_p = \frac{c^2}{v}}$$

This shows that

- $v_p \neq v$
- $v_p = v$ where $v = c$, which is impossible

Wave group / Packet –

Schrodinger Postulated that a moving particle is not equivalent to a single wave by its behaviour / behaves as a wave group or a wave packet.

" An Amplitude Modulated Resultant wave produced by the superposition of two coherent waves is called a wave group / packet."

Group Velocity –

The velocity with which a wave group propagates in the space is called group velocity. It is given by $\boxed{v_g = \frac{d\omega}{dk}}$

- Derivation :- Let there be two coherent waves as under

$$y_1 = A\cos(\omega t - Kx) \quad \text{—— (1)}$$

$$y_2 = A\cos\left[(\omega + d\omega)t - (K + dk)x\right] \quad \text{— (2)}$$

If the two waves superimpose then the resultant is

$$y = y_1 + y_2$$

$$\Rightarrow y = A\cos\underbrace{(\omega t - Kx)}_{D} + A\cos\underbrace{\left[(\omega + d\omega)t - (K + dK)x\right]}_{C}$$

$$\left\{\text{using } \cos C + \cos D = 2\cos\left(\frac{C+D}{2}\right)\cos\left(\frac{C-D}{2}\right)\right\}$$

$$\Rightarrow y = 2A\cos\left[\left(\frac{2\omega + d\omega}{2}\right)t - \left(\frac{2K + dK}{2}\right)x\right]\cos\left(\frac{d\omega}{2}t - \frac{dk}{2}x\right)$$

$$\because \quad 2\omega >> d\omega \quad \& \quad 2K >> dK$$

$$\Rightarrow y = 2A\cos(\omega t - Kx)\cos\left(\frac{d\omega}{2}t - \frac{dk}{2}x\right)$$

$$\Rightarrow y = \underbrace{\left[2A\cos\left(\frac{d\omega}{2}t - \frac{dk}{2}x\right)\right]}_{\text{Amplitude of modulated wave}}\cos(\omega t - Kx) \quad \text{—— (3)}$$

This shows that the resultant is an amplitude modulated wave.

Considering the Amplitude only:

$$\text{Amp.} = 2A\cos\left(\frac{d\omega}{2}t - \frac{dK}{2}x\right)$$

$$= 2A\cos\left[\frac{d\omega}{2}\left(t - \frac{dK}{d\omega}x\right)\right]$$

$$= 2A\cos\left[\frac{d\omega}{2}\left(t - \frac{x}{d\omega/dK}\right)\right]$$

$$= 2A\cos\left[\frac{d\omega}{2}\left(t - \frac{x}{v_g}\right)\right]$$

Here the amplitude modulated resultant propagates with velocity $\boxed{v_g = \frac{d\omega}{dK}}$

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* Relation b/w Group velocity & Particle velocity

Let there be a particle of mass 'm' at velocity 'v'. Then its freq. $\nu = \frac{mc^2}{h}$ & wavelength $\lambda = \frac{h}{mv}$

The angular freq. is given by

$$\omega = 2\pi\nu = 2\pi\frac{mc^2}{h} = \frac{2\pi m_0 c^2}{h} \times \frac{1}{\left(1-\frac{v^2}{c^2}\right)^{1/2}}$$

diff. w.r.t 'v'

$$\frac{d\omega}{dv} = \frac{2\pi m_0 c^2}{h}\frac{d}{dv}\left(1-\frac{v^2}{c^2}\right)^{-1/2} = \frac{2\pi m_0 \cancel{c^2}}{h} \times \left(-\frac{1}{2}\right)\left(1-\frac{v^2}{c^2}\right)^{-3/2} \times \left(-\frac{2v}{\cancel{c^2}}\right)$$

$$\frac{d\omega}{dv} = \frac{\frac{2\pi m_0 v}{h}}{\left(1-\frac{v^2}{c^2}\right)^{3/2}} \quad \text{——— (1)}$$

Now the propagation constant is

$$K = \frac{2\pi}{\lambda} = 2\pi \times \frac{mv}{h} = \frac{2\pi m_0}{h} \times \frac{v}{\left(1-\frac{v^2}{c^2}\right)^{1/2}}$$

diff. w.r.t 'v'

$$\frac{dK}{dv} = \frac{2\pi m_0}{h} \times \frac{d}{dv}\left[v \times \left(1-\frac{v^2}{c^2}\right)^{-1/2}\right]$$

$$= \frac{2\pi m_0}{h} \times \left[\left(1-\frac{v^2}{c^2}\right)^{-1/2} + \left(+\cancel{\tfrac{1}{2}}\right)\left(1-\frac{v^2}{c^2}\right)^{-3/2}\left(\frac{\cancel{2}v^2}{c^2}\right)\right]$$

$$= \frac{2\pi m_0}{h} \times \left(1-\frac{v^2}{c^2}\right)^{-3/2}\left[\left(1-\cancel{\frac{v^2}{c^2}}\right) + \cancel{\frac{v^2}{c^2}}\right]$$

$$\frac{dK}{dv} = \frac{2\pi m_0}{h} \times \frac{1}{\left(1-\frac{v^2}{c^2}\right)^{3/2}} \quad — (2)$$

div. eq^n (1) by (2)

$$\Rightarrow \frac{d\omega/dv}{dK/dv} = \cancel{\frac{2\pi m_0}{h}} \times \frac{v}{\cancel{\left(1-\frac{v^2}{c^2}\right)^{3/2}}} \times \cancel{\frac{h}{2\pi m_0}} \times \cancel{\left(1-\frac{v^2}{c^2}\right)^{3/2}}$$

$$\Rightarrow \frac{d\omega}{dK} = v \quad \Rightarrow \boxed{v_g = v}$$

* if $\nu = \frac{mc^2}{h}$ & $\lambda = \frac{h}{mv}$

we have $v_p = \frac{\omega}{K} = \nu\lambda$

$$= \frac{\cancel{m}c^2}{\cancel{h}} \times \frac{\cancel{h}}{\cancel{m}v}$$

$$v_p = \frac{c^2}{v} = \frac{c^2}{v_g} \quad (\because v_g = v)$$

$$\Rightarrow \boxed{v_p \times v_g = c^2}$$

(A) Relation b/w Group velocity & Phase velocity

we know that the phase velocity is

$$v_p = \frac{\omega}{K} \Rightarrow \omega = v_p K$$

diff. w.r.t 'K'

$$\frac{d\omega}{dK} = v_p + K\frac{dv_p}{dK}$$

$$v_g = v_p + K\frac{dv_p}{d\lambda} \times \frac{d\lambda}{dK}$$

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

we have

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

diff. w.r.t 'K'

$$\frac{d\lambda}{dK} = -\frac{2\pi}{K^2}$$

$$\Rightarrow K\frac{d\lambda}{dK} = \frac{-2\pi}{K} = \frac{-2\pi}{2\pi/\lambda}$$

$$\Rightarrow K\frac{d\lambda}{dK} = -\lambda$$

placing this value in eq^n (1)

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

* for Non-dispersive medium

$$\frac{dv_p}{d\lambda} = 0 \Rightarrow \boxed{v_g = v_p}$$

* for dispersive medium

$$\frac{dv_p}{d\lambda} \neq 0 \Rightarrow \boxed{v_g < v_p}$$

Wave function

" The quantity whose periodic variation describes the propagation of a wave is called wave function. "

For the matter-wave it is denoted by $\boxed{\Psi = \Psi_0 e^{-i\omega t}}$

probability amplitude

Amplitude ~~(const. quantity)~~

- Ψ is often a complex quantity.
- Ψ is always a +ve & real quantity.
- Ψ is also known as the probability amplitude.

Physical Significance of wave function Ψ

Acc. to Max Bond, "wave function Ψ has no physical significance of its own, rather the square of the absolute magnitude of wave function. $|\Psi|^2$ evaluated at a particular point at a particular time instance gives the probability of finding a particle at that point at that time instance."

• $|\psi|^2$ is also known as the probability density.

Condition of acceptability for a wave function

For a function to be accepted as a wave function for a matter wave it should satisfy the following conditions —

• ψ should be continuous, finite & single value at a particular point at a particular time instance.

• ψ should be normalized (i.e)

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

Schrödinger Wave Equation

"Schrodinger wave eqn is a mathematical expression describing the energy & position of a particle in space & time, taking into account its wave nature."

It is expressed in two forms —

* Time-Independent form → $\nabla^2\psi + \frac{2m}{\hbar^2}(E-V)\psi = 0$

* Time-Dependent form → $-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = i\hbar\frac{\partial\psi}{\partial t}$

(where $\hbar = \frac{h}{2\pi}$)

$\nabla^2 \rightarrow$ Laplacian $\rightarrow \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$

Time-Independent form

Proof: Let there be a particle with mass 'm' at velocity 'v' and Potential energy 'V'. Then its total energy is

$$E = K.E + P.E$$

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

$$= \frac{(mv)^2}{2m} + V$$

$$E = \frac{p^2}{2m} + V \Rightarrow p = \sqrt{2m(E-V)}$$

de-broglie's wavelength is

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2m(E-V)}} \quad \text{— (1)}$$

Let us suppose that its wave function is

$$\psi = \psi_0 e^{-i\omega t} \quad \text{--- (2)}$$

We know that general wave eq^n is given as

$$\nabla^2 \psi = \frac{1}{u^2}\frac{\partial^2 \psi}{\partial t^2} \quad \text{--- (3)}$$

(where ψ = wave function
$u = \nu\lambda$; wave speed)

Let us diff^ng eq (2) partially w.r.t 't' we get

$$\frac{\partial \psi}{\partial t} = \psi_0 e^{-i\omega t}(-i\omega)$$

diff^ng again

$$\frac{\partial^2 \psi}{\partial t^2} = \psi_0 e^{-i\omega t}(-i\omega)^2 = -\omega^2\psi \quad \text{--- (4)}$$

placing this value in eq^n (3) we get

$$\nabla^2\psi = -\frac{\omega^2}{u^2}\psi = -\left(\frac{2\pi\cancel{\nu}}{\cancel{\nu}\lambda}\right)^2\psi$$

$$\Rightarrow \nabla^2\psi + \frac{4\pi^2}{\lambda^2}\psi = 0 \quad \text{--- (5)}$$

from eq^n (1), substituting in eq^n (5), we get

$$\nabla^2\psi + \frac{4\pi^2}{h^2} \times 2m(E-V)\psi = 0$$

$$\Rightarrow \boxed{\nabla^2\psi + \frac{2m}{\hbar^2}(E-V)\psi = 0} \quad \text{--- (6)} \qquad \left(\because \hbar = \frac{h}{2\pi}\right)$$

for free space
$V=0$

This is Schrodinger Eq^n in Time-Independent form.

Time-Dependent form

Proof:- We know that wave function is $\psi = \psi_0 e^{-i\omega t}$

diff^ng partially w.r.t 't'

$$\frac{\partial\psi}{\partial t} = -i\omega\psi = -i(2\pi\nu)\psi = -i\left(2\pi \times \frac{E}{h}\right)\psi \qquad (\because E = h\nu)$$

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

$$\Rightarrow E\psi = -\frac{\hbar}{i}\frac{\partial\psi}{\partial t} = i\hbar\frac{\partial\psi}{\partial t} \quad \text{--- (7)}$$

From eqn (6), we have

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

dividing throughout by $-\frac{2m}{\hbar^2}$

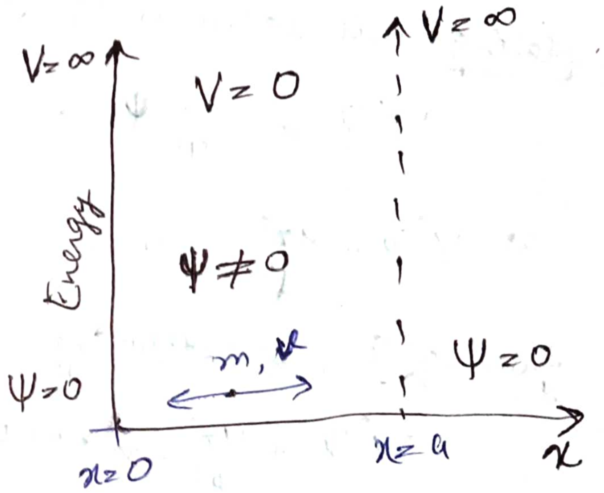
$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi$$

Substituting from eqn (7) in the above, we get

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

This is schrödinger eqn in time-dependent form.

Particle in a Box



Let there be a partical of mass 'm' travelling at velocity 'v' with-in the limits, $0>x>a$, along x-axis only.

ψ is a function of x & t

Now Schrodinger wave eqn in time-independent form is given as

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

for the above particle

$V=0$ $\quad \frac{\partial^2\psi}{\partial x^2} + \frac{2m}{\hbar^2}E\psi = 0$ —— (1)

$$\Rightarrow \frac{\partial^2\psi}{\partial x^2} + \left(\frac{8\pi^2 mE}{h^2}\right)\psi = 0$$

Let $\boxed{K^2 = \frac{8\pi^2 mE}{h^2}}$ (2) where K is arbitrary constant

eqn (1) becomes $\quad \frac{\partial^2\psi}{\partial x^2} + K^2\psi = 0$ —— (3)

General solution to the above eqn would be given as

$\psi = A\sin Kx + B\cos Kx$ (4) where A, B, K - arbitrary constants

Applying boundary condition

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

$\Rightarrow$ eqn (4) becomes

$$0 = A \sin 0 + B \cos 0$$

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

Hence, eqn (4) takes the form $\psi = A \sin Kx$ — (5)

* at $x = a$, $\psi = 0$

placing the above in eqn (5)

$$0 = A \sin(Ka) \Rightarrow \sin(Ka) = 0$$

or, $Ka = n\pi$ $(n = 1, 2, 3 \dots)$

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

Substituting the above in eqn (5)

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

* Now ψ is Normalized in the region $0 > x > a$

i.e $\int_0^a |\psi|^2 dx = 1$

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

$$\Rightarrow \frac{A^2}{2}\left[x - \left(\frac{a}{2n\pi}\right)\sin\left(\frac{2n\pi x}{a}\right)\right]_0^a = 1 \Rightarrow \frac{A^2}{\cancel{1}} \cancel{\times} \frac{a}{2} = 1 \Rightarrow \boxed{A = \sqrt{\frac{2}{a}}}$$

→ Normalized wave function is $\boxed{\psi_n = \sqrt{\frac{2}{a}} \times \sin\left(\frac{n\pi x}{a}\right)}$

Now to find energy let us place the value of K in eqn (2)

$$\frac{8\pi^2 m E}{h^2} = \frac{n^2 \pi^2}{a^2} \Rightarrow \boxed{E_n = n^2 \frac{h^2}{8ma^2}}$$

Eigen function & Eigen values

We have $\psi_n = \sqrt{\frac{2}{a}} \times \sin\left(\frac{n\pi x}{a}\right)$ & $E_n = n^2 \frac{h^2}{8ma^2}$

at $n = 0$, $E_0 = 0$, $\psi_0 = 0$; Particle is at rest / No particle wave

at $n = 1$, $E_1 = \frac{h^2}{8ma^2}$, $\psi_1 = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right)$; ground state of particle wave

at $n = 2$, $E_2 = \frac{h^2}{2ma^2}$, $\psi_2 = \sqrt{\frac{2}{a}} \sin\left(\frac{2\pi x}{a}\right)$; 1st excited state

at $n = 3$, $E_3 = \frac{9}{8} \times \frac{h^2}{ma^2}$, $\psi_3 = \sqrt{\frac{2}{a}} \sin\left(\frac{3\pi x}{a}\right)$; 2nd Excited state