Unit-IV
Quantum Mechanics

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Introduction

- At the end of the nineteenth century, physics consisted essentially of classical mechanics(CM), the theory of electromagnetism(EM), and thermodynamics.

Classical mechanics tells us how everyday objects move. It is the theory of **motion**.

Sir Isaac Newton

1687

1. An object in motion tends to stay in motion.
2. Force equals mass times acceleration.
3. For every action there is an equal and opposite reaction.

Mechanic

Spacecraft

Doctor

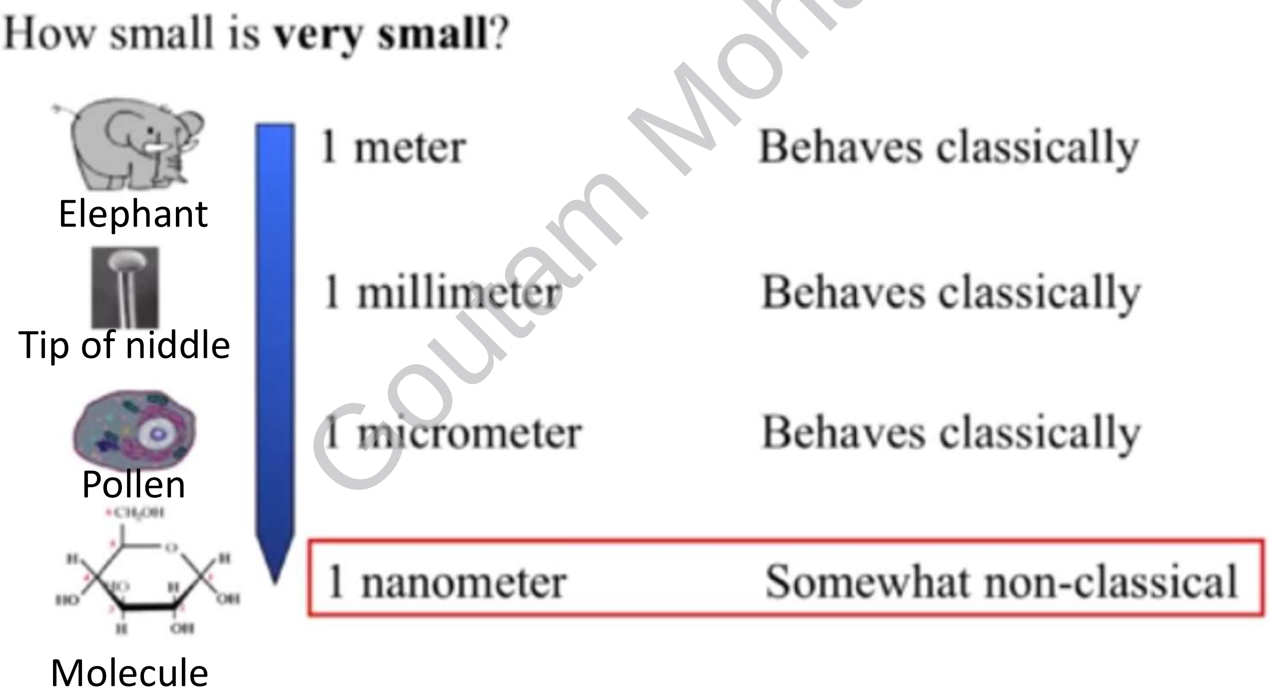
Electrician

- At the end of Nineteenth Century, Several people are reported to have said something like this:

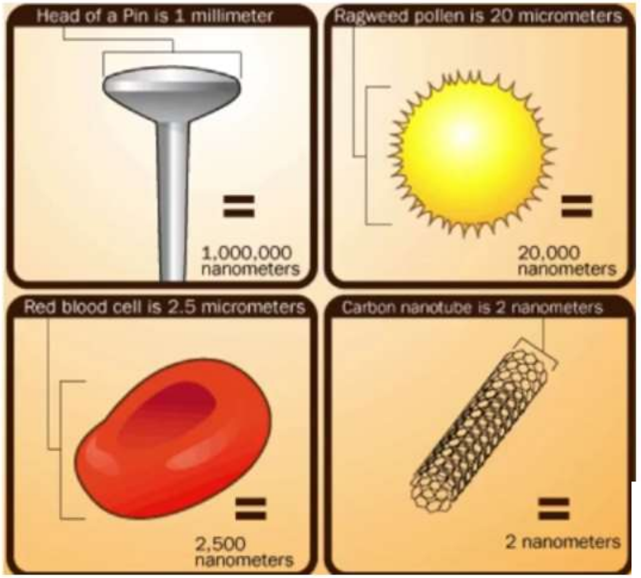
There is nothing new to be discovered in physics now. All that remains is more and more precise measurement !!

- At the turn of the twentieth century, however, classical physics, which had been quite unassailable, was seriously challenged on two major fronts: Relativistic Domain and Microscopic Domain.

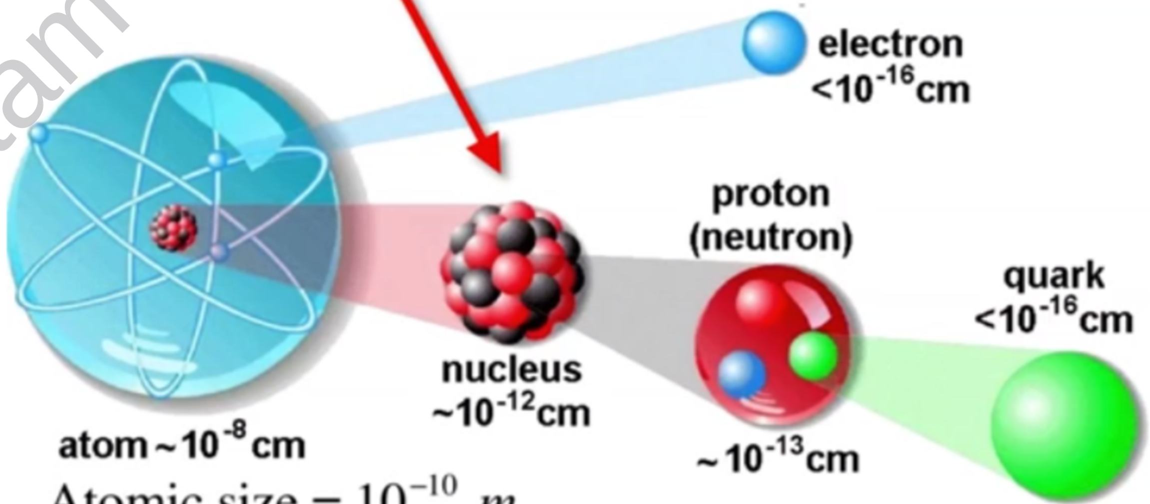
When dealing with very small things:



BIG and SMALL



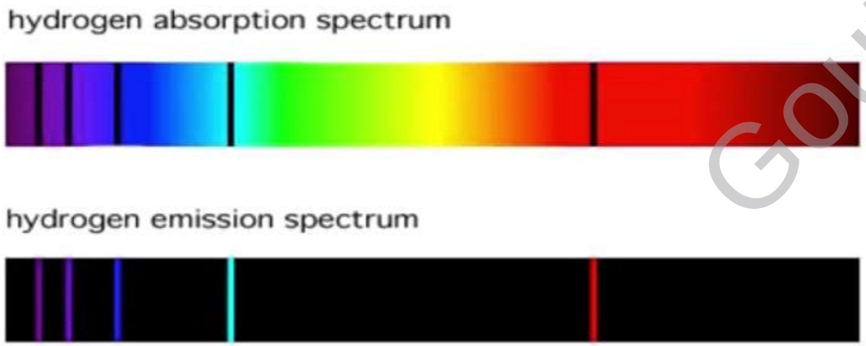
QM IS NEEDED FOR UNDERSTANDING OBJECTS THAT ARE STILL SMALLER



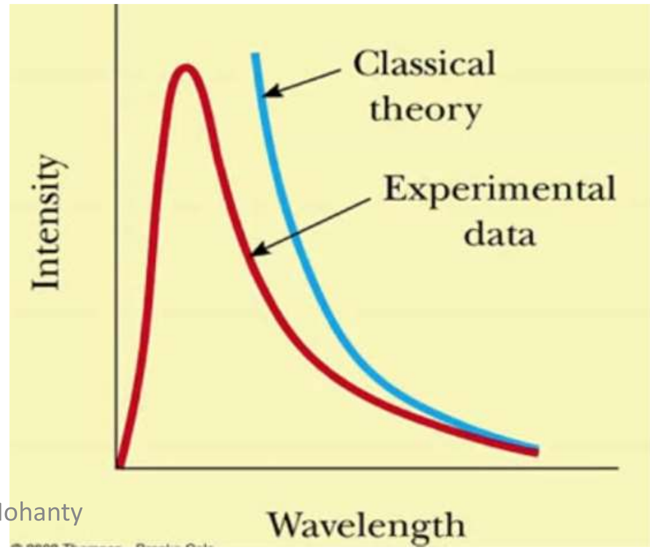
$$\text{Atomic size} = 10^{-10}\ m$$

Few puzzling questions

- Why do atoms absorb or emit light only at particular frequencies?
- Why do not electrons fall into the nucleus?
- Why do not atoms disintegrate on collisions?
- Where does the structure of periodic table come from?
- Why do atoms form chemical bonds?
- If you heat a body it will obviously emit radiate energy. Why is the amount of energy predicted by classical physics completely different from that which is experimentally observed?



This is a strong hint that atoms have quantized in nature.



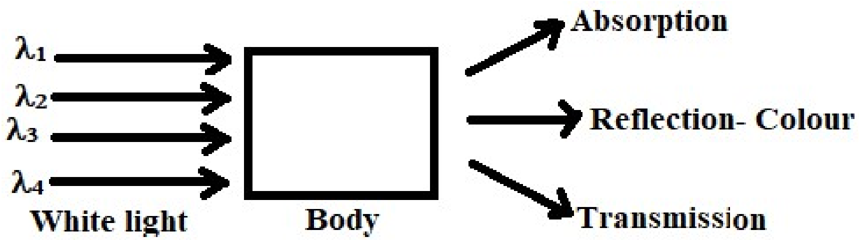
- Classical Mechanics couldn't explain the non relativistic motion of very small particles (i.e. electrons, protons etc.), stability of atoms, spectral distribution of blackbody radiation, photoelectric effect, Compton effect, Raman effect.

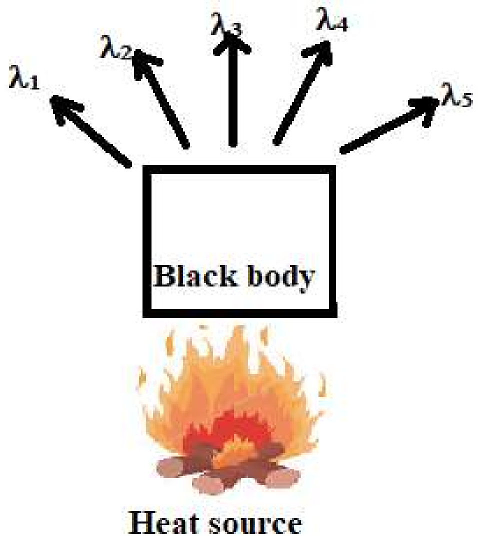
- Thus the failure of CM led to the birth of Quantum Mechanics (QM)

- In 1900, Max Planck introduced the concept of the quantum of energy. Energy exchange between an EM-wave of frequency (ν) and matter occurs only in integer multiples of hν, which he called the energy of a quantum, where h is a fundamental constant called Planck's constant and $h = 6.62 \times 10^{-34}$ J-s. ----→→explain the phenomenon of blackbody radiation.
- In 1905, Einstein explained light is made of discrete bits of energy (or tiny particles), called photons, each of energy hν, where ν is frequency of the light. The experimentally observed by Heinrich Rudolf Hertz.
- In 1913, Neils Bohr explained that that atoms can be found only in discrete states of energy and that the interaction of atoms with radiation, i.e., the emission or absorption of radiation by atoms, takes place only in discrete amounts of hν, because it results from transitions of the atom between its various discrete energy states.-→ Atomic stability and atomic spectroscopy.
- In 1923, Compton made an important discovery that gave the most conclusive confirmation for the corpuscular aspect of light.
- In 1923, De-Broglie introduced another powerful new concept --> Not only radiation does exhibit particle-like behaviour but, conversely, *material particles* themselves display *wave-like* behaviour. This concept was experimentally confirmed by Davisson and Germer (1927).

- Then after a new concept Quantum Mechanics was came in the TWO different forms: Matrix mechanics and wave mechanics
- In 1925, Heisenberg introduced matrix mechanics which describes atomic structure starting from the observed spectral lines. The only allowed values of energy exchange between microphysical systems. He describes the dynamics of microscopic systems using eigen value
- In 1926, Schrödinger described the dynamics of microscopic matter by means of a differential wave equation called the Schrödinger equation.
- In 1927 Max Born proposed his *probabilistic* interpretation of wave mechanics.
- In 1928, combining special relativity with quantum mechanics, Dirac derived an equation which describes the motion of electrons. This equation, known as Dirac's equation.
- In summary, quantum mechanics is the theory that describes the dynamics of matter at the microscopic scale.

Black Body Radiation:

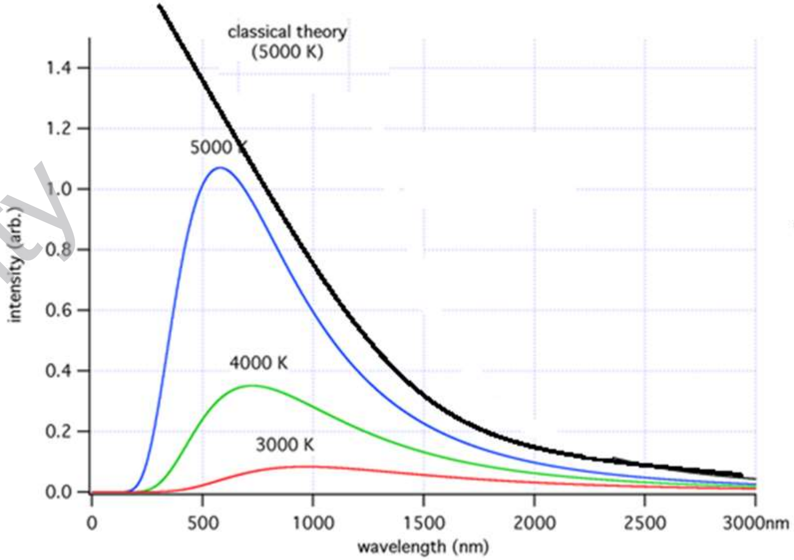




Black Body:

- A Blackbody is a body which absorbs all incident lights. But practically no perfect black body is existing.
- When black body heated it emits all radiations.
- At equilibrium, the emitted radiation has a well defined, continuous energy distribution: to each frequency there corresponds an energy density which depends neither on the chemical composition of the object nor on its shape, but only on the temperature of the cavity's walls.

- At a given temperature, the energy is not uniformly distributed in the radiation spectra blackbody.
- At a given temperature, the intensity of radiation increases with increase in wavelength and at a particular wavelength, its value is maximum. With further increase in wavelength, the intensity of radiation decreases.
- With the increase in temperature, λ_m decreases, where λ_m is the wavelength at which the maximum emission of energy takes place.
- There is increase in energy emission with the increase in temperature corresponding to all the wavelengths.
- The area under each curve gives the total energy emitted for the complete spectrum at a particular temperature. With the increase in temperature, this area increases. It is also observed that the area is directly proportional to the fourth power of the temperature of the blackbody.



$$\lambda_m T = constant$$

$$I_m/T = constant$$

$$I_{total} = \int_0^{\infty} I \, d\lambda = \sigma T^4$$

- Wien's displacement law, $\boxed{\lambda_m T = b = constant}$, $b = 2.89 \times 10^{-3}\, mK$

- Wien's spectral density, $\boxed{u(\lambda)d\lambda = \frac{A}{\lambda^5[e^{B/\lambda T} - 1]} d\lambda,}$

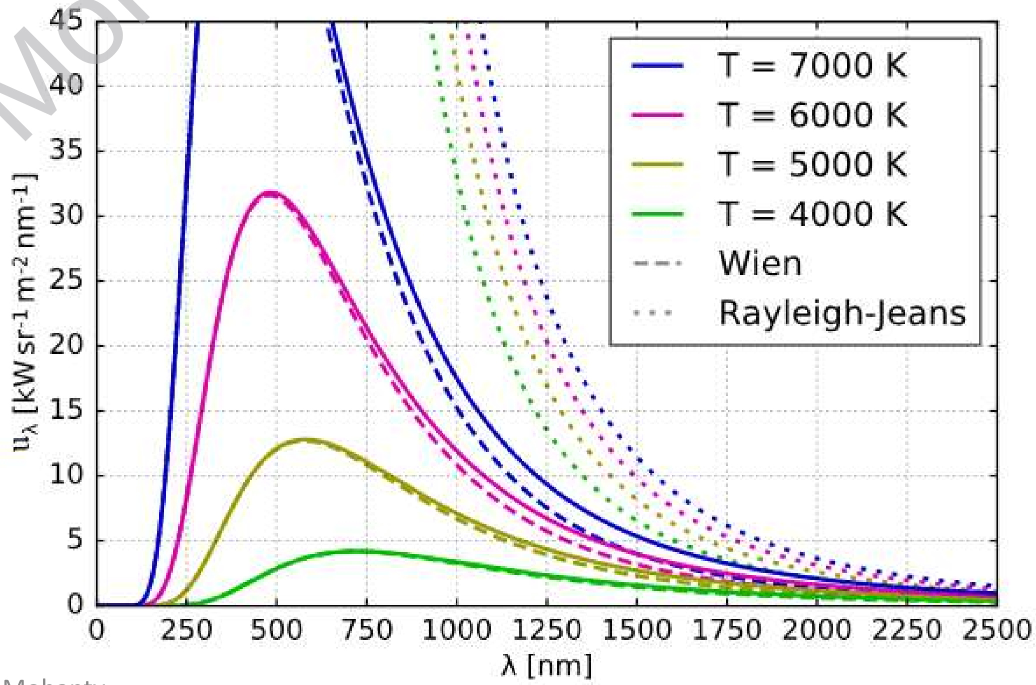
  where A and B are constant

- This Wien's distribution law is valid for short wavelength only

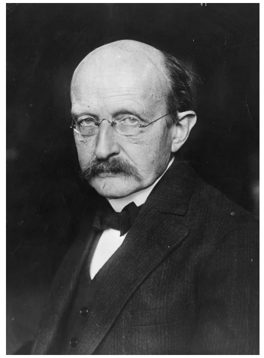
- From classical EM-theory, according to Rayleigh spectral energy density i.e. $\boxed{u(\lambda)d\lambda = \frac{8\pi kT}{\lambda^4} d\lambda}$. This is Rayleigh-Jeans Law

- This law is valid for long wavelength only.

$$\frac{I}{c} = u(\lambda) = spectral\ energy\ density$$



Planck’s Hypothesis

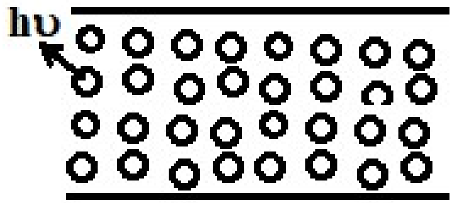


Max Planck

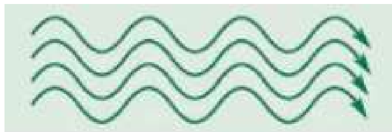
- In 1900, Planck argued that Light is made of packets of energy called quanta--> E = hν, where h= Planck’s constant= 6.626×10^{-34} J-Sec
- Quantum theory began, E = hν =hc/λ
- E(eV) = 1242/λ(nm)= 1242/λ(Å)
- 1eV = 1.6×10^{-19} J
- From Quantum EM-theory, $u(\lambda)d\lambda = \frac{8\pi hc}{\lambda^5[e^{hc/\lambda kT}-1]}d\lambda$

(or) $$\boxed{u(\nu)d\nu = \frac{8\pi\nu^2}{c^3}\frac{h\nu}{e^{h\nu/kT}-1}d\nu,}$$

- This is called Planck’s Radiation Law



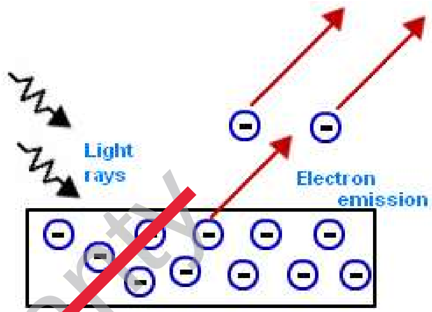
Particle nature



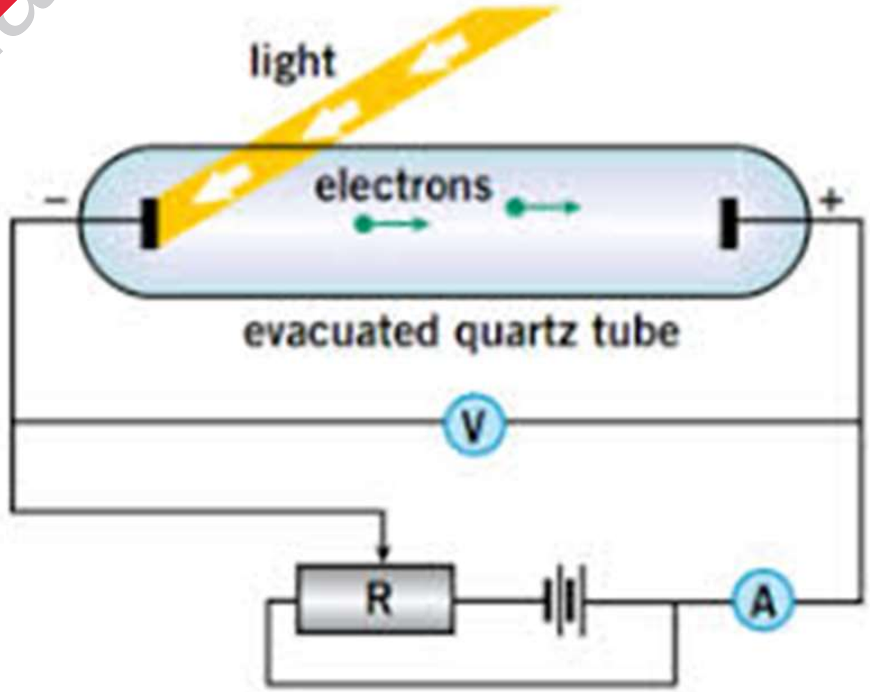
Wave nature

Photoelectric Effect

- The photoelectric effect provides a direct confirmation for the energy quantization of energy.
- In 1887, Hertz discovered the photoelectric effect.
- The emission of electrons from metal surface when illuminated by light or any other radiation of suitable wavelength (or frequency) is known as photoelectric effect.
- The emitted electrons are known as photoelectron and current constituted by these electrons is known as photocurrent.



Heinrich Hertz

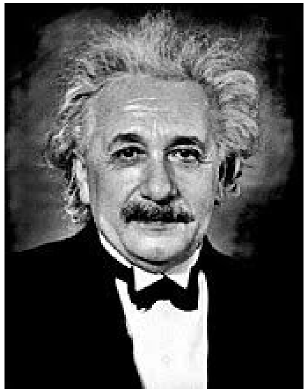


Laws of photoelectric effect:

1. Photoelectric emission starts as soon as radiation falls on metal surface.
2. Minimum frequency (called Threshold frequency, ν_0) is required to eject photoelectrons from metal surface.
3. Photocurrent is proportional to the intensity of the incident light but not frequency of light.
4. The K.E of photoelectron is depend on the frequency of incident light but not intensity of incident light.

These experimental findings cannot be explained using the classical mechanics.

Einstein's photoelectric effect



Einstein

- In 1905, Einstein successfully explained this effect.
- Light consist of photons and each photon has an energy $h\nu$.
- Each photon can eject One electron from the metal surface.
- A part of photon energy is used to eject electron and rest is used to give K.E. to the ejected photoelectrons.
- Governing equation,

$$\boxed{h\nu = \phi + K.E = h\nu_0 + \tfrac{1}{2}(mv^2)}$$, Where ϕ = work function

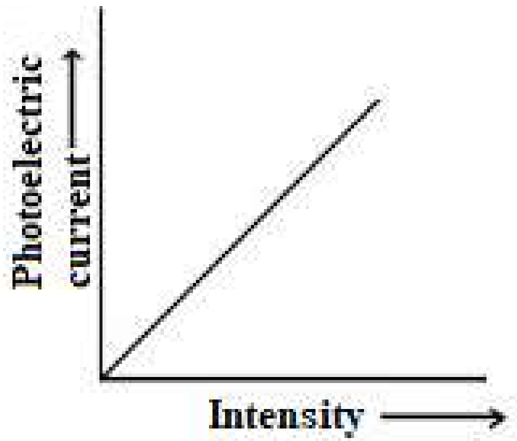
$$\Rightarrow \tfrac{1}{2}(mv^2) = h\nu - h\nu_0$$

$$\Rightarrow eV_s = h\nu - h\nu_0$$

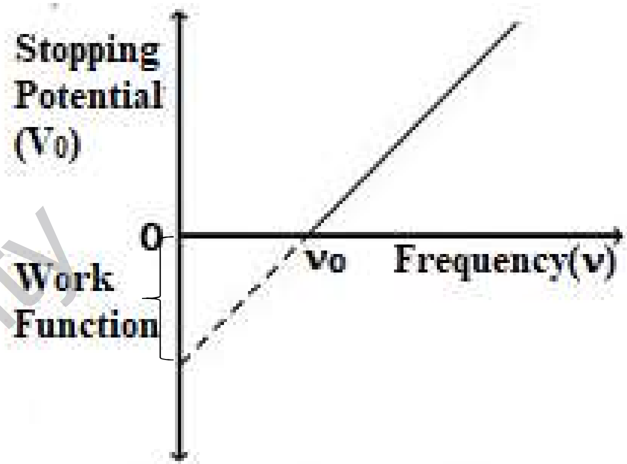
Where V_s is the stopping potential.

According to classical physics,

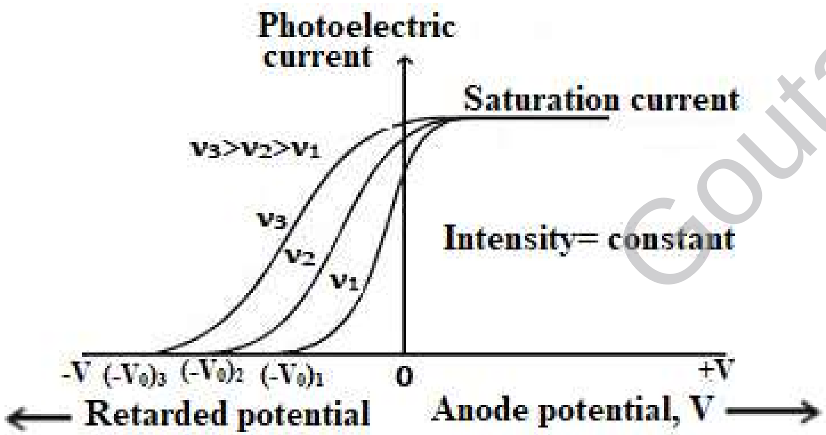
- an electron would keep on absorbing energy-at a *continuous rate*-until it gained a sufficient amount; then it would leave the metal.
- Further experiments showed that an increase in intensity (brightness) alone can in no way dislodge electrons from the metal.



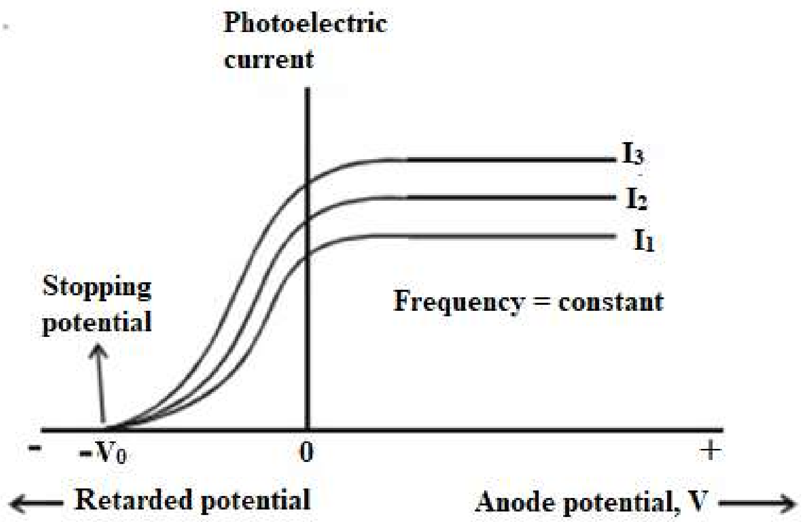
(1. Photocurrent vs Intensity)



(2. Stopping potential vs Frequency)



(3. Photocurrent vs Applied potential with different frequency)



4. Photocurrent vs Applied potential with diff intensity

Wave-Particle duality

- Although it is quite difficult to accept that a radiation will have both wave and particle characters.
- The existing experimental facts, particularly interference, diffraction, and polarisation force us to consider radiation as a wave.
- At the same time, the phenomena like photoelectric effect, Compton effect, black body radiation, and emission and absorption spectra suggest us that radiation has particle nature as well.
- Hence, we can conclude that radiation sometimes behaves as a wave and at other times as a particle, i.e., it has wave-particle duality. Here it is important to remember that radiation cannot exhibit its particle and wave properties simultaneously.

De-Broglie Hypothesis of Matter-Waves

Louis De Broglie

- In 1924, Louis De Broglie suggested that this duality is true not only for radiation but it is also true for all the moving material particles of the universe. It means that like radiation, matter also have wave-particle duality. It is verified experimentally by Davisson and Germer.
- According to de Broglie, a moving particle always has a wave associated with it and the motion of the particle is guided by that wave in the same way as a photon is controlled by a wave. The wavelength of the matter-wave is given by, $\lambda = \frac{h}{mv} = \frac{h}{p}$

Can we realize wavelength of large object??

- Ex-1: For an electron having mass m_e (9.1×10^{-31} kg)moving with velocity 10^6 m/s. then $\lambda = \frac{h}{mv}$ = 725nm
- Ex-2: For an object having mass 0.1 kg with velocity 20m/s, then $\lambda = \frac{h}{mv}$ = 3.3×10^{-25} nm

Different forms of de-Broglie wavelength

- If particle is associated with a K.E (E_k), then $\boxed{\lambda = \frac{h}{\sqrt{2mEk}}}$
- If particle is associated with the help of electrostatic energy, then K.E=qV, so that $\boxed{\lambda = \frac{h}{\sqrt{2mqV}}}$
- When the particles accelerated with the help of thermal energy, then K.E = 3/2 (kT).

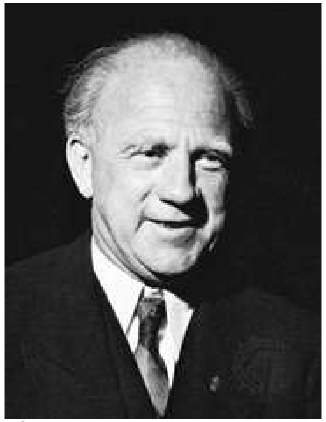
  So that $\boxed{\lambda = \frac{h}{\sqrt{3mkT}}}$
- When the particle is moving with a velocity comparable to that of light, then mass of the particle no longer remains constant. It will vary according to the relation: $\mathrm{m} = \frac{m_0}{\sqrt{1-v^2/c^2}}$

  So $\boxed{\lambda = \frac{h}{mv} = \frac{h\sqrt{1-v^2/c^2}}{m_0 v}}$
- De-Broglie wavelength is associated with electron, i.e $\boxed{\lambda = \frac{12.26}{\sqrt{V}}\,\mathrm{\mathring{A}} = \sqrt{\frac{150}{V}}\,\mathrm{\mathring{A}}}$

Properties of de Broglie matter-waves:

- The lighter particles have greater wavelength than the heavier particles.
- The smaller the velocity of the particle, the greater is the wavelength associated with it.
- From the expression of the de Broglie wavelength, i.e., $\lambda = (h/mv)$, if $v = 0$, then $\lambda = \infty$, whereas if $v = \infty$, then $\lambda = 0$. This shows that the matter-waves are generated only when the particle is in motion.
- Matter-waves are independent of the charge. Thus, they are produced by both charged and uncharged particles. This shows that the matter-waves are not electromagnetic waves; they are entirely different waves.
- The velocity of the matter-waves is not constant. It depends on the velocity of the particle, while the velocity of the electromagnetic wave is constant.
- The velocity of matter wave may be greater than velocity of light.
- The wave and particle aspects of matter never appear simultaneously.
- Wave velocity of matter wave is given in terms of group velocity, $v_{phase} = c^2/v_{group}$
- Wave particle duality introduces the concept of uncertainty.

Heisenberg Uncertainty Principle



Werner Heisenberg

- **Bohr's Model:** The following are the shortcomings
- Valid for single electron species only
- Did not explain splitting of lines: Zeeman effect- due to magnetic field and Stark effect –due to Electric field
- Electrons are moving in a fixed orbit.
- **Heisenberg:** The position and momentum of a microscopic particle (i.e. electron) cann't be exactly determined simultaneously.
- Mathematically, $\boxed{\Delta x \times \Delta px \geq \frac{h}{4\pi}}$, where x= position and p_x = momentum
- $\boxed{\Delta E \times \Delta t \geq \frac{h}{4\pi}}$ (In form of energy and time)
- $\boxed{\Delta J \times \Delta \theta \geq \frac{h}{4\pi}}$ (In form of Angular momentum and angle)

- We know that an object can be seen by illuminating it with light rays consisting of photons. When a beam of light reflected from the surface of the object reaches our eye or any measuring device, the object will become visible.
- According to the principle of optics, the accuracy with which a particle can be located depends upon the wavelength of the light used. The uncertainty in position is $\pm \lambda$.
- Shorter the wavelength, the greater will be accuracy in measuring the position. But shorter wavelength will mean high frequency and high energy of the striking photons
- This means that the striking photons will impart greater momentum to the electrons at the time of impact. This will lead to greater uncertainty in velocity.
- Thus, both the exact position and momentum (velocity) for such particles cannot be measured simultaneously. If we try to have a control on one we lose control over the other and vice versa.

Phase and Group Velocity

- Let us consider a wave whose displacement Y is given as $Y = a\sin(\omega t - kx)$

  Where a = amplitude ,

  $\omega = 2\pi f$ = angular frequency

  $k = 2\pi/\lambda$ = propagation constant

- The ratio of angular frequency and propagation constant is called as phase velocity or wave velocity. i.e. $\boxed{v_p = \frac{\omega}{k}}$
- For a plane of constant phase, $\omega t - kx = constant$

$$\frac{d}{dt}(\omega t - kx) = 0$$

$$\omega - k\frac{dx}{dt} = 0 \quad \Rightarrow \frac{dx}{dt} = v_p = \frac{\omega}{k}$$

Hence , the velocity of propagation of plane of constant phase through a medium is known as phase velocity or wave velocity.

- If velocity of propagation of de-Broglie wave is v_p then we can write,

$v_p = \nu\lambda$, where λ = de Broglie wavelength

The de Broglie wavelength can be written as $\lambda = \frac{h}{mv}$

But we know E = hν and E = mc^2

So we can write $\nu = \frac{mc^2}{h}$

Thus, $\boxed{v_p = \nu\lambda = \frac{mc^2}{h} \times \frac{h}{mv} = \frac{c^2}{v}}$

Group velocity:

- The velocity with which a wave packet or group of waves associated with the moving particle travel is called as group velocity (v_g) where as individual particle velocity is called phase velocity. The group velocity is denoted as v_g and expressed as

$$\boxed{v_g = \frac{d\omega}{dk} = \frac{\omega_1 - \omega_2}{k_1 - k_2}}$$

- Consider TWO waves represented as: $y_1 = a \sin(\omega_1 t - k_1 x)$

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

Their superposition gives

$$y = y_1 + y_2 = a[\sin(\omega_1 t - k_1 x) + \sin(\omega_2 t - k_2 x)]$$

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

$$\therefore \quad y = 2a \cos\left[\frac{(\omega_1 - \omega_2)t}{2} - \frac{(k_1 - k_2)x}{2}\right] \sin(\omega t - kx) \qquad \text{where} \quad \omega = \frac{\omega_1 + \omega_2}{2},\ k = \frac{k_1 + k_2}{2}$$

$$y = 2a \cos\left[\left(\frac{d\omega}{2}\right)t - \left(\frac{dk}{2}\right)x\right] \sin\left[\omega t - kx\right]$$

- Amplitude of the modified wave is

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

$$\text{or} \quad A = 2a \cos \frac{d\omega}{2}\left[t - \frac{dk}{d\omega}x\right]$$

$$A = 2a \cos \frac{d\omega}{2}\left[t - \frac{x}{\upsilon_g}\right]$$

where υ_g is the group velocity.

$$\upsilon_g = \frac{d\omega}{dk}$$

$$\text{or} \quad \boxed{\upsilon_g = \frac{\omega_1 - \omega_2}{k_1 - k_2}}$$

Relation between v_p and v_g:

From the definition of phase velocity, we know that

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

or $$\omega = k v_p$$

Differentiating the above equation, we get

$$d\omega = k\,dv_p + v_p\,dk$$

or $$\frac{d\omega}{dk} = v_p + k\frac{dv_p}{dk}$$

Again we know that

$$v_g = \frac{d\omega}{dk}$$

$$= v_p + k\frac{dv_p}{dk}$$

or $$v_g = v_p + k\frac{dv_p}{d\lambda}\cdot\frac{d\lambda}{dk}$$

Since $k = 2\pi/\lambda$, hence, $d\lambda/dk = -2\pi/k^2$.

Now, we can write

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

- This is the required relation between v_p and v_g in a medium in which phase velocity is frequency dependent.

- For non-dispersive medium $\boxed{v_p = v_g}$