

**Unit-I**

**Quantum mechanics**

**Lecture-1**

# Outline

- Introduction to Quantum Mechanics
- Inadequacy of classical mechanics
- Black body radiation
- Stefan's law
- Wien's law
- Rayleigh-Jeans law
- Limitation of Wien's & Rayleigh law
- Planck's Theory of black body radiation

# Quantum mechanics

- Quantum mechanics deals with the behavior of matter and energy on the scale of atoms and subatomic particles/waves.
- The term “Quantum mechanics” was first coined by Max Born in 1924.

## Inadequacy of classical mechanics

The classical mechanics explain correctly motion of celestial bodies like planet, star and macroscopic. The inadequacies of classical mechanics are given below.

- It does not hold in region of atomic dimension
- It could not explain stability of atoms.
- It could not explained observed spectrum of black body radiation.
- It could not explain observed variation of specific heat of metals and gases.

- It could not explain the origin of discrete spectra of atoms.
- Classical mechanics also could not explain large number of observed phenomena like photoelectric effect ,Compton effect, Raman effect, Anomalous Zeeman effect.

The inadequacy of classical mechanics leads to the development of quantum mechanics.

**What is a black body?**

# Black body

- Black body is that which absorbs completely the electromagnetic radiation of whatever wavelength, that falls on it.
- The term black body was introduced by Kirchhoff in 1860.

**Example:** A perfect black body does not exist in nature and cannot be realized in practice although lamp black and platinum black are good approximations as these absorb 98% of the radiation incident on them.

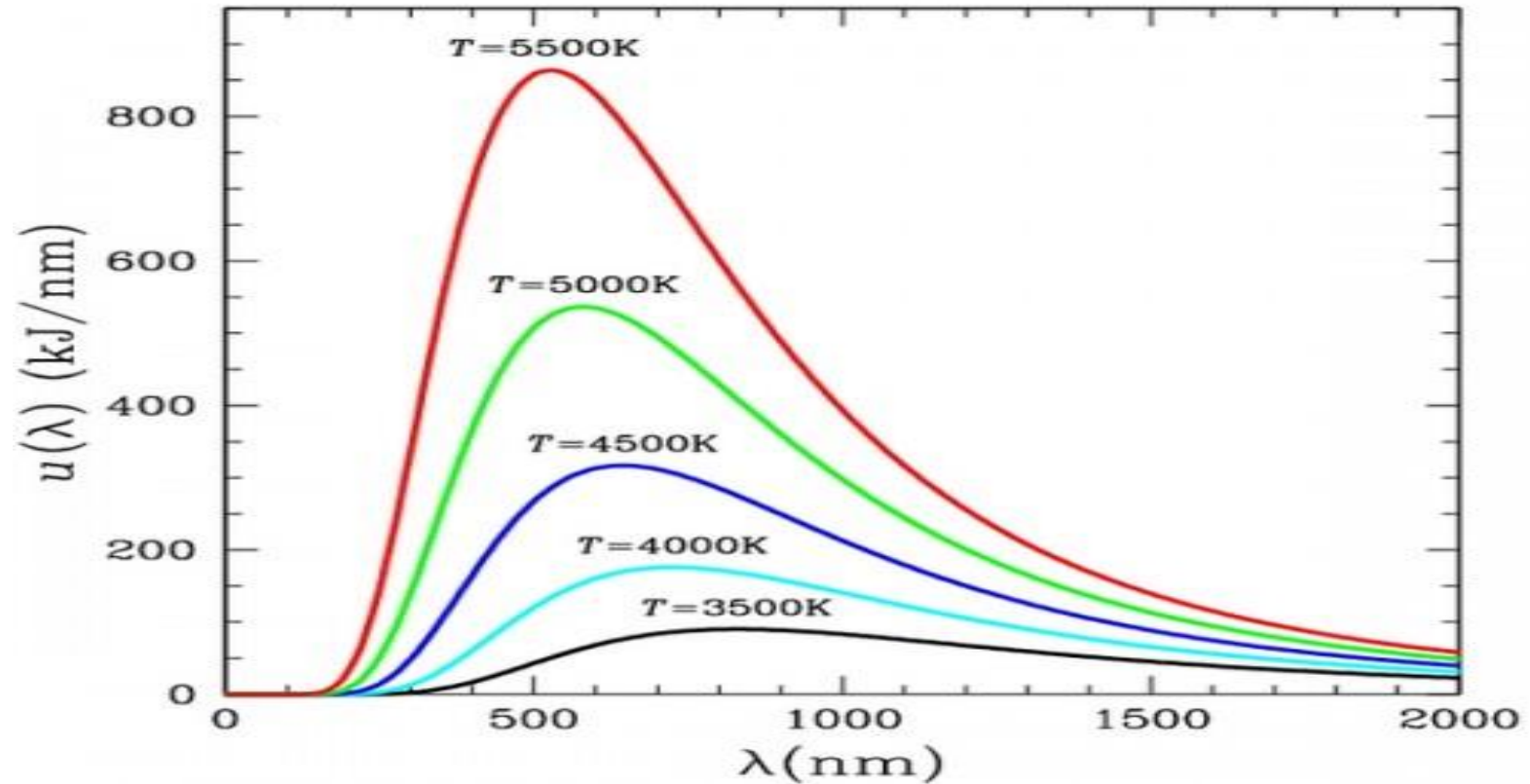
**Describe energy distribution in a black body radiation?**

**(2016-17)**



## Black body spectrum

A graph was obtained between the energy density and wavelength at different temperature as shown in figure.



The experimental results are

1. The emission from black body at any temperature consist radiation of all wavelengths.
2. At a given temperature the energy is not uniformly distributed. As the temperature of black body increases the intensity of radiation for each wavelength increases.
3. The amount of radiant energy emitted is small at very short and very long wavelengths.

4. The wavelength corresponding to the maximum energy represented by the peak of the curve shift towards shorter wavelength as the temperature increases. This is called Wien's displacement law i.e.

$$\lambda_m T = \text{Constant.}$$

**What is Stefan's law of radiation?**

## Stefan's law of radiation

According to Stefan's law, the total amount of the radiant energy by a black body per unit area per unit time due to all wavelengths is directly proportional to the fourth power of absolute temperature.

$$E \propto T^4$$

$$E = \sigma T^4$$

where, the constant of proportionality  $\sigma$  is called the Stefan Boltzmann constant and has a value of  $\sigma = 5.6704 \times 10^{-8}$  watt / (meter<sup>2</sup> Kelvin<sup>4</sup>)

**Explain Wien's law of thermal radiation?**

**(2016-17, 2017-18, 2020-21)**

## Wien's law of thermal radiation

Wien proposed two laws of thermal radiation.

- (1) Wien's first law or Wien's displacement law of radiation
- (2) Wien's second law of radiation

### **(1) Wien's first law or Wien's displacement law of radiation**

- Wien observed that there is wavelength at which radiation has maximum intensity at a given temperature.
- The value of  $\lambda_{\max}$  is inversely proportional to the absolute temperature of the body.

$$\lambda_{\max} \propto \frac{1}{T}$$

$$\lambda_{\max} = \frac{b}{T} \text{ cm-K}$$

$$\lambda_{\max} = \frac{0.2930}{T}$$

where b is known as Wien's constant.

**It is used to determine the temperature of the surfaces of Sun and other stars.**



## (2) Wien's second law of radiation:

According to this law, the total energy density  $E_\lambda d\lambda$  i.e. amount of radiant energy emitted by a black body per unit area per unit time for a given wavelengths range  $\lambda$  and  $\lambda + d\lambda$ , at a given temperature is expressed as:

$$E_\lambda d\lambda = \left( \frac{8\pi hc}{\lambda^5} \right) \left( \frac{d\lambda}{e^{\frac{hc}{\lambda KT}}} \right)$$

$$h = 6.63 \times 10^{-34} (J - S)$$

$$c = 3 \times 10^8 (m / s)$$

$$k = 1.38 \times 10^{-23} (J / K)$$

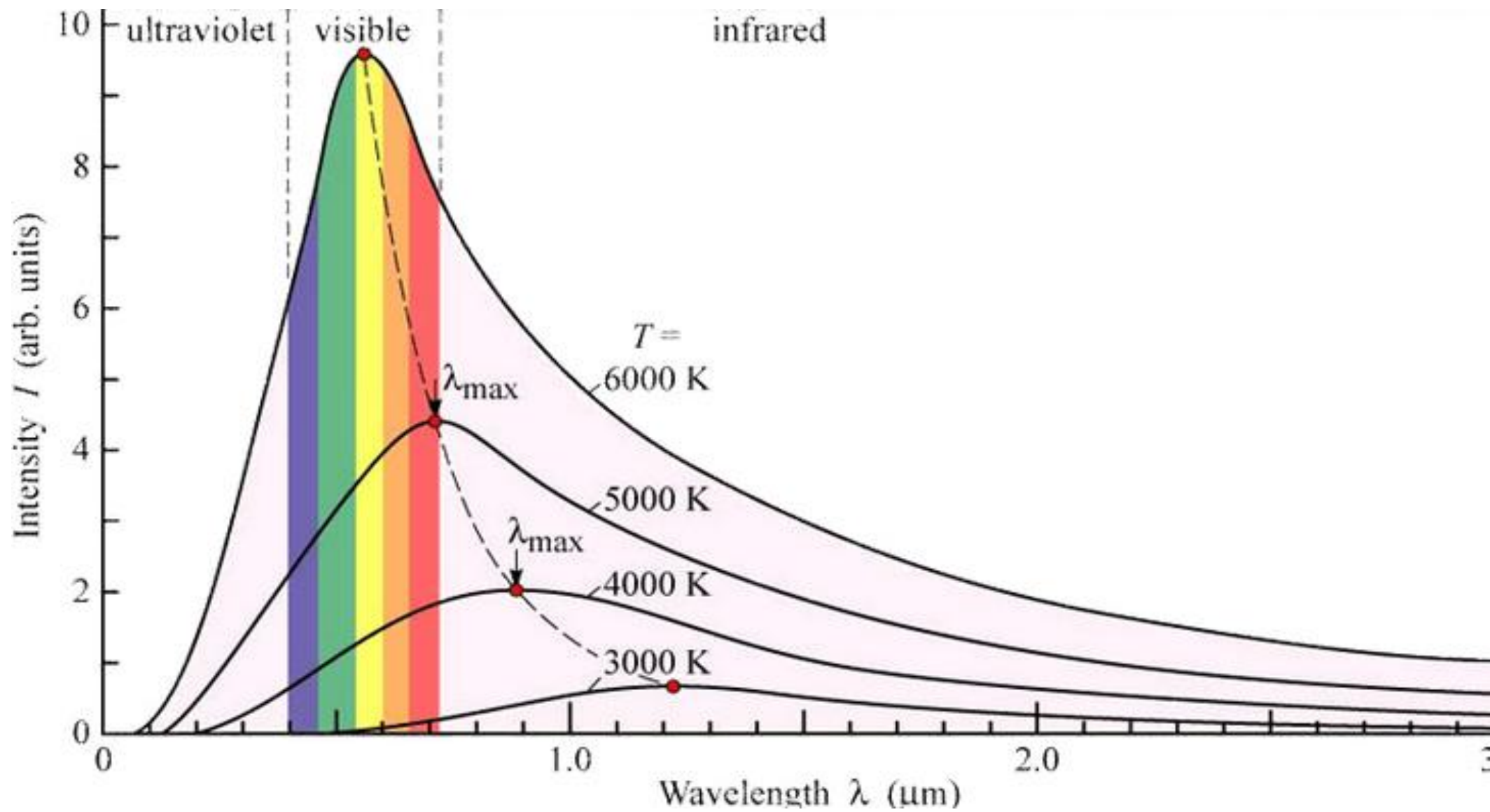
**State Rayleigh Jean's law? (2020-21)**

## Rayleigh Jean's law

Lord Rayleigh used the classical theories of electromagnetism and thermodynamics to show that the blackbody spectral energy distribution is given by:

$$E_{\lambda}d\lambda = \left( \frac{8\pi kT}{\lambda^4} d\lambda \right)$$

where k is Boltzmann's constant.



**What is the limitation of Wien's law and Rayleigh Jeans law?**

## **Limitations of Wien's law**

It is valid for shorter wavelengths, but deviates at long wavelengths.

## **Limitation of Rayleigh Jean's Law**

It is valid for longer wavelengths, but deviates at short wavelengths.

**Why is black best emitter?**

Black is good absorber of all incoming light. According to Kirchhoff's law of radiation good absorber is good emitter. Due to high emissive power black is best emitter.



**Write Planck's law of radiation? (2017-18)**

**Write the assumptions of Planck's hypothesis? (2018-19)**

## Basic assumptions of quantum theory of radiation

1. The energy of an oscillator can have only certain discrete values  $E_n$

$$E_n = nh\nu$$

Where, **n** is a positive integer called the quantum number,  **$\nu$**  is the frequency of oscillation, **h** is Planck's constant.

2. The oscillators emit or absorb energy only in the form of packets of energy ( $h\nu$ ) not continuously, when making a transition from one quantum state to another. The entire energy difference between the initial and final states in the transition is emitted or absorbed as a quantum of radiation,

$$\Delta E = \Delta n h \nu$$

$$E_2 - E_1 = (n_2 - n_1) h \nu$$

**Write Planck's law of radiation. How does it explain Wien's displacement and Rayleigh jeans law. (2018-19)**

## Planck's law

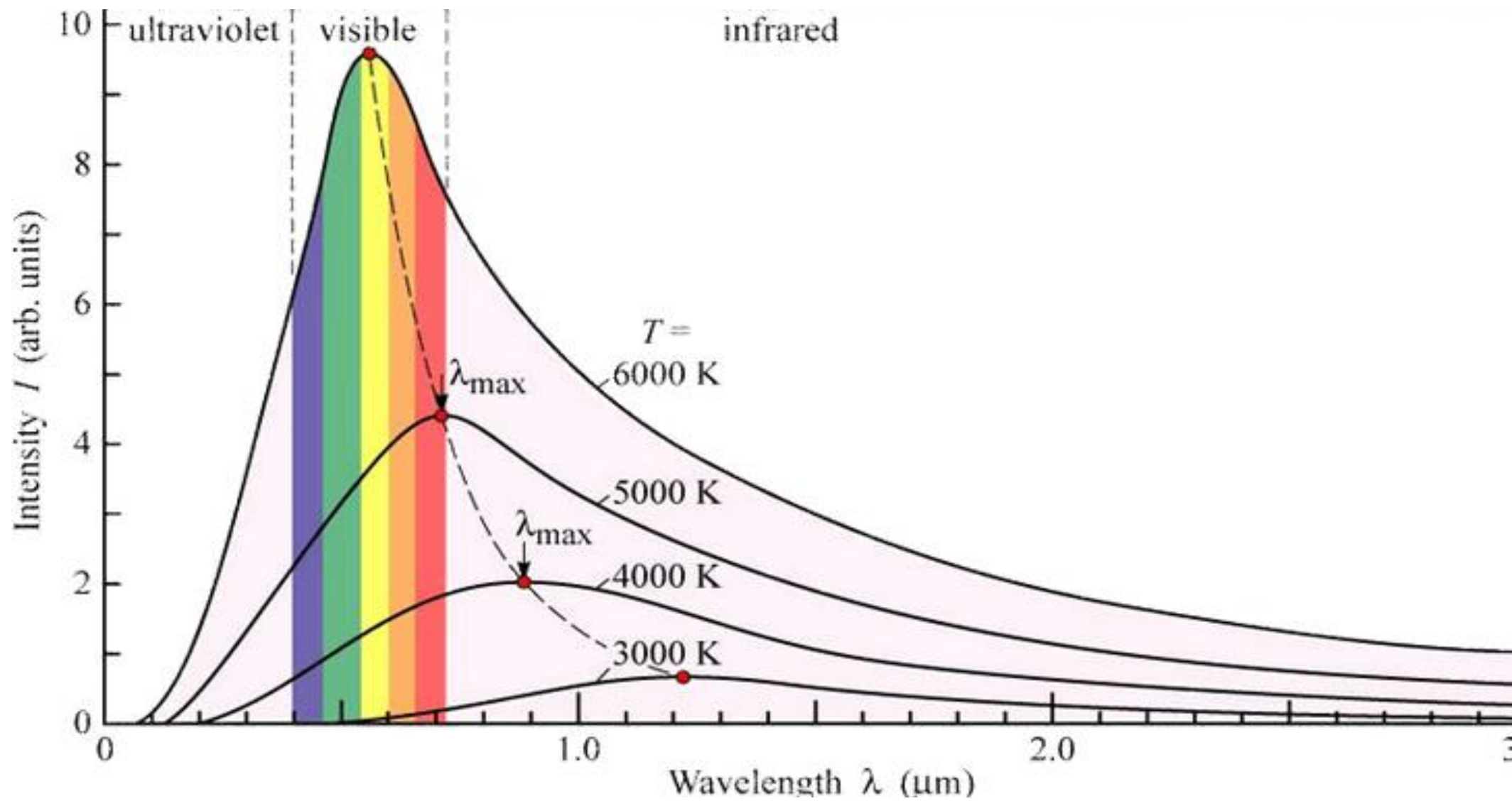
According to Planck, energy density of radiation is given by

$$u_\nu d\nu = \frac{8\pi h\nu^3 d\nu}{c^3} \frac{1}{(e^{\frac{h\nu}{kT}} - 1)} \dots (1)$$

In terms of wavelength, we put

$$\nu = \frac{c}{\lambda} \quad \text{and} \quad d\nu = -\frac{c}{\lambda^2} d\lambda$$

$$u_\lambda d\lambda = \frac{8\pi hc d\lambda}{\lambda^5} \frac{1}{(e^{\frac{hc}{\lambda kT}} - 1)} \dots (2)$$



## Wien's law from Planck's formula:

Planck's radiation formula in terms of wavelength for black body spectrum is given by

$$u_{\lambda}d_{\lambda} = \frac{8\pi hc d\lambda}{\lambda^5} \frac{1}{(e^{\frac{hc}{\lambda kT}} - 1)} \dots (1)$$

For short wavelengths or when  $\lambda$  is small,  $e^{\frac{hc}{\lambda kT}} \gg 1$ , so 1 may be neglected in the denominator of above equation. Thus,

$$u_{\lambda}d_{\lambda} = \frac{8\pi hc}{\lambda^5} e^{-\frac{hc}{\lambda kT}} d\lambda \dots (2)$$

Substituting  $8\pi hc = c_1$  and  $hc/k=c_2$ , equation 2 become

$$U_\lambda d_\lambda = \frac{c_1}{\lambda^5} e^{-\frac{c_2}{\lambda T}} d\lambda$$

*This is Wien's law which agrees with experimental curve at short wavelengths region.*



## Rayleigh-Jeans law from Planck's formula:

For long wavelengths or  $\lambda$  is large,  $e^{\frac{hc}{\lambda kT}} \approx 1 + \frac{hc}{\lambda kT}$  (neglecting terms with higher power of  $\lambda$  in denominator), therefore equation 1 becomes,

$$u_{\lambda}d_{\lambda} = \frac{8\pi hcd\lambda}{\lambda^5(1 + \frac{hc}{\lambda kT} - 1)} = \frac{8\pi kT\lambda}{\lambda^4}$$

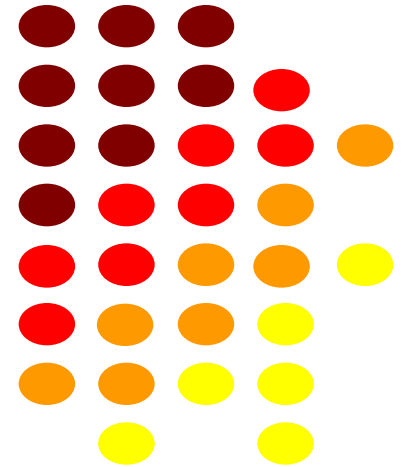
*This is Rayleigh-Jeans law which agrees with experimental curves at long wavelengths region.*

# Unit-I

## Quantum mechanics



### Lecture-2



# Outline

➤ Compton effect

**Explain the modified and unmodified radiations in Compton scattering? (2016 - 17)**

**or**

**What is Compton effect? Derive the necessary expression for Compton shift. (2016 - 17, 2018- 19, 2020 - 21)**

**or**

**What is Compton effect? Derive a suitable expression for Compton shift**  $\lambda' - \lambda = \frac{h}{m_0 c} (1 - \cos\theta)$  . **(2018 - 19)**

**or**

**What is Compton Effect? How does it support the photon nature of light? (2019 - 20)**

## Compton Effect

- In 1921, Professor A.H. Compton discovered that when a monochromatic beam of high frequency radiation is scattered by electrons, the scattered radiation contain the radiations of lower frequency or greater wavelength along with the radiations of unchanged frequency or wavelength.
- The radiations of unchanged wavelength or frequency in the scattered light are called unmodified radiations while the radiations of greater wavelength are called modified radiations.

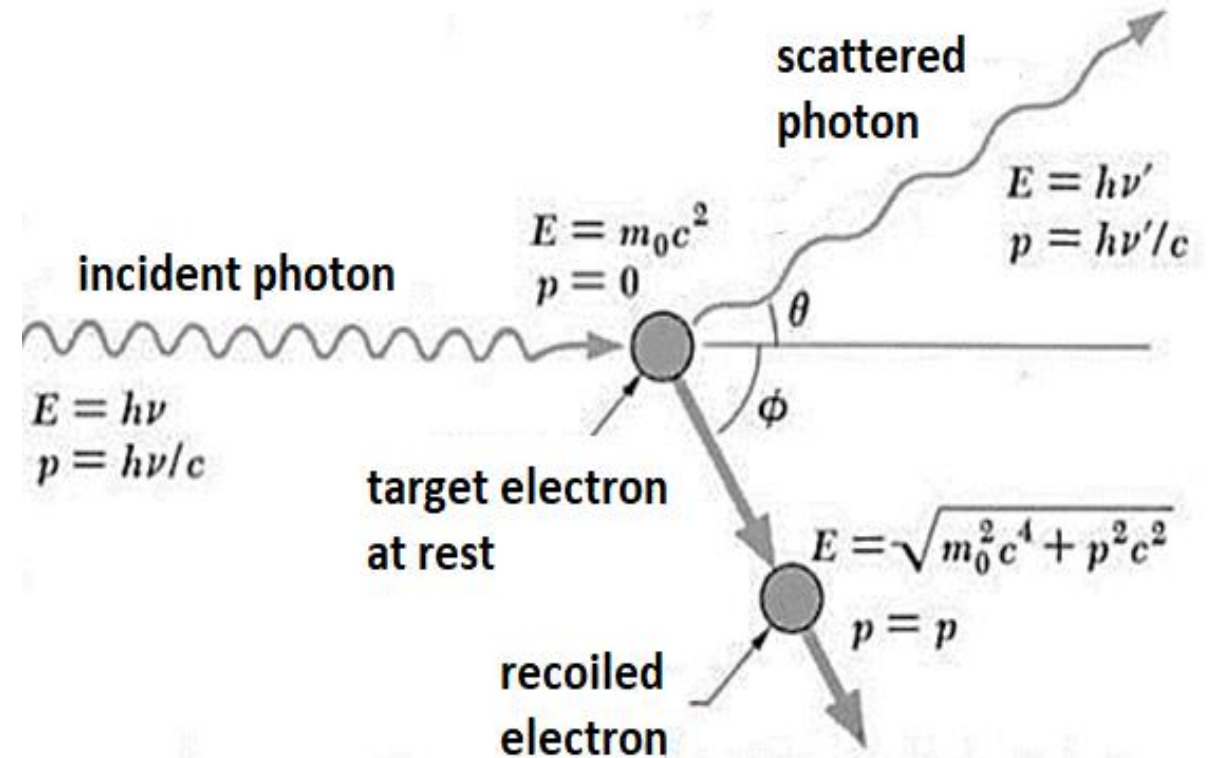
This phenomenon is called the Compton Effect. It provided evidence for the particle nature of light and Planck's postulates.

**Quantum Explanation:** The explanation was given by Compton which was based on Quantum theory of light.

- According to quantum theory when photon of energy  $h\nu$  strikes with the substance some of the energy of photon is transferred to the electrons, therefore the energy (or frequency) of photon reduces and wavelength increases.
- In this way, it support the photon nature of light

Various assumptions were made for explaining the effect these were:

- i. Compton Effect is the result of interaction of an individual particle and free electron of target.
- ii. The collision is relativistic and elastic.
- iii. The laws of conservation of energy and momentum hold good.



The energy of the system before collision =  $h\nu + m_0c^2$

The energy of the system after collision =  $h\nu' + mc^2$

According to the principle of conservation of energy

$$h\nu + m_0c^2 = h\nu' + mc^2$$

$$mc^2 = (h\nu - h\nu') + m_0c^2 \quad \text{.....(1)}$$

According to the principle of conservation of linear momentum along and perpendicular to the direction of incident photon (i.e., along x and y axis).

Along x - axis  $\frac{h\nu}{c} + 0 = \frac{h\nu'}{c} \cos \theta + mv \cos \Phi$

$$mvc \cos \Phi = h\nu - h\nu' \cos \theta \quad \text{.....(2)}$$



Along y – axis

$$0 + 0 = \frac{hv'}{c} \sin \theta - mv \sin \Phi$$

$$mvc \sin \Phi = hv' \sin \theta \quad \dots\dots\dots(3)$$

Squaring (2) and (3) and then adding, we get

$$m^2 v^2 c^2 = (hv - hv' \cos \theta)^2 + (hv' \sin \theta)^2$$

$$m^2 v^2 c^2 = (hv)^2 + (hv' \cos \theta)^2 - 2(hv)(hv') \cos \theta + (hv' \sin \theta)^2$$

$$m^2 v^2 c^2 = (hv)^2 + (hv')^2 ([(\cos \theta)^2 + (\sin \theta)^2] - 2(hv)(hv') \cos \theta$$

$$m^2 v^2 c^2 = (hv)^2 + (hv')^2 - 2(hv)(hv') \cos \theta \quad \dots\dots(4)$$

Squaring equation (1), we get

$$m^2 c^4 = m_o^2 c^4 + (hv)^2 + (hv')^2 - 2(hv)(hv') + 2m_o c^2 (hv - hv') \dots(5)$$

Subtracting (4) from (5), we get

$$m^2 c^4 - m^2 v^2 c^2 = m_o^2 c^4 + 2(hv)(hv')(\cos \theta - 1) + 2m_o c^2 (hv - hv') \dots\dots(6)$$

According to the theory of relativity

$$m = \frac{m_o}{\sqrt{1 - \frac{v^2}{c^2}}} \quad \text{or} \quad m^2 = \frac{m_o^2}{\left(1 - \frac{v^2}{c^2}\right)} \quad \text{or} \quad m^2 \left(1 - \frac{v^2}{c^2}\right) = m_o^2$$

Thus,

$$m^2 c^2 - m^2 v^2 = m_o^2 c^2$$

Multiplying both sides by  $c^2$ , we get

$$m^2 c^4 - m^2 v^2 c^2 = m_o^2 c^4 \quad \dots\dots(7)$$

Using equation (7), equation (6) becomes

$$m_o^2 c^4 = m_o^2 c^4 + 2(h\nu)(h\nu')(\cos \theta - 1) + 2m_o c^2 (h\nu - h\nu')$$

$$0 = 2(h\nu)(h\nu')(\cos \theta - 1) + 2m_o c^2 (h\nu - h\nu')$$

$$2(h\nu)(h\nu')(1 - \cos \theta) = 2m_o c^2 (h\nu - h\nu')$$

$$\frac{(v - v')}{v'v} = \frac{h}{m_0c^2} (1 - \cos \theta)$$

$$\frac{1}{v'} - \frac{1}{v} = \frac{h}{m_0c^2} (1 - \cos \theta) \dots \dots (8)$$

To find the relation in term of wavelength, let us substitute  $v' = \frac{c}{\lambda'}$  and  $v = \frac{c}{\lambda}$ . Thus, we have

$$\Delta\lambda = \lambda' - \lambda = \frac{h}{m_0c} (1 - \cos \theta) \dots \dots (9)$$

Equation (9) represent the expression for Compton shift.

## Cases :

1. When  $\theta = 0$ ;  $\cos \theta = 1$

$$\Delta \lambda = \lambda' - \lambda = 0$$

i.e.  $\lambda' = \lambda$ , the scattered wavelength is same as the incident wavelength in the direction of incidence.

2. When  $\theta = 90^\circ$ ;  $\cos \theta = 0$

$$\Delta \lambda = \lambda' - \lambda = \frac{h}{m_0 c}$$

$$\Delta \lambda = \lambda' - \lambda = \frac{h}{m_0 c} = \frac{6.63 \times 10^{-34}}{9.1 \times 10^{-31} \times 3 \times 10^8} = 0.0243 \text{ \AA}$$

$$= \lambda_c$$

where  $\lambda_c$  is called the **Compton wavelength**

3. When  $\theta = 180^\circ$ ;  $\cos \theta = -1$

$$\Delta \lambda = \lambda' - \lambda = \frac{2h}{m_0 c} = 0.04652 \text{ \AA}$$

**NOTE** : From above equations (8) and (9), following conclusions can be drawn

- The wavelength of the scattered photon  $\lambda'$  is greater than the wavelength of incident photon  $\lambda$ .
- $\Delta \lambda$  is independent of the incident wavelength.
- $\Delta \lambda$  have the same value for all substance containing free electron
- $\Delta \lambda$  only depend on the scattering angle  $\theta$

**Why Compton effect is not observed in visible spectrum?**

The maximum change in wavelength  $\Delta \lambda_{\text{max}}$  is  $0.04652 \text{ \AA}$  or roughly  $0.05 \text{ \AA}$ . This is very small, therefore cannot be observed for wavelength longer than few angstrom units.

For example- For X-ray, the incident radiation is about  $1 \text{ \AA}$ ,  $\Delta \lambda_{\text{max}}$  is  $0.05 \text{ \AA}$ . Therefore, the percentage of incident radiation is about 5% (detectable)

For Visible radiation, the incident radiation is about  $5000 \text{ \AA}$ ,  $\Delta \lambda_{\text{max}}$  is  $0.05 \text{ \AA}$ . Therefore, the percentage of incident radiation is about 0.001% (undetectable)



**What is the kinetic energy and direction of recoiled electron?**

## Kinetic energy of recoiled electron

$$E = h\nu - h\nu'$$

$$E = h \frac{c}{\lambda} - h \frac{c}{\lambda'}$$

$$E = hc \left( \frac{1}{\lambda} - \frac{1}{\lambda'} \right)$$

$$E = hc \left( \frac{\lambda' - \lambda}{\lambda' \lambda} \right)$$

## Direction of recoiled electron

From Compton effect, we get the equation

$$m v c \cos \Phi = h \nu - h \nu' \cos \theta \dots\dots\dots (1)$$

$$m v c \sin \Phi = h \nu' \sin \theta \dots\dots\dots (2)$$

Dividing equation (2) by (1), we get

$$\tan \Phi = \frac{h \nu' \sin \theta}{h \nu - h \nu' \cos \theta}$$

$$\tan \Phi = \frac{v' \sin \theta}{v - v' \cos \theta}$$

$$\tan \Phi = \frac{\frac{c}{\lambda} \sin \theta}{\frac{c}{\lambda} - \frac{c}{\lambda} \cos \theta}$$

$$\tan \Phi = \frac{\lambda \sin \theta}{\lambda' - \lambda \cos \theta}$$

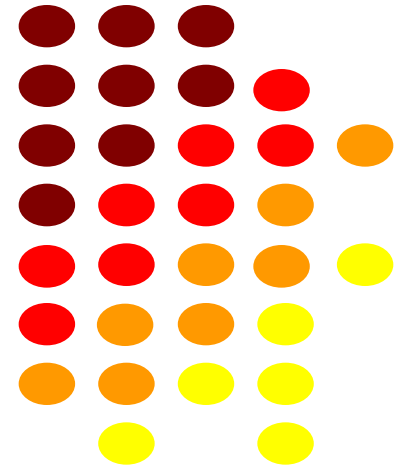
**How Compton Effect support the photon nature of light?**

In the Compton Effect, Compton observed that the scattered radiation has lower frequency than incident radiation. According to wave theory, frequency must be conserved in any scattering process. So we can say that Compton Effect support the photon nature of light.

# Unit-I

## Quantum mechanics

### Lecture-3



# Outline

- de-Broglie matter waves
- Wave particle duality
- Difference between electromagnetic wave and matter wave



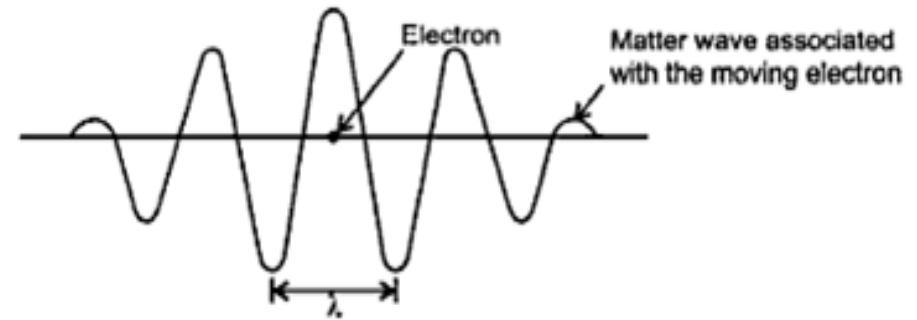
**What is the concept of de-Broglie matter waves?**

**(2017-18, 2020-21)**

## Concept of de-Broglie matter waves

The wave associated with a moving particle is called matter waves or de-Broglie waves. According to de-Broglie's concept (1924), a moving particle always has a wave associated with it.

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



### **Expression for de-Broglie**

According to Planck's theory of radiation, the energy of a photon is given by

$$E = h\nu \dots\dots(1)$$

According to Einstein energy-mass relation

$$E = mc^2 \dots\dots(2)$$

From eqs. (1) & (2), we get

$$h\nu = mc^2$$

$$h\frac{c}{\lambda} = mc^2 \text{ (since } c = v\lambda \text{)}$$

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

$$\lambda = \frac{\mathbf{h}}{\mathbf{mc}}$$

### **For materialistic Particle**

If we consider the case of a material particle of mass  $m$  and moving with a velocity  $v$  then the wavelength associated with this particle is given by

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

**Obtain relation between**

**(1) de-Broglie wavelength and kinetic energy.**

**(2) de-Broglie wavelength and temperature.**

## Relation between de-Broglie wavelength and kinetic energy

If we consider the case of a material particle of mass  $m$  and moving with a velocity  $v$  then the wavelength associated with this particle is given by

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

If  $E$  is then kinetic energy of the material particle, then,

$$E_k = \frac{1}{2} mv^2 = \frac{m^2 v^2}{2m}$$

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

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

**Therefore**

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

## Relation between de-Broglie wavelength and temperature

When a material particle is in thermal equilibrium at a temperature T, then

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

Where  $k$  = Boltzmann's constant =  $1.38 \times 10^{-23}$  J/K

So, de-Broglie wavelength at temperature T is given by

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

$$\lambda = \frac{h}{\sqrt{2m\frac{3}{2}kT}}$$

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

**Obtain de-Broglie wavelength associated with electrons.**

let us consider the case of an electron of rest mass  $m_0$  & charge  $e$  which is accelerated by a potential  $V$  volt from rest to velocity  $v$ , then

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

$$v = \sqrt{2eV/m_0}$$

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

$$\lambda = \frac{h}{m_0 v}$$

$$\lambda = \frac{h}{\sqrt{2eVm_0}}$$



$$\lambda = \frac{6.63 \times 10^{-34}}{\sqrt{2 \times 1.6 \times 10^{-19} \times V \times 1.91 \times 10^{-31}}}$$

$$\lambda = \frac{12.28}{\sqrt{V}} \text{ \AA}$$

**What do you mean by wave particle duality?**

## Wave particle duality

- A particle means an object with a definite position in space which cannot be simultaneously occupied by another particle & specified by their properties such as mass, momentum, kinetic energy, velocity etc.
- On the other hand, a wave means a periodically repeated pattern in space which is specified by its wavelength, amplitude, frequency, energy, momentum etc.

- Two or more waves can coexist in the same region and superimpose to form a resultant wave.
- The particle & wave properties of radiation can never be observed simultaneously.
- Radiation, sometimes behave as a wave (Interference, diffraction, etc.) & at some other time as a particle (Photoelectric effect, Compton Effect), *i.e.*, it has a wave particle dualism.

**What is the difference between electromagnetic wave and matter wave?**

**(2019-20)**

## Difference between electromagnetic and matter wave

- (1) Matter waves are associated with moving particles and does not depend on the charge. On the other hand EM wave are associated with accelerated charge particle.
- (2) Electromagnetic waves are a type of wave that travels through space, carrying electro magnetic radiant energy while matter waves are the waves that consist of particles.

(3) Electromagnetic waves have electric and magnetic fields associated with them, whereas matter waves don't have accelerated electric or magnetic field.

**Why are matter waves associated with a particle generated only when it is motion?**



According to de-Broglie hypothesis

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

When  $v = 0$  then  $\lambda = \infty$ , i.e., wave becomes indeterminate & if  $v = \infty$  then  $\lambda = 0$ . This shows that matter waves are generated by the motion of particles.

**Deduce an expression for de-Broglie wavelength of He-atom having energy at TK.**

de-Broglie wavelength at temperature T is given by

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

For thermal equilibrium at temperature T

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

$$\lambda = \frac{h}{\sqrt{2m \frac{3}{2} kT}}$$

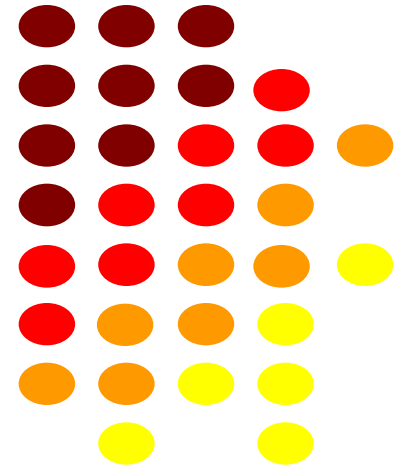
$$\lambda = \frac{h}{\sqrt{3mkT}}$$

# Unit-I

## Quantum mechanics



### Lecture-4



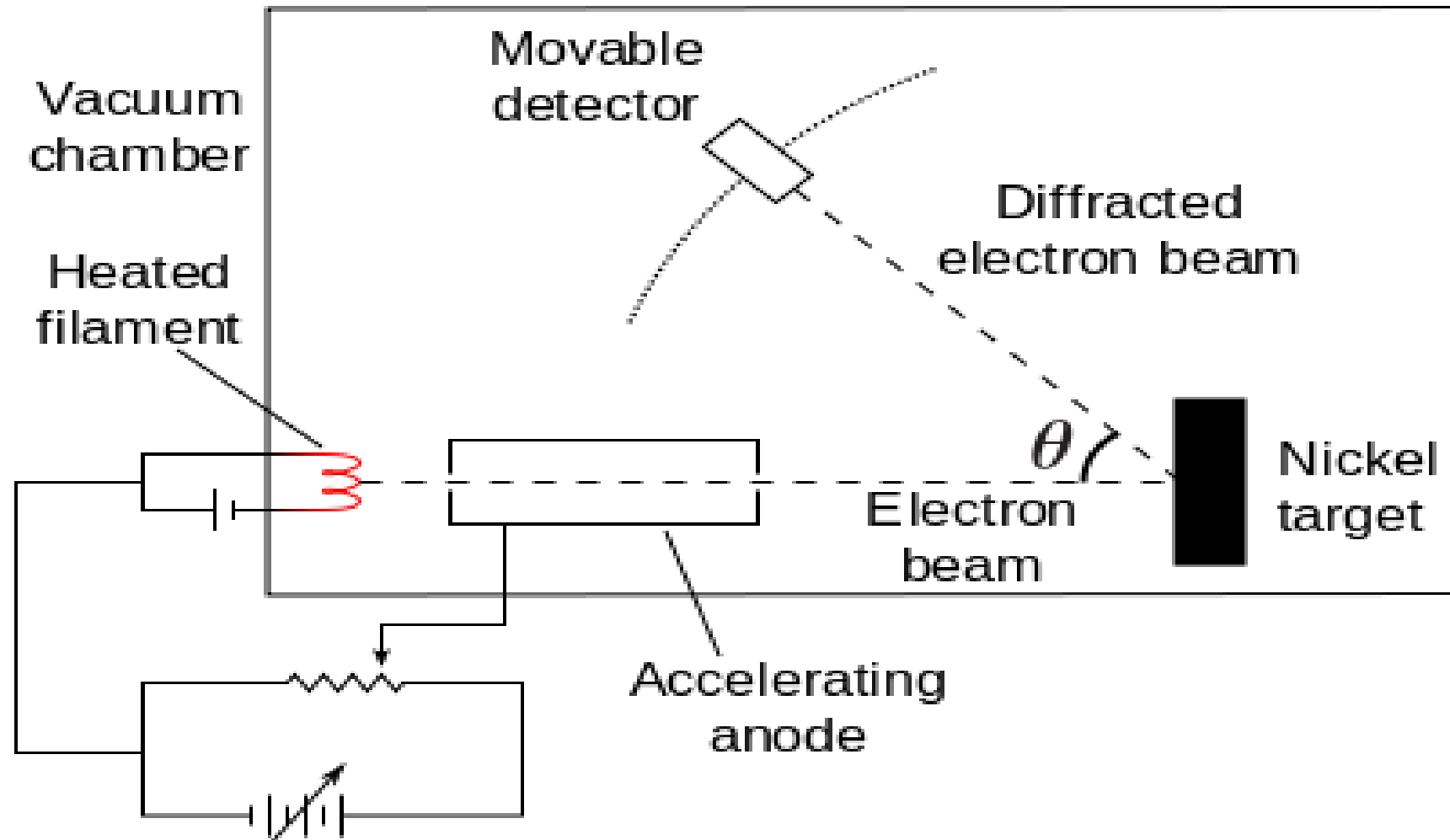
## Outline

➤ Davisson and Germer Experiment

# Davisson and Germer Experiment

- It is the first experimental evidence of material particle was predicted in 1927 by **Clinton Davisson** and **Lester Germer**. This experiment not only confirmed the existence of waves associated with electron by detecting de-Broglie waves but also succeed in measuring the wavelength.
- Davisson and Germer experiment were originally designed for the study of scattering of electrons by a nickel crystal.

# Set up of Davisson - Germer Experiment

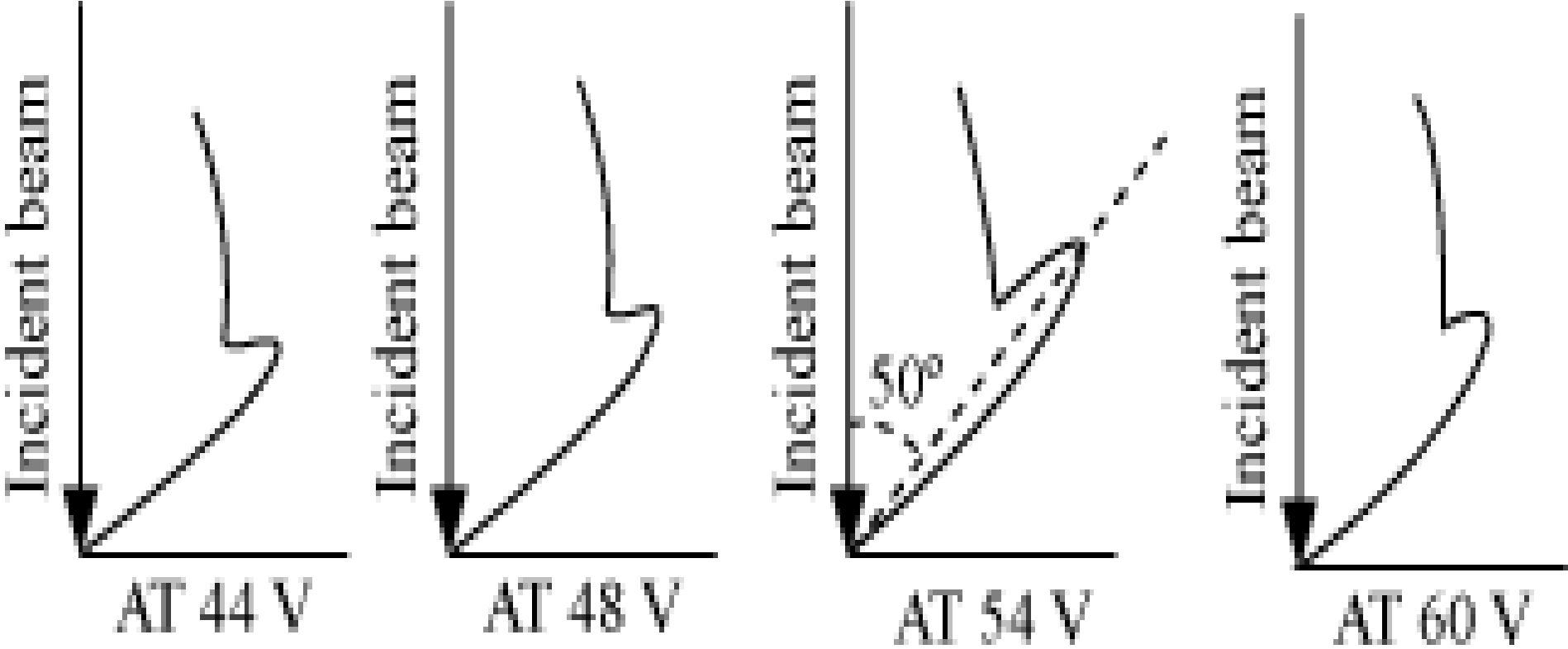


- The electrons are produced by thermionic emission from a tungsten filament F mounted in an electron gun. The ejected electrons are accelerated towards anode in an electric field of known potential difference and collimated into a narrow beam. The whole arrangement used to emit electrons and to accelerate and to focus is called electron gun.
- The narrow beam of electron is allowed to fall normally on the surface of a nickel crystal because their atoms are arranged in a regular pattern/lattice so the surface lattice of the crystal acts as a diffraction grating and electrons are diffracted by crystals in different direction.



- The electrons scattered from target are collected by detector C which is also connected to a galvanometer G and can be moved along a circular scale S.
- The electron are scattered in all direction by atoms in crystal. The intensity of electrons scattered in a particular direction is formed by using a detector. On rotating the detector, the intensity of scattered beams can be measured for different value of angle between incident and scattered direction of electron beam.

The various graphs are plotted between scattering angle and intensity of scattered beam at different accelerating voltage.



## Sailent features observed from the graph

- Intensity of scattered electron depends upon angle of scattering.
- A kink begins to appear in curve at 44 Volts.
- This link moves upward as the voltage increases and become more prominent for 54 Volts at  $50^\circ$
- The size of kink starts decreasing with further increase in accelerating voltage and drops almost to zero at 68 volts.
- The kink at 54 Volts offer evidence for existence of electron waves.

The crystal surface acts like a diffraction grating with spacing  $d$ . The principal maxima for such a grating must satisfy Bragg's equation

$$2d \sin \phi = n\lambda$$

Where  $d$  is interplanar spacing and  $d = 0.91 \text{ \AA}$

$n=1$  for first order

According to Davisson Germer experiment

$$\theta + 2\phi = 180^\circ$$

$$\phi = 90 - \frac{\theta}{2}$$

For  $\theta = 50^\circ$ ,  $\phi = 90 - 25 = 65^\circ$

$$2d \sin \phi = \lambda$$

$$2 \times 0.91 \times 10^{-10} \sin 65 = \lambda$$

$$\lambda = 1.65 \text{Å}$$

Now, for electron having kinetic energy of 54eV

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

$$\lambda = \frac{6.626 \times 10^{-34}}{\sqrt{2 \times 9.1 \times 10^{-31} \times 54 \times 1.6 \times 10^{-19}}}$$

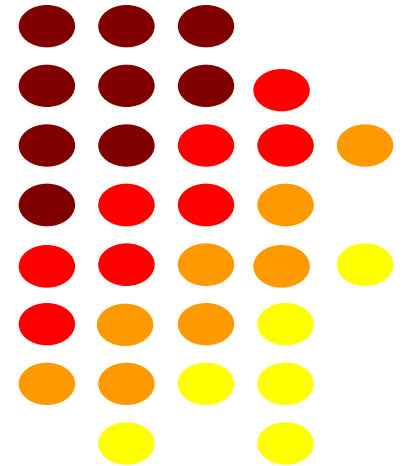
$$\lambda = 1.67 \text{Å}$$

Which agrees well with the observed wavelength of 1.65Å. Thus Davisson and Germer experiment directly verifies de-Broglie hypothesis of wave nature of moving bodies.

# Unit-I

## Quantum mechanics

### Lecture-5



# Outline

- Phase velocity
- Group velocity

**What do you mean by group velocity? (2017-18)**

**Or**

**What is the difference between phase velocity and group velocity? (2013-14)**

**Or**

**What do you mean by phase velocity and group velocity?  
(2014-15)**



## Phase velocity (wave velocity)

When a monochromatic wave (single frequency & wavelength) travels through a medium, its velocity of advancement in the medium is called phase or wave velocity.

Consider a wave whose displacement  $y$  is expressed as,

$$y = a \sin(\omega t - kx)$$

$a$  is amplitude,  $k$  is wave vector,  $\omega$  is angular frequency

For planes of constant phase,  $(\omega t - kx) = \text{constant}$  — (1)

On differentiating above equation with respect to t we get,

$$\omega - k \frac{dx}{dt} = 0$$
$$v_p = \frac{dx}{dt} = \frac{\omega}{k} \quad - (2)$$

Equation (2) represents the phase or wave velocity.

Thus, the wave velocity is the velocity with which the planes of constant phase advance through the medium. Hence is also called phase velocity.

A particle in motion has two velocities : particle velocity (v) and its associated matter wave velocity ( $v_p$ )

**Show that phase velocity of de-Broglie wave greater than velocity of light.**

We know that,

$$E = h \nu = mc^2$$

$$\nu = \frac{mc^2}{h} \quad -(3)$$

$$\& \lambda = \frac{h}{m\nu} \quad -(4)$$

Wave or phase velocity is given by,  $v_p = \nu\lambda$

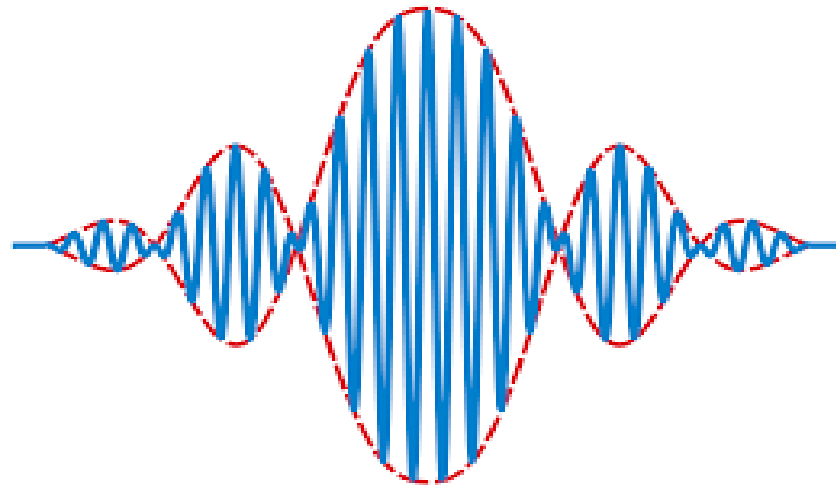
Using eq. (3) & (4) in above equation we have,

$$v_p = \frac{c^2}{\nu}$$

As  $v_p > c$  is not possible as it is in direct contradiction with the special theory of relativity. Thus,  $v_p$  cannot be greater than the velocity of light.

## Group Velocity

**Wave Packet:** A wave packet comprises a group of waves slightly differing in velocity and wavelength such that they interfere constructively over a small region in space where the particle can be located and outside this space they interfere destructively so that the amplitude reduces to zero.



The velocity with which the wave packet obtained by superposition of wave travelling in group is called group velocity ( $v_g$ ).

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

**Establish a relation between phase and group velocity for dispersive medium and non dispersive medium.**

## Relation between group velocity and wave velocity

Wave velocity is given by,  $v_p = \frac{\omega}{k}$   
 $\omega = k v_p$

On differentiating we have,  $d\omega = dk v_p + k dv_p$

$$\frac{d\omega}{dk} = v_p + k \frac{dv_p}{dk} \quad -(1)$$

$$\text{As, } v_g = \frac{d\omega}{dk}$$

Putting in equation (1)



$$v_g = v_p + k \frac{dv_p}{dk} \dots\dots(2)$$

Also,

$$k = \frac{2\pi}{\lambda}$$
$$\Rightarrow dk = \frac{-2\pi d\lambda}{\lambda^2}$$

Substituting in equation (2) we have,

$$v_g = v_p - \lambda \frac{dv_p}{d\lambda} \dots(3)$$

Equation (3) gives the relationship between wave (phase) velocity and group velocity for dispersive medium. Clearly the group velocity is frequency dependent.

For non-dispersive medium:

$$\frac{dv_p}{d\lambda} = 0$$

Putting the above value in equation (3) we have,

$$v_p = v_g$$

## Phase velocity of de-Broglie waves

If  $E$  is the energy of a particle corresponding to matter wave frequency  $\nu$  then,

$$E = h\nu = mc^2$$

$$\Rightarrow \nu = \frac{mc^2}{h} \quad \text{-(1)}$$

Wave vector is given by,  $k = \frac{2\pi}{\lambda}$       -(2)

de – Broglie phase velocity is given by,  $v_p = \frac{\omega}{k} = \frac{2\pi\nu}{k}$       -(3)

Using equation (1) and (2) in (3) we have,

$$v_p = \frac{c^2}{v} \quad - (4)$$

The particle constitutes of all sort of wave groups so,  $v = v_g$

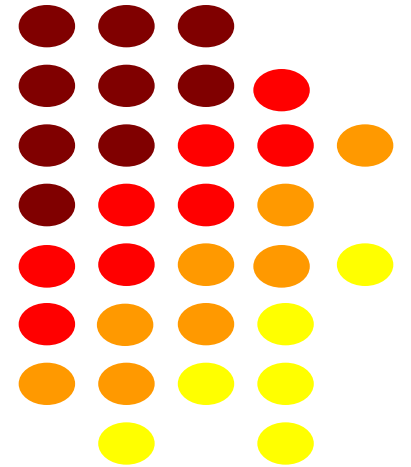
$$v_p v_g = c^2$$

The product of phase and group velocity is equal to the square of velocity of light. As particle(group) velocity is always less than  $c$ , it means phase velocity is greater than speed of light. So, the de-Broglie wave train associated with the particle will travel faster than particle itself and would leave particle behind. This statement is nothing but the collapse of wave description of particle.

# Unit-I

## Quantum mechanics

### Lecture-6

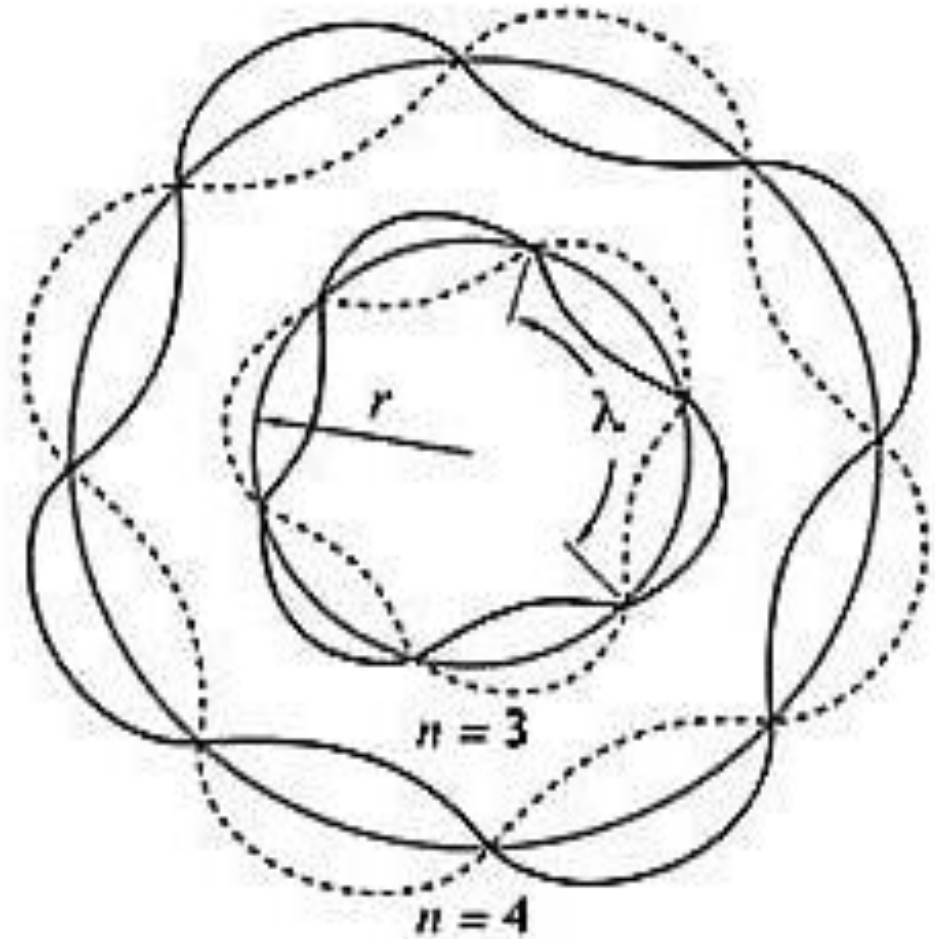


# Outline

- Bohr's quantization rule
- Wave function
- Time dependent Schrödinger wave equation

**Interpret Bohr's quantization rule on the basis of de Broglie concept of matter waves.**

Since the electron does not radiate energy while moving in its orbit, the wave associated with it must be stationary wave in which there is no loss of energy.





Thus the electron forms the stationary wave only when circumference of orbit is integral multiple of wavelength i. e

$$2\pi r = n \lambda \quad (1)$$

We know that,

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

From equation 1,

$$2\pi r = n \frac{h}{mv} \quad (2)$$

$$r = n \frac{h}{2\pi m v} \quad (3)$$

Now angular momentum is given by,

$$L = mvr$$

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

This is Bohr's quantization condition. According to which an electron can revolve only in certain discrete orbits for which total angular momentum of the revolving electron is an integral multiple of  $\frac{h}{2\pi}$ , where h is planck's constant.

**Give physical interpretation of wave function. Also explain eigenvalue and Eigen function. (2016-17, 2018-19)**

## Wave function & its Physical Significance

- The quantity whose variation builds up matter waves is called wave function ( $\psi$ ).
- The value of wave function associated with a moving particle at a particulate point (x, y, z) in space at the time t is related to the possibility of finding the particle there at that time.

## Physical significance of the wave function

- The physical significance of the wave function is that the square of its absolute value at a point is proportional to the probability of experimentally finding the particle described by the wave function in a small element of volume  $d\tau$  ( $dx dy dz$ ) at that point.
- The values of energy for which steady state equation can be solved are called eigenvalues and the corresponding wave functions are called Eigen functions.

**Write some characteristic of wave function? Also write its normalization condition?**

## Characteristics of wave function

1. It must be finite everywhere.
2. It must be single valued.
3. It must be continuous. Its first derivative should also be continuous.

## Normalization condition for wave function

$$\iiint |\Psi|^2 dv = 1$$

**Show that  $\Psi(\mathbf{x},y,z,t) = \Psi(\mathbf{x},y,z,) e^{-i\omega t}$  is a function of stationary state**



If  $\Psi(x,y,z,t)$  is a wave function of stationary state then the value of  $|\Psi(x,y,z,t)|^2$  at each point should be independent of time.

$$\Psi(x,y,z,t) = \Psi(x,y,z) e^{-i\omega t}$$

Complex Conjugate of  $\Psi(x,y,z,t)$

$$\Psi^*(x,y,z,t) = \Psi^*(x,y,z) e^{i\omega t}$$

$$|\Psi(x,y,z,t)|^2 = \Psi(x,y,z,t)\Psi^*(x,y,z,t)$$

$$= \Psi^*(x,y,z) e^{i\omega t} \Psi(x,y,z) e^{-i\omega t}$$

$$|\Psi(x,y,z,t)|^2 = |\Psi(x,y,z)|^2$$

**Obtain Schrodinger time dependent wave equation. (2018-19)**

## Schrodinger time dependent wave equation

The probability of a transition between one atomic stationary state and some other state can be calculated with the aid of the time-dependent Schrödinger equation. The differential equation of a wave motion of a particle in one-dimension can be written as

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 \psi}{\partial t^2} \dots\dots\dots(1)$$

The general solution of eq.(1) is given by

$$\psi(x, t) = A e^{-i\omega[t-(x/v)]} \dots\dots\dots(2)$$

We know that  $\omega = 2\pi\nu$  and  $v = \nu\lambda$ . So, eq.(2) can be written As,

$$\psi(x, t) = Ae^{-2\pi i[\nu t - (x/\lambda)]} \dots\dots\dots(3)$$

Put  $\nu = E/h$  and  $\lambda = h/p$  in eq.(3), we get

$$\psi(x, t) = Ae^{-\left(\frac{2\pi i}{h}\right)(Et - px)} \dots\dots\dots(4)$$

Now, differentiating eq.(4) **twice** with respect to x, we get

$$\frac{\partial^2 \psi}{\partial x^2} = Ae^{-\left(\frac{2\pi i}{h}\right)(Et - px)} \left(\frac{2\pi ip}{h}\right)^2$$

$$= -\frac{4\pi^2 p^2}{h^2} \psi$$

$$p^2 = -\frac{1}{\psi} \frac{h^2}{4\pi^2} \frac{\partial^2 \psi}{\partial x^2} \dots\dots\dots(5)$$

Now, differentiate eq.(4) with respect to t, we get

$$\begin{aligned} \frac{\partial \psi}{\partial t} &= A e^{-\left(\frac{2\pi i}{h}\right)(Et - px)} \left( -\frac{2\pi i E}{h} \right) \\ &= -\frac{2\pi i E}{h} \psi \end{aligned}$$

$$E = -\frac{1}{\psi} \frac{h}{2\pi i} \frac{\partial \psi}{\partial t} = \frac{1}{\psi} \frac{ih}{2\pi} \frac{\partial \psi}{\partial t} \dots\dots\dots(6)$$

If  $E$  &  $V$  be the total & potential energies of the particle respectively, then its kinetic energy  $\frac{1}{2}mv^2$  is given by

$$E = \frac{1}{2}mv^2 + V \quad \text{or} \quad E = \frac{p^2}{2m} + V \quad \dots\dots(7)$$

Putting the values from eqs.(5) & (6) in eq.(7), we get

$$\frac{1}{\psi} \frac{ih}{2\pi} \frac{\partial \psi}{\partial t} = -\frac{h^2}{8\pi^2 m} \frac{1}{\psi} \frac{\partial^2 \psi}{\partial x^2} + V \quad \text{or} \quad -\frac{h^2}{8\pi^2 m} \frac{\partial^2 \psi}{\partial x^2} + V\psi = \frac{ih}{2\pi} \frac{\partial \psi}{\partial t}$$

Substituting  $\hbar = \frac{h}{2\pi}$ , we get

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V\psi = \frac{ih}{2\pi} \frac{\partial \psi}{\partial t} \quad \dots\dots\dots(8)$$

This is the required Schrodinger time dependent equation in one dimension. In threedimension the above equation can be written as-

$$\text{or } \left( -\frac{\hbar^2}{2m} \nabla^2 + V \right) \psi = \frac{i\hbar}{2\pi} \frac{\partial \psi}{\partial t}$$
$$H\psi = E \psi$$

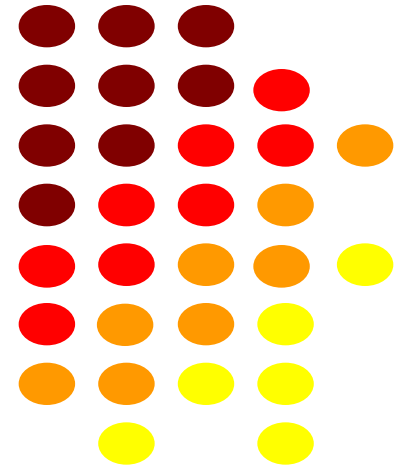
where,  $H = -\frac{\hbar^2}{2m} \nabla^2 + V$ , Hamiltonian operator

$E = \frac{i\hbar}{2\pi} \frac{\partial}{\partial t}$  Energy Operator

# Unit-I

## Quantum mechanics

### Lecture-7





# Outline

- Time independent Schrödinger wave equation
- Solution to stationary state Schrodinger wave equation for **one dimensional particle in a box.**

**Derive time independent Schrodinger wave equation.**

**(2016-17, 2018-19, 2020-21)**

## Schrodinger time independent wave equation

The Schrodinger's time independent equation can be obtained with help of time dependent equation. The differential equation of a wave motion of a particle in one-dimension can be written as

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 \psi}{\partial t^2} \quad \dots\dots\dots(1)$$

The general solution of eq.(1) is given by

$$\psi(x, t) = A e^{-i\omega[t-(x/v)]} \quad \dots\dots\dots(2)$$

We know that  $\omega = 2\pi\nu$  and  $v = \nu\lambda$ . So, eq.(2) can be written as

$$\Psi(x, t) = Ae^{-2\pi i[vt - (x/\lambda)]} \dots (3)$$

Put  $\nu = E/h$  and  $\lambda = h/p$  in eq.(3), we get

$$\Psi(x, t) = Ae^{-\left(\frac{2\pi i}{h}\right)(Et - px)} \dots (4)$$

The wave function can be separated into time dependent and space dependent parts.

$$\Psi(x, t) = Ae^{\left(\frac{2\pi i px}{h}\right)} e^{-\left(\frac{2\pi i Et}{h}\right)}$$

If  $\psi(x) = \psi_0 = Ae^{\left(\frac{2\pi i px}{h}\right)}$  then,

$$\Psi(x, t) = \psi_0 e^{-\left(\frac{2\pi i Et}{h}\right)} \dots (5)$$

Now differentiating equation (5) twice with respect to x, we get

$$\frac{\partial^2 \Psi}{\partial x^2} = \frac{\partial^2 \psi_0}{\partial x^2} e^{-\left(\frac{2\pi i E t}{h}\right)} \dots (6)$$

differentiating equation 5 with respect to t, we get

$$\frac{\partial \Psi}{\partial t} = \psi_0 e^{-\left(\frac{2\pi i E t}{h}\right)} \left(-\frac{2\pi i E}{h}\right) \dots \dots (7)$$

The well known Shrodinger time dependent equation in one dimension is given by-

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

Substituting the values of  $\psi$ ,  $\frac{\partial^2 \psi}{\partial x^2}$  and  $\frac{\partial \psi}{\partial t}$  from equations 5,6,7 in above equation,

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi_0}{\partial x^2} e^{-\left(\frac{2\pi i E t}{h}\right)} + V \psi_0 e^{-\left(\frac{2\pi i E t}{h}\right)} = \frac{i\hbar}{2\pi} \psi_0 e^{-\left(\frac{2\pi i E t}{h}\right)} \left(-\frac{2\pi i E}{h}\right)$$

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi_0}{\partial x^2} + V \psi_0 = E \psi_0$$

$$\frac{\partial^2 \psi_0}{\partial x^2} + \frac{2m}{\hbar^2} (E - V) \psi_0 = 0$$

In general we can write above equation

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

**This is the required** time independent equation in one dimension . In three dimension the above equation can be written as-

$$\nabla^2 \psi + \frac{2m}{\hbar^2} (E - V) \psi = 0 \quad \dots\dots\dots(8)$$

**For a free particle**  $V = 0$ , hence the Schrodinger wave equation for a free particle can be expressed as

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

**Find an expression for the energy states of a particle in one dimensional box? (2017 - 18)**

**or**

**Write down Schrodinger wave equation for particle in a one-dimensional box and solved it to find out the Eigen value and Eigen function. (2019- 20)**

**or**

**A particle is in motion along a line  $X = 0$  and  $X = L$  with zero potential energy. At point for which  $X < 0$  and  $X > L$ , the potential energy is infinite. Solving Schrodinger equation obtain energy eigen values and Normalized wavefunction for the particle. (2018 - 19)**

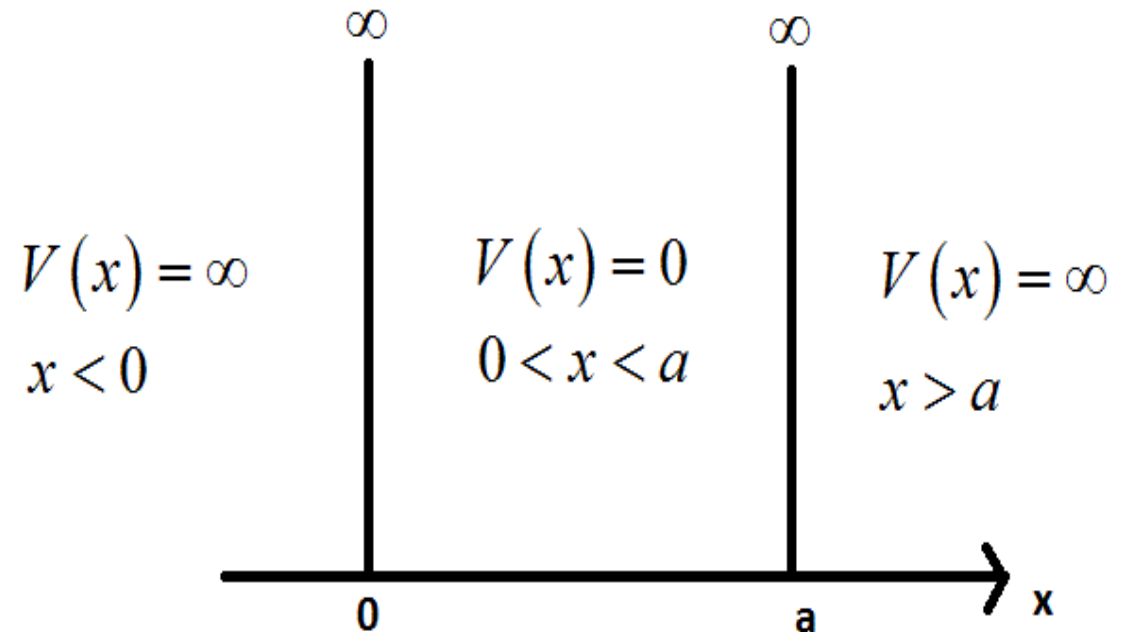


# Particle in one-dimensional Box

Let us consider the case of a particle of mass  $m$  moving along  $x$ -axis between two rigid walls A & B at  $x = 0$  &  $x = a$ . The particle is free to move between the walls. The potential function is defined in the following way:

$$V(x) = 0 \text{ for } 0 < x < a$$

$$V(x) = \infty \text{ for } x \leq 0 \text{ and } x \geq a$$



Under this condition particle is said to move in an infinite deep potential well or infinite square well. The Schrodinger equation for a particle with in the box ( $V = 0$ ) is

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

$$\frac{\partial^2 \psi}{\partial x^2} + k^2 \psi = 0 \quad \dots\dots\dots(2)$$

where

$$k^2 = \frac{2mE}{\hbar^2} \quad \dots\dots\dots(3)$$

The general solution of equation (2) is

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

Apply the boundary condition,  $\psi = 0$  at  $x = 0$  &  $x = a$  to eq.(4). So,

At  $x = 0$ ,  $0 = A \sin k.0 + B \cos k0$



$$B = 0$$

Again at  $x=a$ ,  $0 = A \sin ka$

$$ka = \pm n\pi \quad \text{where } n=1,2,3,\dots \quad \dots(5)$$

$n \neq 0$ , because for  $n=0$ ,  $k=0$

From eq.(3) & eq.(5), we get

$$\sqrt{\frac{2mE}{\hbar^2}}a = \pm n\pi$$

Squaring both side

$$\frac{2mE}{\hbar^2} a^2 = n^2 \pi^2$$

$$E = \frac{n^2 \pi^2 \hbar^2}{2ma^2}$$

Since  $h = \frac{\hbar}{2\pi}$ ,

$$E_n = \frac{n^2 h^2}{8ma^2} \dots\dots\dots(6)$$

From eq.(6), it is clear that the particle can not have an arbitrary energy, but can have certain discrete energy corresponding to  $n = 1, 2, 3, \dots$ . Each permitted energy is called **eigen value** of the particle & constitute the energy level of the system. The corresponding eigenfunction is given by

$$\psi = A \sin kx$$

To find the value of constant A we apply normalization condition,

$$\int_0^a |\psi_n|^2 dx = 1$$

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

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

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

$$\frac{aA^2}{2} = 1$$

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

Therefore, the normalized wavefunction for  $n^{\text{th}}$  state is given by

$$\psi_n = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \dots\dots\dots(7)$$

**Show that the Energy levels are not equally spaced for the particle in one dimensional box.**



We know that the energy of particle in one dimensional box is given by

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

Putting  $n = 1, 2, 3, \dots$  so on, we get

$$E_1 = \frac{1h^2}{8ma^2}$$

$$E_2 = \frac{4h^2}{8ma^2} = 4 E_1$$

$$E_3 = \frac{9h^2}{8ma^2} = 9 E_1$$

$$E_4 = \frac{16h^2}{8ma^2} = 16 E_1$$

$$E_5 = \frac{25h^2}{8ma^2} = 25 E_1$$

The difference between the energy in various states

$$E_2 - E_1 = 3 E_1$$

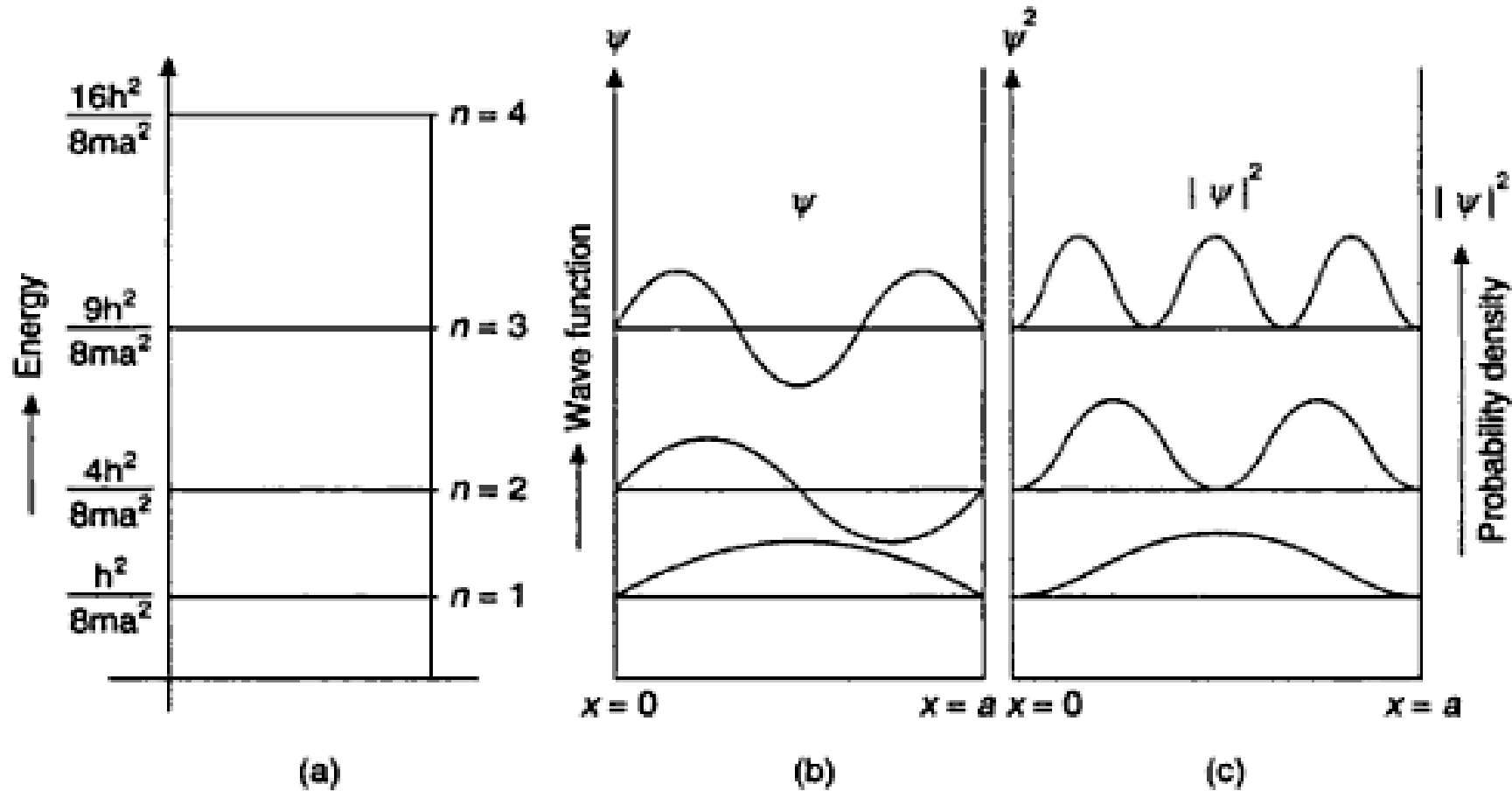
$$E_3 - E_2 = 5 E_1$$

$$E_4 - E_3 = 7 E_1$$

$$E_5 - E_4 = 9 E_1$$

From above equations, it is clear that the difference between energy in consecutive energy states is not constant. This difference increases with an increase in the value of  $n$ .

Therefore it is concluded that that energy levels are not equally spaced as shown in below figure (a).



(a) Energy levels

(b) wave function

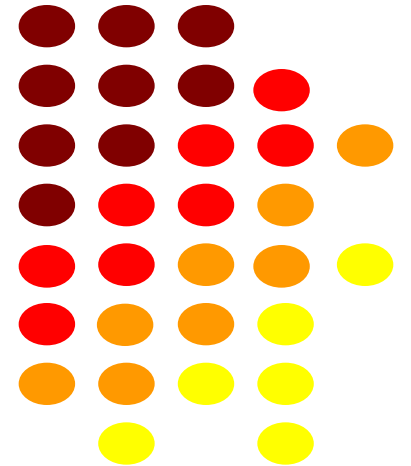
(c) Probability density

# Unit-I

## Quantum mechanics



### Lecture-8



# Outline

➤ Numericals

**Calculate the energy of oscillator of frequency  $4.2 \times 10^{12}$  Hz at  $27^{\circ}$  C treating it as (a) classical oscillator (b) Planck's oscillator.**

**(2018-19)**

$$(i) E_{classical} = kT = 1.4 \times 10^{-23} \times 300 = 4.2 \times 10^{-21} J$$

$$(ii) E_{Planck} = \frac{h\nu}{\left(e^{\frac{h\nu}{kT}} - 1\right)}$$

$$h\nu = 6.6 \times 10^{-34} \times 4.2 \times 10^{12} J = 2.8 \times 10^{-21} J$$

$$\frac{h\nu}{kT} = 0.66 \text{ and } e^{\frac{h\nu}{kT}} - 1 = 0.9348$$

$$\text{Therefore, } E_{Planck} = \frac{h\nu}{\left(e^{\frac{h\nu}{kT}} - 1\right)} = \mathbf{2.99 \times 10^{-21} J}$$

**What is the wavelength of maximum intensity radiation radiated from a source having temperature 3000 K. (IMP)**



According to Wein's law

$$\lambda_m T = b \text{ or } \lambda_m = \frac{b}{T}$$

Given,  $T = 3000 \text{ K}$  and  $b = \mathbf{0.3 \times 10^{-2} \text{ m-K}}$

$$\lambda_m = \frac{\mathbf{0.3 \times 10^{-2}}}{3000} = \mathbf{0.1 \times 10^{-5} \text{ m} = 10,000 \text{ \AA}}$$

**Calculate the wavelength of an  $\alpha$  particle accelerated through a potential difference of 200 volts. (IMP.)**

The de-Broglie's wavelength of an  $\alpha$ -particle accelerated through a potential difference  $V$  is given by,

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

For  $\alpha$ -particle,

$$q = 2e = 2 \times 1.6 \times 10^{-19} \text{ Coulomb}$$

$$\text{mass of } \alpha\text{-particle} = 4 \times \text{mass of proton} = 4 \times 1.67 \times 10^{-27} \text{ kg}$$

$$\lambda = \frac{h}{\sqrt{2 \times 4 \times 1.67 \times 10^{-27} \times 2 \times 200 \times 1.6 \times 10^{-19}}}$$

$$\lambda = 7.16 \times 10^{-13} \text{ m}$$

$$\lambda = 7.16 \times 10^{-3} \text{ \AA} = 0.00716 \text{ \AA}$$

**Show that the de- Broglie wave velocity is a function of wavelength in free space.**

or

**Show that the phase velocity of de-Broglie waves associated with a moving particle having a rest mass  $m_0$  is given by,**

$$v_p = c \sqrt{1 + \left(\frac{m_0 c \lambda}{h}\right)^2}$$

According to the de-Broglie concept of matter wave, the wavelength associated with a particle is given by,

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

$$\lambda = \frac{h}{m_0} \sqrt{\frac{1}{v^2} - \frac{1}{c^2}} \quad (1)$$

Phase velocity of de-Broglie wave is  $v_p = \frac{c^2}{v} \quad (2)$

Putting value of  $\nu$  from (2) in equation (1) we have,

$$\lambda = \frac{h}{m_0} \sqrt{\frac{v_p^2}{c^4} - \frac{1}{c^2}}$$

Solving for  $v_p$  we get  $\mathbf{v_p} = \mathbf{c} \sqrt{\mathbf{1} + \left(\frac{m_0 c \lambda}{h}\right)^2}$

The above equation shows that wave velocity is greater than  $c$  and is a function of wavelength even in free space.

**The de-Broglie wavelength associated with an electron is  $10^{-12}\text{m}$ .  
Find its group velocity and phase velocity.**

From relativistic mass equation,  $\frac{m_0}{m} = \sqrt{1 - \left(\frac{v}{c}\right)^2}$

$$\frac{m_0 c^2}{m c^2} = \sqrt{1 - \left(\frac{v}{c}\right)^2}$$

$$\frac{E_0}{E} = \sqrt{1 - \left(\frac{v}{c}\right)^2}$$

Solving for v we have,  $v = c \sqrt{1 - \left(\frac{E_0}{E}\right)^2}$  -(1)

The total relativistic energy of moving electron is given by,

$$E = \sqrt{(pc)^2 + (E_0)^2}$$



$E_0 = 511\text{keV}$  is the rest mass energy of electron.

$$E = \sqrt{\left(\frac{hc}{\lambda}\right)^2 + (E_0)^2} \quad -(2)$$

Substituting the values of wavelength ,h, c and  $E_0$  in (2) we have,

$$E = 1344.03\text{keV}$$

Putting the values of  $E_0$  and E in equation (1) we have,

$$v = c \sqrt{1 - \left(\frac{511}{1344.03}\right)^2}$$
$$v = 0.925c$$

Phase velocity is given by,  $v_p = \frac{c^2}{v} = \frac{c^2}{0.925c}$

$$v_p = 1.08c$$

**Calculate the de-Broglie wavelength of an neutron having kinetic energy 1ev. (2019-20)**

The rest energy of neutron is  $m_0c^2 = 1.67 \times 10^{-27} \times (3 \times 10^8)^2$   
 $= 1.503 \times 10^{-10}$  joule  
 $= 939.4$  MeV

The Kinetic energy of the given neutron is  $1\text{eV} = 1.6 \times 10^{-19}$  joule , is very small as compared to its rest mass energy, therefore the relativistic consideration may be ignored.

So The de-Broglie's wavelength of an neutron of rest mass  $m_0$  is given by

$$\lambda = \frac{h}{\sqrt{2Em_0}} = \frac{6.63 \times 10^{-34}}{\sqrt{2 \times 1.67 \times 10^{-27} \times 1.6 \times 10^{-19}}} = \mathbf{2.87 \times 10^{-11} \text{ m}}$$

**Determine the probability of finding a particle trapped in a box of length  $L$  in the region from  $0.45L$  to  $0.55L$  for ground state. (2017 - 18)**

The eigen function of a particle trapped in a box of length L is given by

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

Probability of finding the particle between  $x_1$  and  $x_2$  for  $n^{\text{th}}$  state is given by

$$P = \int_{x_1}^{x_2} |\psi_n|^2 dx$$

$$P = \int_{x_1}^{x_2} \frac{2}{L} \sin^2\left(\frac{n\pi x}{L}\right) dx$$

$$P = \frac{2}{L} \int_{x_1}^{x_2} \frac{1}{2} \left(1 - \cos\frac{2n\pi x}{L}\right) dx$$

$$P = \frac{1}{L} \int_{x_1}^{x_2} \left(1 - \cos\frac{2n\pi x}{L}\right) dx$$

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

Here  $x_1 = 0.45 L$ ,  $x_2 = 0.55 L$ , for ground state  $n = 1$

$$P = \frac{1}{L} \left[ \left( 0.55 L - \frac{L}{2\pi} \sin(1.10\pi) \right) - \left( 0.45 L - \frac{L}{2\pi} \sin(0.90\pi) \right) \right]$$

$$P = \left[ \left( 0.55 - \frac{1}{2\pi} \sin(198^\circ) \right) - \left( 0.45 - \frac{1}{2\pi} \sin(162^\circ) \right) \right]$$

$$P = (0.55 - 0.45) - \frac{1}{2\pi} (\sin 198^\circ - \sin 162^\circ)$$

$$P = (0.10) - \frac{1}{2\pi} (\sin 198^\circ - \sin 162^\circ)$$

$$P = 0.10 - \frac{1}{2\pi} (-0.309 - 0.309)$$

$$P = 0.10 - \frac{1}{2\pi} (-0.618)$$

$$P = 0.10 + 0.0984$$

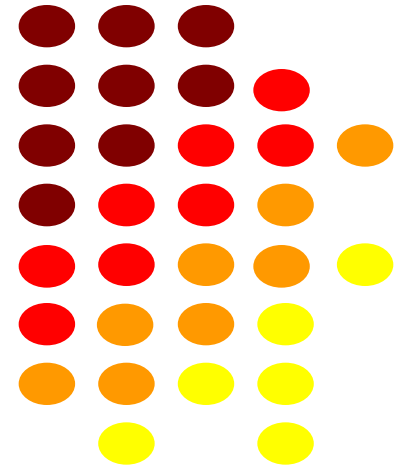
$$P = 0.1984 = 19.84\%$$

# Unit-I

## Quantum mechanics



### Lecture-9





# Outline

➤ Numericals

**An X- ray photon is found to have its wavelength doubled on being scattered through  $90^\circ$  from a material. Find the wavelength of incident photon. (V.IMP)**

If  $\lambda$  and  $\lambda'$  be the wavelength of incident and scattered X-ray of photon respectively then the Compton shift is given by.

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

Here  $\theta = 90^\circ$  and  $\lambda' = 2\lambda$

$$\Delta\lambda = (\lambda' - \lambda) = 2\lambda - \lambda = \lambda$$

$$\text{Thus } \lambda = \frac{h}{m_0 c} = \frac{6.63 \times 10^{-34}}{9.1 \times 10^{-31} \times 3 \times 10^8} = 0.0245 \text{ \AA}$$

**Calculate the wavelength of an electron that has been accelerated through potential difference of 100 volts.**

$$\lambda = \frac{h}{\sqrt{2mqV}} = \frac{12.28}{\sqrt{V}} \text{ \AA}$$

$$= \frac{12.28}{\sqrt{100}} = \frac{12.28}{10}$$

$$= 1.228 \text{ \AA}$$

**Calculate the de- Broglie wavelength associated with a proton moving with a velocity equal to  $(1/20)^{th}$  velocity of light. (M.IMP)**

**Solution:** we know that  $\lambda = \frac{h}{p} = \frac{h}{mv}$

We know that,

$$h = 6.6 \times 10^{-34} \text{ J sec}$$

$$m = 9.1 \times 10^{-31} \text{ kg}, v = c/20 = 3 \times 10^8 / 20$$

$$\lambda = \frac{h}{mv} = 2.643 \times 10^{-14} \text{ m.}$$

**A particle confined to move along x-axis has the wave function  $\psi = ax$  between  $x=0$  and  $x=0.1$  and  $\psi = 0$  elsewhere. Find the probability that the particle can be found between  $x=0.35$  and  $x=0.45$ .**



**Solution-** Probability of finding the particle is given by.

$$P = \int_{-\infty}^{+\infty} |\psi_n|^2 dx$$

$$P = \int_{0.35}^{0.45} (ax)^2 dx = a^2 \int_{0.35}^{0.45} (x)^2 dx$$

$$P = a^2 \left( \frac{x^3}{3} \right) \text{ within limit } 0.35 \text{ to } 0.45.$$

$$P = \frac{a^2}{3} [(0.45)^2 - (0.35)^2] = \frac{a^2}{3} [0.0911 - 0.0428]$$

$$\mathbf{P = 0.0161a^2}$$

**Compare the wavelength of a photon and an electron if the two have same momentum ?**

**Sol.**

The de-Broglie's wavelength of an electron  $\lambda_e = \frac{h}{p_e}$

or momentum  $p_e = \frac{h}{\lambda_e}$  .....(1)

Similarly the momentum of photon

$$p_{ph} = \frac{h}{\lambda_{ph}} \text{ .....(2)}$$

Therefore if photon and an electron have same momentum then from equation 1 and 2, we have

$$\lambda_e = \lambda_{ph}$$

Hence a photon and an electron of same momentum have the same wavelength.

**Show that probability at center of 1-D potential box is minimum for first excited state.**

**Solution.** Since we know that  $\psi_n = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$

For first excited state  $n=2$

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

At center of box  $x = \frac{L}{2}$

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

$$\psi_2 = 0$$

$$\text{Probability } P = \int_0^{L/2} (\psi_2)^2 dx$$

$$P=0$$

**A particle is moving in one dimensional potential box of width  $25 \text{ \AA}$ . Calculate the probability of finding the particle within an interval of  $5 \text{ \AA}$  at the centre of the box when it is in state of least energy.**

## Solution-

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

For lowest energy state  $n=1$ , wave function will be

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

At the centre of box  $x = \frac{L}{2}$  therefore probability of finding the particle at the center of box

$$|\psi_n|^2 = \frac{2}{L} \sin^2 \frac{\pi x}{a} = \frac{2}{L} \sin^2 \frac{\pi \frac{L}{2}}{L} = \frac{2}{L} \sin^2 \frac{\pi}{2} = \frac{2}{L}$$

Probability in the interval is given by,

$$P = |\psi_n|^2 \Delta x = \frac{2}{L} \Delta x$$

Here  $L = 25 \text{ \AA} = 25 \times 10^{-10} \text{ m}$

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

$$P = \frac{2 \times 5 \times 10^{-10}}{25 \times 10^{-10}} = \mathbf{0.4}$$



**Find the two lowest permissible energy states for an electron which is confined in one dimensional infinite potential box of width  $3.5 \times 10^{-9}$  m. (2020 - 21)**

The energy of a particle of mass  $m$  moving in one dimension in an infinitely high potential box of width  $L$  is given by

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

Here,  $m = 9.1 \times 10^{-31}$  kg,  $h = 6.63 \times 10^{-34}$  Joule – sec,  $L = 3.5 \times 10^{-9}$  m

$$E = \frac{n^2 (6.63 \times 10^{-34})(6.63 \times 10^{-34})}{8 \times 9.1 \times 10^{-31} \times (3.5)^2 \times 10^{-18}} = 4.929 \times 10^{-21} n^2$$

Joule

$$E = \frac{(4.929 \times 10^{-21} \text{ n}^2)}{1.6 \times 10^{-19}} = (3.08 \times 10^{-2} \text{ n}^2) \text{ eV}$$

The lowest two permitted energy values of the electron is obtained by putting  $n=1$  and  $n=2$ .

First lowest permitted energy value is (for  $n=1$ ) = **0.038 eV**

Second lowest permitted energy value is (for  $n=2$ ) =  $0.038 \times 4 =$   
**0.152 eV**

**In a Compton scattering experiment X-ray of wavelength  $0.015\text{\AA}$  is scattered at  $60^\circ$ , find the wavelength of scattered X- ray.**

**Solution-** If  $\lambda$  and  $\lambda'$  be the wavelength of incident and scattered X-ray of photon respectively then the Compton shift is given by

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

$$\text{Therefore } \lambda' = \lambda + \frac{h}{m_0 c} (1 - \cos\theta)$$

$$= (0.015 \times 10^{-10}) + \frac{2 \times 6.63 \times 10^{-34}}{9.1 \times 10^{-31} \times 3 \times 10^8} \text{Sin}^2 30^\circ$$

$$= (0.015 \times 10^{-10}) + \frac{2 \times 6.63 \times 10^{-34}}{9.1 \times 10^{-31} \times 3 \times 10^8} (1/2)^2$$

$$= (0.015 \times 10^{-10}) + 0.012 \times 10^{-10}$$

$$\lambda' = \mathbf{0.027 \times 10^{-10} \text{ m} = 0.027 \text{ \AA}}$$

**X-rays of wavelength  $2 \text{ \AA}$  are scattered from a black body and X-rays are scattered at an angle of 45 degree. Calculate Compton shift ( $\Delta\lambda$ ), wavelength of scattered photon  $\lambda'$ . **(2018 - 19)****

Compton shift is given by

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

$$\Delta\lambda = \frac{6.62 \times 10^{-34}}{9.1 \times 10^{-31} \times 3 \times 10^8} (1 - \cos 45^\circ)$$

$$\Delta\lambda = 0.243 \left(1 - \frac{1}{\sqrt{2}}\right)$$

$$\Delta\lambda = \frac{0.0243 \times 0.4142}{1.4142}$$

$$\Delta\lambda = 0.007 \text{ \AA}$$

Wavelength of scattered photon,  $\lambda' = \Delta\lambda + \lambda = (0.007 + 2) \text{ \AA}$

$$\lambda' = 2.007 \text{ \AA}$$

**X-ray with  $\lambda = 1\text{\AA}$  are scattered from a carbon block, the scattered radiation is viewed at  $90^\circ$  to the incident beam. Find the Compton shift and the kinetic energy imparted to the recoiling electron.**

**(IMP)**



Compton shift is given by

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

$$\Delta\lambda = \frac{6.63 \times 10^{-34}}{9.1 \times 10^{-31} \times 3 \times 10^8} (1 - \cos 90^\circ)$$

$$\Delta\lambda = 0.0243 \times 1 = 0.0243 \text{ \AA}$$

Wavelength of scattered photon,  $\lambda' = \Delta\lambda + \lambda = (0.0243 + 1) \text{ \AA}$

$$\lambda' = 1.0243 \text{ \AA}$$

Kinetic energy imparted to the recoiled electron = decrease in the energy of photon, i.e.

$$\begin{aligned} K.E. &= \frac{hc(\lambda' - \lambda)}{\lambda\lambda'} \\ &= \frac{6.63 \times 10^{-34} \times 3 \times 10^8 \times 0.0243 \times 10^{-10}}{10^{-10} \times 1.0243 \times 10^{-10}} \\ &= 4.72 \times 10^{-17} \text{ Joule} \\ &= \frac{4.72 \times 10^{-17}}{1.6 \times 10^{-19}} \text{ eV} \\ &= 295 \text{ eV} \end{aligned}$$

Thank  
you