MODULE-1
MODERN PHYSICS

BLACKBODY RADIATION:

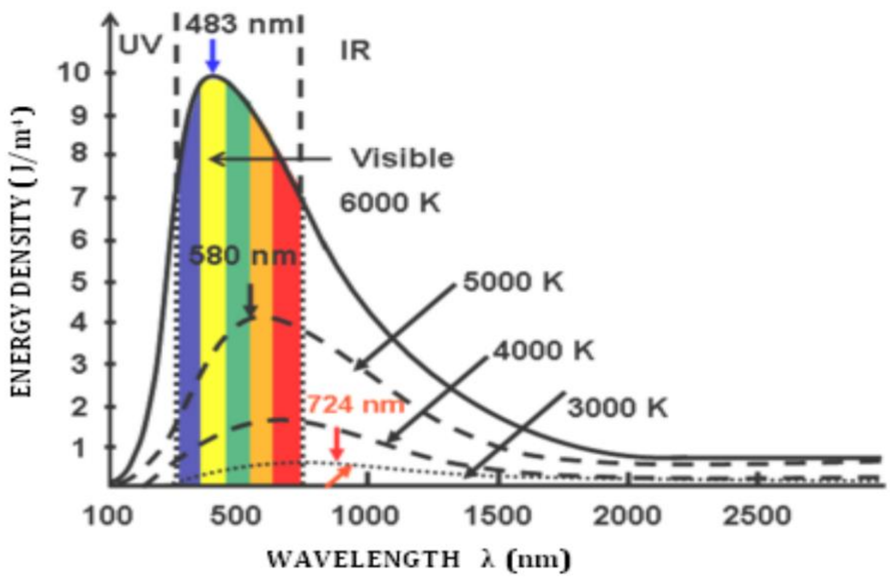
A **black body** in principle absorbs the entire radiations incident on it and also emits all the radiations when it is heated to incandescence. The radiations emitted by such a body are known as **black body radiation**.

1. A black body not only completely absorbs all the radiations falling on it but also behaves as a perfect radiator when heated.

2. The radiation given out by a black body depends only on the temperature and not on the nature of the body.

BLACKBODY RADIATION SPECTRUM AND ITS FEATURES

Following figure illustrates the way in which the energy radiated by a black body is distributed amongst various wavelengths.



The plot had following features:

There are different curves for different temperatures.

There is a peak for each curve. This means that the electromagnetic waves of wavelength corresponding to the peak is emitted to the largest extent at that temperature to which the curve corresponds.

The peak shifts towards the lower wavelength side as higher temperatures are considered.

LAWS GOVERNING THE BLACKBODY RADIATION:

1. Wien's Law
2. Wien's Displacement Law
3. Stefan's Law
4. Rayleigh-Jeans Law
5. Kirchoff's Law
6. Planck's Law

WIEN'S LAW:

Wien's law gives the relation between the wavelength of emitted radiation and the temperature of the source as,

$$E\,d \qquad C_1 \quad {}^{5}e^{\,C_{2}/\;\;T}\,d$$

Where C_1 and C_2 are constants and

$E\,d$ is the energy emitted per unit volume in the wavelength region and +d .

This law is called **Wien's law of energy distribution** in the blackbody radiation spectrum.

Drawbacks of wien's law:

Wien's law holds good only for **shorter values of wavelength** but fails to explain the region in which wavelengths are longer.

RAYLEIGH-JEANS LAW:

In 1900, Lord Rayleigh applied the principle of equipartition of energy to electromagnetic vibrations and deduced an equation for the black body raidiation. This was later modified by Sir James Jeans and came to be called Rayleigh-Jeans law. According to this law the energy density i.e. the amount of energy per unit volume of a blackbody in the wavelength ranging from to +d is given by

$$E\,d \qquad 8\,kT \quad {}^{4}\,d$$

Where, k is Boltzmann constant.

Due to the presence of the factor λ^{-4} in the equation, the energy radiated by the blackbody should rapidly decrease with the increase in wavelength.

Drawbacks of Rayleigh-Jeans law (or Ultraviolet catastrophe):

Rayleigh-Jeans law holds good for **longer values of wavelength** but does not fit the experimental curves for shorter values of wavelength.

This discrepancy between the theoretical conclusion and the experimental result is called **"ULTRAVIOLET CATASTROPHE"**. As per the equation, black body radiates enormously in the shorter wavelength side, but practically black body chiefly radiates in IR or visible range which is the longer wavelength region of the spectrum.

This wrong prediction in the radiation emitted by the body is called Ultraviolet Catastrophe.

<u>PLANCK'S LAW:</u>

In order to explain the energy distribution in the complete spectrum of a blackbody radiation, Max Ludwig Planck in 1900 put forward the quantum theory of radiation. For deriving the equation Planck made certain assumption based on Quantum mechanical consideration.

Assumptions of Quantum theory of radiations are,

1. The walls of the blackbody consist of a very large number of **<u>electrical oscillators.</u>** Each oscillator vibrates with a frequency of its own.

2 Energy is absorbed or emitted by a blackbody in a discrete manner, in the form of small packets called **quanta**.
3. Each quantum has energy that depends only on the frequency of the radiation and is given by **E = nh**
Where h is a constant known as Plank's constant = 6.625 $\times 10^{-34}$ J-sec
and n=0,1,2, …..
4. An oscillator may gain or lose energy when it absorbs or emits radiation of frequency υ given by **υ = ΔE/h**
Where, ΔE is the difference in energies of the oscillator before and after emission or absorption.

Based on the above assumptions, Planck derived an equation which successfully explained the entire spectrum of blackbody radiation. The equation is given by

$$E_\lambda d\lambda = \frac{8\pi hc}{\lambda^5}\frac{1}{e^{h\nu/kT}-1}d\lambda \quad \text{…………(1)}$$

Planck's law explains the spectrum of blackbody radiation successfully in both the shorter wavelength and longer wavelength regions.

REDUCTION OF PLANCK'S LAW TO WIEN'S LAW AND RAYLEIGH-JEANS LAW:

Derivation of Wien's law from Planck's law

- **For shorter wavelengths,** When λ is small,

$\upsilon = c/\lambda$ is large. When υ is large, $e^{h\upsilon/kT}$ is very large.

i.e., $e^{h\upsilon/kT} >> 1$

$e^{h\upsilon/kT} - 1 \approx e^{h\upsilon/kT} \approx e^{hc/\lambda kT}$ (Since $\upsilon = c/\lambda$)

Substituting in Equation (1) we get

$$E\ d \quad \frac{8\ hc}{5} \frac{1}{e^{hc\ \ kT}}\ d$$

$E\ d\ C_1\ ^5 e^{\ C_2/\ T}\ d$ (2) where $C_1\ 8\ hc$ and $C_2\ hc/k$.

This equation is Wien's law of radiation.

Derivation of Rayleigh-Jeans law from Planck's law

- **For longer wavelengths,**

When wavelength λ is large, $\upsilon = \frac{c}{\lambda}$ is small.

Expanding $e^{h\upsilon/kT}$ as power series, we have

$$e^{h\upsilon/kT} = 1 + \mathbf{h\upsilon/kT} + \mathbf{(h\upsilon/kT)^2} + \ldots\ldots$$

Neglecting the higher order terms we get,

$$e^{h\upsilon/kT} \approx 1 + \mathbf{h\upsilon/kT}$$

$\therefore$ $e^{h\upsilon/kT} - 1 \approx h\upsilon/kT \approx hc/\lambda kT$

Substituting in equation (1), we get

$$E\ d \quad \frac{8\ hc}{5} \frac{kT}{hc}\ d$$

$$E\ d \frac{8\ kT}{4}\ d \quad (3)$$

This equation is the Rayleigh-Jeans law of radiation.

COMPTON EFFECT:

In 1923, Arthur H Compton discovered the scattering of X –rays by electrons that are weakly bound to atoms in a target material. Compton Effect confirms the existence of photons and hence proves the particle nature of radiation.

When a beam of monochromatic X- rays is incident on a target material of such as graphite sheet, it undergoes scattering in many directions spanning through 0 to 180^0 leading to the modification in the wavelength. Compton interpreted this interaction as a collision of two particles, a X-ray photon and an electron in the graphite sheet. The scattered X-rays consist of two components. One component called unmodified wavelength denoted by λ (the same wavelength as that of the incident X-rays) and the other component called modified wavelength denoted by λ'(wavelength slightly longer than incident wavelength) . This difference in wavelength **$(\lambda - \lambda') = d\lambda$**, indicates the enhancement in the wavelength is called **Compton Shift.**

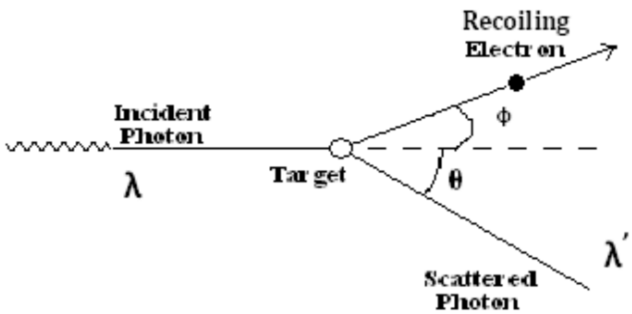
Compton made the measurement by replacing graphite with other materials and found that λ' is independent of the target material, but depends on the angle 'θ' through which the scattering occurs.

The phenomenon in which there is change in wavelength accompanied by a change in the direction of the scattered X-rays compared to the incident X-rays, consequent to the exchange of energy between the X-ray photons and the electrons in the target material, is called Compton Effect.

Compton used Quantum theory to give a satisfactory explanation for the modified wavelength.

- ***EXPLANATION OF COMPTON EFFECT*:**

Compton assumed that during the scattering process, the incident photon from X-rays collides with a free electron in the target material (graphite sheet). As a result, the photon is scattered at an angle 'θ' to the incident direction and its energy reduces from E to E'. To account for the change in energy of the photon, the electron is assumed to recoil at an angle 'φ' to the incident direction of the photon and the photon with reduced energy travels in the direction 'θ' with the original direction.



— (Energy of the photon before the collision) ***E =**

Where,

h is Planck's constant,

c is the velocity of light and

λ is the wavelength of the incident X-rays. and

***E' =** — (Energy of the photon after the collision)

By applying the laws of conservation of momentum, Compton derived an equation for the change in wavelength Δλ of the X-rays. It's given by

$$\Delta\lambda = (\lambda' - \lambda) = \quad \_\_\_ \quad (1 - \cos\theta) \text{ ------------- } (3)$$

where .

m_0 is the rest mass of the electron and c is the velocity of light. This is Compton's equation for Compton shift and the quantity **(** ___) has the dimensions of length and is called Compton wavelength whose value is 2.42 X 10^{-12}m.

PHYSICAL SIGNIFICANCE OF COMPTON EFFECT:

Proves the particle nature of X-rays

Energy exchange between X-ray photon and electron during collision occur as though it is particle-particle collision.

WAVE PARTICLE DUALISM:

The nature of light is not unique i.e. it exhibits both particle nature and wave nature.

Some phenomenon like Interference, Diffraction and Polarization can be explained on the basis of Wave nature of light while other phenomenon like Photoelectric effect and Compton Effect can be explained on the basis of particle nature of light. This property where light behaves both as waves and particles is called dual nature of light or wave particle dualism

Example- X-rays assumes the status of the particles in the Compton Effect experiment and the same X-rays get diffracted by a crystal in few other experiments.

De- BROGLIE'S HYPOTHESIS:

Because of the dual nature observed of radiation and light, Louis de Broglie put forward a bold hypothesis. He reasoned out that nature exhibits a great amount of symmetry. "If the radiation behaves as waves sometimes and as particles at other times then it is expected that entities such as electrons which behave as particles should also exhibit wave like behavior under appropriate circumstances". This is known as de Broglie's hypothesis.

According to this Hypothesis, all material particles in motion are associated with a wave. The waves associated with material particles are called **matter waves** or **de Broglie waves.**

De- BROGLIE WAVELENGTH:

According to de Broglie hypothesis, a moving particle is associated with a wave. The waves associated with the particles of matter like electrons are known as matter waves or de Broglie waves.

When a particle has momentum 'p' ,its motion is associated with called **De Broglie wavelength.** It is given by

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

The above equation is known as de Broglie wave equation.

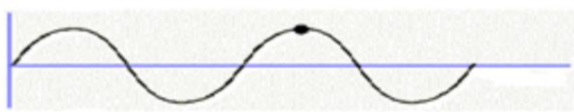
Hence de Broglie wavelength depends upon the mass of the particle and its velocity.

PHASE VELOCITY AND GROUP VELOCITY:

Phase Velocity (v_{phase}):

Phase velocity is the velocity of the individual waves. The velocity with which each phase in a wave moves is called the phase velocity.

If we consider a point to be marked on a travelling wave, then that point represents a particular phase of the wave, and the velocity with which it is transported owing to the motion of the wave is called Phase velocity.



Here, the point on the wave represents the phase $\frac{\pi}{2}$ Phase velocity is given by

$$v_{phase} = k$$

Where ω is the angular frequency and k is the wave number.

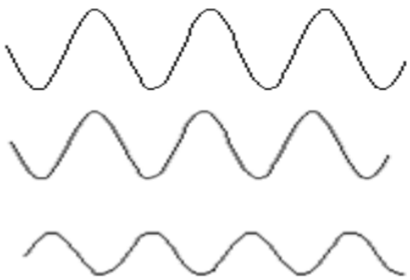
Group Velocity (v_{group}):

When a group of two or more waves of different wavelengths and different velocities are superimposed on each other, the amplitude of the resultant wave is varied, which forms a wave group or wave packet. The velocity with which the envelope enclosing the wave packet is transported is called the group velocity.

In other words the velocity with which the energy in the wave group is transmitted is called group velocity. Group Velocity is represented by

$$v_{group} = \frac{d}{dk}$$

where dω is the change in angular frequency dk is the change in wave number.



Individual waves

Wave packet

RELATION BETWEEN PHASE VELOCITY AND GROUP VELOCITY:

We know that

$$v_{group} = \frac{d}{dk} \quad \text{-----------} \ (1)$$

$$v_{phase} = \frac{}{k} \quad \text{------------} \ (2)$$

Eq. (2) can be written as

$$= k \, . \, v_{phase}$$

On differentiating, $\frac{d}{dk} = v_{phase}\frac{dk}{dk} + k \, . \, \frac{dv_{phase}}{dk}$

$$v_{group} = v_{phase} + k \, . \, \frac{dv_{phase}}{dk}$$

$$v_{group} = v_{phase} + k. \, . \, \frac{dv_{phase}}{d} \; \frac{d}{dk} \; ....(3)$$ (divide and multiply by d)

We know that,

$$k = \frac{2}{} \qquad \frac{dk}{d} \qquad \frac{2}{2} \qquad \text{(upon differentiation)}$$

$$\frac{d^2}{dk2}$$

Substituting in Eqn (3) we get,

$$\frac{2dV_{phase}}{d} \quad \frac{2}{2}$$

$$\boxed{\mathbf{Vgroup} = \mathbf{Vphase} - \frac{dv_{phase}}{d}}$$

RELATION BETWEEN GROUP VELOCITY AND PARTICLE VELOCITY:

We have the equation for group velocity as

$$v_{group} = \frac{d}{dk} \qquad \text{-----------} \ (1)$$

But, $= 2\,\upsilon = \frac{2\ E}{h}$ since $E = h\upsilon$ $\upsilon = \frac{E}{h}$

Upon differentiation we get,

$$d = \frac{2}{h} dE \qquad \text{------------} \ (2)$$

Also we have $k = \frac{2}{\ }$ $k = \frac{2}{h} p$ since $= \frac{h}{p}$

$$dk = \frac{2}{h}.dp \qquad \text{-------------} \ (3)$$

Dividing (2) by (3), we have

$$\frac{d}{dk} = \frac{dE}{dp} \qquad \text{-------------} \ (4)$$

We know that $E = \frac{p^2}{2m}$,

Where ,p is the momentum of the particle.

Upon differentiation we get,

$$dE = \frac{2pdp}{2m} = \frac{pdp}{m}$$

$$\frac{dE}{dp} = \frac{p}{m} = \frac{mv_{particle}}{m}$$

$$\frac{dE}{dp} = v_{\text{particle}} \qquad \text{------------------} \ (5)$$

From (1), (4) & (5) we have

$v_{group} = \frac{d}{dk} = \frac{dE}{dp} = v$ particle $\therefore$ **$v_{group} = v_{particle}$**

The velocity of a de Broglie wave group associated with a particle is equal to the velocity of the particle itself.

RELATION BETWEEN PHASE VELOCITY, GROUP VELOCITY AND VELOCITY OF LIGHT:

The equation for phase velocity is

$$v_{phase} = \frac{\;}{k} \quad \text{----------------} \ (1)$$

We know that $\quad = 2\ \upsilon = \frac{2\ E}{h}$ $\quad$ and $\quad k \quad \frac{2}{h} p$

Substituting for ω and k in equation (1), we get

$$v_{phase} = \frac{\frac{2\ E}{h}}{\frac{2}{h}\ p} \quad \frac{E}{p}$$

$$v_{phase} = \frac{mc^2}{mV_{particle}} \quad \frac{mc^2}{mV_{group}}$$

$$\boxed{v_{phase} \,.\, v_{group} = c^2}$$

v_{phase} is always greater than the velocity of light.

CHARACTERISTICS OF MATTER WAVES:

[1]Matter waves are the waves that are associated with a moving particle. The wavelength and energy of the matter waves are given by.

$$= \frac{h}{p} \ \textbf{and } \mathbf{E = h\,\upsilon}$$

Where, p is the momentum of the particle and υ is the frequency of the waves.

(2) Group velocity of the matter waves is equal to the velocity of the moving particle.

(3) Phase Velocity of the matter waves is greater than the velocity of the Light (c).

We have $\mathbf{v_{phase}} = \frac{c^2}{V_{group}} \quad \frac{c^2}{V} c$

(4) Phase Velocity of different matter waves may be different.

(5) The amplitude of the matter waves at a particular region and time

depends on the probability density of the particle at that region and time.

END

QUANTUM MECHANICS

Quantum Mechanics is a new branch of study in physics which is indispensable in understanding the mechanics of particles or bodies in the atomic and the subatomic scale**.** The term quantum mechanics was first introduced by Max Born in1924.Within the field of engineering, quantum mechanics plays an important role. The study of quantum mechanics has lead to many new inventions that include the laser, the diode, the transistor, the electron microscope, and magnetic resonance imaging. Flash memory chips found in USB drives also use quantum ideas to erase their memory cells. The entire science of Nanotechnology is based on the quantum mechanics.

HEISENBERG'S UNCERTAINTY PRINCIPLE:

One of the fundamental principles of quantum mechanics is the "Heisenberg's uncertainty principle".
The principle was formulated in 1927 by German physicist Werner Heisenberg. It is also called the indeterminacy principle.
Statement:

"It is impossible to determine precisely and simultaneously both the position and momentum of a particle."

Further, "in any simultaneous determination of the position and momentum of a particle, the product of the corresponding uncertainties in the measurement is equal to, or greater than (h/4π)".

$$\mathbf{x}\ \mathbf{p}\quad {}^{h}\!/_{4}$$

Where **x** represents the uncertainty in the measurement of the position of the particle and **p** represents the uncertainty in the measurement of its momentum.

Heisenberg's uncertainty principle could also be expressed in terms of the uncertainties involved in the measurement of the physical variable-pair, **energy (E) and time (t) and also angular displacement (θ) and angular**

momentum (L).

If E and t are the uncertainties involved in determining the energy and time respectively, then

$$\mathbf{E\ t}\quad {}^{h}\!\big/_{4}$$

Similarly, if and L are the uncertainties involved in determining the angular displacement and angular momentum of the particle respectively, then

$$\mathbf{L}\quad {}^{h}\,4\big/$$

where, the notation associated with the respective variables indicates the minimum uncertainty involved in the measurement of the corresponding variable.

<u>PHYSICAL SIGNIFICANCE OF HEISENBERG'S PRINCIPLE:</u>

It signifies that one should not think about accurate values for the position and momentum of a particle. Instead one should think about only the probable values for the position and momentum.

The estimation of such probabilities are made by mathematical functions named probability density functions.

<u>APPLICATION OF HEISENBERG'S UNCERTAINTY PRINCIPLE:</u>

<u>Non-existence of electrons in the nucleus:</u>

As an application of Heisenberg's uncertainty principle, we consider the case of "Non-existence of electrons in the nucleus". This is based on the observations regarding the emission of β–rays during nuclear decay.

. Becquerel demonstrated that β-rays are actually streams of **electrons**. During β decay process it was found that the emitted β-rays travelled with different velocities. Becquerel demonstrated that β-rays are actually streams of **electrons** Their kinetic energy varied from very low values to a maximum value of about 3-4 MeV. Hence the obvious question, ***"is it possible that electrons exist inside the nucleus with certain energy, and the same energy appears as their kinetic energy when they are emitted?"***

The proof for this is presented below:

We know by the theory of relativity that, the energy E of a body is expressed as,

$$E = mc^2 = \frac{m_0 c^2}{\sqrt{1 - \frac{v^2}{c^2}}}$$

where ‘m_o’ is the rest mass of the body and ‘m’ is the mass while its velocity is v.

Squaring on both sides, we get

$$E^2 = \{ \ \}^2 = \ = \frac{m_o^2 c^6}{c^2 - v^2} \text{ ………….. (1)}$$

Also, we know that, momentum p of the body is given by,

$p = mv =$

or, $p^2 =$ $=$

Multiplying by c^2, we have,

$p^2 c^2 =$ …………..(2)

Subtracting eq. (3) by (2), we get,

$E^2 - p^2 c^2 =$

$E^2 = p^2c^2 +$

$E^2 = c^2 [p^2 + m_o^2 c^4]$ ....(3)

This is Einstein’s relativistic energy-momentum equation,

where m_0 = rest mass of electron = 9.1×10^{-31} kg,

p = momentum and

c = speed of light = 3×10^8 m/s.

Now, for an electron to exist inside the nucleus, the uncertainty Δx in its position cannot be greater than the nuclear radius. The nuclear radius is in the order of 5×10^{-15} m. We can take this value to be approximately the maximum space of confinement. Thus the maximum value for uncertainty in position can be taken as

$$(\Delta x)_{max} \leq 5 \times 10^{-15} \text{ m}$$

By uncertainty principle,

$$\Delta \cdot \Delta \geq \frac{h}{4}$$

$$(\Delta\ )_{min} \quad \frac{h}{4\pi} \frac{1}{\Delta x}$$

$$\therefore \quad \Delta \geq \frac{6.63 \quad 10^{34}}{4 \quad 3.14 \quad 5 \quad 10 \quad 15}$$

$$(\Delta p)_{min} \geq 1.1 \quad 10^{-20} \text{ Ns} \quad \ldots\ldots\ldots\ldots\ldots(4)$$

This is the uncertainty in the momentum of the electron. But since the momentum of the electron must atleast be equal to the uncertainty in the momentum, we can take

$$(p_x)_{min} \geq 1.1 \quad 10^{-20} \text{ Ns} \quad \ldots\ldots\ldots(5)$$

We know that the rest mass of the electron is $m_o = 9.11 \times 10^{-31}$ kg.

Using the inequality (5) in equation (3), we can say that for the electrons to exist inside the nucleus, its energy E must be such that

$$E^2 \geq c^2 [p^2 + m_o^2 c^4]$$

$(E)_{min} \geq (3 \times 10^8)^2 [(1.1 \times 10^{-20})^2 + (9.11 \times 10^{-31})^2 (3 \times 10^8)^4]$ Since the second term inside the bracket is too small, it is neglected.

$$\mathbf{(E)_{min} \geq 20.6 \text{ MeV}}$$

This means to say that, for electrons to exist inside the nucleus, it must have a minimum energy of about 20.6 MeV. But beta-decay studies indicate that the kinetic energy of β-particles is of the order of 3 to 4 MeV. Hence, we can conclude that electrons cannot exist inside the nucleus.

WAVE FUNCTION:

In quantum mechanics, because of the wave-particle duality, the properties of particles can be described by a wave. Therefore its quantum state can be represented by a wave of any arbitrary shape. This is called a **Wave function.**

The variable quantity characterizing matter waves is known as **wave function.** It gives complete information about the system .It is also called state function as it speaks about the physical state of the system.

Wave function is obtained by solving a fundamental equation called

Schrodinger equation.

It varies w.r.t position and time.

It is denoted by a symbol (Ψ)

Ψ itself cannot be an observable quantity hence, Ψ has no direct physical significance

Ψ can have real values or imaginary(complex).

<u>Properties of wave function</u>

Property 1: ψ is single valued everywhere.

A function f(x) which is not single valued over a certain interval is shown in Fig. 1. Here f(x) has three values, f_1, f_2 and f_3 for the same value of P at x = P. Since f1≠ f2 ≠ f3, it means to say that, if f(x) were to be wave function, then the probability of finding the particle has three different values at the same location P which is absurd. Hence this wave function is not acceptable.

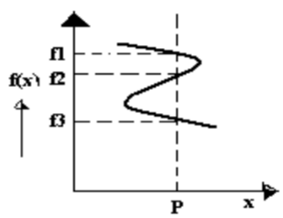


Figure:1

Property 2: ψ is finite everywhere.

A function f(x) which is not finite at x = R is shown in Fig.2. At x = R, f(x) = ∞. Thus, if f(x) were to be a wave function, it signifies a large probability of finding the particle at a single location (x = R), which violates the uncertainty principle. Hence the wave function becomes unacceptable.

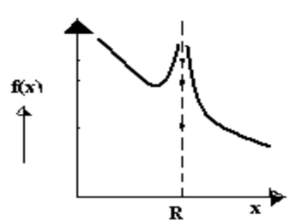


Figure: 2

***Property 3: ψ and its first derivatives with respect to its variable are continuous everywhere*.**

A function f(x) which is discontinuous at Q is shown in Fig. 3. At x = Q, f(x) is truncated at A, and restarts at B. The function is not defined between A & B. If f(x) is taken to be a wave function, then the state of the system at x = Q cannot be ascertained. Hence the wave function is not acceptable.

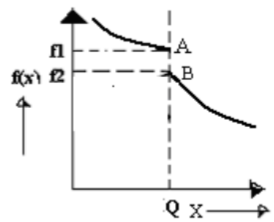


Figure: 3

Also, when ψ is not continuous, its first derivatives will not be finite. The first derivatives should also be continuous, because, if they are not continuous, the second derivatives of ψ will not be finite.

Property 4: For bound states, ψ must vanish at infinity. If ψ is a complex function, then ψ* ψ must vanish at infinity.

The wave functions that possess all the above properties are called **Eigen functions**.

<u>Physical significance of wave function ( ):</u>

a) It gives the idea about the probability of finding a particle.

b) Let us consider a system of electrons. If is the wave function associated with that system, then ^{2} gives measure of density of electrons.

c) If we consider an electron to be present in the region of volume V then ^{2}**dV** gives the probability of finding the electron in the region of volume dV

d) The certainty of finding the electron in the entire region of volume V is given by

$$\int {}^2 dV = 1.$$

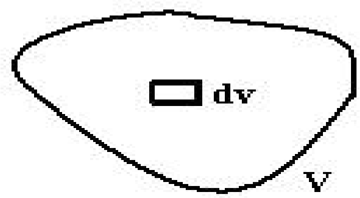
This is known as normalization.

Probability density:

According to Max born approximation, probability of locating a particle at a point is directly propotional to ^{2}. This is called **probability density.**

If $^2 = 1$; then we are sure that particle is present .

If $^{2} = 0$; then the particle is completely absent.



Consider a particle inside the volume V. Let dV be the infinitesimally small element in V. If ψ is the wave function associated with the particle, then ^{2} is the probability per unit volume of space, centered at a point where ψ is evaluated at that time

Thus, the probability of finding a particle is

$$P = \int \ ^{2} dV$$

Here, the product of ψ. ψ* is real and is written as ^{2}, where ψ* is the complex conjugate of ψ.

Probability density is given by

$$^{2} = \quad ^{*}, \text{ where } \quad ^{*} \text{ is the complex conjugate of } .$$

Normalization condition:

Further, if we are certain that the particle is present in a particular region or space of volume V, then

$$\int \quad ^{2} \quad . dV = 1$$

This value 1 for probability means, it is clearly a certainty. However, if we are not certain about locating the particle anywhere in the given volume, then it is expected to be present somewhere in space. Then the probability of finding the particle somewhere in the universe must be unity. Thus

$$_{-\infty}^{+\infty} \quad ^{2} \quad \int . dV = 1$$

This condition is known as the normalization condition.

A wave function that satisfies the above condition is said to be normalized.

Eigen function and eigen value

Eigen functions are those functions which possess the properties of that they are single valued & finite everywhere and also their first derivatives with respect to their variables are continuous everywhere..

To find ψ Schrodinger's wave equation has to be solved. Since it is a second order differential equation, hence it has many numbers of solutions. But all of them may not be the correct solutions in such a case we have to choose only a permitted function. These permitted functions are called Eigen function the corresponding energy values are called **Eigen values**

Operator.

An operator($\hat{A}$) is a symbol or a code which directs one to perform an operation on the Eigen function (ψ)to get the information (Eigen value)(λ)

$$\hat{\mathbf{A}} = \lambda$$

Schrodinger's Wave Equation:

Schrodinger equation is a fundamental wave equation in quantum mechanics capable of determining the wave function ψ for different physical conditions.

Time independent Schrodinger Wave Equation:

According to de- Broglie theory, for a particle of mass 'm' moving with a velocity 'v', the wave length λ is given by,

$\lambda = \frac{h}{p} = \frac{h}{mv}$ ----------------(1) where , p is the momentum of the particle.

The de- Broglie wave equation for a particle travelling in positive x-direction can be written in complex form as

$$\Psi = A e^{i(kx-\omega t)} \text{ ----------------- } (2)$$

where, A is the amplitude of the wave, ω is angular frequency of the wave, ψ is the total wave function and k is the wave number.

The space independent part in equation (2) can be represented as a wave function,

$$\Psi = \psi A e^{-i\omega t} \text{ ----------------- } (3)$$

Differentiate (3) twice wrt x. Since Ψ depends on x, we get

$$\frac{d^2}{dx^2} e^{-i\omega t} . \frac{d^2}{dx^2} \quad (4)$$

Now again differentiate (3) w.r.t. time 't' twice, we get

$$\frac{d}{dt}(-i\omega)\, Ae^{i(kx-\omega t)}\, \psi$$

$$\frac{d^2}{dt^2} = (-i\omega)(-i\omega)\, Ae^{i(kx-\omega t)}\, \psi$$

$$\frac{d^2}{dt^2} = -\omega^2 e^{-i\omega t}\, \psi \text{ ------------- (5)}$$

The equation for a travelling wave in differential form can be written as,

$$\frac{d^2y}{dx^2} \quad \frac{1}{v^2}\frac{d^2y}{dt^2}$$

Then by analogy**,** the wave equation for a de Broglie wave for the motion of a free particle can be written as

$$\frac{d^2}{dx^2} \quad \frac{1}{v^2}\frac{d^2}{dt^2} \text{ ----------------- (6)}$$

This equation represents the waves propagating along x-axis with a velocity 'v', and 'x' is the displacement at time 't'.

Substituting equations (4) and (5) in the above equation, we get

$$e^{-i\omega t} . \frac{d^2}{dx^2} \quad \frac{1}{v^2} . (\; ^2 e^t)$$

$$\frac{d^2}{dx^2} \quad \frac{2}{v^2}$$

But, we know that = 2 ν and v = υ . Substituting for ω and v, we get

$$\frac{d^2\psi}{dx^2} = \frac{-4\pi^2\nu^2}{\nu^2\lambda}\psi = \frac{-4\pi^2}{\lambda}\psi \text{------- (7)}$$

But, we have, = $\frac{h}{}$ = $\frac{h}{}$. Then eq.(7) becomes

$$\frac{d^2\psi}{dx^2} + \frac{4\pi^2 m^2 v^2}{h^2}\psi = 0 \text{ -------------(8)}$$

We know that,

Total Energy = Kinetic Energy + Potential Energy

E=KE+PE

E = ____ ² +

²

² ² = 2 (−) ----------(9)

Substitute eq. (9) in (8), then

$$\frac{d^2\psi}{dx^2} + \frac{4\pi^2 2\,(\;-\;)}{h^2}\psi = 0$$

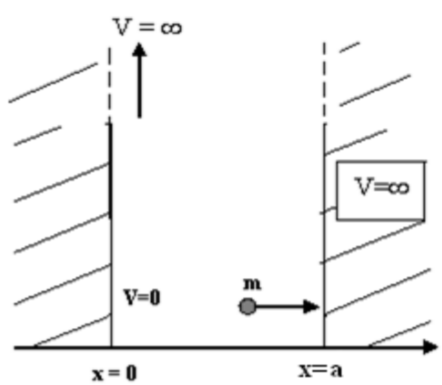
(−) + =

This is known as time independent Schrodinger wave equation in one dimension.

<u>Applications of Schrodinger's Equation:</u>

<u>(1) Particle in one dimensional potential well of infinite height:</u>

Consider a particle of mass '**m**' moving inside a box along the X – direction between two rigid walls A and B. The particle is free to move between the walls of the box at x = o and x = a. The potential energy of the particle is considered to be zero inside the box and infinity at all points outside the box. This means that



1. PE, V=0 for 0 < x < a

2. PE,V=   for x   0 and x   a

The particle is always inside the box and therefore the probability of finding the particle outside the box is zero. Therefore the wave function is zero for x 0 and x a.

The Schrodinger's equation for a particle is given by

$$\frac{\quad}{\quad} + \frac{(\ - \ )}{\quad} =$$

Since, V = 0 inside the box between the walls, the above equation reduces to

$$\frac{d^2}{dx^2} \quad \frac{8\ ^2 mE}{h^2} 0 \text{ ---------- } \mathbf{(1)}$$

Take, $\frac{8\pi^2}{h^2} = k^2$ **--------------- (1A)**

Then, equation (1) becomes

$$\frac{\quad}{\quad} + \quad = \quad \text{..............( )}$$

The general solution for equation (2) is of the form

= A Sin kx + B Cos kx --------------- (3)

where A and B are constants. The values of these constants can be evaluated by applying the following boundary conditions. The particle cannot penetrate the walls. Hence

(i)   = 0 at x = 0

(3) 0 = A sin 0 + B cos 0

0=0+B $\boxed{\mathbf{B = 0}}$

= A **Sinkx** ------------- (4)

Again, (ii) = 0 at x = a

(3) 0 = A Sin ka

But A ≠ 0 ; because if A = 0, then the entire function will become zero.

Therefore, Sin ka = 0 = Sin nπ

ka = n , n = 0,1,2,3,.....

= — -------------- (5)

Equation (4) becomes

$\psi_n = A \sin\left(\frac{n\pi}{a}\right)x$ --------------- (6)

Substituting equation (5) in (1A) , we get

$\frac{n^2 \pi^2}{a^2} = \frac{8\pi^2 mE_n}{h^2}$

$E_n = \frac{n^2 h^2}{8ma^2}$ -------------------- (7)

where n = 1, 2, 3.......

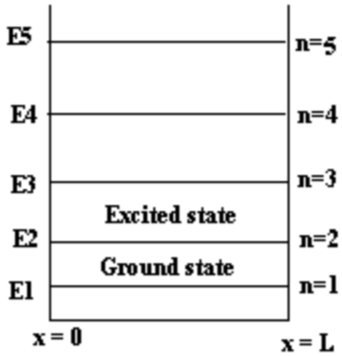
When n = 1 is the lowest energy level given by

$E_1 = \frac{\mathbf{h}^2}{\mathbf{8m}a^2}$

This energy is called the zero-point energy. Also,

$E_1 = \frac{h^2}{8ma^2} E_0$, $E_2 = \frac{4h^2}{8ma^2}$, $E_3 = \frac{9h^2}{8ma^2}$ ......

For each value of 'n' there is an energy level. The possible allowed values of energy obtained from equation (7) i.e., E_1, E_2, E_3 etc are called **Eigen values** and the corresponding wave function ψ_n is called the Eigen function.



The energy corresponding to n = 1 is called ground state energy or zero point energy and the energy levels for n = 2,3,4,5,…., are called excited states.

Inside the well, the particles can have discrete set of values of energy and it is quantized i.e.,

$E_2 = 4E_0$, $E_3 = 9E_0$, $E_4 = 16E_0$, and so on.

Normalization of wave function (evaluation of the value of A):

We have,

$$_n = A \sin\left(\frac{n\pi}{a}\right)x$$

The constant A of this equation can be obtained by applying the normalization condition i.e.,

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

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

We know that $\sin^2\theta = \frac{1-\cos 2\theta}{2}$.

Then

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

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

$$\Rightarrow \frac{A^2}{2}[\;]_0^a - \frac{A^2}{2}\left[\frac{\sin 2n\pi x}{a}\right]_2 = 0$$

$\Longrightarrow A^2 a - A^2 a \; [\mathrm{Sin}\,2n\pi a] \qquad = 0 \Rightarrow \mathrm{Sin}(2n\pi) = 0$

$\frac{A^2 a}{2} = 1 \Rightarrow A = \sqrt{2} \ldots\ldots\ldots (8)$

$\psi_n = \sqrt{a} \sin a$

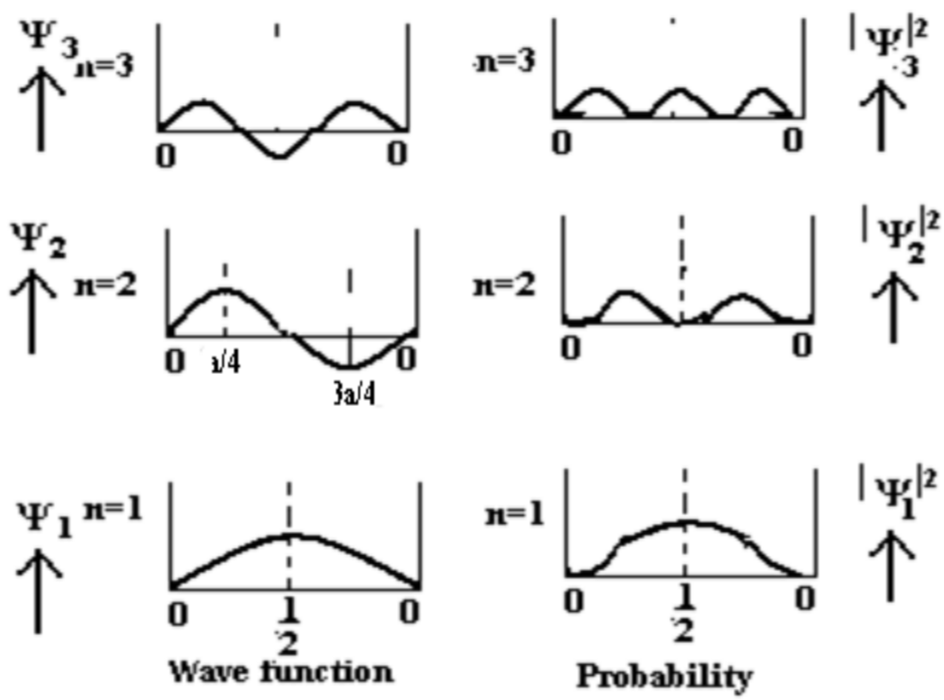
The normalized wave function of the particle is

$$\psi = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}$$

Wave functions, probability densities and energy eigen values for a particle in a box:

The first three energy levels (Eigen Values) E_1, E_2, E_3 and their corresponding wave function is 1, 2, 3 and probability densities corresponding to n = 1,2, & 3 respectively.

Figure



Case (1)

For n = 1,   the eigen function is

$= A \sin \frac{\pi}{a} x$ $_1$

$_1$ is maximum at x = a/2.

Thus a plot of $_1$ versus x will be as shown in figure and a plot of probability density $_1$ ^{2} versus x is as shown in figure. The probability of finding the particle is zero both at x = 0 and

x = a. It is maximum at x = a/2. This means that in the ground state, the probability of finding the particle is maximum at the center of the box.

Also, the ground state energy, $E_1 = \frac{h^2}{8ma^2} E_0$.

Case (2)

At n=2, the eigen function for the first excited state

is $_2$ = A $\sin \frac{2\pi}{a} x$

$_2$ = 0 at x = 0, a/2 and a.

$_2$ is maximum at the positions x = a/4 and 3a/4.

The plot of $_2$ versus x and the probability density $_2$ ^{2} versus x is as shown in fig.

Since $_2$ ^{2} = 0 at x = 0, a/2 and a, this means in the first excited state the particle cannot be observed either at the walls or at the center.

Here, the energy of the first excited state is $E_2 = \frac{4h^2}{8ma^2}$

= 4E_0 **Case (3)**

At n=3 ; the second excited state, the eigen function for the second excited state is given by

$_3$ = A $\sin \frac{3}{a} x$,

$_3$ = 0 for x = 0, a/3, 2a/3 and a.

$_3$ has maximum value for x = a/6, a/2 and 5a/6.

A plot of $_3$ versus x and probability density $_3$ ^{2} versus x is as shown in fig.

For each value of n there is an energy level as obtained from equation (1).

Here, $E_3 = \frac{9h^2}{8ma^2} = 9E_0$

Hence, the energy levels are discrete. Each energy value of E_n is called Energy Eigen value. The Eigen value for the corresponding wave function $_n$ is called the Eigen function. The energy values that are permissible in any system are obtained from the solution of the Schrodinger's equation and are called Eigen Values.

2) Energy Eigen value for a free particle

Free particle means a particle that is not under the influence of any electric field or force. For a free particle, V=0.

∴ Schrodinger wave equation becomes

$$\frac{d^2}{dx^2} \quad \frac{8\ ^2 m(E \quad 0)}{h^2} \qquad 0 \qquad \textbf{(V=0)}$$

$$\frac{d^2}{dx^2} \quad \frac{8\ ^2 mE}{h^2} \qquad 0 \text{ ---------- } \textbf{(1)}$$

+= ....( )

where $\frac{8\pi^2}{h^2}$ $= k^2$ ---------- (3)

The solution for the above equation is of the form

= A sin kx + B cos kx

For a free particle there are no boundary conditions. Therefore there are no values for the constants A, B and K.

Hence Equation (3) becomes $E=\frac{K^2 h^2}{8\ ^2 m}$

Thus for a free particle energy values are not quantized and the problem is dealt in classical mechanics. Thus a free particle is a classical entity.

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QUESTION BANK

1) What are the basic postulates of quantum theory of radiation? Explain how Planck's theory overcomes the drawbacks of weins law and Rayleigh jeans law

2) What is a blackbody? Draw the blackbody radiation spectrum. Mention its features

3) Show that group velocity is equal to particle velocity.i.e ($V_{group} = V_{particle}$)

4) State Heisenberg's Uncertainty Principle and P.T non existence of electron in nucleus using Uncertainty principle

5) Find the Eigen values and Eigen functions for an electron in one dimensional potential well of infinite height.

6) Set up the time independent Schrodinger wave equation.