UNIT-01

MODERN PHYSICS

Introduction

The classical concept of particle, space and time stood unchallenged for more than two hundred years and it had achieved many spectacular successes particularly in celestial mechanics. But in the early years of the twentieth century, the outcome of revolutionary theories like quantum theory and theory of relativity swept away the classical concept of particle, space and time given by Newton. A new set of laws of quantum physics and relativistic physics replaced the laws of classical physics.

In classical physics it is assumed that light consists of minute particles called corpuscles, which is responsible for various processes and phenomenon associated with light; however, after the discovery of phenomenon like interference, diffraction and polarization, it is proved beyond doubt that light is a form of wave, more correctly electromagnetic wave and these phenomena are successfully explained on the basis of Huygens wave theory of light. The observed phenomena like Compton Effect and explanation of spectrum of black body radiation required description of radiation in terms of particles of energy-photons. Thus dual nature of light is a fact of experimental evidence.

Overview of Unit-01

This unit consists of three lessons of teaching. In the first lesson, we will study spectrum of black body radiation, significance of Quantum theory. In the second lesson, we will study Compton Effect and its significance; in the third lesson, we will study dual nature of radiation and de-Broglie concept of matter waves and numericals.

Objectives of Unit 01

At the end of this unit we shall understand that:

- The emission and absorption of energy is not continuous, but discrete.
- A particle in motion is associated with waves called matter waves.
- Matter has dual characteristics i.e. it exhibits both wave and particle properties.
- Both wave properties and particle properties of moving objects cannot appear together at the same time because there is a separable link.
- De-Broglie waves are pilot waves and not electromagnetic waves.
- A moving particle is described in terms of wave packet.
- The dual nature of radiation has made position of a particle uncertain.

Introduction:

In this unit we will study about the failure of classical physics to explain the spectrum of black body radiation leading to discovery of Quantum theory of radiation, which signifies the particle nature of radiation thereby opening new way of understanding physics. Hence physics developed from the year 1901 is called Modern Physics and most of the phenomena are satisfactorily explained on the basis of Quantum theory of radiation. Later it became a tool to study particles of sub atomic world. And there was a need for new mechanics to explain experimentally verified atomic phenomena.

Objectives:

At the end of lesson you shall understand that:

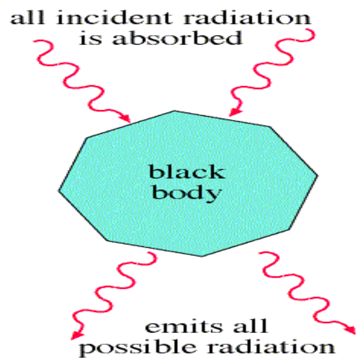
The classical physics cannot explain spectrum of black body radiation, which has lead to discovery of Quantum theory of radiation, hence radiation cannot be emitted continuously as predicted in classical physics.

Introduction:

In this lesson we will study spectrum of black body radiation and various laws put forward to explain the energy distribution in the spectrum, their failure and success.

Introduction to Black Body Radiation Spectrum

A perfect black body is the one which absorbs the entire radiations incident on it, it neither reflects nor transmits radiations, and hence it appears perfectly black. But there are no perfect black bodies. For all practical purposes we take **lamp black** as black body, because when a body coated with lamp black exposed to radiations, it absorbs 99 percent of it, and also when it is heated, it emits radiations containing almost all wavelengths.



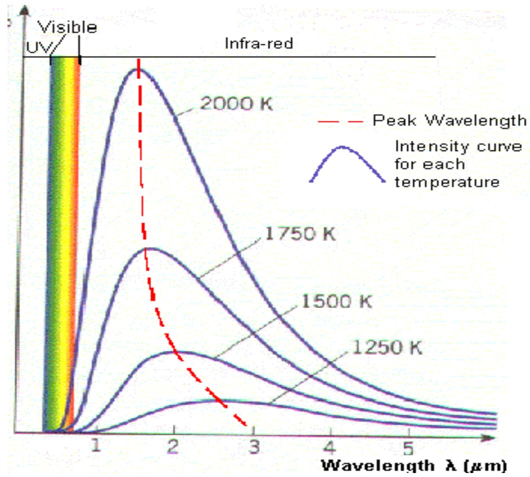
The black body radiation is characteristic of its temperature; hence it is important to know how the energy is distributed among various wavelengths at different temperatures.

Number of scientists carried out experiments on this energy distribution. Among them two scientists namely Lummer and Pringsheim found that when a graph of energy density is plotted against wavelength, curves are obtained as shown in the figure. These curves are known as radiation curves or spectrum of black body radiation.

The following conclusions can be drawn from the radiation curves.

1) The energy is not uniformly distributed in the spectrum of black body radiation.
2) At a given temperature, energy density increases with wave length, becomes maximum for a particular wavelength and then decreases as wavelength increases.
3) As temperature increases, intense radiation represented by peak of the curve shifts towards shorter wavelength region.

Spectrum of Black Body Radiation or Radiation Curves



Laws of black body radiation

In order to explain the spectrum of black body radiation, number of laws have been put forward, notable among them are Stefan's law of Radiation, Rayleigh-Jeans Law of energy distribution, Wien's Law of energy distribution and Planck's Law of Radiation.

Stefan's law of radiation

The Stefan's law states that energy radiated per second per unit area is directly proportional to thefourth power of absolute temperature. $E \propto T^4$, or $E = \sigma T^4$ where σ is Stefan's constant, though this law is experimentally verified, it does not explain the energy distribution in the spectrum of black body radiation.

Wien's law of radiation

In the year 1893, Wien assumed that black body radiation in a cavity is supposed to be emitted by resonators of molecular dimensions having Maxwellian velocity distribution and applied law of kinetic theory of gases to obtain formula for energy distribution as $U_\lambda d\lambda = C_1\lambda^{-5}e^{-(C_2/\lambda T)}d\lambda$, where $U_\lambda d\lambda$ is the energy /unit volume for wavelengths in the range, λ and $\lambda + d\lambda$, and C_1 and C_2 are constants.

Drawbacks of Wien's Law: This law explains the energy distribution only in shorter wavelengths & fails to explain the energy distribution in longer wavelength region. Also according to this law, when temperature is zero, energy density is finite. This is a contradiction to Stefan's law.

Lord Rayleigh –Jeans law of Radiation:

Lord Rayleigh–Jeans considered the black body radiations full of electromagnetic waves of all wavelengths, between 0 and infinity, which due to reflection, form standing waves. They calculated number of possible waves having wavelengths between λ and $\lambda+d\lambda$ and by using law of equi-partition of energy, they established distribution law as: $U_\lambda d\lambda = 8\pi kT\lambda^{-4}d\lambda$.Because of the presence of the factor λ^{-4}in the equation, the energy radiated by the black body should rapidly decrease with increasing wavelength.

Drawbacks of Rayleigh–Jeans law: It is found that, Lord Rayleigh–Jeans law holds good only for longer wavelengths region and fails to explain energy distribution in shorter wavelength region, moreover; as per this law, as wavelength decreases, energy density increases enormously deviating from the experimental observations. The failure of the Rayleigh–Jeans law to explain the aspect of very little emission of radiation beyond the violet region towards the lower wavelength side of the spectrum is particularly referred to as **Ultra-violet Catastrophe.**

Planck's Law of Radiation

In the year 1901, Max Planck of Germany put forward Quantum Theory of Radiation to explain Black Body Radiation spectrum. The following are the assumptions of Planck law of radiation.

1) The black body radiations in a cavity are composed of tiny oscillators having molecular dimensions, which can vibrate with all possible frequencies.
2) The frequency of radiations emitted by oscillators is same as the frequency of its vibrations.
3) An oscillator cannot emit energy in a continuous manner, but emission and absorption can take place only in terms of small packet of energy called Quanta, the oscillator can have only discrete energy values E given by $nh\nu$

ν = Frequency of radiations, n = integer and 'h' is Planck's constant, h= 6.625 x 10^{-34}Js.

Planck using above assumptions derived a formula to explain black body radiation spectrum as,

$$U_\lambda \, d\lambda = \frac{8\pi hc}{\lambda^5}\left[\frac{1}{e^{h\nu/kT}-1}\right]d\lambda \quad \text{[Since, } \nu=c/\lambda\text{] ----------- (1)}$$

This is called **Planck's radiation law** and explains the entire spectrum of black body radiation. From this law, we can also obtain Stefan's law, Wien's law and Rayleigh-Jean law under suitable conditions.

1. **Reduction of Planck's radiation law to Wien's law for shorter wavelengths:**

   For shorter wavelengths, $\nu=c/\lambda$ is large, When ν is large, $e^{h\nu/kT}$ is very large

$e^{h\nu/kT}>>1$.

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

Making use of this in (1)

$$U_\lambda\, d\lambda = \frac{8\pi hc}{\lambda^5}\left[\frac{1}{e^{h\nu/kT}}\right] d\lambda,$$

$=C_1\lambda^{-5}e^{-C2/\lambda T}d\lambda$ where $C_1=8\pi hc$ and $C_2=(hc/k)$.

This equation is Wien's law of radiation.

2. **Reduction of Planck's radiation law to Rayleigh-Jeans law for longer wavelengths:**

For longer wavelengths, $\nu= c/\lambda$ is small,
When ν is small, $h\nu/kt$ will be very small.
Expanding $e^{h\nu/kT}$ as power series, we have,

$e^{h\nu/kT}=1+ (h\nu/kt) + (h\nu/kt)^2+\ldots..$

$\approx$ $1+h\nu/kt$ [since $h\nu/kt$ is very small, its higher power terms could be neglected]

$(e^{h\nu/kT}-1)$ $h\nu/kt = hc/\lambda kt$

Substituting in (1)

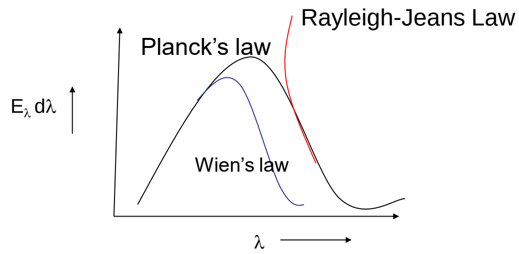
$$U_\lambda\, d\lambda = \frac{8\pi hc}{\lambda^5}\left[\frac{1}{hc/\lambda kt}\right] d\lambda$$

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

This equation is Rayleigh-Jeans law of radiation.

Thus Wien's law and Rayleigh-Jeans law are special cases of Planck's law.

Energy distribution curves



Summary of Lesson –01

Here we have learnt that classical physics cannot explain black body radiation spectrum. The emission and absorption of energy takes place only in terms of quanta and not continuously as predicted in classical physics. Quantum theory of radiation has opened a new concept of understanding physics.

LESSON-2

Objectives:

At the end of lesson you shall understand that:

- Light rays consists of invisible particles called photons.
- A single electron in metal cannot absorb one photon of energy hυ.
- Compton scattering is different from classical scattering.
- Compton effect signifies particle nature of radiation.

Introduction

In this lesson, we will study Compton Effect which signifies particle nature of radiation, thereby strengthening the fact that radiation has dual characteristics.

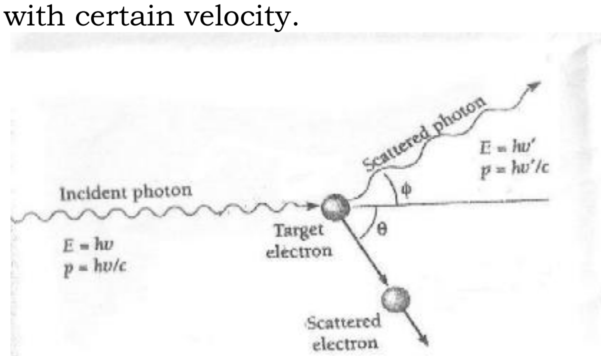
COMPTON EFFECT

In the year 1924, Compton discovered that when monochromatic beam of very high frequency radiation such as X-rays or Gamma rays is made to scatter through a substance, the scattered radiation found to contain two components; one having same frequency or wavelength as that of incident radiation, known as unmodified radiation; and the other, having lower frequency or longer wavelength than incident radiation known as modified radiation. This is called

Compton scattering, during the process an electron recoils with certain velocity. This phenomenon is called Compton Effect.

The Compton Effect is explained on the basis of Quantum theory of radiation, in which it is assumed that, radiation is composed of small packets of energy called Quanta or photons having energy $h\upsilon$. According to Compton, when a photon of energy $h\upsilon$ of momentum h/λ moving with velocity equal to velocity of light, obeying laws of conservation of energy and momentum, strikes an electron which is at rest, there occurs an elastic collision between two particles namely photon and electron.

When photon of energy $h\upsilon$ strikes the electron at rest, photon transfers some of its energy to electron, therefore photon loses its energy, hence, its frequency reduces to υ^1 and wavelength changes to λ^1, the scattered photon makes an angle ϕ with the incident direction, during the process an electron gains kinetic energy and recoils with certain velocity.



Compton by applying laws of conservation of energy and momentum showed that, the change in wavelength is given by formula,

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

where m_o = rest mass of electron.

The change in wavelength $\lambda' - \lambda$ is called Compton shift. This shows that the change in wavelength (Compton shift) depends neither on the incident wavelength nor the scattering material, but depends only on the angle of scattering.

When the angle of scattering is 90^o, the Compton shift is found to be 0.0243 Å. This value is in agreement with theoretical value obtained from Compton formula.

Physical significance of Compton Effect

The phenomena of Compton effect is explained by Compton on the basis of Quantum theory of radiation, in which it is assumed that radiation is composed of small packets of energy called Quanta. The Compton Effect is an elastic collision between two particles namely photon and electron in which exchange of energy takes place as if it is a particle–particle collision. Also it is assumed that photon and electron obey laws of conservation of energy and momentum. Hence Compton Effect signifies particle nature of radiation.

Summary of Lesson -02

The Compton Effect signifies particle nature of radiation.

LESSON-3

Objectives

- At the end of this lesson we will learn that:

- Any particle in motion exhibits wave like properties.
- Matter waves are generated due to motion of the particle not by the charge carried by them.
- Wave properties and particle properties do not appear together.
- Dual nature of radiation has put the position of the particle uncertain.

Introduction:

In this lesson we shall study dual characteristics of matter waves and de-Broglie concept that all particles in motion exhibit wave properties and also de-Broglie equation.

Wave Particle Dualism and de-Broglie concept of Matter Waves

Before we discuss wave particle dualism, we must know the concept of particle and the concept of wave. The concept of particle is easy to understand, because it has mass and occupies certain fixed position in space and particle in motion has definite momentum; when slowed down, it gives out energy. Therefore particle is specified by its mass, momentum, energy and position.

The concept of wave is bit difficult to understand, because a wave is a disturbance spread over a large area. We cannot say wave is coming from here or going there. No mass is associated with wave and the wave is characterized by its wavelength, frequency, amplitude and phase.

Considering the above properties of particle and wave, it is difficult to accept the dual nature of radiation, but the acceptance is necessary because, the phenomenon like interference and diffraction has shown beyond doubt the wave nature of light radiation. And successfully explained by Huygens wave theory of light, however, experimental phenomenon like Photo electric effect, Compton Effect are successfully explained by Quantum theory of radiation, which signifies particle nature of radiation. Hence we can conclude that radiation has dual characteristics i.e. sometimes behaving like a wave and at other time as a particle, but radiation cannot exhibit both wave and particle properties simultaneously.

De-Broglie concept of matter waves

L. de-Broglie in the year 1924 put forward the concept of matter waves. According to this concept the dual characteristics of radiation is not confined only to electromagnetic waves, but also holds good for all material particles in motion i.e. all the particles like electrons, protons, neutrons, molecules, atoms etc. exhibit dual characteristics. His theory is based on the fact that nature loves symmetry that means when waves exhibits particle like properties then particle also should possess wave like properties.
According to de-Broglie the particle in motion is associated with a group of waves and controlled by the wave. This wave is known as matter wave or de Broglie wave and wavelength associated with it is called de Broglie wavelength.

De-Broglie wavelength of a free particle

For a free particle, total energy is same as its kinetic energy given by,

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

$$E = m^2v^2/2m \quad (\text{But } p = mv)$$

$$E = p^2/2m$$

Hence,

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

By de Broglie hypothesis,

$\lambda = h/p$

Therefore, $\lambda = h/\sqrt{2mE} = h/\sqrt{2meV}$ (since $E = eV$) where V is the accelerating potential on an electron.

Substituting the constants, we get, $\lambda = 12.27/\sqrt{V}$ Å.

Characteristics of Matter Waves

- Matter waves are the waves associated with a moving particle.
- The lighter the particle larger the wavelength.
- Smaller the velocity of particle larger the wavelength.
- The amplitude of the matter wave at a given point determines the probability of finding the particle at that point at a given instant of time.
- The wavelength of a particle is given by, $\lambda = h/p = h/mv$

Summary of Lesson

The material particle in motion exhibits wave like properties. The de - Broglie waves are pilot waves and are not electro-magnetic waves. Wave properties and particle properties cannot appear together.The dual nature of radiation has put position of particle uncertain.

Solved Examples

1. Calculate the momentum of the particle and de Broglie wave length associated with an electron with a KE of 1.5KeV.

Solution: Data p=?

$\lambda = ?$

$K E = 1.5 \times 10^{3}$ eV

$p^2 = 2mE$

$= 2 \times 9.1 \times 10^{-31} \times 1.5 \times 10^{3} \times 1.6 \times 10^{-19}$

$= 2.08 \times 10^{-23}$ kgms^{-1}

$\lambda = h/p$

$= 6.625 \times 10^{-34}/2.08 \times 10^{-23}$

= $\mathbf{3.10 \times 10^{-11}}$ **m.**

2. Calculate the wave length of the wave associated with an electron of 1eV.

Solution:

$\lambda = h/p$

$= h/\{2mE\}^{1/2}$

$= 6.625x10^{-34}/\{2x9.1x10^{-31}x1.6x10^{-19}\}^{1/2}$

$=$ **$1.23x10^{-9}$ m**

3. Find de Broglie wave length associated with a proton having velocity equal to $1/30^{th}$ of that light. Given, mass of proton as$1.67x10^{-27}$kg.

Solution: $v = 1x3x10^8/30 = 10^7$ m/s

$\lambda = h/mv$

$= 6.625x10^{-34}/1.67x10^{-27}x10^{7}$

$=$ **$3.9x10^{-14}$ m/s**

4. The velocity of an electron of a hydrogen atom in the ground state is $2.19x10^6$m/s. Calculate the wave length of the deBroglie waves associated with motion.

Solution: $\lambda = h/mv$

$= 6.625x10^{-34} / 9.11x10^{-31}x2.19x10^6$

$=$ **$3.31x10^{-10}$ m**

5. Estimate the potential difference through which a proton is needed to be accelerated so that its deBroglie wave length becomes equal to 1Å. Given that it's mass is $1.673x10^{-27}$kg.

Solution: $eV = 1/2\ mv^2$

$= p^2/2m$

$= h^2/2m\lambda^2\{v^2 = h^2/m^2\lambda^2\}$

$= h^2/2me\lambda^2$

$= \{6.625x10^{-34}\}^2/2x1.67x10^{-27}x1.6x10^{-19}x(10^{-10})^2$

$=$ **0.082 V**

6. Compare the energy of a photon with that of a neutron when both are associated with wave length of 1 Å. Given the mass of the neutron is 1.67 x 10^{-27}Kg.

Solution: $E_1 = h\nu$

$= hc/\lambda_1$

$= 1.989\times10^{-15} / 10^{-10} \times 1.6\times10^{-19}$eV

$=12411$ eV

$E_2 = h^2/2m\lambda_2^2$

$= 0.08$ eV

$E_1/E_2 = 12411/0.08$

$=$ **1.5×10^5**

7. Find the KE of an electron with de Broglie wave length of 0.2nm.

Solution: $p = h/\lambda$

$= 6.625\times10^{-34}/0.2\times10^{-9}$

$= 3.313\times10^{-24}$ n-s

$E = p^2/2m$

$= (3.313\times10^{-24})^2/2\times9.1\times10^{-31} = 37.69$ eV

QUANTUM MECHANICS

Over view

This unit consists of five lessons, in first lesson we will study Heisenberg's uncertainty principle and its physical significance. In lesson two, we will study the applications of uncertainty principle and show that it is not possible for an electron to exist inside the nucleus. In lesson three, we will study wave function, its properties and physical significance and also we will study probability density and normalized wave functions, Eigen values, Eigen functions. In lesson four we will study Schrödinger matter wave equation and in the last lesson we will study particle in a box, energy values and wave functions.

Objectives

At the end of unit we would understand that:

- In sub atomic world, it is impossible to determine precise values of two physical variables of particular pair which describes atomic system.
- Both wave properties and particle properties are essential to get clear picture of atomic system.
- Wave properties and particle properties are complimentary to one another.
- In our daily life, we cannot realize quantum conditions.
- Particle in a box is a quantum mechanical problem and the probable position of a particle can be estimated by evaluating the value of $|\psi|^2$.

- Quantum mechanics is an important tool to study atomic and sub atomic state.

LESSON –1

Introduction

In this lesson we will study uncertainty principle, its related equations derived from concept of wave packet and also we will study the physical significance of uncertainty principle.

Objectives

At end of lesson we understand that:

- It is impossible to determine precise values of physical variables which describes atomic system. Hence we should always think of probabilities of estimating those values.
- Both wave properties and particle properties of moving objects cannot appear together at the same time.
- Wave properties and particle properties of moving objects are complimentary to one another.
- From uncertainty principle it is clear that, inaccuracy inherently present in its measurements.

HEISENBERG'S UNCERTAININITY PRINCIPLE

In the year 1927, Heisenberg proposed very interesting principle known as uncertainty principle, which is a direct consequence of dual nature of matter.

In the classical physics the moving particle has fixed position in space and definite momentum. If the initial values are known final values can be determined. However in Quantum Mechanics the moving particle is described by a wave packet. The particles should be inside wave packet, hence when wave packet is small; position of the particle may be fixed, but particle flies off rapidly due to very high velocity; hence, its momentum cannot be determined accurately. When the wave packet is large, velocity or momentum may be determined but position of particle becomes uncertain.

In this way, certainty in position involves uncertainty in momentum and certainty in momentum involves uncertainty in position. Therefore, it is impossible to say where exactly the particle inside the wave packet is and what its exact momentum is.

According to uncertainty principle it is impossible to determine precisely and simultaneously, the exact values of both members of particular pair of physical variables which describes atomic system.

In any simultaneous determination of position and momentum of a particle, the product of corresponding uncertainties inherently present in the measurements is equal to or greater than $h/4\pi$

$$\Delta p.\Delta x \geq h/4\pi$$

These are the other uncertainty relations:

$$\Delta E.\Delta t \geq h/4\pi$$

$$\Delta L.\Delta\theta \geq h/4\pi$$

Δx = uncertainty in measurement of position

Δp = uncertainty in measurement of momentum

ΔE = uncertainty in measurement of energy

Δt = uncertainty in measurement of time

ΔL = uncertainty in measurement of angular momentum

$\Delta\theta$ = uncertainty in measurement of angular distance

Note**:** Heisenberg's uncertainty principle could also be expressed in terms of uncertainty involved in the measurements of physical variable pair like angular displacement (θ) and angular momentum (L).

Summary
It is impossible to determine the values of both members of a particular pair of physical variables which describes atomic system. Hence we should always think of probability to estimate those values. However precise may be the method of measurement there is no escape from these uncertainties because it is an inherent limitation of nature on the measurement.

LESSON-2
Objectives:

At the end of lesson we shall understand that the electron cannot exist inside the nucleus of an atom and we can determine frequency of radiation emitted by atom and radius of electronic orbit and binding energy of electron.

Introduction
In this lesson we will study applications of uncertainty principle, mainly to show that it is not possible for an electron to stay inside the nucleus of an atom.

Applications of Heisenberg's Uncertainty Principle

- Non-existence of electrons in nucleus of atoms
- Calculation of frequency of radiation emitted by atom
- Calculation of binding energy of an electron in an atom
- Determination of radius of Bohr electronic orbit

Here we will discuss first two important applications.

Non-existence of electrons in nucleus of atoms

The diameter of nucleus of atom is of the order 10^{-14} m. If an electron exists in nucleus of atom then maximum uncertainty in determining position of electron must be 10^{-14} m.

$$(\Delta x)_{max} = 10^{-14} \text{ m}$$

From uncertainty principle $(\Delta x)_{max} (\Delta p)_{min} = h/4\pi$

$$10^{-14} (\Delta p)_{min} = h/4\pi$$

If an electron exists in nucleus then it should possess minimum momentum of 0.528×10^{-20} kg-m/sec particle of having this momentum must be moving with velocity equal to velocity of light, then it must be a relativistic problem. Hence energy of the particle is given by $E = mc^2$ or $E = (mc)(c)$

$$E = pc = (0.528 \times 10^{-20} \text{ kg-m/sec})(3 \times 10^8 \text{m}) \text{ J}$$

$$E = 0.990346 \times 10^7 \text{ eV}$$

$$E = 10 \text{ MeV}$$

If an electron exists in nucleus of atom then it should have minimum energy of 10 MeV, but beta decay experiments has shown that energy possessed by beta particle from nucleus of an atom has maximum energy of 2 to 3 MeV. Hence we can conclude that it is not possible for an electron to exist inside the nucleus of an atom.

Physical significance of Heisenberg's uncertainty principle

- Non-existence of electrons inside the nucleus of atoms.
- Calculation of frequency of radiation emitted by an atom.
- Calculation of binding energy of an electron in an atom.
- Determination of radius of Bohr electronic orbit.
- The wave and particle properties are complimentary to one another.
- It is impossible to determine precisely and simultaneously values of physical variables which describes the atomic system.

Summary

The negatively charged particle electron cannot exist inside the nucleus. The wave and particle properties are complimentary to one another rather than contradictory.

LESSON-3

Objectives

At end of lesson we shall understand that:

- The wave function by itself has no physical significance
- The wave function is a complex quantity
- The value of $|\psi|^2$ evaluated at a point gives the probability of finding the particle at that point

Introduction

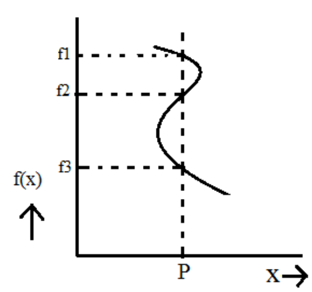
In this lesson we will study the wave function and its characteristics, physical significance, probability densities, and normalization of a wave function.

Wave Function, Probability Density and Normalized Functions

The concept of wave function was introduced by Schrödinger in the matter wave equation. It is denoted by ψ, it is a variable whose variations constitutes matter wave. Wave Function is related to position of particle. The following are some characteristics of wave function.

1) The wave function by itself has no direct physical significance.
2) The wave function cannot be interpreted by an experiment.
3) The wave function is complex quantity consisting of both real and imaginary parts.
4) With the knowledge of the wave function we can establish angular momentum, energy and position of particle.
5) The value of $|\psi|^2$ evaluated at point gives the probability of finding particle at that point.

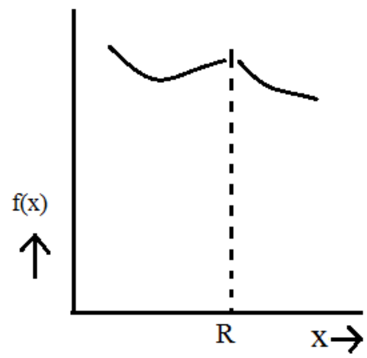
Properties of Wave function:
Property 1:ψ is single valued everywhere.



MULTIVALUED FUNCTION

A function f(x) which is not single valued over a certain interval as shown in the above figure, has 3 values f1,f2,f3 for the same value of P at x=P. Since f1≠f2≠f3, it says that the probabilities of finding the particle have 3 different values at the same location. Hence such wave functions are not acceptable.

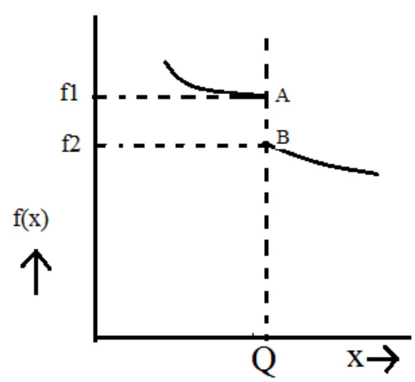
Property 2:ψ is finite everywhere.



FUNCTION NOT FINITE AT A POINT

A function f(x) which is not finite at x=R as shown the above figure. At x=R, f(x)=infinity. Thus if f(x) were to be a wave function, it signifies large probability of finding the particle at a single location at x=R, which violates the uncertainty principle. Hence such wave functions are not acceptable.

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



Discontinuous function

A function which is discontinuous at Q as shown in the above figure, at x=Q, f(x) is truncated at A and restarts at B. Between A and B it is not defined and f(x) at Q cannot be ascertained. Hence such wave functions are not acceptable.

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 these four properties are named in quantum mechanics as Eigen functions.

Probability Density

The wave function is a complex quantity consisting of both real and imaginary parts. Hence it can be expressed as follows:

$\psi = a + ib$ where a and b are real functions of (x, y, z) and 't'.

Complex conjugate of ψ is,

$$\psi^* = a - ib$$

The product of ψ and ψ* is $\psi\psi^* = a^2 + b^2$, which is called Probability density denoted by $P = |\psi|^2$,

Where ψ and ψ* are real and positive and also if $\psi \neq 0$.

Normalized functions

The value of $|\psi|^2$ evaluated at point gives the probability of finding a particle at that point, hence the probability of finding the particle in an element of volume δv is given by:

$$|\psi|^2\delta v$$

Since the particle must be somewhere in space, the total probability of finding the particle should be equal to 1 i.e

$$|\psi|^2\delta v = 1$$

Any function which obeys this condition is said to be normalized Wave function. Normalized wave functions should satisfy following conditions:

1. It should be single valued function.
2. It should be finite everywhere.
3. It should be continuous and it should have continuous first derivative

ψ tends to zero when x, y, z tends to 0.

Eigen functions and Eigen values of energy

In Quantum mechanics, the state of a system is defined by its energy, position and momentum. These quantities can be obtained with the knowledge of wave function ψ.

Hence to define the state of a system we have to solve Schrödinger wave equation, but Schrödinger equation is a second order equation. It has several solutions, and only few of them are acceptable which gives physical meaning, these acceptable solutions are called proper functions or Eigen functions.

These are single valued, finite and continuous functions.

Eigen functions are used in Schrödinger equation to solve for energy of a system, since there can only be certain restricted Eigen functions and hence only few restricted values of energy, these values of energy is called Eigen values of energy.

Summary

The wave function is a variable quantity, whose variations constitute matter waves.

The wave function is related to position of particle.

With the knowledge of wave function we can establish energy, angular momentum and position of particle.

Lesson 4

Objectives

At the end of the lesson we will understand that:

The Schrödinger Wave Equation is useful in obtaining wave function, which is related to position of a particle. We will also understand that energy of free particle is not quantized.

Introduction

In this lesson we study, which is fundamental equation of quantum mechanics and free particle.

Schrödinger Time Independent Wave Equation

According to de Broglie concept of matter waves, a particle in motion is associated with group of waves called matter waves, the wavelength is given by $\lambda = h/mv$.

If the particle behaves like a wave then there should be some sort of wave equation which describe behavior of wave, and this equation is called Schrödinger Time Independent Wave Equation.

Consider a system of stationary waves, a particle of coordinates (x,y,z,) and wave function ψ. The wave equation of wave motion in positive x – direction is given by,

$$\Psi = Ae^{i(kx-\omega t)} = \dots\dots\dots\dots 1$$

The time independent part is given by,

$$\psi = Ae^{ikx} \text{.......................}2$$

$$\Psi = \psi e^{-i\omega t} \text{.....................}3$$

Let us differentiate Ψ twice with respect to x,

We get,

$$\frac{\partial^2 \Psi}{\partial x^2} = e^{-i\omega t} \frac{\partial^2 \psi}{\partial x^2} \text{...........}4$$

Let us differentiate Ψ twice with respect to t,

$$\frac{\partial^2 \Psi}{\partial t^2} = -\omega^2 e^{-i\omega t} \psi \text{.........}5$$

We have the equation for a travelling as,

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

where y is the displacement and v is the velocity of the wave.

By analogy, we can write the motion of a free particle as,

$$\frac{d^2 \Psi}{dx^2} = \frac{1}{v^2} \frac{d^2 \psi}{dt^2} \text{...............}6$$

The above equation represents waves propagating along x–axis with a velocity v and Ψ is the displacement at the instant t. Substituting 4 and 5 in 6 we get,

$$\frac{d^2 \Psi}{dx^2} = \frac{-\omega^2}{v^2} \psi \text{...............}7$$

$$\frac{d^2 \Psi}{dx^2} = \frac{-4\pi^2}{\lambda^2} \psi$$

$$\text{or } 1/\lambda^2 = -\frac{1}{4\pi^2 \psi} \frac{d^2 \psi}{dx^2} \text{...............}8$$

We have KE = $p^2/2m$

Put $\lambda = h/p$, KE $= h^2/2m.\ 1/\lambda^2$ 9

Substituting 7 in 9 we get,

$KE = -h^2/8\pi^2 m.\ \ 1/\psi\ .d^2\psi/dx^2$...............10

$E = KE + PE = -h^2/8\pi^2 m.\ \ 1/\psi\ .d^2\psi/dx^2 + V$

$E - V = -h^2/8\pi^2 m\ \ 1/\psi\ \ d^2\psi/dx^2$

$d^2\psi/dx^2 + 8\pi^2 m/h^2\ (E - V)\ \psi = 0$

This is Schrödinger time independent wave equation.

Summary

The Schrödinger matter wave equation is basic equation of quantum mechanics. And it is one of the important tools to study subatomic world. The energy of free particle is not quantized.

Lesson 5

Objectives

At the end of the lesson we shall learn that:

- The energy levels for a particle in a box are quantized and hence cannot have arbitrary values.
- The energy corresponding to n=1 is called ground state energy or zero point energy and all other energy states are called excited states.
- The energy difference between successive levels is quite large.
- The electron cannot jump from one level to the other level on the strength of thermal energy, hence quantization of energy plays important role in case of electron.

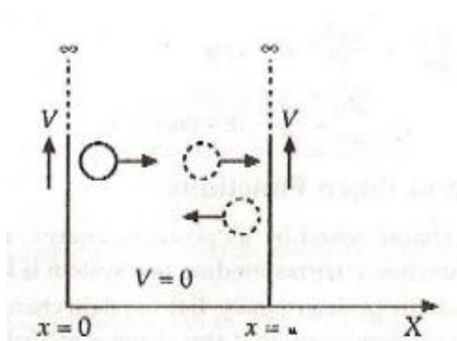
Introduction

In this lesson we will study one of the important applications of Schrödinger wave equation, that is particle in a box of infinite depth and solve for Eigen values and Eigen functions. We will also study wave functions, probability densities and energy values of a particle in a box.

Particle in a box of infinite depth

Considered a particle of mass' 'm' moving along 'x' axis between two rigid walls of infinite length at x=0 and x= a. The particle is said to be moving inside potential well of infinite depth and potential inside box is zero and rises to infinity outside box.

i.e V=0 for $0 \le x \le a$, V= ∞ for $0 \ge x$ $x \ge a$



Schrödinger wave equation for particle in a box

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

but V=0 for $0 \le x \le a$

$$\frac{\delta^2\psi}{\delta x^2} + \frac{8\pi^2 m}{h^2}(E)\,\psi = 0$$

or $E\,\psi = -\,h^2/\,8\pi^2 m\,.\,(\delta^2\psi/\,\delta x^2)$

put, $$\frac{8\pi^2 mE}{h^2} = K^2$$

$$\frac{\delta^2\psi}{\delta x^2} + K^2\psi = 0$$

The general solution for above equation is of the type,

$\Psi(x) = A\sin Kx + B\cos Kx$

'A' and 'B' are constants to be determined by applying suitable boundary conditions.

The particle cannot exist outside the box and cannot penetrate through walls, hence the wave function $\Psi(x)$ must be zero for x=o and x= a.

i) Applying boundary conditions $\Psi(x)=0$ at $x = 0$,

We get $0 = A\sin K(0) + B\cos K(0)$

$0 = A(0) + B(1)$

ie $B = 0$,

Substituting in above equation, $\Psi(x) = A\sin Kx$

ii) Applying boundary conditions $\Psi(x) = 0$ at $x = a$,

$0 = A\sin Ka$

Since, $A \neq 0$, $\sin Ka = 0$

Hence $ka = 0, \pi, 2\pi, 3\pi, 4\pi, 5\pi,$ ------$n\pi$

$Ka = n\pi$

or $K = n\pi/a$.

The wave function is $\Psi(x) = A\sin\left(\frac{n\pi}{a}\right)x$ for $n = 1,2,3,4,5,6,7,8$----

Energy $$\frac{8\pi^2 m E}{h^2} = K^2$$

Hence, $\frac{8\pi^2 mE}{h^2} = \frac{n^2\pi^2}{a^2}$

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

From the above equation it is clear that particle in a box cannot have arbitrary value for its energy, but it can take values corresponding to n = 1,2,3,4, --- these values are called Eigen values of energy.

EIGEN VALUES FOR ENERGY

When n = 1, $E_1 = \frac{h^2}{8ma^2} = E_o$-is called ground state energy

E_o or zero point energy or lowest permitted energy.

When n = 2, $E_2 = \frac{4h^2}{2ma^2} = 4E_o$ - this is first excited energy state

When n = 3, $E_3 = \frac{9h^2}{8ma^2} = 9E_o$ - this is second excited energy state

To evaluate A in Ψ (x) = A sin(nπ/a)x, We have to perform normalization of wave function. As the particle is inside the box at any time, we can write,

$$\int_0^a |\psi|^2 \delta x = 1$$

Substituting for ψ [from Ψ(x) = A sin (nπ/a)]

We get, $$\int_0^a A^2 \sin^2 (n\pi/a)x \, \delta x = 1$$

Solving we get, $A = \sqrt{2/a}$

Substituting in the equation for Ψ(x) = A sin(nπ/a)x

We get,

$\Psi(x) = \sqrt{2/a} \sin(n\pi/a)x$

ENERGY EIGEN FUNCTIONS

For n=1,

$\Psi_1 = \sqrt{2/a} \sin (\pi/a) x$. Here $\Psi_1 = 0$ for x = 0 & x = a. And maximum for x = a/2.

For n=2,

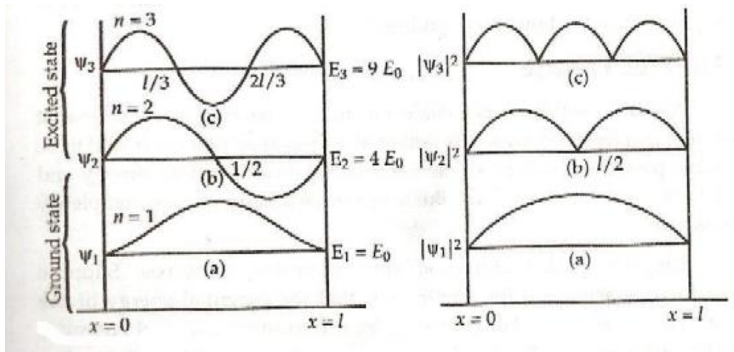
$\Psi_2 = \sqrt{2/a} \sin (2\pi/a)x$. Here $\Psi_2 = 0$ for x=0, a/2 and a.

And maximum for x=a/4 and 3a/4.

For n=3,

$\Psi_3 = \sqrt{2/a}\, \sin(3\pi/a)x$. Here $\Psi_3 = 0$ for x=0, a/3, 2 a/3 and a.

And maximum for x=a/6, a/2 and 5a/6. The plot of $|\psi(x)|^2$ versus x is as shown in the figure below, for n=1,2 and 3.



Summary:

The particle in a box is quantum mechanical problem. The most probable position of a particle at different energy levels can be estimated by solving for its Eigen functions. The existence of zero point energy is in conformity with Heisenberg uncertainty principle.

Solved problems

1. An electron has a speed of 300m/s accurate to 0.01% with what fundamental accuracy can we locate the position of the electron?

Solution: Given, v= 300m/s, Δv=0.01% of v.

$\Delta v = (0.01/100) \times 300 = 0.03$m/s.

We know that uncertainty relation is $\Delta x.\Delta p \geq h/4\pi$

For the given uncertainty in speed, Δp is minimum

Uncertainty in the position is given by,

$\Delta x = h/4\pi\Delta p = h/4\pi m\Delta v$

$= 6.632\times10^{-34} / 4\times 3.14\times 9.11\times10^{-31}\times3\times10^{-2}$

$=$**1.93×10^{-3}m/s**

2. An electron of energy 20 eV is passed through a circular hole of radius10^{-6} m. what is the uncertainty introduced in the angle of emergence?

Solution: Given E= 250eV= $250\times1.6\times10^{-19}$J

$r=10^{-6}$m

$\Delta x=2x10^{-6}$

We know that energy $E=p^2/2m$ and

$p=\sqrt{2mE}$

$=\sqrt{(2x9.11x10^{-31}x40x10^{-18})}= 8.853x10^{-24}Kgm/s.$

$\Delta p= h/4\pi\Delta x$

$=6.632x10^{-34} / 4x\ 3.14x\ 2x10^{-6} = 0.263x10^{-28}Kgm/s$

Angle of emergence, $\theta=\Delta p/p$

$=0.263x10^{-28} /8.853x10^{-24}$

$=$**$0.0309x10^{-4}$radian**

3.The average time an atom retains excess excitation energy before re-emitting it in the form of electromagnetic radiation is 10^{-8} sec. calculate the limit of accuracy with which the excitation energy of the emitted radiation can be determined?

Solution: Given $\Delta t=10^{-8}$ sec

According to uncertainty principle, $\Delta E.\Delta t= h/4\pi$

$\Delta E = h/4\pi\Delta t$

$=6.632x10^{-34} / 4x\ 3.14x\ 10^{-8}$

$= 0.5x10^{-26}$ J

$=0.5x10^{-26}/1.6x10^{-19}eV$

$\Delta E=$**$0.3x10^{-7}$eV.**

4. Using Heisenberg uncertainty relation, calculate the kinetic energy of an electron in a hydrogen atom?

Solution: The uncertainty in the coordinate of an electron inside the atom is equal to the radius of the atom. The Bohr radius, r= 0.053nm,is the reasonable estimate for the uncertainty in position Δp.

We know from Heisenberg uncertainty principle.

$\Delta x.\ \Delta p=h/4\pi$

$\Delta p= h/4\pi\Delta x$

But $\Delta x=r$ (Bohr radius)

Now energy, $E=p^2/2m= h^2/16\pi^2r^2\ 2m$

$=(6.632x10^{-34})^2/\ (4x\ 3.14x0.053x\ 10^{-9})^2x2x9.1x10^{-31}$

$=5.45 x 10^{-19}$ J = **3.4 eV**

5. An electron is constrained in a 1-dimensional box of side 1nm. Calculate the first Eigen values in electron volt.

Solution: Given a=1nm

The Eigen values are given by

$E_n=n^2h^2/8ma^2$

The first Eigen value given by

$E1= (6.632x10^{-34})^2 / 8x9.11x10^{-31}x (1x 10^{-9})^2{}_J$

=0.377eV

E1=0.377eV

Second Eigen value, $E^2= 2^2x\ 0.377=$ **1.508 eV**

Third Eigen value, $E^2= 3^2x\ 0.377=$ **3.393 eV**

Fourth Eigen value, $E^2= 4^2x\ 0.377=$ **6.5032 eV**

6. Is it possible to observe energy states for a ball of mass 10 grams moving in a box of length 10cm.

Solution: The Energy is given by

$E_n=n^2h^2/8ma^2$

$E1= n^2(6.632x10^{-34})^2 / 8x9.11x10^{-31}x (0.1)^2$

$=38x10^{-18}\ n^2$

When n=1, 2 , 3etc energies are $38x10^{-18}$ eV, $152.6x10^{-18}$eV,

343.35×10^{-18}eV.

The energies states are so near that they appear as continuous.

7.A spectral line of wavelength 5461 Å has a width of 10^{-4} Å. Evaluate the minimum time spent by the electrons in the upper energy state between the excitation and de-excitation processes?

Solution: Wavelength of the spectral line, $\lambda=5461x10^{-10}$m

Width of the spectral line $\Delta\ \lambda=10^{-14}$m

Minimum time spent by the electron, $\Delta t=?$

We have the equation, $E = h\nu= hc/ \lambda$

$\Delta E = hc\ \Delta(1/\lambda)$
$\Delta E = hc\ (\Delta\lambda/\lambda^2)$ ------ (1)
As per uncertainty principle,
$\Delta E\ \Delta t \geq h/4\pi$

$\Delta t \geq h/4\pi\Delta E$ ------ (2)

From (1) the right hand side of (2) can be written as

$h/4\pi\Delta E = h\ \lambda^2/4\pi\ (hc\ \Delta\lambda) = \lambda^2/4\pi c\Delta\lambda$

$= (5461 \times 10^{-10})2/4\pi \times 3 \times 10^{8} \times 10^{-14}$

$=0.8X10^{-8}s$

From equation (2), we have $\Delta t = 0.8X10^{-8}$ second.

Therefore the minimum time spent by the electron is $\geq 0.8X10^{-8}$ second.

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