UNIT-3

QUANTUM PHYSICS

PART-A QUESTION

Level-I

1) Quantum mechanics deals with the behavior of

a) Macroscopic particle b) **Microscopic particle** c) both a&b d)none of the above

2) In Black body radiation, Wine's displacement law holds well only for,

a) Longer wavelength b) **Shorter Wavelength** c) Medium Wavelength d) all the above

3) In Black body radiation, Rayleigh-Jeans law holds well only for,

a) **Longer wavelength** b) Shorter Wavelength c) Medium Wavelength d) all the above

4) According to wine's displacement law, $\lambda_m T=$

a) 0 b) 1 c) **Constant** d) variable

5) According to wien's displacement law, the maximum energy is directly proportional to the

a) $\mathbf{T^5}$ b) T^3 c) T^6 d) T^4

6) In Compton shift, When $\theta=0$, $\Delta\lambda=$?

a) **0** b) 0.02424Å c) 0.04848Å d) 0.0538Å

7) In Compton shift, When $\theta=\pi/2$, $\Delta\lambda=$?

a) 0 b) **0.02424Å** c) 0.04848Å d) 0.0538Å

8) In Compton shift, When θ=π,   Δλ=?

a) 0   b) 0.02424Å   c) **0.04848Å**   d) 0.0538Å

9) The nature of light radiation is

a) Wave nature   b) Particle nature   c) **both a&b**   d) none of the above

10) SEM stands for

a) **Scanning electron microscope** b) scattered electron microscope c) Scanning emission microscope   d) Scattered emission microscope

11) In SEM, the scattered electrons are converted into light signal is done by

a) Scanning coil   b) Photomultiplier   **c) Scintillator** d) Magnetic condensing lenses

12) The resolving power of SEM is

a) **10-20 nm**   b) 20-30nm   c)15-25nm   d)25-35nm

Level-II

13) The expression for Compton shift is

a)**dλ=**$\mathbf{\frac{h}{m_0 c}(1-\cos\theta)}$ b)λ= $\frac{h}{m_0 c}(1-cos\theta)$ c)dλ= h/m_0c d)λ=h/mv

14) The scattered wave which is having the same frequency as that of the incident radiation in Compton Effect is called

a)Modified radiation   b)**Unmodified radiation**   c)scattered radiation d) None of the above

15) The scattered wave which is having the lower frequency as that of the incident radiation in Compton Effect is called

a) **Modified radiation** b) Unmodified radiation c) scattered radiation d) none of the above

16) The scattered wave which is having the same wavelength as that of the incident radiation in Compton Effect is called

a)Modified radiation b)**Unmodified radiation** c)scattered radiation d) None of the above

17) The scattered wave which is having the higher wavelength as that of the incident radiation in Compton Effect is called

a) **Modified radiation** b) Unmodified radiation c) scattered radiation d) none of the above

18) de-Broglie wavelength in terms of kinetic energy

a) h/mv b) $\frac{h}{\sqrt{2m_eV}}$ c) $\boldsymbol{\frac{h}{\sqrt{2mE}}}$ d)none of the above

19) de-Broglie wavelength in terms of Voltage

a) h/mv b) $\boldsymbol{\frac{h}{\sqrt{2m_eV}}}$ c) $\frac{h}{\sqrt{2mE}}$ d) none of the above

20) For a free particle, the schroedinger one dimensional time independent wave equation becomes

a) $\boldsymbol{\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar}E\psi=0}$ b) $\nabla^2\psi + \frac{2m}{\hbar}E\psi = 0$ c) $\nabla^2\psi + \frac{2m}{\hbar}E\psi=0$ d) $\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar}[E-v]\psi=0$

21) For a free particle, the schroedinger three dimensional time independent wave equation becomes

a) $\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar}E\psi=0$ b) $\nabla^2\psi + \frac{2m}{\hbar}E\psi = 0$ c) $\boldsymbol{\nabla^2\psi + \frac{2m}{\hbar}E\psi=0}$ d) $\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar}[E-v]\psi=0$

Level-III

22) Photons are

a) Electrons b) Energetic Particle c) **Energy Waves** d) all the above

23) Compton shift is depends on

a) Wavelength of the incident radiations b) nature of the scattering substance c) **Angle of scattering** d) all the above

24) Which particle does not have the particle wave duality?

a) The Proton b) The electron c) The Photon d) **none of the above**

25) Schroedinger wave equation can be applied for

a) Macroscopic particle b) Microscopic particle c) **both a&b** d) none of the above

26) $\int_{-\infty}^{\infty} |\psi| 2 d\tau$ =

a) 0 **b)1** c)-1 d)both a&b

27) If the various combination of quantum number describes the same Eigen value and same Eigen function are called

a)Degenerate state b) **non-degenerate state** c) Normal state d) all the above

28) If the various combination of quantum number describes the same Eigen value and different Eigen function are called

a) **Degenerate state** b) non-degenerate state c) Normal state d) all the above

29) If a particle present within a one dimensional box, then the probability of finding the particle is

a) 0 b) **1** c) 0.7 d) none of the above

30) In microscopic, resolving power is inversely proportional to

a) Pressure b) Energy c) **Wavelength d**) all the above

PART-B QUESTION

Level-I

1) Explain Planck's hypothesis (or) what are the postulates of Planck's quantum theory?

(i) The electrons in the black body are assumed as simple harmonic oscillators.
(ii) The oscillators will not emit energy continuously.
(iii) They emit radiation in terms of quanta's of magnitude 'hv' discreetly.
i.e., E=n hv where n=1,2,3…

2) What is a black body radiation?

A perfect black body is the one which absorbs and also emits the radiations completely.

In practice no body is perfectly black. We have to coat the black colour over the surface to make a black body.

Black body is said to be a perfect absorber, since it absorbs all the wavelength of the incident radiation. The black body is a perfect radiator, because it radiates all the wavelength absorbed by it. This phenomenon is also called black body radiation.

3) Define Rayleigh-jeans law. Give its limitation.

It is defined as "The energy (E) is directly proportional to the absolute temperature and inversely proportional to the fourth power of the Wavelength"

$$E_\lambda \propto \frac{T}{\lambda^4}$$

$$E_\lambda = \frac{8\pi K_b T}{\lambda^4}$$

Limitation .It holds good only for longer wavelength.

4) Define Wien's displacement law. Give its limitation.

It is defined as "The Product of the wavelength (λ_m) of maximum energy emitted and the absolute temperature (T) is a constant".

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

Limitation .It holds good only for shorter wavelength.

5) Define Compton Effect and Compton shift.

When a photon of energy 'hv' collides with a scattering element, the scattered beam has two components, viz one of the same frequency (or) wavelength as that of the incident radiation and the other has lower frequency (or) higher wavelength compared to incident frequency (or) wavelength. This effect is called Compton Effect. The change in wavelength is called Compton shift.

6) State the principle of electron microscope.

In an electron microscope a stream of electron are passed through the object and the electron which carry the information about the object are focused by electric and magnetic lenses (or) electromagnetic lenses.

7) Mention the application of electron microscope

[i] It has a very wide area of applications in the field of physics, chemistry, medicine and engineering.

[ii]It is used to determine the complicated structure of crystals.

[iii]It is used to determine the structure of micro organisms such as virus, bacteria, etc

8) State the principle of SEM?

Electron beam is made to fall on the various portions of the specimen by the scanning coils for scanning the sample. From the secondary electron or back scattered electrons or X-rays that are produced by incoming incident electrons are used to get the information about the specimen's surface, topography, composition etc

9) Mention the application of Scanning electron microscope

[i] This microscope also has wide range of applications in various fields of physics, chemistry, biology, industry and engineering etc.

[ii]It is used to examine the structure of specimens in a three dimensional view.

Level-II

10) What is Compton Wavelength? Give its value.

The shift in wavelength corresponding to the scattering angle of 90° is called Compton wavelength.

We know Compton shift $\Delta\lambda = \frac{h}{m_0 c}(1 - cos\theta)$

When θ=90°; cosθ=0

$$\Delta\lambda = \frac{6.625X10^{-34}}{(9.11X10^{-31})X(3X10^{8})}$$

Δλ=0.02424Å

11) State de-Broglie's hypothesis (or) Explain the concept of wave nature

The light exhibits the dual nature (i.e) it can behave both as a particle and the wave debroglie suggested that an electron, which is particle can also behave as a wave and exhibits the dual nature.

Thus the waves associated with a material particle are called as matter waves.

If v is the velocity and m is the mass of the particle then

de-Broglie wavelength $\lambda = \frac{h}{mv}$

12) What is the physical significance of a wave function?

[i] The probability of finding a particle in space at any given instant of time is characterized by a function Ψ(x.y,z), called wave function.

[ii] It relates the particle and the wave statistically.

[iii] It gives the information about the particle behavior.

[iv]It is a complex quantity.

[v] $|\Psi|^2$ represents the probability density of the particle, which is real and positive.

13) Write down the schroedinger wave equation and give any two application of it.

[i] schroedinger time dependent wave equation, given by

$$E\psi=H\psi$$

Where E= Total energy of the particle

H=Hamiltonian operator

ψ= Wave function

[ii] schroedinger time independent wave equation , given by

$$\Delta^2\psi+\frac{2m}{\hbar}[E\text{-}v]\psi=0$$

Where E= Total energy of the particle

V=Potential energy of the particle

m =Mass of the particle

Application

[i] It is used to find the electron in the metal.

[ii]It is used to find the energy level of an electron in an infinite deep potential well.

14) What is meant by degenerate and non-degenerate state?

Degenerate state

For various combinations of quantum numbers if we get same Eigen value but different Eigen function, then it is called degenerate state.

Non- degenerate state

For various combinations of quantum numbers if we get same Eigen value but same Eigen function, then it is called Non -degenerate state.

Level-III

15) What is meant by photon? Give any two properties.

Photons are discrete energy values in the form of small quanta's of definite frequency

(or) wavelength.

Properties

[i] They do not have any charge and they will not ionize.

[ii] The energy and momentum of the photon is given by

$$E= h\nu \quad \text{and } p=mc$$

Where ν=frequency h=Planck's constant

m- Mass of photon c=velocity of photon

16) What is meant by wave function?

Wave function is a variable quantity that is associated with a moving particle at any position (x.y, z) and at any time‘t’. It relates the probability of finding the particle at that point at that time.

17) Write down the one dimensional schroedinger time independent equation and write the same for a free particle.

The one dimensional schroedinger time independent equation is given by

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar}[E\text{-}v]\psi = 0$$

For a free particle, the potential energy is zero. Therefore it becomes

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

18) Define normalisation process and write down the normalised wave function for an electron in a one dimensional potential well of length ‘a’ metres

Normalisation is the process by which the probability of finding a particle inside any potential well can be done.

For a one dimensional potential well of length ‘a’ metre the normalised wave function is given by

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

19) Define Eigen value and Eigen function.

Eigen value is defined as energy of the particle (E_n).

Eigen function is defined as wave function of the particle (ψ_n).

20) Define Magnifying power

$$\text{Magnifying power (M)} = \frac{\text{Angle subtended by the final image at eye}(\beta)}{\text{Angle subtented by the object at eye kept at the near point}(\alpha)}$$

QUANTUM PHYSICS
PART –C QUESTION

Level-I

With the concept of quantum theory of black body radiation derive an expression for energy distribution and use it to prove wine's displacement law and Rayleigh –Jeans law

Assumptions

Planck derived an expression for the energy distribution, with the following assumptions.

(i) A black body radiator contains electrons (or) so called simple harmonic oscillators, which are capable of vibrating with all possible frequencies.

(ii) The frequency of radiation emitted by an oscillator is the same as that of the frequency of its vibration.

(iii) The oscillators (electrons) radiate energy in a discrete manner and not in a continuous manner.

(iv) The oscillators exchanges energy in the form of either absorption or emission within the surroundings interms of quanta of magnitude '$h\nu$'.

$$\text{(i.e.,)} \quad E = n\,h\nu$$

where $n = 0, 1, 2, 3 \ldots$

This implies that the exchange of energy will not take place continuously but are limited to a dicrete set of values say $0, h\nu, 2h\nu, 3h\nu, 4h\nu, \ldots n\,h\nu$.

Planck's Radiation Law

To derive the Planck's radiation law, let us consider 'N' Number of oscillators with their total energy as E_T.

Then, the average energy of an oscillator is given by

$$\overline{E} = \frac{E_T}{N} \qquad \ldots (1)$$

If $N_0, N_1, N_2, N_3, \ldots N_r$ are the oscillators of energy $0, E, 2E, 3E \ldots rE$ respectively then we can write

(i) The total number of oscillators $N = N_0 + N_1 + N_2 + N_3 + \ldots + N_r \quad \ldots (2)$

and (ii) Total energy of oscillators $E_T = 0\,N_0 + EN_1 + 2EN_2 + 3EN_3 + \ldots + rEN_r \quad \ldots (3)$

According to Maxwell's distribution formula, the number of oscillator having an energy rE is given by

$$N_r = N_0 e^{-rE/K_BT} \quad \text{... (4)}$$

Where K_B is called Boltzmann constant and $r = 0, 1, 2, 3 \ldots$

$\therefore$ For various of r, i.e., $r = 0, 1, 2 \ldots r$, the number of oscillators $N_0, N_1, N_2, N_3, \ldots N_r$ can be got as follows:

(i) For $r = 0$; $N_0 = N_0 e^0$

(ii) For $r = 1$; $N_1 = N_0 e^{-1E/K_BT}$

(iii) For $r = 2$; $N_2 = N_0 e^{-2E/K_BT}$

(iv) For $r = 3$; $N_3 = N_0 e^{-3E/K_BT}$

Similarly for $r = r$; $N_r = N_0 e^{-rE/K_BT}$

$\therefore$ The total number of oscillators can be got by substituting the values of $N_0, N_1, N_2, N_3 \ldots N_r$ in equation (2)

$$\therefore N = N_0 e^0 + N_0 e^{-E/K_BT} + N_0 e^{-2E/K_BT} + N_0 e^{-3E/K_BT} + \ldots + N_0 e^{-rE/K_BT}$$

$$\text{(or)} \quad N = N_0 [1 + e^{-E/K_BT} + e^{-2E/K_BT} + e^{-3E/K_BT} \ldots + e^{-rE/K_BT}] \quad \text{... (5)}$$

We know, $1 + x + x^2 + x^3 + \ldots = \frac{1}{1-x}$. Therefore we can write equation (5) as

$$\text{The total number of oscillators} \quad N = N_0 \left[\frac{1}{1 - e^{-E/K_BT}} \right] \quad \text{... (6)}$$

Similarly by substituting the values of $N_0, N_1, N_2, N_3 \ldots N_r$ in equation (3), the total energy can be written as

$$E_T = 0N_0e^0 + E\,N_0\,e^{-E/K_BT} + 2E\,N_0e^{-2E/K_BT} + 3\,EN_0\,e^{-3E/K_BT} + \ldots + rE\,N_0e^{-rE/K_BT}$$

$$E_T = N_0\,[0 + E\,e^{-E/K_BT} + 2E\,e^{-2E/K_BT} + 3E\,e^{-3E/K_BT} + \ldots + rEe^{-rE/K_BT}]$$

$$E_T = N_0\,Ee^{-E/K_BT}\,[0 + 1 + 2e^{-E/K_BT} + 3e^{-2E/K_BT} + \ldots + re^{-(r-1)E/K_BT}] \quad \text{... (7)}$$

$\therefore$ Energy density ($E_\nu d\nu$) (or) Total energy per unit volume $\Big\}$ = No. of oscillators per unit volume × Average energy of an oscillator

$$\text{i.e., } E_\nu d\nu = N\bar{E} \quad \text{... (12)}$$

Substituting equations (10) and (11) in equation (12) we get

$$E_\nu \, d\nu = \frac{8\,\pi\nu^2}{c^3} d\nu \frac{h\nu}{e^{(h\nu/K_BT)} - 1} \quad \text{... (13)}$$

$$\text{(or) } E_\nu = \frac{8\,\pi\,h\,\nu^3}{c^3\,(e^{h\nu/K_BT} - 1)} \quad \text{... (14)}$$

Equation (14) represents the ***Planck's radiation law interms of frequency.***

Planck's radiation law interms of wavelength (λ)

We know $\nu = \frac{c}{\lambda}$

Wien's Displacement Law

We know Wien's displacement law holds good only for ***shorter wavelengths.***

(i.e.,) If T is less, $\frac{1}{T}$ will be greater $\therefore \; e^{hc/\lambda K_BT} >> 1$

Since $e^{hc/\lambda K_BT} >> 1$, we can write $e^{hc/\lambda K_BT} - 1 = e^{hc/\lambda K_BT}$

$\therefore$ Equation (1) becomes

$$E_\lambda = \frac{8\pi hc}{\lambda^5 (e^{hc/\lambda K_BT})}$$

$$\text{(or)} \quad E_\lambda = 8\pi\, hc\, \lambda^{-5}\, e^{-hc/\lambda\, K_BT}$$

$$E_\lambda = C_1\, \lambda^{-5}\, e^{-C_2/\lambda T}$$

where C_1 and C_2 are constants given by $C_1 = 8\pi hc$ and $C_2 = \frac{hc}{K_B}$

Equation (8) represents the ***Wien's displacement law.***

Thus we got Wiens displacement law from Planck's radiation law using Quantum theory of black body radiation.

Rayleigh-Jean's law

We know *Rayleigh-Jeans law holds good only for* ***longer wavelength.***

i.e., If T is greater; $1/T$ will be lesser.

We know $e^{hc/\lambda K_BT} = 1 + \frac{hc}{\lambda K_BT} + \frac{1}{2}\left(\frac{hc}{\lambda K_BT}\right)^2 + ...$

For large values of T, the value $\left(\frac{hc}{\lambda K_B T}\right)^2 + \ldots$ will be very small and hence the higher terms can be neglected.

$$\therefore e^{hc/\lambda K_B T} = 1 + \frac{hc}{\lambda K_B T}$$

$\therefore$ Equation (1) becomes

$$E_\lambda = \frac{8\pi hc}{\lambda^5 \left[1 + \frac{hc}{\lambda K_B T} - 1\right]}$$

(or) $$E_\lambda = \frac{8\pi hc\, \lambda K_B T}{\lambda^5 hc}$$

$$\text{(or)} \quad E_\lambda = \frac{8\pi K_B T}{\lambda^4}$$

Equation (9) represents the ***Rayleigh-Jean's law.***

Thus we have deduced Rayleigh-Jeans law from the Planck's radiation law using Quantum theory of black body radiation.

2) What are matter waves? Explain de-Broglie waves.

de-Broglie concept of Dual Nature

The universe is made of Radiation (light) and matter (particles). The light exhibits the dual nature (i.e.,) it can behaves both as a wave (Interference, diffraction phenomenon) and as a particle (Compton effect, photo-electric effect etc).

Since the nature loves symmetry, in 1924 Louis de-Broglie suggested that an electron (or) any other material particle must exhibit wave like properties in addition to particle nature.

*The waves associated with a material particle are called as **Matter waves***

de-Broglie Wavelength

From the theory of light, considering a photon as a particle the total energy of the photon is given by $E = mc^2$. ... (1)

where $m \rightarrow$ Mass of the particle

$c \rightarrow$ Velocity of light

Considering the photon as a wave, the total energy is given by $E = h\nu$ ... (2)

where $h \rightarrow$ Planck's constant

$\nu \rightarrow$ Frequency of radiation

From equations (1) and (2) we can write $E = mc^2 = h\nu$ ... (3)

We know momentum $=$ mass $\times$ velocity

Other forms of de-Broglie Wavelength

(i) de-Broglie wavelength interms of Energy

We know kinetic energy $E = \frac{1}{2} mv^2$

Multiplying by 'm' on both sides we get

$$Em = \frac{1}{2} m^2 v^2$$

$$\text{(or)} \quad m^2 v^2 = 2Em$$

$$mv = \sqrt{2Em}$$

mat
part

$$\therefore \textit{de-Broglie wavelength } \lambda = \frac{h}{\sqrt{2mE}} \quad \text{... (6)}$$

(ii) de-Broglie Wavelength interms of voltage

If a charged particle of charge 'e' is accelerated through a potential difference 'V'

Then the kinetic energy of the particle $= \frac{1}{2} mv^2$ ... (7)

Also we know energy $= eV$ ... (8)

Equating equations (7) and (8) we get

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

Multiplying by 'm' on both sides we get

$$m^2v^2 = 2meV$$

$$\text{(or)} \quad mv = \sqrt{2meV} \qquad \text{...(9)}$$

Substituting equation (9) in (5), we get

$$\textit{de-Broglie wavelength } \lambda = \frac{h}{\sqrt{2meV}} \qquad \text{... (10)}$$

(iii) de-Broglie wavelength interms of Temperature

When a particle like neutron is in thermal equilibrum at temperature T, then they possess Maxwell distribution of velocities.

$$\therefore \text{ Their kinetic energy } E_k = \frac{1}{2} mv_{rms}^2 \qquad \text{... (11)}$$

where v_{rms} is the Root mean square velocity of the particle.

$$\text{Also, we know Energy } = \frac{3}{2} K_B T \qquad \text{... (12)}$$

where K_B is the Boltzmann constant.

$\therefore$ Equating equations (11) and (12) we get

$$\frac{1}{2}mv^2 = \frac{3}{2} K_B T$$

(or)

$$m^2v^2 = 3m\, K_B T$$

$$mv = \sqrt{3mK_B T}$$

$$\therefore \quad \text{de-Broglie wavelength } \lambda = \frac{h}{mv} = \frac{h}{\sqrt{3mK_B T}} \qquad \text{... (13)}$$

Level-II

3) Deduce schroedinger's time independent and time dependent equation

Schroedinger describes the wave nature of a particle in mathematical form and is known as ***Schroedinger wave equation***. There are two types of wave equations, *viz.*

(i) Time dependent wave equation.

(ii) Time independent wave equation.

Time dependent wave equation

According to classical mechanics, if 'x' is the position of the particle moving with the velocity 'v', then the displacement of the particle at any time 't' is given by

$$y = A\, e^{-i\omega(t - x/v)}$$

where ω is the Angular frequency of the particle.

Similarly, in Quantum Mechanics the wave function $\Psi(x, y, z, t)$ represents the position (x, y, z) of a moving particle at any time 't' and is given by

$$\Psi(x, y, z, t) = A\, e^{-i\omega(t - x/v)} \quad \ldots (1)$$

We know angular frequency $\omega = 2\pi\nu$

$\therefore$ Equation (1) becomes

$$\Psi(x, y, z, t) = A\, e^{-2\pi i\left(\nu t - \frac{\nu x}{v}\right)} \quad \ldots (2)$$

We know $E = h\nu$ (or) $\nu = \frac{E}{h}$ ... (3)

Also, if 'v' is the velocity of the particle behaving as a wave, then the frequency $\nu = \frac{v}{\lambda}$ (or) $\frac{\nu}{v} = \frac{1}{\lambda}$ ... (4)

Substituting equations (3) and (4) in equation (2), we get,

$$\Psi(x, y, z, t) = A\, e^{-2\pi i\left(\frac{E}{h}t - \frac{x}{\lambda}\right)} \quad \ldots (5)$$

If 'p' is the momentum of the particle, then the de-Broglie wavelength is given by $\lambda = \frac{h}{mv} = \frac{h}{p}$ ... (6)

Substituting equation (6) in (5) we get

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

$$\text{(or)}\quad \Psi(x, y, z, t) = A\, e^{-\frac{2\pi i}{h}(Et - px)}$$

Since $\hbar = \frac{h}{2\pi}$, we can write $\boxed{\Psi(x, y, z, t) = A\, e^{-\frac{i}{\hbar}(Et - px)}}$ ...(7)

Differentiating equation (7) partially with respect to 'x' we get

$$\frac{\partial \Psi}{\partial x} = A e^{\frac{-i}{\hbar}(Et - px)}\left(\frac{ip}{\hbar}\right)$$

Differentiating once again partially with respect to 'x' we get

$$\frac{\partial^2\Psi}{\partial x^2} = Ae^{\frac{-i}{\hbar}(Et-px)}\left(\frac{i^2p^2}{\hbar^2}\right)$$

Since $\Psi(x, y, z, t) = Ae^{\frac{-i}{\hbar}(Et-px)}$ and $i^2 = -1$, we can write

$$\frac{\partial^2\Psi}{\partial x^2} = \Psi(x, y, z, t)\cdot\left(\frac{-p^2}{\hbar^2}\right)$$

(or)

$$p^2\Psi = -\hbar^2\frac{\partial^2\Psi}{\partial x^2} \quad ...(8)$$

Differentiating equation (7) partially with respect to 't', we get

$$\frac{\partial\Psi}{\partial t} = Ae^{\frac{-i}{\hbar}(Et-px)}\left(\frac{-iE}{\hbar}\right)$$

(or) $\frac{\hbar}{-i}\frac{\partial\Psi}{\partial t} = \Psi(x, y, z, t)\,E$ $\left[\because \Psi(x, y, z, t) = A\,e^{-\frac{i}{\hbar}(Et-px)}\right]$

or

$$E\Psi = i\hbar\frac{\partial\Psi}{\partial t} \quad ...(9)$$

A particle can behave as a wave only under motion. So, it should be accelerated by a potential field. Therefore, the total energy (E) of the particle is equal to the sum of its potential energy (V) and kinetic energy.

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

$$\text{(or)} \quad E = V + \frac{1}{2}\frac{m^2v^2}{m}$$

$$\text{(or)} \quad E = V + \frac{p^2}{2m} \qquad [\because p = mv]$$

$$\text{(or)} \quad E\Psi = V\Psi + \frac{p^2}{2m}\Psi \quad ...(10)$$

Substituting equations (8) and (9) in equation (10), we get,

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

(or)

$$\frac{i\hbar\partial}{\partial t}\Psi = \left[V - \frac{\hbar^2}{2m}\frac{\partial}{\partial x^2}\right]\Psi \quad \text{...(11)}$$

Equation (11) represents the ***one dimensional*** *(along 'x' direction)* ***Schroedinger time dependent equation***. It is called time dependent wave equation, because here the wave function $\Psi(x, y, z, t)$ depends both on position (x, y, z) and time (t).

Similarly, the ***3-dimensional Schroedinger time dependent wave equation*** can be written as

$$i\hbar \frac{\partial \Psi}{\partial t} = \left[V - \frac{\hbar^2}{2m}\nabla^2\right]\Psi \quad \text{... (12)}$$

where, $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$

Equation (12) can also be written as

$$E\Psi = H\Psi \quad \text{...(13)}$$

where E is the ***energy operator*** given by $E = i\hbar\frac{\partial}{\partial t}$ and

H is called ***Hamiltonian Operator***, given by $H = V - \frac{\hbar^2}{2m}\nabla^2$

8.13 SCHROEDINGER TIME INDEPENDENT WAVE EQUATION

It is convenient to use the time independent wave equation rather than using time dependent wave equation, because of the following reason.

In Schroedinger time dependent wave equation the wave function 'Ψ' depends on time, but in Schroedinger time independent wave function ψ does not depend on time and hence it has many applications.

We know that time dependent wave function

$$\Psi(x, y, z, t) = Ae^{-\frac{i}{\hbar}(Et - px)}$$

Splitting the RHS of this equation into two parts, *viz.,* (i) Time dependent factor and (ii) Time independent factor, we get

$$\text{(i.e.,)} \quad \Psi(x, y, z, t) = A\, e^{-\frac{}{\hbar}} \cdot e^{\frac{}{\hbar}}$$

$$\text{(or)} \quad \Psi(x, y, z, t) = A\, \psi\, e^{-\frac{iEt}{\hbar}} \qquad \text{... (1)}$$

where ψ *represents the time independent wave function* (i.e.,) $\psi = e^{\frac{ipx}{\hbar}}$

Differentiating equation (1) partially with respect to 't' we get

$$\frac{\partial \Psi}{\partial t} = A\, \psi\, e^{-\frac{iEt}{\hbar}} \left(\frac{-iE}{\hbar} \right) \qquad \text{... (2)}$$

Differentiating equation (1) partially with respect to 'x' we get,

$$\frac{\partial \Psi}{\partial x} = A\, e^{\frac{-iEt}{\hbar}} \frac{\partial \psi}{\partial x}$$

Differentiating once again partially with respect to 'x' we get

$$\frac{\partial^2 \Psi}{\partial x^2} = A\, e^{\frac{-iEt}{\hbar}} \frac{\partial^2 \psi}{\partial x^2} \qquad \text{... (3)}$$

We know the Schroedinger time dependent wave equation (one dimensional) is

$$i\hbar \frac{\partial \Psi}{\partial t} = V\Psi - \frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} \qquad \text{... (4)}$$

We can get the Schroedinger time dependent wave equation, just by substituting equations (1), (2) and (3), which has relation between the time dependent wave function (Ψ) and time independent wave function (ψ), in equation (4).

$\therefore$ Substituting equations (1), (2) and (3) in equation (4) we get

$$i\hbar\, A\, \psi\, e^{\frac{-iEt}{\hbar}} \left(\frac{-iE}{\hbar} \right) = VA\, \psi\, e^{\frac{-iEt}{\hbar}} - \frac{\hbar^2}{2m} A\, e^{\frac{-iEt}{\hbar}} \cdot \frac{\partial^2 \psi}{\partial x^2}$$

$$\text{(or)} \quad i\hbar \left(\frac{-iE}{\hbar} \right) \psi = V\psi - \frac{\hbar^2}{2m} \cdot \frac{\partial^2 \psi}{\partial x^2}$$

$$\text{(or)} \quad -(i)^2 E\psi = V\psi - \frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2}$$

$$\text{(or)} \quad E\psi - V\psi = \frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}$$

$$\text{(or)} \quad \frac{\partial^2\psi}{\partial x^2} = \frac{-2m}{\hbar^2}[E\,\psi - V\psi]$$

$$\text{(or)} \quad \frac{\partial^2\psi}{\partial x^2} + \frac{2m}{\hbar^2}[E\,\psi - V\psi] = 0$$

(or)

$$\boxed{\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - V)\,\psi = 0} \quad \ldots (5)$$

Equation (5) represents the ***one dimensional*** *(x- direction) Schroedinger time independent wave equation, because, in this equation the wave funtion* ψ *is independent of time. Similarly the* ***three dimensional Schroedinger time independent wave equation*** *can be written as*

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

where $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$

Note:

For a free particle, *the potential energy* $V = 0$

$\therefore$ *Schroedinger time independent wave equation becomes*

$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}E\psi = 0,$ *[for one dimension]*

and $\nabla^2\psi + \frac{2m}{\hbar^2}E\psi = 0$ *[for 3 dimension].*

4) Explain the construction and working of an electron microscope. Mention their merits and application

It is an instrument that uses highly energetic electron beam to examine a very small specimen.

Principle: The high energy electron beam is allowed to fall over the specimen and image formed due to the transmitted electron beam from the specimen is examined.

Construction

Essential parts of the electron microscope

i) An electron source
ii) Electro magnetic lenses
iii) Metal aperture
iv) Object holder
v) Screen

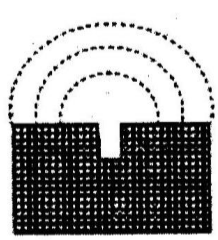

Fig. 3.13

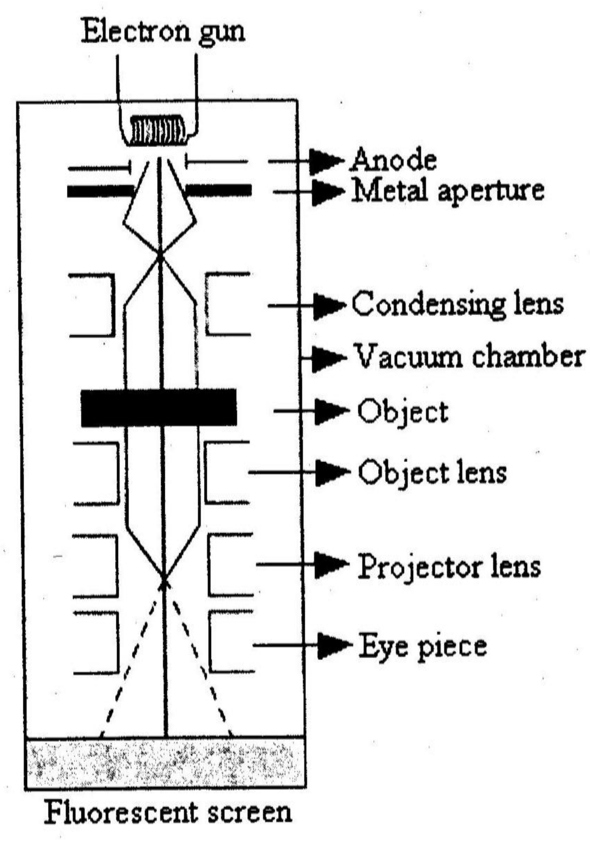

Fig. 3.14

Description

Electron gun is made of tungsten filament. Electrons which are emitted due to thermionic emission by the filament are accelerated by a large potential applied to the electrodes of the electron gun.

Electro magnetic lenses are made of coils enclosed inside the iron shield which has a gap at the middle as shown in the Fig. 3.13. If the gaps of the two electromagnetic lenses are faced with each other uniform magnetic field is produced. Similarly if the gaps of the two electromagnetic lenses are slightly disturbed non-uniform magnetic field is produced. Electron beam can be focused by the electromagnetic lens.

In this system we have three magnetic lenses.

i) Condensing lens which is used to condense the electron beam.

ii) Objective lens which is used to resolve the structures of the object.

iii) Projector lens which is used to enlarge the object.

Metal aperture is used to get a narrow beam and object holder holds the object. Enlarged image of the object is seen through the fluorescent screen.

The whole arrangement is kept inside a vacuum chamber as shown in the Fig. 3.14.

Working

Streams of electrons from the electron gun are accelerated by the positive anode potential. The electron beam is then confined to a narrow beam by the metal aperture (slit) and the condensing lens. Then the electron beam is passed through the object.

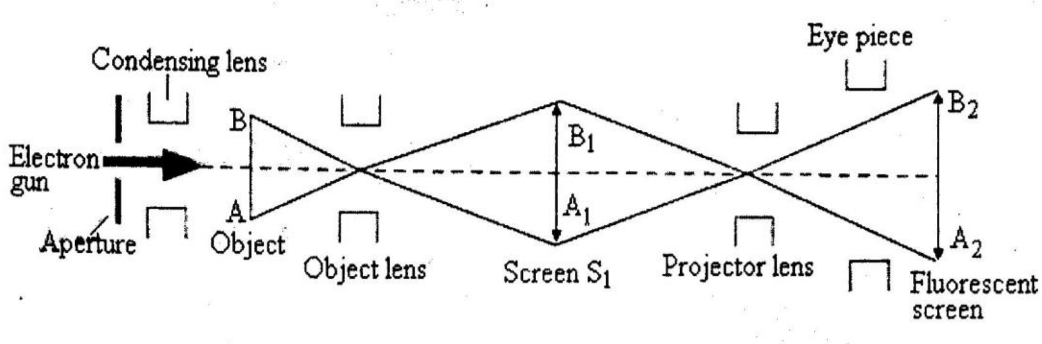

Fig. 3.15

An interaction between the electron beam and the object occurs and the transmitted electron beam carries the image of the object. Then it is passed through the magnifying objective lens as shown in Fig. 3.15. This lens magnifies the images of the object more than 100 times. Then the image is made to fall on the screen S_1 and the electron beam is passed through the magnifying projector lens. It also magnifies the image of the object again more than 10 times. Finally the image of the object is made to fall on a fluorescent screen. The image formed on the fluorescent screen is viewed through an optical lens which is attached with the eyepiece. It also magnifies the image 10 times. Therefore total magnification in the order of more than 10^5 times is achieved.

Merits

i) The magnification is 100000X.

ii) Focal length of the microscope can be varied.

Applications

i) It is used to determine the complicated structure of the crystal.

ii) It is used to study the disease due to virus and bacteria.

iii) It is used to study and analysis of colloidal particles.

iv) It is used to study the composition of papers, paints etc.

5) Explain the Principle, construction and working of a Scanning electron microscope. Mention their merits and application

Principle

Electron beam is made to fall on the various portions of the specimen by the scanning coils for scanning the sample. From the secondary electrons or back scattered electrons or x-rays that are produced by the incoming incident electrons are used to get the information about the specimen's surface, topography, composition etc.

Construction

The schematic diagram of the SEM is shown in the Fig. 3.16. It consists of an electron gun to produce high energy electron beam. Metal aperture is used to get a narrow beam and a magnetic condensing lenses are used to condense the electron beam. A beam deflector is placed between magnetic condensing lens and the magnetic objective lens. A set of scanning coils are placed inside the objective lens to scan the sample. The electron detector (scintillator) is used to collect the secondary electrons and can be converted into electrical signals by the detector (photomultiplier tube). These signals containing information about the scanned sample are then passed into the CRO. Finally the image is viewed on the CRO screen (image viewing screen).

Working

Streams of electrons are produced by the electron gun. These electrons are accelerated by the anode. These accelerated electron beams are confined to a narrow beam by the metal aperture and the first magnetic condensing lens. It is then passed through the second condenser lens to get thin, light coherent electron beam. Beam deflector effectively focuses the electron beam on the desired portion of the specimen. Again it is passed through the objective lens which focuses the coherent electron beam on the object. When electron beam strikes the specimen the specimen is scanned and the specimen-beam interactions can take place as shown in the Fig. 3.17.

In SEM the secondary electrons from the specimen are selectively attracted towards the detector. Detector consists of a positive potential at the front and scintillating coating at the back. Hence the secondary electrons are attracted towards the positive potential and finally converted into light pulses by the scintillating coating.

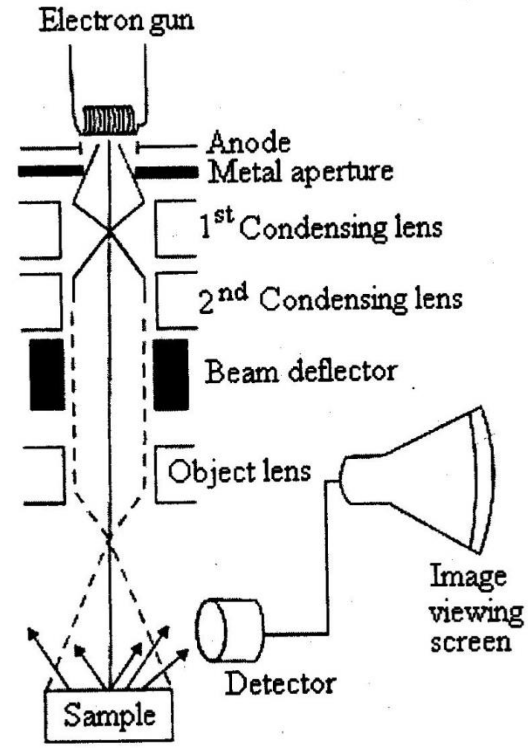

Fig. 3.16

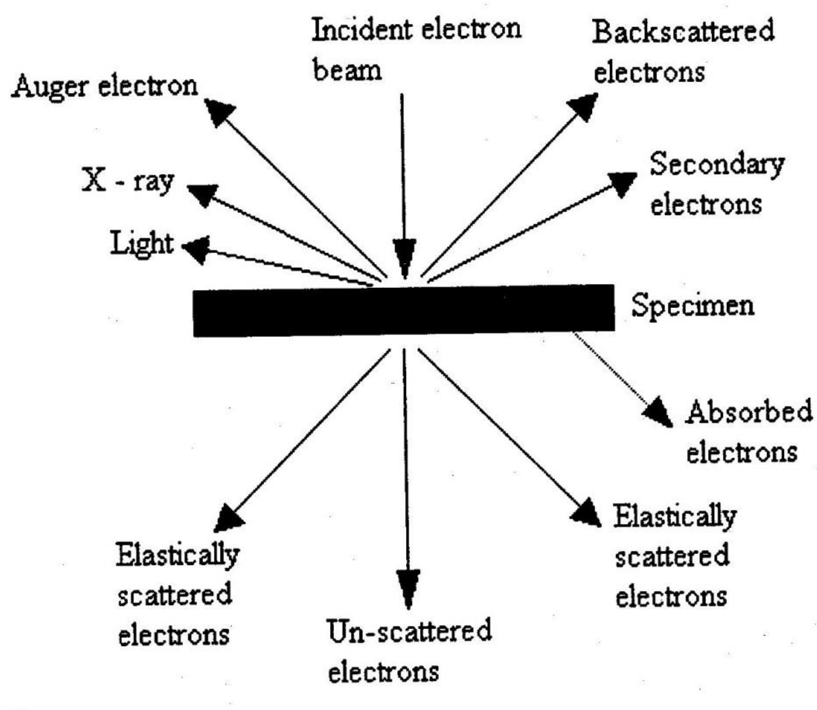

Fig. 3.17

The photomultiplier tube in the detector converts the light pulses into voltage signals. This voltage signal is then processed and amplified by an electronic circuit to get a point of brightness on the screen of the CRO. Thus the image is built up simply by scanning the electron beam across the specimen.

Advantages

i) Magnification is 300000X.
ii) It has large depth of focus.

Applications

i) It is used to study the disease causing agent like virus and bacteria.
ii) Used in microstructure analysis of ceramic materials.
iii) It is used to measure the thickness of thin coating.

LEVEL-III

6) Define Compton Effect, Compton shift and Compton wavelength; also explain how it can be verified experimentally?

Ass

with

Compton effect: *When a beam of monochromatic radiation such as X-rays, $\gamma-$ rays etc., of high frequency is allowed to fall on a fine scatterer, the beam is scattered into two components viz.*

(i) One component having the same frequency (or) wavelength as that of the incident radiation, so called ***unmodified radiation.***

and (ii) The other component having lower frequency (or) higher wavelength compared to incident radiation, so called ***modified radiation.***

This effect of scattering is called ***Compton effect.***

Compton Shift: *When a photon of energy 'hν' collides with an electron of a scatterer at rest, the photon gives its energy to the electron. Therefore the scattered photon will have lesser energy (or) lower frequency (or) higher wavelength compared to the wavelength of incident photon. Since the electron gains energy, it recoils with the velocity 'v'. This effect is called Compton effect and the shift in wavelength is called* ***Compton shift.***

Thus as a result of compton scattering, we get (i) Unmodified radiations (ii) Modified radiations and (iii) a recoil electron.

THEORY OF COMPTON EFFECT

Principle

In Compton scattering the collision between a photon and an electron is considered. Then by applying the laws of conservation of energy and momentum, the expression for compton wavelength is derived.

We know $e^{hc/\lambda K_B T} = 1 + \frac{hc}{\lambda K_B T} + \frac{1}{2}\left(\frac{hc}{\lambda K_B T} \right) + ...$

During the collision process, a part of energy is given to the electron, which inturn increases the kinetic energy of the electron and hence it recoils at an angle of ϕ as shown in Fig. 8.4. The scattered photon moves with an energy $h\nu'$ (lesser than $h\nu$), at an angle θ with respect to the original direction.

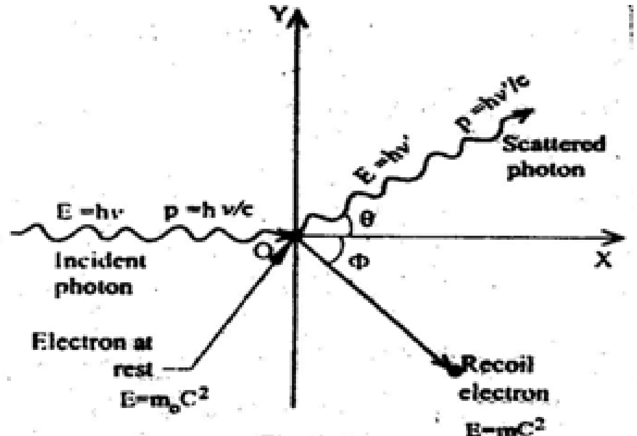

Fig. 8.4

Let us find the energy and momentum components before and after collision process.

Energy before collision

(i) Energy of the incident photon $= h\nu$.

(ii) Energy of the electron at rest $= m_0 c^2$

where m_0 is the rest mass energy of the electron.

$$\therefore \textit{Total Energy before Collision} = h\nu + m_0 c^2 \quad \text{... (1)}$$

Energy after collision

(i) Energy of the scattered photon $= h\nu'$

(ii) Energy of the recoil electron $= mc^2$

where m is the mass of the electron moving with velocity 'v'

$$\therefore \textit{Total energy after collision} = h\nu' + mc^2 \quad \text{... (2)}$$

We know according to the law of conservation of energy

Total energy before collision = Total energy after collision

$\therefore$ Equation (1) = Equation (2)

$$\text{(i.e.,)} \quad h\nu + m_0 c^2 = h\nu' + mc^2 \quad \text{... (3)}$$

X-Component of Momentum Before Collision

(i) X-component momentum of the incident Photon $= \dfrac{h\nu}{c}$

(ii) X-component momentum of the electron at rest $= 0$

$$\therefore \textit{Total X-component of momentum before Collision} = \frac{h\nu}{c} \quad \text{... (4)}$$

Component of momentum After collision

(i) From Fig. 8.5, In ΔOAE, $\sin\theta = \dfrac{M_y}{h\nu'/c}$

$\therefore$ Y-Component momentum of the scattered photon $= \dfrac{h\nu'}{c}\sin\theta$

(ii) From fig 8.5, In $\Delta\, OCD$, $\sin\phi = \dfrac{-M_y}{mv}$

$\therefore$ Y-Component momentum of the recoil electron $= -mv\sin\phi$

Total Y-Component of momentum after collision $= \dfrac{h\nu'}{c}\sin\theta - mv\sin\phi$ (8)

According to the law of conservation of momentum,

Equation (7) = Equation (8)

$$\therefore 0 = \frac{h\nu'}{c}\sin\theta - mv\sin\phi \quad \text{...(9)}$$

From equation (6), we can write

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

$$\text{(or)}\ mcv\cos\phi = h(\nu - \nu'\cos\theta) \quad \text{... (10)}$$

From equation (9) we can write

$$mcv\sin\phi = h\nu'\sin\theta \quad \text{... (11)}$$

Squaring and adding Equation (10) and (11) we get

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

Since $\cos^2\phi + \sin^2\phi = 1$ and $h^2(\nu')^2[\cos^2\theta + \sin^2\theta] = h^2(\nu')^2$ we get

$$\text{(or)}\ m^2c^2v^2 = h^2[\nu^2 - 2\nu\nu'\cos\theta + (\nu')^2] \quad \text{... (12)}$$

From equation (3), we can write

$$mc^2 = m_0c^2 + h(\nu - \nu')$$

Squaring on both sides we get

$$m^2c^4 = m_0^2c^4 + 2h\,m_0c^2(\nu - \nu') + h^2[\nu^2 - 2\nu\nu' + (\nu')^2] \quad \text{... (13)}$$

Subtracting equation (12) from equation (13), we get

$$m^2c^2(c^2 - v^2) = m_0^2c^4 + 2h\,m_0c^2(\nu - \nu') - 2h^2\nu\nu'(1 - \cos\theta) \quad \text{...(14)}$$

$\therefore$ *Total X-Component of momentum before collision* $= 0$ ... (7)

From the theory of relativity, the relativistic formula for the variation of mass with the velocity of the electron is given by

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

Squaring, we get $m^2 = \frac{m_0^2}{\left(1 - \frac{v^2}{c^2}\right)}$ (or) $m^2 = \frac{m_0^2 c^2}{c^2 - v^2}$

(or) $m^2 (c^2 - v^2) = m_0^2 c^2$ ... (15)

In order to make this equation, similar to LHS of equation (14) multiply it by c^2 on both sides.

$$\therefore \text{ We get } \quad \boxed{m^2 c^2 (c^2 - v^2) = m_0^2 c^4} \qquad \text{... (16)}$$

Equating equations (16) and (14), we can write

$$m_0^2 c^4 = m_0^2 c^4 + 2\, h\, m_0\, c^2 (\nu - \nu') - 2\, h^2 \nu\, \nu' (1 - \cos\theta)$$

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

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

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

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

Multiplying both sides by 'c', we get

$$\frac{c}{\nu'} - \frac{c}{\nu} = \frac{hc}{m_0 c^2} (1 - \cos\theta) \qquad \text{... (17)}$$

Since $\lambda = \frac{c}{\nu}$ and $\lambda' = \frac{c}{\nu'}$ we can write equation (17) as

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

or) *Change in wavelength* $\boxed{\Delta\lambda = \frac{h}{m_0 c} (1 - \cos\theta)}$ .... (18)

Equation (18) represents the shift in wavelength, i.e., ***Compton Shift*** which is independent of the incident radiation as well as the nature of the scattering substance.

Thus the shift in wavelength (or) Compton Shift purely depends on the angle of scattering.

SPECIAL CASES

Case (i) When $\theta = 0$; $\cos\theta = 1$

$\therefore$ **Equation (18) becomes** $\boxed{\Delta\lambda = 0}$

This implies that at $\theta = 0$ the scattering is absent and the outcoming radiation has the same wavelength (or) frequency as that of the incident radiation. Thus we get the output as a single peak. [Refer fig. 8.7]

Case (ii) When $\theta = 90°$; $\cos\theta = 0$

$\therefore$ Equation (18) becomes $\Delta\lambda = \frac{h}{m_0 c}$

Substituting the values of h, m_0 and c we get

$$\Delta\lambda = \frac{6.625 \times 10^{-34}}{(9.11 \times 10^{-31})(3 \times 10^{8})}$$

(or) $\boxed{\Delta\lambda = 0.02424 \text{ Å}}$

This wavelength is called **COMPTON WAVELENGTH,** *which has a good agreement with the experimental results.* [Refer fig. 8.7]

Case (iii) When $\theta = 180°$, $\cos\theta = -1$

$\therefore$ Equation (18) becomes $\Delta\lambda = \frac{h}{m_0 c}[1 - (-1)]$

(or) $$\Delta\lambda = \frac{2h}{m_0 c}$$

Substituting the values of h, m_0 and c we get

$$\boxed{\Delta\lambda = 0.04848 \text{ Å}}$$

Thus for $\theta = 180°$ the shift in wavelength is found to be maximum. [Refer fig. 8.7]

$\therefore$ When the angle of scattering (θ) varies from 0 to 180°, the wavelength shifts from λ to $\lambda + \frac{2h}{m_0 c}$

EXPERIMENTAL VERIFICATION OF COMPTON EFFECT

Principle

When a photon of energy 'hν' collides with a scattering element, the scattered beam has two components, viz., one of the same frequency (or) wavelength as that of the incident radiation and the other has lower frequency (or) higher wavelength compared to incident frequency (or) wavelength. This effect is called Compton effect and the shift in wavelength is called Compton shift.

Construction

It consists of an X-ray tube for producing X-rays. A small block of carbon C (scattering element) is mounted on a circular table as shown in Fig. 8.6.

A Bragg's spectrometer (B_s) is allowed to freely swing in an arc about the scattering element to catch the scattered photons. Slits S_1 and S_2 helps to focus the X-rays onto the scattering element.

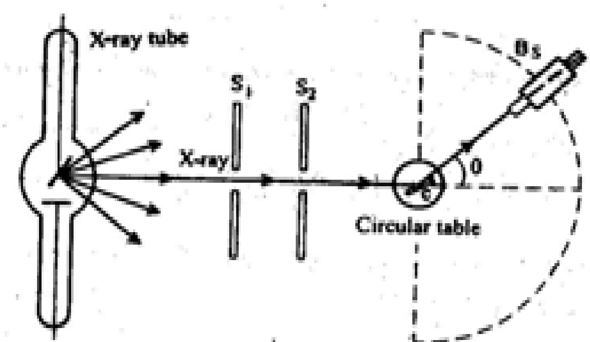

Fig. 8.6

The interactive animation of this concept can be viewed in the CD.

Working

X-rays of monochromatic wavelength 'λ' is produced from an X-ray tube and is made to pass through the slits S_1 and S_2. These X- rays are made to fall on the scattering element. The scattered X-rays are received with the help of the Bragg's spectrometer and the scattered wavelength is measured.

The experiment is repeated for various scattering angles and the scattered wavelengths are measured. The experimental results are plotted as shown in Fig. 8.7.

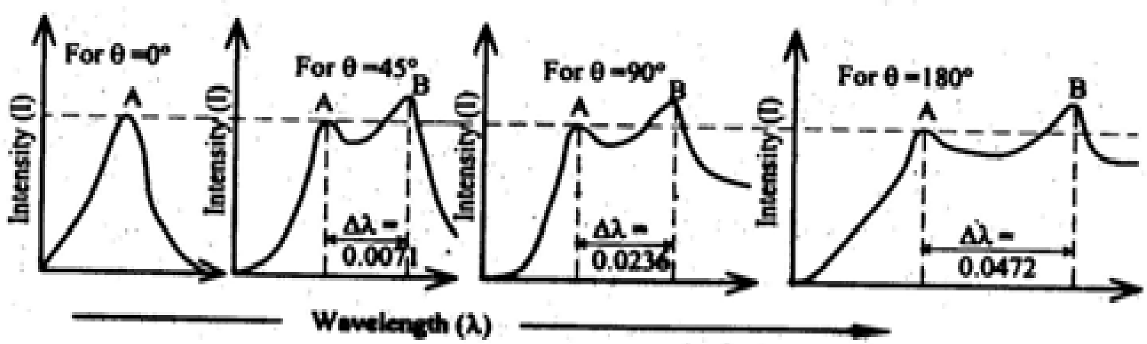

Fig. 8.7

In this figure when the scattering angle $\theta = 0°$, the scattered radiation peak will be the same as that of the incident radiation Peak '*A*'. Now, when the scattering angle is increased, for one incident radiation peak *A* of wavelength (λ) we get two scattered peaks *A* and *B*. Here the peak '*A*' is found to be of same wavelength as that of the incident wavelength and the peak '*B*' is of greater wavelength than the incident radiation.

The shift in wavelength (or) difference in wavelength ($\Delta\lambda$) of the two scattered beams is found to increase with respect to the increase in scattering angle.

At $\theta = 90°$, the $\Delta\lambda$ is found to be $0.0236 \approx 0.02424$, which has good agreement with the theoretical results. Hence *this wavelength is called Compton wavelength and the shift in wavelength is called* **Compton shift**.

7) List out the physical significance of wave function. Explain the application of Schroedinger wave equation to one dimensional potential well.

PHYSICAL SIGNIFICANCE OF A WAVE FUNCTION [Ψ]

Wave function: *It is the variable quantity that is associated with a moving particle at any position (x, y, z) and at any time 't' and it relates the probability of finding the particle at that point and at that time.*

» It relates the particle and the wave statistically

$$\text{(i.e.,)}\ \Psi(x, y, z, t) = A\, e^{-i\omega(t - x/v)}$$

$$\boxed{\text{(or)}\ \Psi = \psi\, e^{-i\omega t}}$$

» Wave function gives the information about the particle behaviour.

» Ψ is a complex quantity and individually it does not have any meaning.

» $|\Psi|^2 = \Psi^* \Psi$ is real and positive, it has physical meaning. This concept is similar to light. In light, amplitude may be positive (or) negative but the Intensity, which is the square of amplitude is real and is measurable.

» $|\Psi|^2$ represents the probability density (or) probability of finding the particle per unit volume.

» For a given volume $d\tau$, the probability of finding the particle is given by

$$\text{Probability } (P) = \iiint |\Psi|^2\, d\tau$$

where $d\tau = dx \cdot dy \cdot dz$

» The probability will have any value between zero to one. (i.e.,)

(i) If $P = 0$ then there is no chance for finding the particle (i.e.,) there is no particle, within the given limits.

(ii) If $P = 1$ then there is 100% chance for finding the particle (i.e.,) the particle is definitely present, within the given limits.

(iii) If $P = 0.7$, then there is 70% chance for finding the particle and 30% there is no chance for finding the particle, within the given limits.

Example: If a particle is definitely present within a one dimensional box (*x*-direction) of length '*l*', then the probability of finding the particle can be written as

$$P = \int_0^l |\Psi|^2 dx = 1$$

The application of Schrodinger wave equation to one dimensional potential well.

Let us consider a particle (electron) of mass '*m*' moving along *x*-axis, enclosed in a one dimensional potential box as shown in fig. 8.8.

Since the walls are of infinite potential the particle does not penetrate out from the box.

Also, the particle is confined between the length '*l*' of the box and has *elastic collisions* with the walls. *Therefore, the potential energy of the electron inside the box is constant and can be taken as zero for simplicity.*

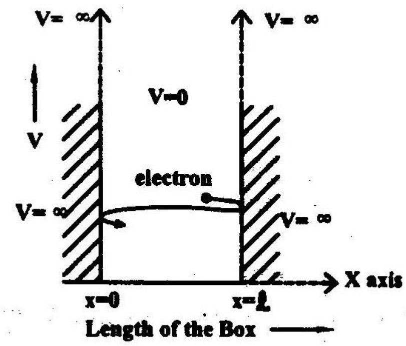

Fig. 8.8

The interactive animation of this concept can be viewed in the CD.

∴ *We can say that* ***Outside the box*** *and* ***on the wall of the box****, the potential energy V of the electron is ∞.*

Inside the box *the potential energy (V) of the electron is zero.*

In other words we can write the ***boundary conditions*** as

$$V(x) = 0 \text{ when } 0 < x < l$$

$$V(x) = \infty \text{ when } 0 \geq x \geq l$$

Since the particle cannot exist outside the box the wave function $\psi = 0$ when $0 \geq x \geq l$.

To find the wave function of the particle within the box of length '*l*', let us consider the schroedinger one dimensional time independent wave equation (i.e.,)

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}[E - V]\,\psi = 0$$

Since the potential energy inside the box is zero [(i.e) $V = 0$], the particle has kinetic energy alone and thus it is named as a free particle (or) free electron.

$\therefore$ For a *free particle (electron)*, the Schroedinger wave equation is given by

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} E\,\psi = 0$$

(or)
$$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \qquad \text{... (1)}$$

where $k^2 = \dfrac{2mE}{\hbar^2}$ ... (2)

Equation (1) is a second order differential equation, therefore, it should have solution with two arbitrary constants.

$\therefore$ The solution for equation (1) is given by

$$\boxed{\psi(x) = A \sin kx + B \cos kx} \qquad \text{... (3)}$$

where A and B are called as arbitrary constants, which can be found by applying the boundary conditions.

(i.e.,) $V(x) = \infty$ when $x = 0$ and $x = l$

Boundary condition (i) at $x = 0$, potential energy $V = \infty$, $\therefore$ There is no chance for finding the particle at the walls of the box, $\therefore$ $\psi(x) = 0$

$\therefore$ Equation (3) becomes

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

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

$$\therefore \mathbf{B = 0}$$

Boundary condition (ii) at $x = l$, potential energy $V = \infty$, $\therefore$ There is no chance for finding the particle at the walls of the box, $\therefore$ $\psi(x) = 0$

$\therefore$ Equation (3) becomes

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

Since $B = 0$ (from 1st Boundary condition), we have

Since $A \neq 0$; $\sin kl = 0$

We know $\sin n\pi = 0$

Comparing these two equations, we can write $kl = n\pi$

where n is an integer.

$$\text{(or)}\ k = \frac{n\pi}{l} \qquad \text{... (4)}$$

Substituting the value of B and k in equation (3) we can write the wave function associated with the free electron confined in a one dimensional box as

$$\psi_n(x) = A \sin\frac{n\pi x}{l} \qquad \text{...(5)}$$

Energy of the particle (Electron)

We know from equation (2)

$$k^2 = \frac{2mE}{\hbar^2}$$

$$= \frac{2mE}{(h^2/4\pi^2)} \qquad \left[\because \hbar^2 = \frac{h^2}{4\pi^2}\right]$$

$$\text{(or)}\ k^2 = \frac{8\pi^2 mE}{h^2} \qquad \text{... (6)}$$

Squaring equation (4) we get

$$k^2 = \frac{n^2\pi^2}{l^2} \qquad \text{... (7)}$$

Equating equation (6) and equation (7), we can write

$$\frac{8\pi^2 mE}{h^2} = \frac{n^2\pi^2}{l^2}$$

$$\therefore \textit{Energy of the particle (electron)}\ E_n = \frac{n^2h^2}{8ml^2} \qquad \text{...(8)}$$

$\therefore$ From equations (8) and (5) we can say that, for each value of 'n', there is an energy level and the corresponding wave function.

*Thus we can say that, each value of E_n is known as **Eigen value** and the corresponding value of ψ_n is called as **Eigen function**.*

Energy levels of an electron

For various values of '*n*' we get various energy values of the electron. ***The lowest energy value (or) ground state energy value*** can be got by substituting $n = 1$ in equation (8)

$$\therefore \text{When } n = 1 \text{ we get } E_1 = \frac{h^2}{8ml^2}$$

Similarly we can get the other energy values

$$\text{(i.e.,) When } n = 2 \text{ we get } E_2 = \frac{4h^2}{8ml^2} \Rightarrow 4E_1$$

$$\text{When } n = 3 \text{ we get } E_3 = \frac{9h^2}{8ml^2} \Rightarrow 9E_1$$

$$\text{When } n = 4 \text{ we get } E_4 = \frac{16\,h^2}{8\,ml^2} \Rightarrow 16\,E_1$$

$\therefore$ In general we can write the energy eigen function as

$$\boxed{E_n = n^2 E_1} \qquad ...(9)$$

It is found from the energy levels E_1, E_2, E_3 etc the energy levels of an electron are ***Discrete.***

This is the great success which is achieved in quantum mechanics than classical mechanics, in which the energy levels are found to be continuous.

The various energy eigen values and their corresponding eigen functions of an electron enclosed in a one dimensional box is as shown in fig. 8.9. Thus we have discrete energy values.

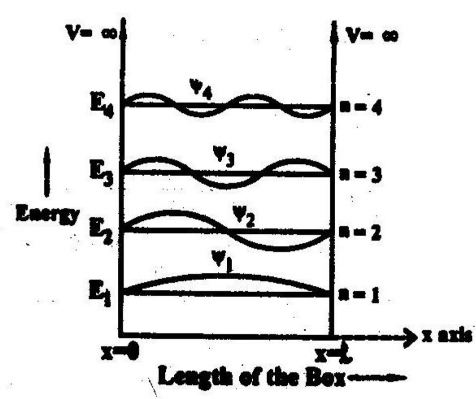

Fig. 8.9

Normalisation of the wave function.

Normalisation: It is the process by which the probability (P) of finding the particle (electron) inside the box can be done.

We know that the total probability (P) is equal to 1 means then there is a particle inside the box.

∴ For a one dimensional potential box of length 'l', the probability

$$P = \int_0^l |\psi|^2 \, dx = 1 \quad \left(\begin{array}{l} \text{Since the particle is present inside the well between the} \\ \text{length 0 to1 the limits are chosen between 0 to 1} \end{array} \right) \qquad (10)$$

Substituting equation (5) in equation (10), we get

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

$$\text{(or)} \quad A^2 \int_0^l \left[\frac{1 - \cos 2n\pi x/l}{2} \right] dx = 1$$

$$A^2 \left[\frac{x}{2} - \frac{1}{2} \frac{\sin 2n\pi x/l}{2n\pi/l} \right]_0^l = 1$$

$$A^2 \left[\frac{l}{2} - \frac{1}{2} \frac{\sin 2n\pi l/l}{2n\pi} \right] = 1$$

$$A^2 \left[\frac{l}{2} - \frac{1}{2} \frac{\sin 2n\pi}{2n\pi} \right] = 1 \qquad ...(11)$$

We know $\sin n\pi = 0$ ∴ $\sin 2n\pi$ is also $= 0$

∴ Equation (11) can be written as

$$\frac{A^2 l}{2} = 1$$

(or) $$A^2 = \frac{2}{l}$$

(or) $$A = \sqrt{\frac{2}{l}}$$

Substituting the value of 'A' in equation (5),

The normalised wave function can be written as

$$\psi_n = \sqrt{\frac{2}{l}} \sin\frac{n\pi x}{l}$$

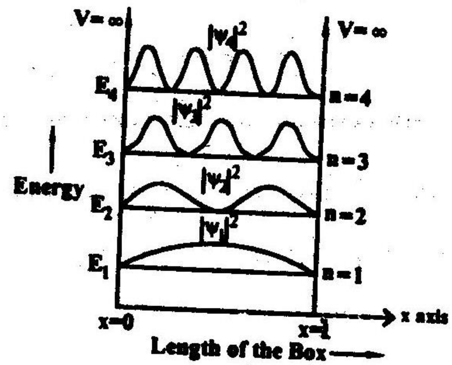

Fig. 8.10

The interactive animation of this concept can be viewed in the CD.

The normalised wave function and their energy values are as shown in fig. 8.10.

8.16 THREE DIMENSIONAL POTENTIAL BOX

The solution of one-dimensional potential box can be extended for a three dimensional potential box. In a three dimensional potential box, the particle (electron) can move in any direction in space. Therefore instead of one quantum number 'n', we have to use three quantum number n_x, n_y and n_z corresponding the three co-ordinate axis (ie) x, y and z respectively.

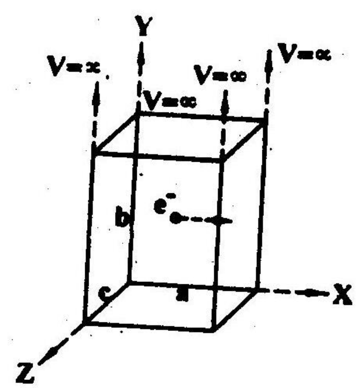

Fig. 8.11

∴ If a, b, c are the length of the box as shown in figure 8.11 along x, y and z axis, then the

The energy of the particle $= E_x + E_y + E_z$

$$\text{(i.e.,) } E_{n_x, n_y, n_z} = \frac{n_x^2 h^2}{8ma^2} + \frac{n_y^2 h^2}{8mb^2} + \frac{z^2 h^2}{8mc^2}$$

If $a = b = c$ (i.e.,) for a ***cubical box.***

Energy Eigen value is $$E_{n_x, n_y, n_z} = \frac{h^2}{8ma^2}[n_x^2 + n_y^2 + n_z^2] \quad \text{...(1)}$$

The corresponding normalized wave function of an electron in a cubical box can be written as

$$\psi_{n_x n_y n_z} = \sqrt{\frac{2}{a} \times \frac{2}{a} \times \frac{2}{a}} \cdot \sin \frac{n_x \pi x}{a} \sin \frac{n_y \pi y}{a} \sin \frac{n_z \pi z}{a}$$

$$\therefore \quad \psi_{n_x n_y n_z} = \sqrt{\frac{8}{a^3}} \cdot \sin \frac{n_x \pi x}{a} \sin \frac{n_y \pi y}{a} \sin \frac{n_z \pi z}{a} \quad \text{... (2)}$$

From equations (1) and (2) we can note that, several combinations of the three quantum numbers (n_x, n_y and n_z) leads to different energy eigen values and eigen functions.