UNIT – III QUANTUM MECHANICS

PART – A QUESTIONS

1. What is black body?

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

2. What is black body radiation?

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

3. State Planck's quantum theory (or) State Planck's hypothesis (or) What are the postulates of Planck's quantum theory? (or) What are the assumptions of quantum theory of black body radiation? (or) Give the special features of Quantum theory.

(i) The electrons in the black body are assumed as simple harmonic oscillators.
(ii) The oscillators will not emit energy continuously.
(iii) The emit radiation in terms of quantas of magnitude 'hυ', discretely.
i.e. $E = nh\nu$, where $n = 0, 1, 2, 3, \ldots$..

4. Give the importance of Planck's radiation formula.

- It explains all regions of black body radiation.
- It is based on quantum theory.
- It is used to derive other laws related to black body radiation.

5. State Wien's displacement law. Give its limitation.

The product of wavelength (λ_m) of maximum energy emitted and the absolute temperature (T) is a constant.

$$\lambda_m T = Constant.$$

Limitation: It holds good only for shorter wavelength.

6. State Rayleigh-Jeans law. Give its limitation.

The energy is directly proportional to the absolute temperature and is inversely proportional to the fourth power of the wavelength.

$$\boxed{E_\lambda \ \alpha \ \frac{T}{\lambda^4}}$$

Limitation: It holds good only for longer wavelength.

7. What is meant by photon?

Photons are discrete energy values in the form of small quantas of definite frequency or wavelength.

8. State the properties of photon.

- Photons are similar to that of electrons.
- They do not have any charge.
- They do not ionize.
- They are not affected by electric and magnetic fields.

9. Define Compton shift and Compton Effect.

When a beam of high frequency radiation (x – rays or γ – rays) is scattered by a fine scatterer, the scattered beam contains two components.

(i) One component has the same wavelength as incident radiation (unmodified radiation)

(ii) The other component has slightly higher wavelength than incident radiation (modified radiation).
The change in wavelength is called Compton shift.
This phenomenon is called Compton Effect.

10. What is Compton wavelength? Calculate its value.

The shift in wavelength corresponding to the scattering angle of 90^0 is called Compton wavelength.

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

When $\theta = 90^0$, $\cos\theta = 0$

$$\textit{Compton Shift } \Delta\lambda = \frac{h}{m_0 c}$$

$$\textit{Compton Shift } \Delta\lambda = \frac{6.625\times10^{-34}}{(9.11\times10^{-31})\times(3\times10^{5})}$$

$$\boxed{\Delta\lambda = 0.02424 \text{ Å}}$$

11. What is wave function?

Wave function (ψ) 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 and at that time.

12. Mention the physical significance of wave function of matter waves (or) de Broglie waves.

(i) A variable quantity which characterizes waves is known as 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) Ψ represents the probability density of the particle which is real and positive.

13. State de-Broglie hypothesis (or) Explain the concept of wave nature (or) What is meant by matter waves? (or) Give the origin of concept of matter waves.

The light exhibits the dual nature. It can behave as a particle and the wave. de Broglie suggested that an electron which is a particle can also behave as a wave and exhibits the dual nature.

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

If 'v' is the velocity and 'm' is the mass of the particle,

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

14. For a free particle moving within a one dimensional potential box, the ground state energy cannot be zero. Why?

For a free particle moving within a one dimensional potential box, when $n = 0$, the wave function is zero for all values of x, i.e., it is zero even within the potential box. This would mean that the particle is not present within the box. Therefore the state with $n = 0$ is not allowed. As energy is proportional to n^2, the ground state energy cannot be zero since $n = 0$ is not allowed.

15. Define Eigen value and Eigen function.

Eigen value is defined as energy of the particle. It is denoted by E_n.

Eigen function is defined as the wave function of the particle. It is denoted by ψ_n.

16. What is photoelectric Effect?

When a photon hits an electron on a metal surface, the electron can be emitted. The emitted electrons are called photoelectrons. The effect is called Photoelectric Effect.

17. Write down the Schroedinger time dependent wave equation.

$$E\psi = H\psi$$

Where E – Total energy of the particle
H – Hamiltonian operator
ψ - Wave function

18. Write down the Schroedinger time independent wave equation.

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

Where E – Total energy of the particle
V – Potential energy of the particle
m – Mass of the particle
$\hbar = \frac{h}{2\pi}$ - Planck's Constant

19. Mention the applications of Schroedinger wave equation.

- It is used to find the electrons in metals.
- It is used to find energy levels of an electron in an infinite deep potential well.

20. What are meant by a degenerate state and Non-degenerate state?

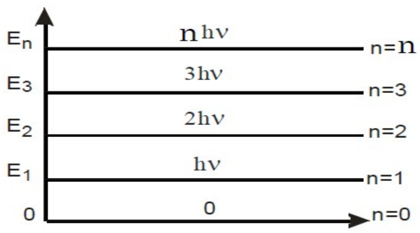
For various combinations of quantum numbers, if we get same eigen value but different eigen functions, it is called degenerate state.

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

PART – B QUESTIONS

1. Using Quantum theory, derive an expression for the average energy emitted by a black body and arrive at Planck's radiation law in terms of frequency. State the assumptions before starting the derivation.

Assumptions



1. The electrons in the black body are assumed as simple harmonic oscillators.

2. They do not emit energy continuously.
3. They emit energy in terms of quanta of magnitude 'hv' discretely.

$$E = nhv, \quad n = 0, 1, 2, 3, \ldots$$

To calculate average energy

Consider a black body with large number of oscillators.

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

$\overline{E}$ – Average energy

E_T – Total energy

N – Number of oscillators.

$$N = N_0 + N_1 + N_2 + N_3 + \ldots\ldots\ldots N_r \qquad \text{------------ (2)}$$

$$E_T = 0N_0 + EN_1 + 2EN_2 + 3EN_3 + \ldots\ldots\ldots rEN_r \qquad \text{------------- (3)}$$

According to Maxwell distribution law,

$$N_r = N_0 e^{-rE/K_BT} \qquad r = 0, 1, 2, 3, \ldots$$

$$r = 0, \quad N_0 = N_0 e^{-0E/K_BT} \Rightarrow N_0$$

$$r = 1, \quad N_1 = N_0 e^{-E/K_BT}$$

$$r = 2, \quad N_2 = N_0 e^{-2E/K_BT}$$

$$r = 3, \quad N_3 = N_0 e^{-3E/K_BT}$$

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$$r = r, \quad N_r = N_0 e^{-rE/K_BT}$$

Sub. $N_0, N_1, N_2, N_3, \ldots$ values in (2)

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

$$N = N_0 [1 + e^{-E/K_BT} + e^{-2E/K_BT} + e^{-3E/K_BT} + \ldots\ldots]$$

Put $x = e^{-E/K_BT}$

$$N = N_0 [1 + x^2 + x^3 + x^4 + \ldots\ldots]$$

$$N = N_0\left[\frac{1}{1-x}\right] \qquad \text{------------ (4)}$$

[By Binomial series $1 + x^2 + x^3 + x^4 + \ldots = \left[\frac{1}{1-x}\right]$

Sub. $N_0, N_1, N_2, N_3, \ldots$ values in (3)

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

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

Put $x = e^{-E/K_BT}$

$E_T = N_0E[x + 2x^2 + 3x^3 + \ldots\ldots]$

$E_T = N_0Ex[1 + 2x + 3x^2 + \ldots\ldots]$

$$E_T = N_0Ex\left[\frac{1}{(1-x)^2}\right] \quad \text{------------- (5)}$$

[By Binomial series, $1+2x+3x^2+\ldots = \left[\frac{1}{(1-x)^2}\right]$]

Sub. (4) & (5) in (1)

$$\overline{E} = \frac{N_0Ex\left[\frac{1}{(1-x)^2}\right]}{N_0\left[\frac{1}{1-x}\right]}$$

$$\overline{E} = \frac{Ex}{1-x}$$

Sub. $x = e^{-E/K_BT}$

$$\overline{E} = \frac{Ee^{-E/K_BT}}{1-e^{-E/K_BT}} \quad \text{----------- (6)}$$

Divide by e^{-E/K_BT} in numerator & denominator

$$\overline{E} = \frac{\frac{Ee^{-E/K_BT}}{e^{-E/K_BT}}}{\frac{1}{e^{-E/K_BT}} - \frac{e^{-E/K_BT}}{e^{-E/K_BT}}}$$

$$\overline{E} = \frac{E}{\frac{1}{e^{-E/K_BT}} - 1}$$

$$\overline{E} = \frac{h\nu}{e^{E/K_BT} - 1} \quad \text{------------- (7)} \qquad [E = h\nu]$$

Energy density $E_\nu d\nu = N\overline{E}$

N – Number of oscillators per unit volume

$\overline{E}$ – Average energy

$$N = \frac{8\pi\nu^2}{c^3}d\nu$$

$$\overline{E} = \frac{h\nu}{e^{E/K_BT} - 1}$$

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

$$E_\nu = \frac{8\pi h\nu^3}{c^3\left(e^{h\nu/K_BT}-1\right)} \qquad \text{------------- (9)}$$

(9) is the expression for Planck's law of radiation in terms of frequency.

W.K.T., $\nu = \frac{c}{\lambda}$

$$d\nu = \frac{-c}{\lambda^2}d\lambda \Rightarrow \frac{c}{\lambda^2}d\lambda$$

Sub. the values of ν & $d\nu$ in (8)

$$E_\lambda d\lambda = \frac{8\pi\frac{c^2}{\lambda^2}}{c^3}\frac{c}{\lambda^2}d\lambda\frac{h\frac{c}{\lambda}}{e^{hc/\lambda K_BT}-1}$$

$$E_\lambda = \frac{8\pi hc}{\lambda^5}\frac{1}{\left(e^{hc/\lambda K_BT}-1\right)} \qquad \text{------------- (10)}$$

(10) is the expression for Planck's law of radiation in terms of wavelength.

2. Deduce Wien's displacement law and Rayleigh-Jean's law from Planck's law of radiation.

Planck's law of radiation $E_\lambda = \frac{8\pi hc}{\lambda^5}\frac{1}{\left(e^{hc/\lambda K_BT}-1\right)}$ ---------- (1)

Deduction of Wien's displacement law

When λ is very small, ν is large, hence $\frac{h\nu}{K_BT} >> 1$ and $e^{h\nu/K_BT}$ is large when compared to 1 hence 1 is neglected in the denominator of (1)

(1) becomes $E_\lambda = \frac{8\pi hc}{\lambda^5}\frac{1}{\left(e^{hc/\lambda K_BT}\right)}$

Thus we get Wein's displacement law, from Planck's Radiation Law

Deduction of Rayleigh-Jean's law

When λ is very large, ν is very small,

hence $\frac{h\nu}{K_BT} << 1$ and $e^{h\nu/K_BT} = 1 + \frac{h\nu}{K_BT} + \ldots$ (using exponential series and neglecting higher order terms).

(1) can be written as

$$E_\lambda = \frac{8\pi hc}{\lambda^5} \cdot \frac{1}{1+\frac{hc}{\lambda K_B T} - 1}$$

$$E_\lambda = \frac{8\pi hc}{\lambda^5 \frac{hc}{K_B T \lambda}}$$

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

Thus we get Rayleigh-Jeans Law from Planck's Radiation Law.

3. **What is Compton Effect? Give the theory of Compton Effect and show that the Compton shift is** $\Delta\lambda = \frac{h}{m_0 c}(1 - \cos\theta)$.

(or)

Derive an expression for the change in wavelength suffered by an X-ray photon when it collides with an electron.

Compton Effect

When a beam of high frequency radiation (x – rays or γ – rays) is scattered by a fine scatterer, the scattered beam contains two components.

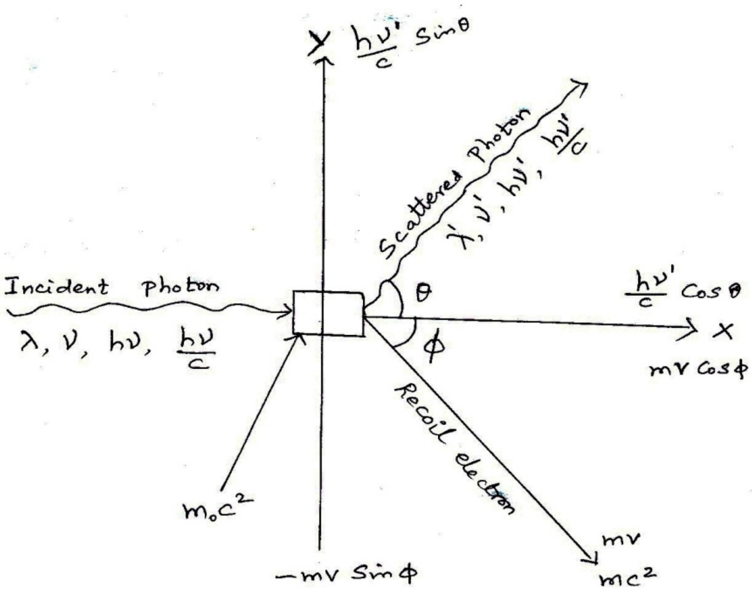
(i) One component has the same wavelength as incident radiation (unmodified radiation)

(ii) The other component has slightly higher wavelength than incident radiation (modified radiation).

The change in wavelength is called Compton shift.

This phenomenon is called Compton Effect.

Diagram



Theory

Before Collision

λ – Wave length of incident wave
ν – Frequency of incident wave
$\frac{h\nu}{c}$ – Momentum of incident wave
$h\nu$ – Energy of incident wave
m_0c^2 – Rest mass energy
m_0 – Rest mass of electron
c – Velocity of light

After collision

λ' – Wave length of scattered wave
ν' – Frequency of scattered wave
$\frac{h\nu'}{c}$ – Momentum of scattered wave
$h\nu'$ – Energy of scattered wave
mc^2 – Energy of recoil electron
mv – Momentum of recoil electron
$\frac{h\nu'}{c}\cos\theta$ – Momentum of scattered wave along x-axis
$\frac{h\nu'}{c}\sin\theta$ – Momentum of scattered wave along y-axis
$mv\cos\phi$ – Momentum of recoil electron along x-axis
$-mv\sin\phi$ – Momentum of recoil electron along y-axis

According to conservation law of energy

Energy before collision = Energy after collision

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

According to conservation law of momentum

Momentum before collision = Momentum after collision

x – axis

$$\frac{h\nu}{c} = \frac{h\nu'}{c}\cos\theta + mv\cos\phi$$
$$mv\cos\phi = \frac{h\nu}{c} - \frac{h\nu'}{c}\cos\theta$$
$$= \frac{h}{c}(\nu - \nu'\cos\theta)$$
$$\boldsymbol{mvc\cos\phi = h(\nu - \nu'\cos\theta)} \qquad \text{--------------- (2)}$$

y – axis

$$0 = \frac{hv'}{c}\sin\theta - mv\,sin\phi$$

$$\frac{hv'\sin\theta - mvc\sin\phi}{c} = 0$$

$$hv'\sin\theta - mvc\sin\phi = 0$$

$$hv'\sin\theta = mvc\sin\phi \Rightarrow mvc\sin\phi = \boldsymbol{hv'sin\theta} \quad \text{------------- (3)}$$

Squaring (2) & (3) and adding

$$(mvc\,cos\phi)^2 + (mvc\sin\phi)^2 = h^2 (v - v'\cos\theta)^2 + h^2v'^2 sin^2\theta$$

$$m^2v^2c^2 cos^2\phi + m^2v^2c^2 sin^2\phi = h^2 (v^2 - 2vv'cos\,\theta + v'^2cos^2\theta) + h^2v'^2sin^2\theta$$

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

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

$$\boldsymbol{m^2v^2c^2 = h^2 (v^2 - 2vv'\cos\theta + v'^2)} \quad \text{-------------- (4)}$$

Squaring (1) on both sides

$$m^2 c^4 = [h (v - v') + m_0c^2]^2$$

$$m^2c^4 = h^2 (v - v')^2 + 2h (v - v') m^0c^2 + m^0c^4$$

$$\boldsymbol{m^2 c^4 = h^2 (v^2 - 2v\,v' + v'^2) + 2h (v - v') m_0 c^2 + m_0 c^4} \quad \text{--------------- (5)}$$

(5) – (4)

$$m^2 c^4 - m^2v^2c^2 = h^2 (v^2 - 2v\,v' + v'^2) + 2h (v - v') m_0 c^2 + m_0 c^4 - h^2 (v^2 - 2vv'\cos\theta + v'^2)$$

$$m^2c^2 (c^2 - v^2) = h^2 v^2 - 2 h^2 v\,v' + h^2 v'^2 + 2h (v - v') m_0 c^2 + m_0 c^4 - h^2 v^2 + 2 h^2vv'\cos\theta - h^2v'^2)$$

$$m^2c^2 (c^2 - v^2) = - 2 h^2 v\,v' + 2h (v - v') m_0 c^2 + m_0 c^4 + 2 h^2vv'\cos\theta$$

$$\boldsymbol{m^2c^2 (c^2 - v^2) = -2h^2 v\,v' (1 - \cos\theta) + 2h (v - v') m_0c^2 + m_0^2c^4} \quad \text{-------------- (6)}$$

From theory of relativity, $\boldsymbol{m^2c^2 (c^2 - v^2) = m_0^2c^4}$ ------------- (7)

Sub. (7) in (6)

$$m_0^2c^4 = -2h^2 v\,v' (1 - \cos\theta) + 2h (v - v') m_0c^2 + m_0^2c^4$$

$$2h^2 v\,v' (1 - \cos\theta) = 2h (v - v') m_0c^2$$

$$h\,v\,v' (1 - \cos\theta) = (v - v') m_0c^2$$

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

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

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

X by 'c' on both sides

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

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

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

$$\Delta\lambda = \frac{h}{m_0 c}(1-\cos\theta) \qquad \text{---------------} \ (8)$$

(8) represents the expression for shift in wavelength.

Special cases:

Case :1 When $\theta = 0^o$

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

$$\Delta\lambda = \frac{h}{m_0 c}(1-\cos 0^0) \Rightarrow \frac{h}{m_0 c}(1-1)$$

$$\Delta\lambda = \mathbf{0}$$

Case :2 When $\theta = 90^o$

$$\Delta\lambda = \frac{h}{m_0 c}(1-\cos 90^0)$$

$$\Delta\lambda = \frac{h}{m_0 c}(1-0) \Rightarrow \frac{h}{m_0 c}$$

$$\Delta\lambda = \mathbf{0.0243\ \mathring{A}}$$

This is known as Compton wavelength.

Case :3 When $\theta = 180^o$

$$\Delta\lambda = \frac{h}{m_0 c}(1-\cos 180^0)$$

$$\Delta\lambda = \frac{h}{m_0 c}[1-(-1)] \Rightarrow \frac{2h}{m_0 c}$$

$$\Delta\lambda = \mathbf{0.0485\ \mathring{A}}$$

The change in wavelength is maximum at $\theta = 180^o$.

4. Explain the experimental verification of Compton Effect.

Compton Effect

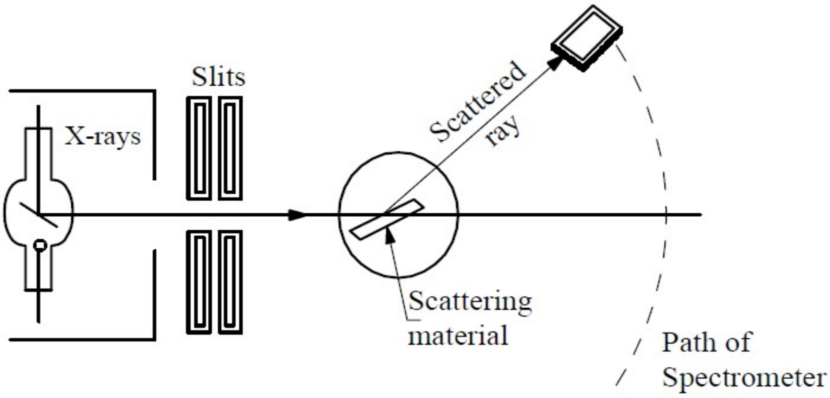
When a beam of high frequency radiation (x – rays or γ – rays) is scattered by a fine scatterer, the scattered beam contains two components.

(i) One component has the same wavelength as incident radiation (unmodified radiation)

(ii) The other component has slightly higher wavelength than incident radiation (modified radiation).

The change in wavelength is called Compton shift.
This phenomenon is called Compton Effect.

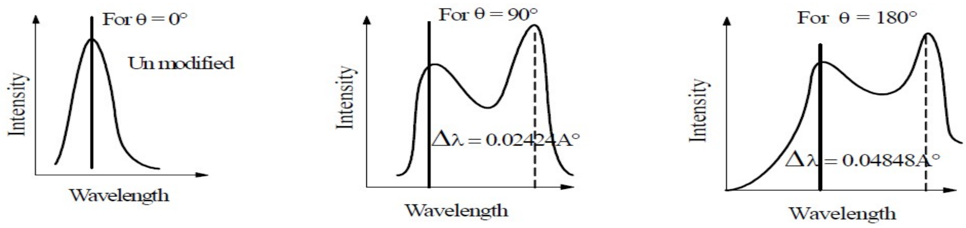
Construction



1. It consists of X-ray tube for producing X-rays.
2. A small scattering substance (carbon) is mounted on a table.
3. A Bragg spectrometer is used to receive scattered X-rays.
4. The slits are used to focus the X-rays towards the scattering substance.

Working

1. A beam of monochromatic X-rays is made to fall on the scattering element.
2. The scattering element scatters the X-rays.
3. The scattered X-rays are received by the Bragg spectrometer.
   λ – Wavelength of incident X-rays
   λ' – Wavelength of scattered X-rays
4. The experiment is repeated for various angles and the graph is plotted for the results.
5. In the graph, two peaks are observed,
   Peak 'A' – Unmodified radiation
   Peak 'B' – Modified radiation

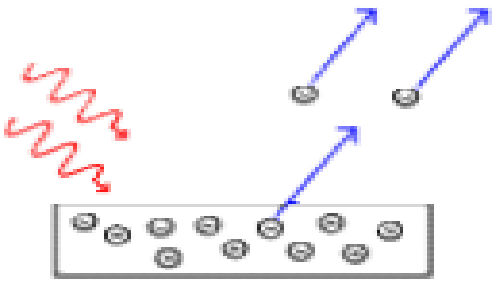


6. The difference between two peaks is called Compton Shift.

5. What is Photo electric effect? Deuce Einstein's equation for the same.

Photo electric Effect

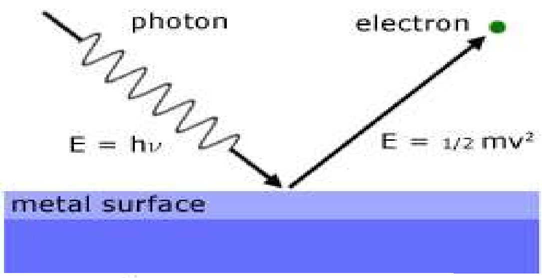
Electromagnetic radiation is made of a series of particles called photons. When a photon hits an electron on a metal surface, the electron can be emitted. The emitted electrons are called photoelectrons. The effect is called Photoelectric Effect.

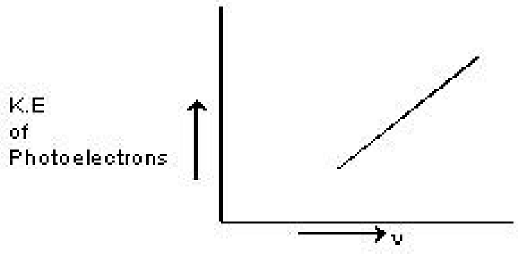


- The photoelectric effect explained the quantum nature of light and electrons.
- The concept of wave–particle duality was developed because of the photoelectric effect.
- Albert Einstein proposed the Laws of Photoelectric Effect and Won the Nobel Prize for Physics, 1921.

Einstein's equation:

- Light must have stream of energy particles or quanta of energy (hv).
- Suppose, the threshold frequency of light required ejecting electrons from a metal is n_0, when a photon of light of this frequency strikes a metal it imparts its entire energy (hv_0) to the electron.





"This energy enables the electron to break away from the atom by overcoming the attractive influence of the nucleus". Thus each photon can eject one electron. If the frequency of light is less than v_0 there is no ejection of electron. If the frequency of light is higher than v0 (let it be v), the photon of this light having higher energy (hv), will impart some energy to the electron that is needed to remove it from the atom. The excess energy would give a certain velocity (i.e, kinetic energy) to the electron.

$hv = hv_0 + K.E$

$hv = hv_0 + \frac{1}{2} mv^2$

$\frac{1}{2} mv^2 = hv - hv_o$

Where, v = frequency of the incident light

v_0 = threshold frequency

hv_0 is the threshold energy (or) the work function denoted by $\Phi = hv_0$ (minimum energy of the photon to liberate electron). It is constant for particular metal and is also equal to the ionization potential of gaseous atoms.

The kinetic energy of the photoelectrons increases linearly with the frequency of incident light. Thus, if the energy of the ejected electrons is plotted as a function of frequency, it result in a straight line whose slope is equal to Planck's constant 'h' and whose intercept is hn_0.

6. **Derive the expression for de Broglie wavelength.**

From the theory of light, considering a photon as a particle the total energy of the photon is given by

$$E=mc^2 \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots 1$$

Where m is the mass of the particle and c is the velocity of light

Considering the photon as a wave, the total energy is given by

$$E = h\nu \text{ --------------------------}2$$

Where h is the Planck's constant, ν is the frequency of the radiation.

From equations (1) and (2)

$$E = mc^2 = h\nu \text{ -----------------}3$$

We know Momentum = Mass × velocity, $p = mc$, $h\nu = pc$

$$\frac{h}{p} = \frac{c}{\nu} = \lambda \ldots\ldots\ldots\ldots\ldots 4$$

De-Broglie suggested that the equation 4 can be applied both for photons and material particles. If m is the mass of the particle and v is the velocity the particle, then

Momentum $p = mv$

De-Broglie wavelwngth, $\lambda = \frac{h}{mv}$ ---------5

This is expression for wavelength of matter waves.

De-Broglie wavelength in terms of energy

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

Multiply by m on both sides, $2mE = m^2v^2$--------6

Subs. eqn. 6 in 5 we get, $\lambda = \frac{h}{\sqrt{2mE}}$ -----------7

De-Broglie wavelength in terms of voltage

If an electron of charge e is accelerated by a potential difference of V volts, then the electron gains a velocity v and hence, Work done on the electron = eV-----------8

Kinetic energy of electron = $\frac{1}{2}mv^2$--------9

$\frac{1}{2}mv^2$= eV ,mv^2= 2eV, m^2v^2=2meV------10

Subs. eqn 10 in eqn 5 we get, $\lambda = \frac{h}{\sqrt{2meV}}$ -------11

De-Broglie wavelength in terms of temperature

According to M.B statistics, an electron is considered as gas.

Kinetic energy of electron gas = $\frac{3}{2}kT$----------12

Kinetic energy of electron, $= \frac{1}{2}mv^2$-----------13

$\frac{1}{2}mv^2 = \frac{3}{2}kT$, mv^2=3kT, m^2v^2=3mkT---------14

Subs. eqn 14 in eqn 5 we get, $\lambda = \frac{h}{\sqrt{3mkT}}$ ------15

7. Deduce Schrodinger time dependent wave equation.

A particle can behave as a wave only under motion. In order to achieve a wave motion, the particle should be accelerated by a potential field.

E – Total energy of the particle
V – Potential energy of the particle
$\frac{1}{2}mv^2$ – Kinetic energy of the particle
m – Mass of the particle
v – Velocity of the particle
p – Momentum of the particle $(p = mv)$
x – Position of the particle at time *'t'*.

Total energy = Potential energy + Kinetic energy

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

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

$$E = V + \frac{1}{2m}(mv)^2$$

$$E = V + \frac{1}{2m}(p)^2 \qquad [mv = p]$$

$$E = V + \frac{p^2}{2m}$$

x by ψ on both sides

$$E\psi = V\psi + \frac{p^2}{2m}\psi \quad \text{---------------} (1)$$

Time dependent wave function

$$\psi = Ae^{-\frac{i}{\hbar}(Et-px)} \quad \text{------------------} (2)$$

Differentiate (2) w.r.to 'x'

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

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

Again differentiate w.r.to 'x'

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

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

$$\frac{\partial^2\psi}{\partial x^2} = -Ae^{-\frac{i}{\hbar}(Et-px)}\frac{p^2}{\hbar^2} \quad \text{---------------} (3) \qquad [\because i^2 = -1]$$

Sub. (2) in (3)

$$\frac{\partial^2\psi}{\partial x^2} = -\frac{p^2}{\hbar^2}\psi$$

$$p\psi = -\hbar\frac{\partial^2\psi}{\partial x^2} \quad \text{---------------} (4)$$

Differentiate (2) w.t. 't'

$$\frac{\partial\psi}{\partial t} = Ae^{-\frac{i}{\hbar}(Et-px)}\left(-\frac{i}{\hbar}E\right) \quad \text{---------------} (5)$$

Sub. (2) in (5)

$$\frac{\partial\psi}{\partial t} = -\frac{i}{\hbar}E\psi$$

$$E\psi = -\frac{\hbar}{i}\frac{\partial\psi}{\partial t}$$

$$E\psi = -\frac{i\hbar}{i^2}\frac{\partial \psi}{\partial t}$$

$$E\psi = i\hbar\frac{\partial \psi}{\partial t} \quad \text{---------------- (6)}$$

Sub. (4) & (5) in (1)

$$i\hbar\frac{\partial \psi}{\partial t} = V\psi - \frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} \quad \text{--------------- (7)}$$

$$i\hbar\frac{\partial \psi}{\partial t} = \left[V - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right]\psi \quad \text{--------------- (8)}$$

In 3 – dimensional

$$i\hbar\frac{\partial \psi}{\partial t} = \left[V - \frac{\hbar^2}{2m}\nabla^2\right]\psi \quad \text{--------------- (9)}$$

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

(9) can be written as

$$E\psi = H\psi \quad \text{--------------- (10)}$$

(7), (8), (9) & (10) are known as Schroedinger time dependent equation.

8. Derive Schrodinger independent wave equation.

In Schrodinger time independent wave equation, the wave function ψ does not depend on time.

Time dependent wave function

$$\psi = Ae^{-\frac{i}{\hbar}(Et-px)} \quad \text{------------- (1)}$$

$-\frac{iE}{\hbar}$ – Time dependent factor

$\frac{ip}{\hbar}$ – Time independent factor

$$\psi = Ae^{-\frac{iEt}{\hbar}}e^{\frac{ipx}{\hbar}} \quad \text{-------------- (2)}$$

Put $\psi_0 = e^{\frac{ipx}{\hbar}}$

(2) becomes $\psi = A\psi_0 e^{-\frac{iEt}{\hbar}}$ --------------- (3)

Differentiate (3) w.r.to '*x*'

$$\frac{\partial \psi}{\partial x} = Ae^{-\frac{iEt}{\hbar}}\frac{\partial \psi_0}{\partial x}$$

Again differentiating w.r.to *'x'*

$$\frac{\partial^2 \psi}{\partial x^2} = A e^{-\frac{iEt}{\hbar}} \frac{\partial^2 \psi_0}{\partial x^2} \quad \text{------------- (4)}$$

Differentiate (3) w.r.to *'t'*

$$\frac{\partial \psi}{\partial t} = A \psi_0 e^{-\frac{iEt}{\hbar}} \left(-\frac{iE}{\hbar} \right) \quad \text{------------- (5)}$$

Sub. (3), (4) & (5) in Scroedinger time dependent wave equation

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

$$i\hbar \left[A \psi_0 e^{-\frac{iEt}{\hbar}} \left(-\frac{iE}{\hbar} \right) \right] = V \left[A \psi_0 e^{-\frac{iEt}{\hbar}} \right] - \frac{\hbar^2}{2m} \left[A e^{-\frac{iEt}{\hbar}} \frac{\partial^2 \psi_0}{\partial x^2} \right]$$

$$i\hbar A e^{-\frac{iEt}{\hbar}} \left[\psi_0 \left(-\frac{iE}{\hbar} \right) \right] = A e^{-\frac{iEt}{\hbar}} \left[V [\psi_0] - \frac{\hbar^2}{2m} \left[\frac{\partial^2 \psi_0}{\partial x^2} \right] \right]$$

$$-\frac{i^2 \hbar \psi_0 E}{\hbar} = V [\psi_0] - \frac{\hbar^2}{2m} \left[\frac{\partial^2 \psi_0}{\partial x^2} \right]$$

$$E \psi_0 = V \psi_0 - \frac{\hbar^2}{2m} \left[\frac{\partial^2 \psi_0}{\partial x^2} \right]$$

$$E \psi_0 - V \psi_0 = -\frac{\hbar^2}{2m} \left[\frac{\partial^2 \psi_0}{\partial x^2} \right]$$

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

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

$$\frac{\partial^2 \psi_0}{\partial x^2} + \frac{2m}{\hbar^2} (E - V) \psi_0 = 0 \quad \text{--------------- (6)}$$

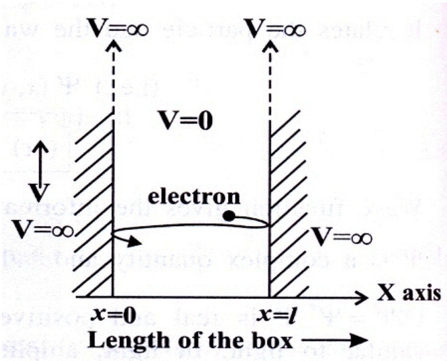
In 3 – dimensional

$$\nabla^2 \psi_0 + \frac{2m}{\hbar^2} (E - V) \psi_0 = 0 \quad \text{---------------- (7)}$$

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

(6) & (7) are known as Schroedinger time independent wave equation.

9. Solve Schroedinger wave equation for a particle in a box and obtain the energy eigen values.



- Consider a one dimensional potential box.
- A particle is moving inside the box.
- *m* – Mass of the particle.
- The walls of the box have infinite height.
- Hence the particle cannot come out from the box.
- *l* – Length of the box.
- Potential energy inside the box is zero.
- Potential energy outside the box and on the wall is infinity.

Boundary conditions

V (x) = 0   *when 0<x<l*

V(x) = ∞   *when 0>x>l*

To find the wave function

Schroedinger time independent wave equation

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

Inside the box potential energy V= 0

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

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

where $k^2 = \frac{2mE}{\hbar^2}$ -------------- (2)

The solution of (1) is

$$\psi(x) = A \sin kx + B \cos kx \quad \text{-------------- (3)}$$

A & B – Constants

Boundary condition (i), at $x=0$, $\psi(x) = 0$

(3) becomes, $0 = A \sin 0 + B \cos 0$

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

$$B = 0$$

Boundary condition (ii), at $x = l$, $\psi(x) = 0$

(3) becomes, $0 = A \sin kl + B \cos kl$

$$0 = A \sin kl \qquad (B = 0)$$

$$A \neq 0, \sin kl = 0$$

$$\sin n\pi = 0$$

Comparing above two equations,

$$kl = n\pi$$

$$k = \frac{n\pi}{l} \quad \text{------------ (4)}$$

Sub. the value of B & k in (3),

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

(5) is the expression for wave function (or) eigen function of the particle.

To find the eigen value

From (2), $$k^2 = \frac{2mE}{\hbar^2}$$

$$k^2 = \frac{2mE}{\frac{h^2}{4\pi^2}}$$

[$\because \hbar = \frac{h}{2\pi} \Rightarrow \hbar^2 = \frac{h^2}{4\pi^2}$]

$$k^2 = \frac{8\pi^2 mE}{h^2} \quad \text{-------------- (6)}$$

Squaring (4)

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

Compare (6) & (7)

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

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

$$E_n = \frac{n^2 h^2}{8ml^2} \qquad \text{---------------- } \mathbf{(8)}$$

(5) is the expression for energy (or) eigen value of the particle.

By applying the normalization condition, the value of constant $A = \sqrt{\frac{2}{l}}$.

Sub. in (5), $$\psi_n(x) = \sqrt{\frac{2}{l}} \sin \frac{n\pi x}{l} \qquad \text{---------------- (9)}$$

(9) is the expression for wave function of the particle.