QUANTUM PHYSICS

Black body:

A perfect black body is one which absorbs all the radiation of heat falling on it and emits all the radiation when heated in an isothermal enclosure.

The heat radiation emitted by the black body is called black body radiation.

Laws of Black body radiation:

Wien's displacement law:

This law states that the product of the maximum wavelength (λ_m) corresponding to the maximum energy and the absolute temperature is a constant.

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

$$\lambda_m = \frac{\text{constant}}{T}$$

$$\lambda_m \propto \frac{1}{T}$$

i.e. when the temperature increases the wavelength corresponding to the maximum energy decreases.

Wien's radiation law:

The maximum energy radiated at peak wavelength is directly proportional to the fifth power of the absolute temperature (T^5).

i.e.

$$E_\lambda \propto T^5$$

$$E_\lambda = \text{Constant}\, T^5$$

The energy density is derived as

$$\boldsymbol{E_n = 8\pi hc\lambda^{-5}\, e^{\frac{-hc}{\lambda kT}}.}$$

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

, Where C_1 and C_2 are constants.

$$C_1 = 8\pi hc \text{ , and } C_2 = \frac{hc}{k}.$$

Limitation: This law holds well only for the short wavelength and not for the longer wavelength.

Raleigh – Jean's Law:

This law states that the energy distribution is directly proportional to absolute temperature (T) and inversely proportional to the fourth power of wavelength (λ^4).

i.e. $E_\lambda \propto \frac{T}{\lambda^4}$

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

Limitation: This law holds well only for the longer wavelength and not for the shorter wavelength.

Planck's quantum theory of black body radiation:

Planck's theory:

1. A black body contains a large number of oscillating particles:
2. Each particle is vibrating with a characteristic frequency.
3. The frequency of radiation emitted by the oscillator is the same as the oscillator frequency.
4. The oscillator can absorb energy in multiples of small unit called quantum.
5. This quantum of radiation is called photon.
6. The energy of a photon is directly proportional to the frequency of radiation emitted. $E \propto \nu$ or $E = h\nu$
7. An oscillator vibrating with frequency can only emit energy in integral multiples of $h\nu$. $E_n = nh\nu$, where n= 1, 2, 3, 4…….n. n is called quantum number.

Planck' law of radiation:

The energy density of radiations emitted by a black body at a temperature T in the wavelength range λ to $\lambda + d\lambda$ is given by

$$E_\lambda d\lambda = \frac{8\pi hC}{\lambda^5 \left(e^{\frac{h\nu}{kT}} - 1\right)} d\lambda$$

$h = 6.625\times10^{-34}Js^{-1}$ - Planck's constant.

$C = 3\times10^{8}$ ms-1 -velocity of light

K = 1.38x 10-23 J/K -Blotzmann constant

T is the absolute temperature in kelvin.

Derivation of Planck's law:

- Consider a black body with a large number of atomic oscillators.
- Average energy per oscillator is

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

- E is the total energy of all the oscillators and N is the number of oscillators.
- Let the number of oscillators in ground state is be N_0.
- According to Maxwell's law of distribution, the number of oscillators having an energy value E_N is givenby

$$N_n = N_0 e^{-\frac{E_n}{kT}} ------(2)$$

- T is the absolute temperature. K is the Boltzmann constant.
- Let N_0 be the number of oscillators having energy E_0,
  - N_1 be the number of oscillators having energy E_1,
  - N_2 be the number of oscillators having energy E_2 and so on.
- Then

$$N = N_0 + N_1 + N_1 + \cdots .. ------- (3)$$

$$N = N_0 e^{-\frac{E_0}{kT}} + N_0 e^{-\frac{E_1}{kT}} + N_0 e^{-\frac{E_2}{kT}} + \cdots .. ------ (4)$$

- From Planck's theory, E can take only integral values of hν.
- Hence the possible energy are 0, hν, 2hν,3 hν……. and so on.
- $i.e. E_n = nh\nu, where\ n = 0,1,2,3$

  $E_0 = 0,\ E_1 = h\nu,\ E_2 = 2h\nu,\ E_3 = 3h\nu$, and so on.

$$N = N_0 e^0 + N_0 e^{-\frac{h\nu}{kT}} + N_0 e^{-\frac{2h\nu}{kT}} + N_0 e^{-\frac{3h\nu}{kT}} \ldots ..$$

- $N = N_0 + N_0 e^{-\frac{h\nu}{kT}} + N_0 e^{-\frac{2h\nu}{kT}} + N_0 e^{-\frac{3h\nu}{kT}} \ldots..(5)$

Putting

$$x = e^{-\frac{h\nu}{kT}} \; in \; (5)$$

$$N = N_0 + N_0 x + N_0 x^2 + N_0 x^3 \ldots..(6)$$

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

$N = \frac{N_0}{(1-x)} \ldots\ldots\ldots\ldots 7)$ (using Binomial expansion)

- The total energy

$$\mathrm{E = E_0\ N_0 + E_1\ N_1 + E_2\ N_2 + E_3\ N_3} \ldots (8)$$

- Substituting the value for $E_0\ E_1\ E_2\ E_3\ \ etc$ and

$$\boldsymbol{N_0 + N_1 + N_2 \ldots\ldots in\ (7)}$$

$$\boldsymbol{E = 0XN_0 + h\nu N_0 e^{-\frac{h\nu}{kT}} + 2h\nu N_0 e^{-\frac{2h\nu}{kT}} + 3h\nu N_0 e^{-\frac{3h\nu}{kT}} \ldots. +}$$

$$\boldsymbol{E = h\nu\ N_0 e^{-\frac{h\nu}{kT}} + 2h\nu\ N_0 e^{-\frac{2h\nu}{kT}} + \cdots. \pm ------ (9)}$$

- Putting $\boldsymbol{x = e^{-\frac{h\nu}{kT}}\ in\ (8)}$

$$\boldsymbol{E = h\nu\ N_0 x + 2h\nu\ N_0 x^2 + \cdots. \pm --- (10)}$$

$$\boldsymbol{E = h\nu N_0[x + 2x^2 + \ \ldots +]}$$

$$\boldsymbol{E = h\nu N_0 x[1 + 2x + \ \ldots +]}$$

$$\boldsymbol{E = \frac{h\nu\ N_0 x}{(1-x)^2} ------ (11)}$$

$$\boldsymbol{Since\ \left\{\frac{1}{(1-x)^2} = (1-x)^{-2} = 1 + 2x + \cdots\right\}}$$

- Substituting (11) and (7) in (1)

$$\overline{E} = \frac{\left(\frac{h\nu N_0 x}{(1-x)^2}\right)}{\frac{N_0}{(1-x)}}$$

$$\overline{E} = \frac{h\nu x}{(1-x)}$$

$$\overline{E} = \frac{h\nu x}{x\left(\frac{1}{x}-1\right)}$$

$$\overline{E} = \frac{h\nu}{\left(\frac{1}{x}-1\right)}$$

- Substituting the value for x

$$\overline{E} = \frac{h\nu}{\left(\frac{1}{e^{-\frac{h\nu}{kT}}}-1\right)}$$

$$\overline{E} = \frac{h\nu}{\left(e^{\frac{h\nu}{kT}}-1\right)} ----(12)$$

- The number of oscillators per unit volume in the wavelength range λ and λ+dλ is given by

$$\frac{8\pi d\lambda}{\lambda^4} --------(13)$$

- Hence the energy density of radiation between the wavelength range λ and λ+dλ is $E_\lambda d\lambda$= No. of oscillator per unit volume in the range λ and λ+dλ X Average energy.

$$E_\lambda d\lambda = \frac{8\pi d\lambda}{\lambda^4} X \frac{h\nu}{\left(e^{\frac{h\nu}{kT}} - 1\right)} - - - - (1)$$

$$E_\lambda d\lambda = \frac{8\pi d\lambda}{\lambda^4} \frac{hC/_\lambda}{\left(e^{\frac{h\nu}{kT}} - 1\right)}$$

$$E_\lambda d\lambda = \frac{8\pi d\lambda}{\lambda^5} \frac{hC}{\left(e^{\frac{h\nu}{kT}} - 1\right)}$$

$$E_\lambda d\lambda = \frac{8\pi d\lambda}{\lambda^5} \frac{hC}{\left(e^{\frac{h\nu}{kT}} - 1\right)}$$

$$E_\lambda d\lambda = \frac{8\pi hC}{\lambda^5} \frac{1}{\left(e^{\frac{h\nu}{kT}} - 1\right)} d\lambda - - - - - (15)$$

$$E_\lambda = \frac{8\pi hC}{\lambda^5} \frac{1}{\left(e^{\frac{h\nu}{kT}} - 1\right)} - - - - - - - - 16$$

- The equation (16) represents Planck's law of radiation.
- Planck's law can also be represented in terms of frequencies.

$$E_\nu d\nu = \frac{8\pi h\nu^3}{C^3} \frac{1}{\left(e^{\frac{h\nu}{kT}} - 1\right)} d\nu - - - - - - - - 17$$

Deductions of Radiation laws from Planck's Law:

I. Wien's Law:

1) Wien's law holds good when wavelength λ is small.(ν is large)
2) Therefore $\frac{h\nu}{kT} > 1$ and $e^{\frac{h\nu}{kT}}$ is very large compared to 1.
3) Neglecting 1 in equation (16)

$$E_\lambda = \frac{8\pi hC}{\lambda^5} \frac{1}{e^{\frac{h\nu}{kT}}} ----(18)$$

4) Equation (18) represents Wien's law.
5) Thus Planck's law reduces to Wien's law at shorter wavelength.

II. Raleigh- Jean's law:

1) Raleigh- jean's law holds good when wavelength λ is large.(ν is small).
2) Therefore $\frac{h\nu}{kT} < 1$ and expanding $e^{\frac{h\nu}{kT}}$ we get **(1+$\frac{h\nu}{kT}$)**
3) Substituting in (16)

$$E_\lambda = \frac{8\pi hC}{\lambda^5} \frac{1}{\left(1 + \frac{h\nu}{kT} - 1\right)}$$

$$E_\lambda = \frac{8\pi hC}{\lambda^5} \frac{1}{\frac{h\nu}{kT}}$$

=

$$= \frac{8\pi kThC}{\lambda^5} \frac{1}{h\nu}$$

=

$$= \frac{8\pi kThC}{\lambda^5} \frac{1}{hC/\lambda}$$

=

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

4) Thus Planck's law reduces to Raleigh- jean's law at longer wavelength.

Scattering of X-Rays:

Two Kinds:

1. Coherent scattering or classical scattering or Thomson scattering
2. Incoherent scattering or Compton scattering

Coherent scattering:

1. X rays are scattered without any change in wavelength.
2. Obeys classical electromagnetic theory

Compton scattering:

1. Scattered beam consists of two wavelengths.
2. One is having same wavelength as the incident beam
3. The other is having a slightly longer wavelength called modified beam.

Compton scattering:

QUANTUM PHYSICS

1. When a beam of high frequency radiation is scattered by a substance of low atomic number the scattered radiations consists of two lines.
2. One is having the same wavelength λ as the incident beam
3. The other is having slightly longer wavelength.
4. This change in wavelength of the scattered X rays is known as the Compton shift.
5. This effect is called Compton Effect.

Theory of Compton Effect:

1. Compton treated this scattering as the interaction between X ray and the matter as a particle collision between X ray photon and loosely bound electron in the matter.
2. Consider an X ray photon of frequency ν striking an electron at rest.
3. This Photon is scattered through an angle θ to x-axis.
4. Let the frequency of the scattered photon be ν'.
5. During collision the photon gives energy to the electron.
6. This electron moves with a velocity V at an angle ϕ to x axis.
7. <u>Total energy before collision</u>:

   Energy of the incident photon $= \mathbf{h\nu}$

   Energy of the electron at rest = $= \boldsymbol{m_0 C^2}$ where m_0 is the rest mass of electron and C the velocity of light.

   Therefore total energy before collision = $= \boldsymbol{h\nu + m_0 C^2}$

   <u>Total energy after collision:</u>

   Final energy of the photon= $= \mathbf{h\nu'}$

   Final energy of the scattered photon = mC^2, where m is the mass of electron and C the velocity of light.

   Therefore total energy after collision = $h\nu' + mC^2$

   By the law of conservation of energy,

   Total energy before collision = Total energy after collision

   i.e. $\boldsymbol{h\nu + m_0 C^2 = h\nu' + mC^2}$

   $$mC^2 = h\nu - h\nu' + mC_0^2$$

   $$\boldsymbol{mC^2 = h(\nu - \nu') + m_0 C^2 ----(1)}$$

8. Total momentum along X axis before collision:

   Initial momentum of photon along x axis = $= \frac{h\nu}{c}$

   Initial momentum of electron along x axis = 0

   Total momentum before collision along x axis= $= \frac{h\nu}{c}$

9. Total momentum along x axis after collision:

   The momentum is resolved along x axis and y axis.

   Final momentum of momentum along x axis $= \frac{h\nu'}{c} cos\theta$

   Final momentum of electron along x axis = $= mVcos\phi$

   Total final momentum along s axis = $= \frac{h\nu'}{c} cos\theta + mVcos\phi$

   Applying the law of conservation of momentum,

   Momentum before collision = momentum after collision

$$\frac{h\nu}{C} = \frac{h\nu'}{C} cos\theta + mvcos\phi \ldots \ldots .2)$$

$$\frac{h\nu}{C} - \frac{h\nu'}{C} cos\theta = mvcos\phi$$

$$\frac{h}{C}(\nu - \nu' cos\theta) = mvcos\phi$$

$$h(\nu - \nu' cos\theta) = mvCcos\phi$$

$$mvCcos\phi = h(\nu - \nu' cos\theta) \ldots \ldots \ldots .3)$$

10. Total momentum along y axis before collision:

    Initial momentum of photon along y axis = 0

    Initial momentum of electron along y axis = 0

    Total momentum before collision along y axis= 0

11. Total momentum along y axis after collision:

    Final momentum of photon along y axis = $= \frac{h\nu'}{c} sin\theta$

Final momentum of electron along y axis == $-\boldsymbol{mvsin\phi}$ (along the negative Y direction)

Total momentum after collision along y axis= $= \frac{\boldsymbol{h\nu'}}{\boldsymbol{C}}\boldsymbol{sin\theta - mvsin\phi}$

Applying the law of conservation of momentum,

Momentum before collision = momentum after collision

$$\boldsymbol{0 = \frac{h\nu'}{C} sin\theta - mvsin\phi}$$

$$\boldsymbol{mvCsin\phi = h\nu' sin\theta \ldots\ldots(4)}$$

Squaring (3) and (4) and adding,

$$\boldsymbol{m^2v^2C^2cos^2\phi + m^2v^2C^2sin^2\phi}$$
$$\boldsymbol{= h^2(\nu - \nu' cos\theta)^2 + h^2\nu'^2 sin^2\theta \ldots\ldots(5)}$$

LHS of the equation is: $= \boldsymbol{m^2v^2C^2cos^2\phi + m^2v^2C^2sin^2\phi}$

$$\boldsymbol{= m^2v^2C^2(sin^2\phi + cos^2\phi)}$$

$= m^2v^2C^2$ since $(sin^2\phi + cos^2\phi) = 1$

$$h^2(\nu - \nu' cos\theta)^2 + h^2\nu'^2 sin^2\theta$$

RHS of the equation: =

$$h^2(\nu - \nu' cos\theta)^2 + h^2\nu'^2 sin^2\theta$$
$$= h^2(\nu^2 - 2\nu\nu' cos\theta + \nu'^2 cos^2\theta) + h^2\nu'^2 sin^2\theta$$
$$h^2(\nu^2 - 2\nu\nu' cos\theta + \nu'^2 cos^2\theta + \nu'^2 sin^2\theta)$$
$$h^2(\nu^2 - 2\nu\nu' cos\theta + \nu'^2)$$

Equating LHS and RHS,

$$m^2v^2C^2 = h^2(\nu^2 - 2\nu\nu' cos\theta + \nu'^2) ----(6)$$

Squaring (1) ,

$$m^2C^4 = (h(\nu - \nu') + mC_0^2)^2 ----(7)$$
$$m^2C^4 = (h^2(\nu - \nu')^2 + 2h(\nu - \nu')m_0 C^2 + m_0^2C^4)$$

$$m^2C^4 = \left(h^2(\nu^2 - 2\nu\nu' c + \nu'^2) + 2h(\nu - \nu')m_0 C^2 + m_0^2C^4\right) — (8)$$

(8)-(6)

$$m^2C^4 - m^2v^2C^2$$
$$= h^2\left(\nu^2 - 2\nu\nu' cos\theta + \nu'^2\right) + 2h(\nu - \nu')m_0\, C^2 + m_0^2C^4$$
$$- \; h^2\left(\nu^2 - 2\nu\nu' cos\theta + \nu'^2\right)$$
$$m^2C^4 - m^2V^2C^2 = -2h^2\,\nu\nu' + 2h^2\,\nu\nu' cos\theta + 2h(\nu - \nu')m_0\, C^2 + m_0^2C^4$$
$$m^2C^2(C^2 - v^2) = -2h^2\,\nu\nu'(1 - cos\theta) + 2h(\nu - \nu')m_0\, C^2 + m_0^2C^4 - - - (9)$$

From the theory the variation of mass with velocity is given by

$$m = \frac{m_0}{\sqrt{1 - \frac{v^2}{C^2}}} - -(10)$$

Squaring (10)

$$m^2 = \frac{{m_0}^2}{1 - \frac{v^2}{C^2}} = \frac{{m_0}^2}{\frac{C^2 - v^2}{C^2}} = \frac{{m_0}^2C^2}{C^2 - v^2}$$
$$i.e.\, m^2(C^2 - v^2) = {m_0}^2C^2$$

Multiplying on both sides by C^2

$$m^2C^2(C^2 - v^2) = {m_0}^2C^4 - - - (11)$$

Substituting in (10)

$${m_0}^2C^4 = -2h^2\,\nu\nu'(1 - cos\theta) + 2h(\nu - \nu')m_0\, C^2 + m_0^2C^4$$
$$2h^2\,\nu\nu'(1 - cos\theta) = 2h(\nu - \nu')m_0\, C^2$$
$$\frac{(\nu - \nu')}{(\nu\nu')} = \frac{h}{m_0\, C^2}(1 - cos\theta)$$
$$\frac{\nu}{\nu\nu'} - \frac{\nu\,'}{\nu\nu'} = \frac{h}{m_0\, C^2}(1 - cos\theta)$$
$$\frac{1}{\nu'} - \frac{1}{\nu} = \frac{h}{m_0\, C^2}(1 - cos\theta)$$

Multiplying by C on both the sides,

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

Therefore the change in wavelength is given by

$$d\lambda -= \frac{h}{m_0\, C}(1 - cos\theta) - - - -12$$

- The change in wavelength dλ does not depend on the
  i. wavelength of the incident photon
  ii. Nature of the scattering material.
- It depends only on the scattering angle.

Case (1) When θ=0 then,

$$d\lambda -= \frac{h}{m_0\, C}(1 - 1\,) = 0$$

Case (2) When θ=0 then,

$$d\lambda -= \frac{h}{m_0\, C}(1 - 0) = \frac{h}{m_0\, C}$$

Substituting the values for h,m_0 and C

$$d\lambda -= \frac{h}{m_0\, C} = \frac{6.63x10^{-34}}{9.11x10^{-31}x3x10^{8}} = 0.0243\ A^0$$

Case(3) When θ=180 then, $d\lambda -= \frac{h}{m_0\, C}(1 - (-1)\,)$

$$d\lambda -= \frac{h}{m_0\, C}x2 = 0.485A^0$$

The change in wavelength is maximum at 180^0

Experimental verification of Compton Effect.

1. The experimental set up is as shown in the fig.
2. A beam of mono chromatic X ray beam is allowed to fall on the scattering material.
3. The scattered beam is received by a Bragg spectrometer.
4. The intensity of the scattered beam is measured for various angles of scattering.
5. A graph is plotted between the intensity and the wavelength.
6. Two peaks were found.
7. One belongs to unmodified and the other belongs to the modified beam.
8. The difference between the two peaks gives the shift in wavelength.

9. When the scattering angle is increased the shift also gets increased in accordance with

$$d\lambda - = \frac{h}{m_0\, C}(1 - cos\theta) - - - -12$$

10. The experimental values were found to be in god agreement with that found by the formula.

Matter WAVES:

De Broglie's Hypothesis:

1. Waves and particles are the modes of energy propagation.
2. Universe of composed of matter and radiations.
3. Since matter loves symmetry matter and waves must be symmetric.
4. If radiation like light which is a wave can act like particle some time, then materials like particles can also act like wave some time.

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De Broglie waves and wavelength:

- From Planck's theory $E = h\nu - - - -(1)$
- According to Einstein's theory, $E = mc^2 - - - (2)$

  Equation (1) and (2)

$$h\nu = mc^2 - - - (3)$$

-

$$\frac{hC}{\lambda} = mc^2$$

- Therefore

$$\lambda = \frac{hC}{mc^2}$$

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

$$\lambda = \frac{h}{p} = \frac{h}{mV} - - - - - - (4)$$

Where p is the momentum of the particle.

De Broglie wavelength in terms of energy

We know that Kinetic energy

$$E = \frac{1}{2}mv^2 - - - (5)$$

Multiplying by m on both sides

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

$$m^2v^2 = 2Em$$

$$\sqrt{m^2v^2} = \sqrt{2Em}$$

$$mv = \sqrt{2Em} - - - (6)$$

Substituting in (4)

$$\lambda == \frac{h}{\sqrt{2Em}} - - - - - - (7)$$

Schrodinger wave equation

QUANTUM PHYSICS

Schrodinger equation is basic equation of matter waves.

The two forms of the wave equation are:

1. Time independent wave equation
2. Time dependent wave equation

I. Schrodinger time independent equation:

- Consider a wave associated with a particle.
- Let x,y,z be the coordinates of the particle.
- Let ψbe the displacement for the de Broglie wave at any time,
- The 3D wave equation for wave motion is given by:

$$\frac{\partial^2\Psi}{\partial x^2}+\frac{\partial^2\Psi}{\partial y^2}+\frac{\partial^2\Psi}{\partial z^2}=\frac{1}{v^2}\frac{\partial^2\Psi}{\partial t}---(1)$$

- v is the velocity of the wave.
- Equation is rewritten as

$$\nabla^2\Psi=\frac{1}{V^2}\frac{\partial^2\Psi}{\partial t}---(2)$$

- Where

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

- ∇ is a Laplacian's operator.
- The solution equation of this equation is of the form

$$\Psi(x,y,z,t)=\Psi_0(x,y,z,t)e^{-i\omega t}$$
$$\Psi=\Psi_0 e^{-i\omega t}----(3)$$

- $\Psi_0(\mathrm{x},\mathrm{y},\mathrm{z},\mathrm{t})$ is a function of x,y,z,t and gives the amplitude with respect to time t.
- Differentiating twice with respect to t

$$\frac{\partial\Psi}{\partial t}=-i\omega\Psi_0\mathrm{e}^{-\mathrm{i}\omega\mathrm{t}}$$
$$\frac{\partial^2\Psi}{\partial t^2}=(-i\omega)(-i\omega)\Psi_0 e^{-i\omega t}$$
$$\frac{\partial^2\Psi}{\partial t^2}=(i^2\omega^2)\Psi_0 e^{-i\omega t}$$

$$\frac{\partial^2 \Psi}{\partial t^2} = -\omega^2 \Psi_0 e^{-i\omega t}$$

$$\frac{\partial^2 \Psi}{\partial t^2} = -\omega^2\ \Psi - - - (4)$$

Since

$$\Psi_0 e^{-i\omega t} = \Psi_0$$

- Substituting (4) in (2),

$$\nabla^2 \Psi = -\frac{\omega^2}{v^2} \Psi$$

$$\nabla^2 \Psi + \frac{\omega^2}{v^2} \Psi = 0 - - - (5)$$

- Angular frequency is

$$\omega = 2\pi\nu = 2\pi \frac{v}{\lambda}$$

- Therefore

$$\frac{\omega}{v} = \frac{2\pi}{\lambda} - - - (6)$$

- Squaring (6)

$$\frac{\omega^2}{v^2} = \frac{4\pi^2}{\lambda^2} - - - (7)$$

- Substituting (7) in (5), $\nabla^2\Psi + \frac{4\pi^2}{\lambda^2}\Psi = 0 - - - -(8)$
- Putting $\lambda = \frac{h}{mv}$, in equation (8)

$$\nabla^2 \Psi + \frac{4\pi^2}{\frac{h^2}{m^2 v^2}} \Psi = 0 - - -$$

$$\nabla^2 \Psi + \frac{4\pi^2 m^2 v^2}{h^2} \Psi = 0 - - - (9)$$

- If E is the energy of the particle and V is the potential energy and ½ mv^2 is the kinetic energy, then Total energy (E)= potential energy (V) + kinetic energy (½ mv^2).

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

- Multiplying by on both sides,

$$m^2v^2 = 2m(E - V) - - - (10)$$

- Substituting (10) in (9),

$$\nabla^2\Psi + \frac{4\pi^2 2m(E - V)}{h^2}\Psi = 0$$
$$\nabla^2\Psi + \frac{8\pi^2 m(E - V)}{h^2}\Psi = 0 - - - - (11)$$

- This equation is called Schrodinger Time independent equation.
- Substituting $\hbar = \frac{h}{2\pi}$,

$$\hbar^2 = \frac{h^2}{4\pi^2} - - - (12)$$

, where $\hbar$ is called reduced Planck's constant.

- Substituting (12) in (11),

$$\nabla^2\Psi + \frac{2m(E - V)}{\hbar^2}\Psi = 0 - - - - (13)$$

- Equation (13) has no term representing time and hence it is called Time independent Schrodinger equation.

Special case:

The one-dimensional equation is represented as

$$\frac{\partial^2\Psi}{\partial x^2} + \frac{2m(E - V)}{\hbar^2}\Psi = 0 - - - (15)$$

II. Schrodinger time independent equation:

- Consider a wave associated with a particle.
- Let x,y,z be the coordinates of the particle.
- Let ψbe the displacement for the de Broglie wave at any time,

- The 3D wave equation for wave motion is given by: $\frac{\partial^2\Psi}{\partial x^2}+\frac{\partial^2\Psi}{\partial y^2}+\frac{\partial^2\Psi}{\partial z^2}=\frac{1}{v^2}\frac{\partial^2\Psi}{\partial t}---(1)$

v is the velocity of the wave. The solution equation of this equation is of the form

$$\Psi(x,y,z,t)=\Psi_0(x,y,z,t)e^{-i\omega t}$$
$$\Psi=\Psi_0 e^{-i\omega t}----(2)$$

- Differentiating twice with respect to t

$$\frac{\partial\Psi}{\partial t}=-i\omega\Psi_0\mathrm{e}^{-\mathrm{i}\omega\mathrm{t}}$$
$$\frac{\partial\Psi}{\partial t}=-i(2\pi\nu)\Psi_0 e^{-i\omega t}$$
$$\frac{\partial\Psi}{\partial t}=-i(2\pi\nu)\Psi---(3)$$
$$\frac{\partial\Psi}{\partial t}=-2\pi i\frac{E}{h}\Psi \qquad \left\{since\ E=h\nu, \qquad h=\frac{E}{\nu}\right\}$$
$$\frac{\partial\Psi}{\partial t}=-\ i2\pi\frac{E}{h}\Psi$$

$$\frac{\partial\Psi}{\partial t}=-\ i\frac{E}{\frac{h}{2\pi}}\Psi$$
$$\frac{\partial\Psi}{\partial t}=-\ i\frac{E}{\hbar}\Psi---(4)$$

Multiplying by "i" on both sides

$$i\frac{\partial\Psi}{\partial t}=-\ iXi\frac{E}{\hbar}\Psi=-i^2\frac{E}{\hbar}\Psi$$
$$i\frac{\partial\Psi}{\partial t}=\frac{E}{\hbar}\Psi$$
$$E\Psi=i\hbar\frac{\partial\Psi}{\partial t}---(5)$$

Schrodinger time independent equation(6)

$$\nabla^2\Psi+\frac{2m(E-V)}{\hbar^2}\Psi=0---(6)$$

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

Substituting (5) in the above equaton

$$\nabla^2\Psi + \frac{2m}{\hbar^2}\left\{i\hbar\frac{\partial\Psi}{\partial t} - V\Psi\right\} = 0)$$

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

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

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

$$\left[\frac{-\hbar^2}{2m}\nabla^2 + V\right]\Psi = i\hbar\frac{\partial\Psi}{\partial t} - - - - (7)$$

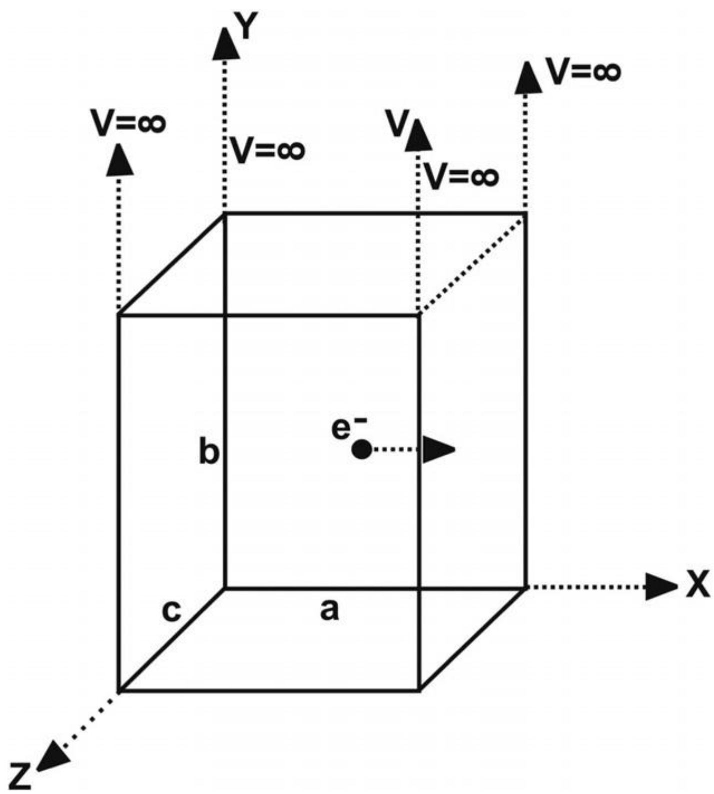
$$\mathrm{H}\Psi = \mathrm{E}\Psi - - (8)$$

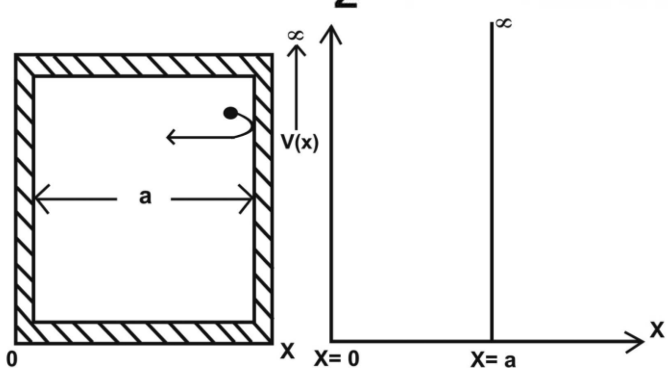
$H \rightarrow \left[\frac{-\hbar^2}{2m}\nabla^2 + V\right]$ is Hamiltonian operator and $E \rightarrow i\hbar\frac{\partial}{\partial t}$ is energy operator.

Equation (8) is called time dependent Schrodinger equation.

Physical significance of the wave function ψ

- The variable ψ characterizes the de Broglie waves is called wave function.
- The wave function connects the particle nature and the associated wave nature statistically.
- It gives the probability of finding the particle at any instant.
- The probability 1 corresponds to the certainty of finding the particle at a point at any instant.
  $\iiint \psi^*\psi d\tau = 1$, means the particle is present
- The probability 0 corresponds to the certainty of not finding the particle at a point at any instant.
  $\iiint \psi^*\psi d\tau = 0$, means the particle is not present.
- The wave function is a complex quantity that cannot be measured.
- The probability density is given by $P(\vec{r}, t) = |\psi(\vec{r}, t)|^2 = \psi^*\psi$


Y
V=∞
V=∞
V
V=∞
V=∞
b
e⁻
X
c
a
Z


∞
V(x)
a
0
X
X= 0
X= a
X
∞

Particle in a box

1. Consider a particle of mass "m" moving inside a one dimensional box.
2. The walls of the box are between x=0 and x=a.
3. The potential energy (V) is assumed to be 0 inside the box.
4. The potential function is : $V(x) = 0 \; for \; 0 < x < a$ and $V(x) = \infty \; for \; 0 \geq x \geq a$
5. This function is known as the square well potential.
6. The value of ψ the wave function of the particle is found by applying the boundary conditions to the one dimensional Schrodinger equation.
7. The Schrodinger equation is

$$\frac{\partial^2 \Psi}{\partial x^2} + \frac{2m(E-V)}{\hbar^2}\Psi = 0 --- (1)$$

8. Since V is 0 between the walls ,

$$\frac{\partial^2 \Psi}{\partial x^2} + \frac{2mE}{\hbar^2}\Psi = 0 --- (2)$$

9. Substituting

$$\frac{2mE}{\hbar^2} = k^2 \;\; in \; (2)$$

$$\frac{\partial^2 \Psi}{\partial x^2} + k^2\Psi = 0 --- (3)$$

10.The general solution is of the form$\Psi(x) = Asin \; kx + B \; cos \; kx --- (4)$

11.A and B are unknown constants.

12.Applying the boundary condition (i) ψ=0 at x=0, to (4)

$$0 = Asin \; kx + B \; cos \; kx --- (4)$$

$$0 = A \; X \; 0 + B \; X \; 1$$

$$Hence \; B = 0$$

$$Therefore \;\;\; 0 = Asin \; ka$$

That is either A=0 or sin ka=0.

14.Since B is already zero, A cannot be zero. Therefore sin ka = 0.

15.Hence ka = nπ, where n = 1,2,3,........ or,

$$k = \frac{n\pi}{a} - - - (5)$$

16.Substituting (5) in (4),

$$\Psi(x) = A\, sin \frac{n\pi}{a} x - - - - (6)$$

17.Squaring (5)

$$k^2 = \frac{n^2\pi^2}{a^2} - - - (7)$$

18.From (2)

$$k^2 = \frac{2mE}{\hbar^2} = \frac{2mE}{\frac{h^2}{4\pi^2}} = \frac{8\pi^2 mE}{h^2} - - (8) since\ \hbar^2 = \frac{h^2}{4\pi^2}$$

19.Equating (7) & (8)

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

$$E_n = \frac{n^2h^2}{8ma^2} \quad - - - (9)$$

20.For each value of n,(n=1,2,3..) there is an energy level.

21. Thus the particle in a box can have only a discrete energy level given by (9).

22.Each energy value is called Eigen value and the corresponding wave function is called Eigen function.

"Eigenvalue" and "eigenvector" come from the meaning "inherent, characteristic"

Normalization of Wave function:

Probability density is =$\psi^*\psi$

The eigen function is

$$\Psi(x) = A\, sin \frac{n\pi}{a} x \quad from\ (6)$$

Therefore

$$\psi^*\psi = A\, sin\frac{n\pi}{a}x \quad X\, A\, sin\frac{n\pi}{a}x$$

$$\psi^*\psi = A^2\, sin\left[\frac{n\pi}{a}x\right]^2 \;---\; (10)$$

The probability of finding the particle anywhere inside the box is given by:

$$\int_0^a \psi^*\psi\, dx = 1$$

Substituting the value from (1) in (2)

$$\int_0^a A^2\, sin\left[\frac{n\pi}{a}x\right]^2 dx = 1$$

$$A^2\int_0^a \frac{1 - cos2\frac{n\pi}{a}x}{2}dx = 1$$

$$A^2\left[\int_0^a \frac{1}{2}dx - \frac{1}{2}\int_0^a cos2\frac{n\pi}{a}x\, dx\right] = 1$$

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

$$A^2\left[\frac{x}{2}\right]_0^a = 1$$

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

Therefore

$$A^2 = \frac{2}{a} \;\; or\; A = \sqrt{\frac{2}{a}} \;----(11)$$

Substituting in (6) , the eigen function ψ_n belonging to is eigen values E_n is expressed as

$$\Psi_n(x) = \sqrt{\frac{2}{a}}\, sin\frac{n\pi}{a}x --- (12)$$

Equation (12) is called Normalized wave function.

Special Cases:

<u>Case1:</u> For n=1,

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

$$\Psi_1(x) = \sqrt{\frac{2}{a}}\, sin\frac{\pi}{a}x$$

<u>Case2:</u> For n=2,

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

$$\Psi_2(x) = \sqrt{\frac{2}{a}}\, sin\frac{2\pi}{a}x$$

<u>Case3:</u> For n=3,

$$E_2 = \frac{9h^2}{8ma^2} = 9E_1$$

$$\Psi_2(x) = \sqrt{\frac{2}{a}}\, sin\frac{3\pi}{a}x$$

Electron microscope

Types:

1. Transmission electron microscope (TEM)
2. Scanning electron microscope (SEM)
3. Scanning transmission electron microscope (STEM)

1. Transmission electron microscope (TEM)

Principle:

1. Accelerated primary electrons are made to pass through the specimen.
2. The image formed by using the transmitted beam or diffracted beam.
3. The transmitted beam produces bright field image
4. The diffracted image is used to produce dark field image.

Construction:

1. Electron gun:
    i. Electron gun produces a high energy electron beam by thermionic emission.
    ii. These electrons are accelerated by the anode towards the specimen

2. Magnetic condensing lens:
    1. These are coils carrying current.
    2. The beam of electrons passing between two can be made to converge or diverge.
    3. The focal length can be adjusted by varying the current in the coils
    4. The electron beam can be focused to a fine point on the specimen.

3. Magnetic projector lens:
    i. The magnetic projector lens is a diverging lens.
    ii. It is placed in before the fluorescent screen
4. Fluorescent (Phosphor) screen or Charge coupled device (CCD)
    1. The image can be recorded by using florescent or Phosphor or charge coupled device.

Working:

1. The electron beam produced by the electron gun is focused on the specimen.
2. Based on the angle of incident the beam is partially transmitted and partially diffracted.
3. Both the beams are combined to form phase contrast image.

4. The diffracted beam is eliminated to increase the contrast and brightness.
5. The magnified image is recorded in the florescent screen or CCD.

Advantages:

1. High resolution image which cannot be obtained in optical microscope.
2. It is easy to change the focal length of the lenses by adjusting the current.
3. Different types of image processing are possible.

Limitations:

1. TEM requires an extensive sample preparation.
2. The penetration may change the structure of the sample.
3. Time consuming process.
4. The region of analysis is too small and may not give the characteristic of the entire sample.
5. The sample may get damaged by the electrons.

Applications:

1. It is used in the investigation of atomic structure and in various field of science.
2. In biological applications, TEM is used to create tomographic reconstruction of small cells or a section of a large cell.
3. In material science it is used to find the dimensions of nanotubes.
4. Used to study the defects in crystals and metals.
5. High resolution TEM (HRTEM) is used to study the crystal structure directly.

2. Scanning electron microscope (SEM)

<u>Principle:</u>

1. Accelerated primary electrons are made to strike the object.
2. The secondary electrons emitted from the objects are collected by the detector to give the three dimensional image of the object.

Construction:

1. Electron gun:
    i. This produces a high energy electron beam by thermionic emission
    ii. These electrons are accelerated by the anode towards the specimen.
2. Magnetic condensing lens:
    i. These are coils carrying current.
    ii. The beam of electrons can be made to converge or diverge.
    iii. The focal length can be adjusted by varying the current in the coils
    iv. The electron beam can be focused to a fine point on the specimen.
3. Scanning coil:
    i. This coil is placed between the condensing lens and the specimen.
    ii. This is energized by a varying voltage.
    iii. This produces a time varying magnetic field.
    iv. This field deflects the beam and the specimen can be scanned point by point.

4. Scintillator:
    i. This collects secondary electrons and converts into light signal.
5. Photomultiplier:
    i. The light signal is further amplified by photomultiplier.
6. CRO.
    i. Cathode ray oscilloscope produces the final image.

Working:

1. The primary electrons from the electron gun are incident on the sample after passing through the condensing lenses and scanning coil.
2. These high speed primary electrons falling on the sample produce secondary electrons.
3. The secondary electrons are collected by the Scintillator produces photons.
4. Photomultiplier converts these photons into electrical signal.
5. This signal after amplification is fed to the CRO, which in turn produces the amplified image of the specimen.

Advantages:

1. SEM can be used to examine large specimen.
2. It has a large depth of focus.
3. Three dimensional image can be obtained using SEM.
4. Image can be viewed directly to study the structural details.

Limitations:

1. The resolution of the image is limited to 10-20 nm and hence it is poor

Applications:

1. SEM is used to study the structure virus, and find the method to destroy it.
2. It is used in the study of bacteria.
3. Chemical structure and composition of alloys, metals and semiconductors can be studied.
4. SEM is used in the study of the surface structure of the material.