Lecture : 1) **Quantum Physics** ① Date : 08.08

(Unit - I)

Lectures by Dr. Tanushree Basak

Syllabus :— Black body radiation — Planck's law (without derivation) — Wien's displacement law and Rayleigh - Jeans' law from Planck's theory — Compton effect (Theory and experimental verification) — wave-particle duality — Uncertainty principle — Matter waves — Schrodinger's wave eqn. — Time independent and time - dependent eqn. — Physical significance of wave function — particle in a one dimensional box.

Why quantum mechanics is necessary for describing molecular properties ?

We know that all molecules are made of atoms which, in turn, contain nuclei and electrons. The eqns. that govern the motions of electrons and of nuclei are not the familiar Newton's eqn. $\vec{F} = m\vec{a}$, but a new set of eqns. called Schrödinger eqns. When Scientists studied the behaviour of electrons and nuclei, they tried to interpret their experimental findings in terms of Classical Newtonian motions, but such attempts eventually failed.

A brief history of QM :—

1900 (Planck) :— Max Planck proposed that light with freq. ν is emitted in quantized lumps of energy that come in integral multiples of the quantity,

$$E = h\nu = \hbar\omega$$

where, $h \simeq 6.63 \times 10^{-34}$ J.s (Planck's con-stant)

and $\hbar = h/2\pi = 1.06 \times 10^{-34}$ J.s.

In late 19th century, one of the puzzles in physics was the blackbody radiation problem. Planck's hypothesis of quantized radiation not only got rid of the problem, but also correctly predicted the shape of the spectrum.

1905 (Einstein) :— Albert Einstein stated that the quantization was in fact inherent to the light and the energy packet can be interpreted as "photons". This proposal was a result of his work on "photoelectric effect", which deals with the absorption of light and the emission of electrons from metal.

1913 (Niels Bohr) :— Niels Bohr stated that electrons in atoms have wavelike properties. This correctly explained the energy levels of hydrogen atoms, which where quantized.

1924 (De Broglie) :— Louis de Broglie proposed that all particles are associated with waves, where the frequency and wavenumber are given by, $E = \hbar\omega$ and $p = \hbar k$

The Larger the E & p are, the larger ω and k are. This is referred to as "wave - particle" duality.

1925 (Heisenberg) :— Werner Heisenberg formulated a version of quantum mechanics that made use of matrix mechanics.

1926 (Schrödinger) :— Erwin Schrödinger formulated a version of QM that was based on waves, more commonly known as Schrödinger's eqn.

1926 (Born) :— Max Born correctly interpreted Schrödinger's eqn. as a probability amplitude. By "amplitude" we mean the probability of finding a particle at a given location

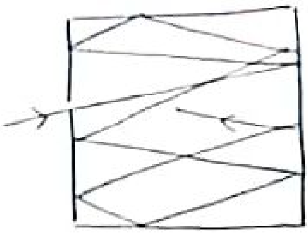
1926 (Dirac) :— Paul Dirac showed that Heisenberg's and Schrödinger's versions of QM were equivalent, in that they could both be derived from a more general version of quantum mechanics.

Blackbody radiation :—

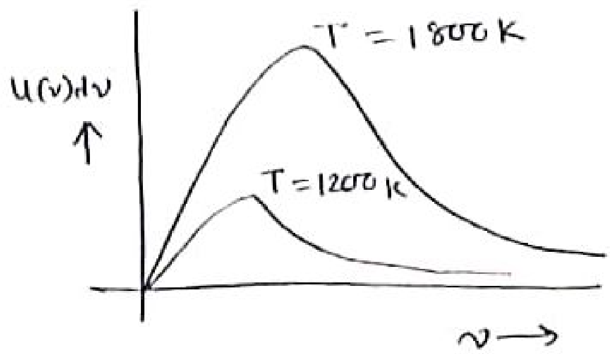
An ideal object that is a perfect absorber and a perfect emitter of light of all possible wavelengths.

The ability of a body to radiate is closely related to its ability to absorb radiation. This is to be expected since a body at a const. temperature is in thermal equilibrium with its surroundings and must absorb energy from them at the same rate as it emits energy. It is convenient to consider as an ideal body one that absorbs all radiation incident upon it, regardless of frequency. Such a body is called a "blackbody".

In the Laboratory a blackbody can be approximated by a hollow object with a very small hole leading to its interior. Any radiation striking the hole enters the cavity, where it is trapped by reflection back and forth until it is absorbed. The cavity walls are constantly emitting and absorbing radiation.



A blackbody radiates more when it is hot than when it is cold.



Blackbody spectra

The spectral distribution of energy in the radiation depends only on the temperature of the body. The higher the temp., the greater the amount of radiation and the higher the frequency at which the maximum emission occurs.

Rayleigh-Jeans formula :- $u(\nu)\,d\nu = \frac{8\pi kT}{c^3}\nu^2 d\nu$

where, $k = 1.381 \times 10^{-23}$ J/K (Boltzmann's const.)

→ the total energy $u(\nu)d\nu$ per unit volume in the cavity in the frequency interval from ν to $\nu+d\nu$.

It shows that the radiation rate is proportional to this energy density. The formula predicts that the energy density should increase as ν^2.

$$\lim_{\nu \to \infty} u(\nu)d\nu \longrightarrow \infty$$

In reality of course, the energy density falls to 0 as $\nu \longrightarrow \infty$. This discrepancy became known as the <u>"ultraviolet catastrophe"</u> of classical physics.

In 1900 Max Planck came up with a formula for the spectral energy density of a blackbody radiation,

$$\boxed{u(\nu)d\nu = \frac{8\pi h}{c^3} \frac{\nu^3 d\nu}{e^{h\nu/kT} - 1}}$$

<u>Solution</u>:— The oscillators in the cavity walls could not have a continuous distribution (as in classical physics) of possible energies, but must have only the specific energies,

$$\epsilon_n = nh\nu \quad , \quad n = 0, 1, 2, \cdots$$

Planck's law in terms of wavelength :—

We know, $\nu = c/\lambda$

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

Substituting this we obtain,

$$u(\lambda)\, d\lambda = \frac{8\pi h}{\cancel{c^3}} \frac{\cancel{c^3}/\lambda^3}{e^{hc/\lambda kT} - 1} \left(-\frac{c}{\lambda^2}\right) d\lambda$$

$$\Rightarrow \boxed{u(\lambda)\, d\lambda = -\frac{8\pi hc\, \lambda^{-5}}{e^{hc/\lambda kT} - 1}\, d\lambda}$$

This relation has been derived on the basis of these assumptions,

1. A black body consists of large no. of oscillators whose energies are quantized and in the form, $E_n = nh\nu$ $(n = 0, 1, 2, \ldots)$

2. A vibrating particle can emit energy only when it goes from one quantized state to lower quantized states

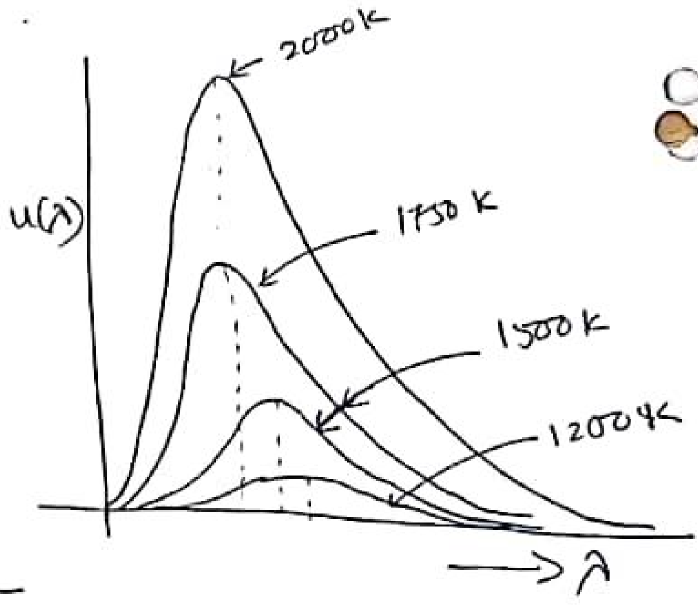
3. The absorption and emission of a energy by oscillating particle is always in discrete form.

Nature of the black body spectrum :—

1. The distribution of the radiated energy is not uniform

2. For a particular wavelength, the intensity of the radiated energy first increase with increase in temperature and become highest at a certain value of the wavelength, thereafter it decreases with increase in temperature.

3. Rate of emission of black body radiation (area under the $u(\lambda) - \lambda$ curve) increases with increase in a temperature of the black body.



4. The peak of the curve shifted towards shorter wavelength (higher frequencies) as the temperature of the black body increases.

5. The radiations emitted from the blackbody are independent of the nature of the body.

Rayleigh - Jeans formula from Planck's radiation formula :—

For small x,

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots$$

become, $e^x \simeq 1 + x$

At Low frequency, $h\nu \ll kT$ or, $\frac{h\nu}{kT} \ll 1$

Therefore, we obtain,

$$\frac{1}{e^{h\nu/kT} - 1} \approx \frac{1}{\cancel{1} + \frac{h\nu}{kT} - \cancel{1}} = \frac{kT}{h\nu}$$

Substituting this in Planck's radiation formula,

$$u(\nu)d\nu \approx \frac{8\pi h}{c^3} \frac{\nu^3 d\nu}{h\nu/kT} \approx \frac{8\pi kT}{c^3} \nu^2 d\nu$$

which is the Rayleigh - Jeans formula.

Wien's displacement Law :—

$$\lambda_{max} T = \frac{hc}{4.965k} = 2.898 \times 10^{-3} \text{ m.K}$$

→ It quantitatively expresses the empirical fact that the peak in the blackbody spectrum shifts to progressively shorter wave-lengths (higher frequencies) as the temperature is increased

Derivation of Wien's Law from Planck's formula:

To find the peak of the black body radiation curve, we take the derivative,

$$\frac{d}{d\lambda}\left[\frac{1}{\lambda^5}\,\frac{1}{e^{a/\lambda T}-1}\right]=0 \qquad \left(a=\frac{hc}{k}\right)$$

$$\Rightarrow -\frac{5}{\lambda^6}\,\frac{1}{e^{a/\lambda T}-1}+\frac{1}{\lambda^5}\,\frac{-e^{+a/\lambda T}\left(\frac{-a}{\lambda^2 T}\right)}{\left(e^{a/\lambda T}-1\right)^2}=0$$

$$\Rightarrow -\frac{5}{\cancel{\lambda^6}}\,\cancel{\frac{1}{(e^{a/\lambda T}-1)}}=\frac{1}{\cancel{\lambda^5}}\,\frac{e^{+a/\lambda T}}{(e^{a/\lambda T}-1)^{\cancel{2}}}\,\frac{a}{\lambda^2 T}$$

$$\Rightarrow \lambda T=\frac{a}{5}\left(\frac{1}{1-e^{-a/\lambda T}}\right)$$

which must be solved numerically to give,

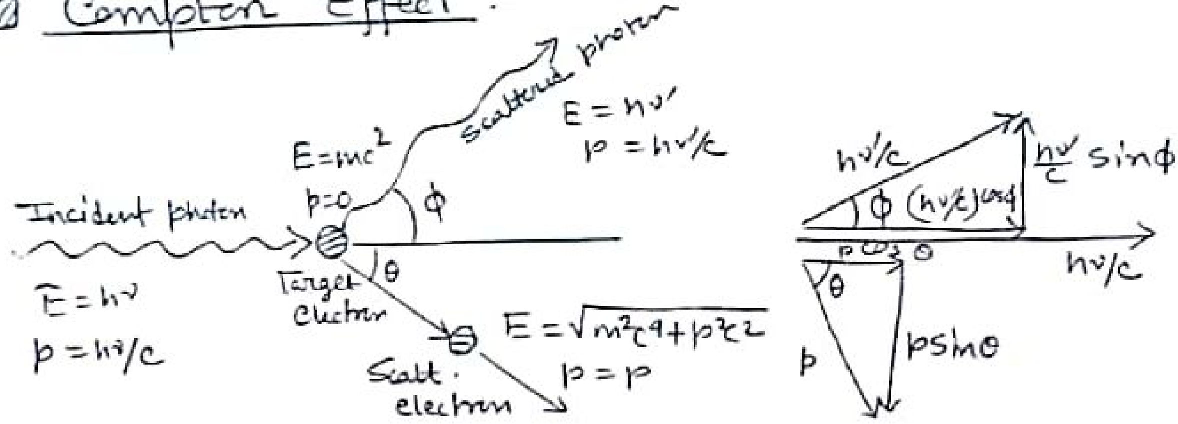
$$\lambda_{max} T = 2.898\times10^{-3}\ m\cdot K$$

Lecture: 3

Particle properties of wave :—

(i) Compton Effect
(ii) X-rays
(iii) Photoelectric effect

Compton Effect :—



A photon strikes an electron (initially at rest in the Laboratory frame) and is scattered away from its original direction of motion while the electron receives an impulse and begins to move. We can think of the photon as losing energy in the collision that is as same as the kinetic energy gained by the electron.

IF the initial photon has freaquency ν and the scattered photon has a lower freaquency ν', then,

Loss in photon energy = Gain in e^- energy

$$h\nu - h\nu' = KE \quad \text{—(1)}$$

According to special relativity the energy of a particle having mass 'm' and momentum 'p' is, $E = \sqrt{m^2c^4 + p^2c^2}$

Now for a massless particle, $m = 0$,

$$E = pc$$

Therefore, the initial photon momentum is,

$$p = E/c = \frac{h\nu}{c}$$

The angle ϕ is that between the directions of the initial and scattered photons, and θ is that between the directions of the initial photon and recoil electron.

By momentum conservation, in the original photon direction,

Initial mom. = Final momentum

$$\frac{h\nu}{c} + 0 = \frac{h\nu'}{c}\cos\phi + p\cos\theta \qquad \text{—(2)}$$

and perpendicular to this direction,

$$0 = \frac{h\nu'}{c}\sin\phi - p\sin\theta \qquad \text{—(3)}$$

Multiply both eqns. (2) & (3) by c,

$$pc\cos\theta = h\nu - h\nu'\cos\phi$$

$$pc\sin\theta = h\nu'\sin\phi$$

Squaring each of these eqns. and adding we obtain,

$$p^2c^2 = (h\nu)^2 + (h\nu')^2 - 2(h\nu)(h\nu')\cos\phi \qquad \text{—(4)}$$

Next we equate two expressions for the total energy,

$$E = KE + mc^2 \qquad (\text{Rest energy} = mc^2)$$

$$E = \sqrt{m^2c^4 + p^2c^2}$$

to give,

$$(KE + mc^2)^2 = m^2c^4 + p^2c^2$$

$$\Rightarrow p^2c^2 = KE + 2(KE)mc^2$$

Now, since, $KE = h\nu - h\nu'$

we have,

$$p^2c^2 = (h\nu)^2 - 2(h\nu)(h\nu') + (h\nu')^2 + 2mc^2(h\nu - h\nu') \qquad \text{—(5)}$$

Substituting this value of p^2c^2 in (4), we finally obtain,

$$\cancel{(h\nu)^2} - 2(h\nu)(h\nu') + \cancel{(h\nu')^2} + 2mc^2(h\nu - h\nu')$$

$$= \cancel{(h\nu)^2} - 2(h\nu)(h\nu')\cos\phi + \cancel{(h\nu')^2}$$

$$\Rightarrow \boxed{mc^2(h\nu - h\nu') = (h\nu)(h\nu')(1 - \cos\phi)} \qquad \text{—(6)}$$

Use the relation between frequency and wavelength, $\nu/c = 1/\lambda$ and $\nu'/c = 1/\lambda'$

From eqn. (6),

$$\cancel{h}c\left(\frac{1}{\lambda} - \frac{1}{\lambda'}\right) = \frac{h^{\cancel{2}}}{m\cancel{c^2}}\left(\frac{\cancel{c}}{\lambda}\right)\left(\frac{\cancel{c}}{\lambda'}\right)(1-\cos\phi)$$

$$\Rightarrow \frac{\lambda' - \lambda}{\cancel{\lambda\lambda'}} = \frac{h}{mc}\left(\frac{1}{\cancel{\lambda\lambda'}}\right)(1-\cos\phi)$$

$$\Rightarrow \boxed{\lambda' - \lambda = \frac{h}{mc}(1-\cos\phi)} \quad —(7)$$

→ This eqn. was derived by Arthur H. Compton in the early 1920's and the phenomenon it describes is known as the "<u>Compton effect</u>".

- Compton wavelength :— $\boxed{\lambda_c = \frac{h}{mc}}$

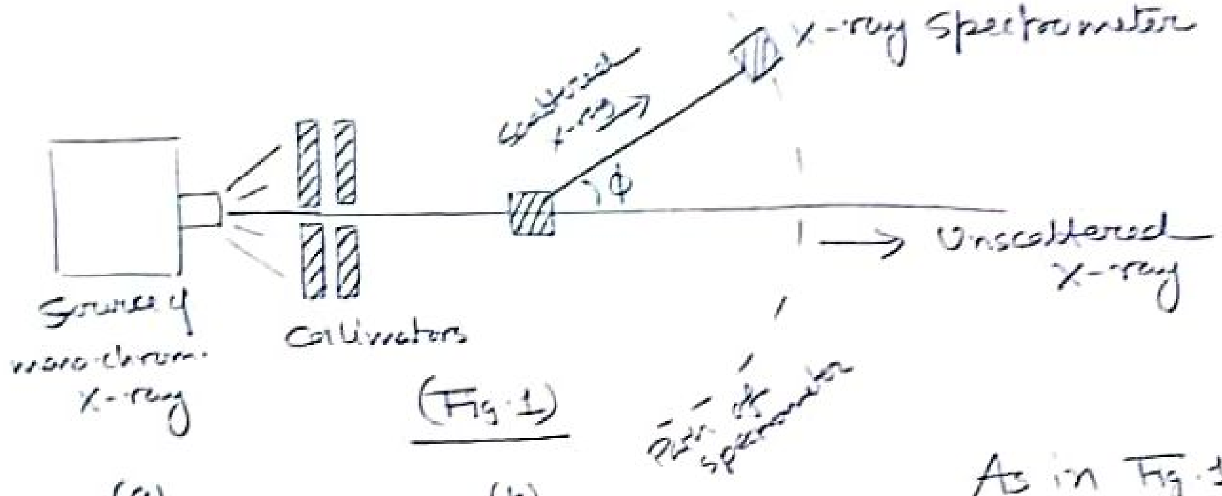
(For an electron, $\lambda_c = 2.426 \times 10^{-12}$ m)

<u>Compton effect</u> :— $\boxed{\lambda' - \lambda = \lambda_c(1-\cos\phi)}$ —(8)

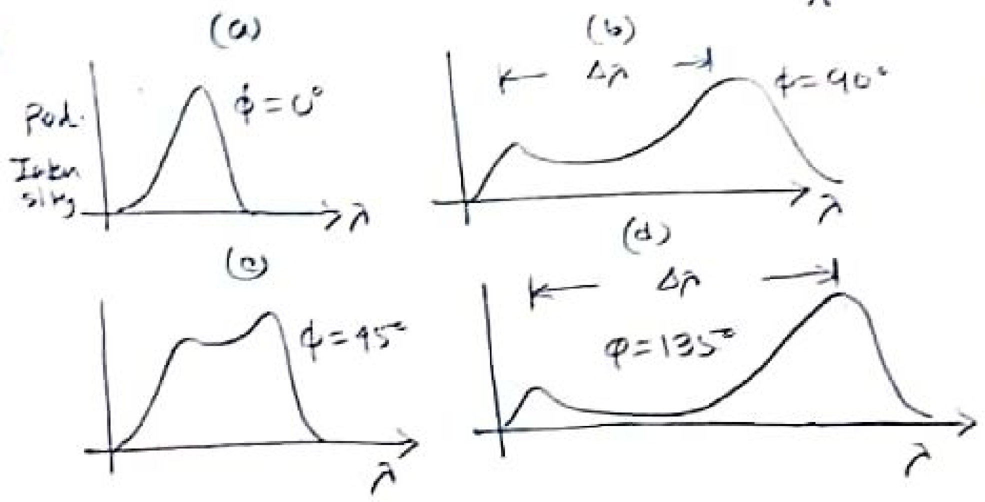
→ change in the wavelength of the photon.

For, $\boxed{\phi = 180°}$, <u>maximum change</u> in wavelength occurs. The compton effect is the chief means by which x-rays lose energy when they pass through matter. For, $\boxed{\phi = 0}$, there is <u>no compton shift</u> observed.

Experimental Demonstration of Compton effect:



(Fig. 1)



(Fig. 2)

As in Fig. 1, a beam of X-rays of a single, known wavelength is directed at a target, and the wavelengths of scattered X-rays are determined at various angles ϕ.

The results are shown in Fig. 2. In deriving eqn (7) it was assumed that the scattering particle is able to move freely, which is reasonable since many of the electrons in matter are only loosely bound to the parent atoms. The greater the scattering angle, the larger the wavelength change. But some electrons are tightly bound to the atom. Therefore it results in the recoil of the entire atom when struck by a photon. The ~~Sc~~ resulting Compton shift is accordingly so small to be detected since, mass of the atom is almost thousand times greater than me.

Compton Effect (Definition) :— When a monochromatic beam of high frequency radiations (e.g. x-rays and γ-rays) is Scattered by a substance of less atomic number, the scattered radiations contain the radiations of higher wavelength (lower frequency) along with the radiations of unchanged wavelength (or lower frequency). This phenomenon is called the Compton Effect.

Lecture : 4

Problems on Compton Effect :—

1. Calculate λ_c for electrons.

$\lambda_c = \frac{h}{mc}$ where $h = 6.63 \times 10^{-34}$ J.s
$c = 3 \times 10^8$ s
$m = 9.1 \times 10^{-31}$ kg

$\Rightarrow \boxed{\lambda_c = 2.43 \times 10^{-12} m}$

$= 2.43$ pm $\quad (1 \text{ pm} = 10^{-12} m)$

2. X-rays of wavelength 10.0 pm are scattered from a target. (a) Find the wavelength of the x-rays scattered through 45°. (b) Find the maximum wavelength present in the scattered x-rays. (c) Find the maximum kinetic energy of the recoil electrons.

(a) $\lambda' - \lambda = \lambda_c (1 - \cos\phi)$

$\Rightarrow \lambda' = \lambda + \lambda_c (1 - \cos\phi)$
$= 10.0 \text{ pm} + 2.43 \text{ pm} \times (0.293)$
$= 10.7$ pm

(b) $\lambda' - \lambda$ is a maximum when $\phi = 180°$, $(1 - \cos\phi) =$

In that case, $\lambda' = \lambda + 2\lambda_c = (10.0 + 4.86)$ pm
$= 14.86$ pm

(c) The maximum recoil kinetic energy is equal to the difference between the energies of the incident and scattered photons, so

$$K.E_{max} = h(\nu - \nu') = hc\left(\frac{1}{\lambda} - \frac{1}{\lambda'}\right)$$

where λ' is given in (b).

$$K.E_{max} = \frac{(6.626 \times 10^{-34}\ J.s) \times (3 \times 10^{8}\ m/s)}{10^{-12}\ m}\left(\frac{1}{10.0} - \frac{1}{14.86}\right)$$

$$= 6.54 \times 10^{-15}\ J$$

Wien's displacement law :—

- What is the maximum wavelength of a black-body of temperature 35°c.

We know that, $\lambda_{max} T = 2.898 \times 10^{-3}\ m.K$

Now, $T = 35°c = 308\ K$

$$\therefore \lambda_{max} = \frac{2.898 \times 10^{-3}\ m.K}{308\ K} = 9.41 \times 10^{-6}\ m$$

$$= 9.41\ \mu m$$

$$\left(1\ \text{Joule} = 6.241 \times 10^{18}\ eV\right)$$

De-Broglie Hypothesis :-

In 1924, Louis de Broglie extended the wave-particle dualism of light to the material particles. A moving body behaves in certain ways as though it has a wave nature. This is known as "de Broglie hypothesis".

According to de Broglie hypothesis any moving particle is associated with a wave. The wave associated with particles are known as de Broglie waves or matter waves.

A photon of light of frequency ν has the momentum,

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

$$\Rightarrow \boxed{\lambda = \frac{h}{p}}$$

A particle with mass 'm' moving with a velocity 'v', must be associated with a wave of wavelength,

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

Properties :-

1. $\lambda \rightarrow \infty$ when $v = 0$, means that matter waves are detectable only for moving particles.
2. Lighter the particle, Longer is the wave-length.
3. Smaller the velocity of micro-particle, the longer is the wavelength.

VI De Broglie wavelength associated with particles in thermal equilibrium

If the particle is in thermal equilibrium at temperature T, then kinetic energy is,

$$K.E = \frac{3}{2}KT$$

We know that, $KE = \frac{P^2}{2m}$

$$\Rightarrow P = \sqrt{2m(KE)}$$

$$\therefore \lambda = \frac{h}{\sqrt{2m(\frac{3}{2}KT)}} = \frac{h}{\sqrt{3mKT}}$$

VII De Broglie waves are insignificant in case of macro-bodies :—

As the mass of the body increases, the wavelength tends to be insignificant, even at very low velocities,

Example :— If we consider a cricket ball of mass 500 gm flying with velocity 50 km/hr, its wavelength becomes,

$$\lambda = \frac{6.62 \times 10^{-34} J.s}{0.5 kg \times 13.9 m/s} = 10^{-34} m = 10^{-24} Å$$

$(1 Å = 10^{-10} m)$

On the other hand, if we consider the case of an electron having energy 100 eV, the

∴ de Broglie wavelength of the electron becomes,

$$\lambda = \frac{h}{\sqrt{2m(K.E)}} \quad , \quad K.E = eV$$

$$= \frac{6.62 \times 10^{-34} \text{ J.s}}{\sqrt{2 \times 9.1 \times 10^{-31} \text{ Kg} \times 1.6 \times 10^{-19} \text{ C} \times 100 \text{ V}}}$$

$$= 1.33 \text{ Å}$$

The size of an electron is about 10^{-5} Å, which is far smaller than the wavelength of 1.33 Å. It means that the electron behaves more as a wave than a particle under the circumstances.

Problem :— An enclosure filled with He^4 is heated to 400 K. Calculate the de Broglie wavelength corresponding to He^4 atoms. Mass of He^4 atom is 6.7×10^{-27} kg.

Ans:— $$\lambda = \frac{h}{\sqrt{2mKT}} = \frac{6.63 \times 10^{-34} \text{ J.s}}{\sqrt{2 \times 6.7 \times 10^{-27} \times 1.38 \times 10^{-23} \times 400}}$$

$(K = 1.38 \times 10^{-23} \text{ m}^2 \text{ kg s}^{-2} \text{K}^{-1})$ $$= 0.769 \text{ Å}$$

Lecture 5 (27)

Heisenberg's Uncertainty Principle :-

Statement : It is impossible to know both the exact position and exact momentum of an object at the same time.

$$\boxed{\Delta x \, \Delta p \geq \frac{\hbar}{2}}$$

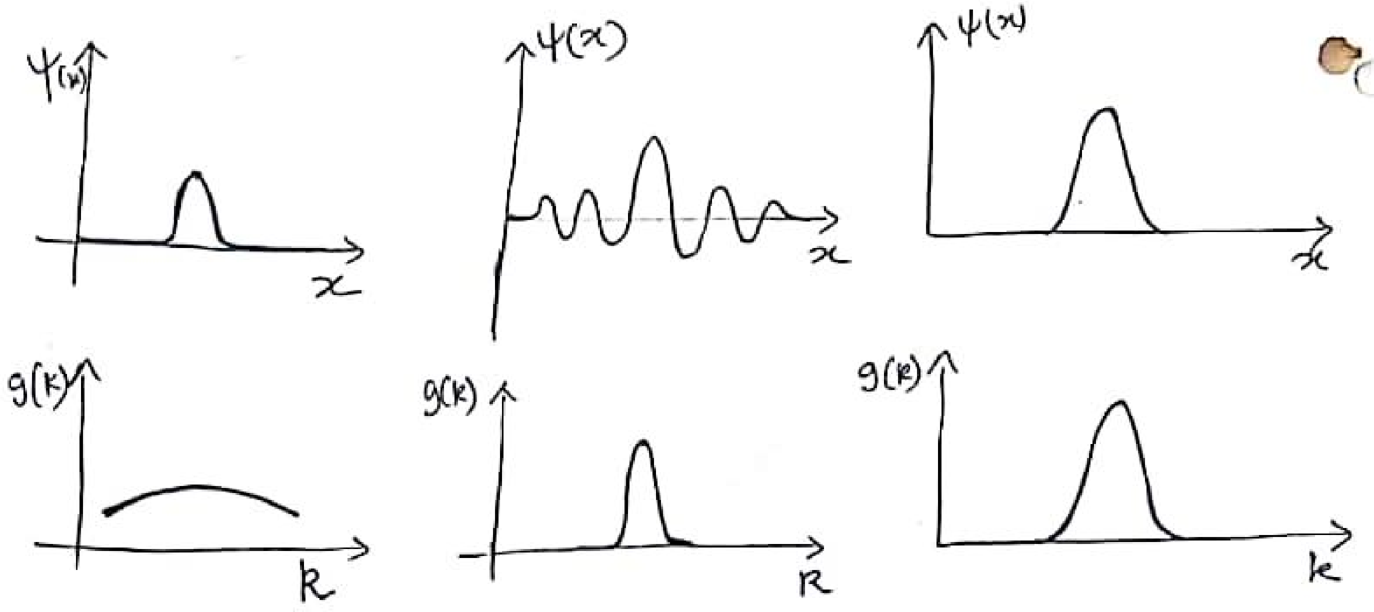
where, Δx is the uncertainty in position and Δp is the uncertainty in the momentum ~~position~~ component in x-direction.

In terms of wave number 'k',

$$p = \hbar k$$

therefore,

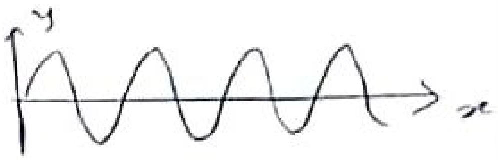
$$\boxed{\Delta x \, \Delta k \geq \frac{1}{2}}$$



Pulse | Wave group | Gaussian distribution

Schrödinger's wave Equation :—

Any wave function $y(x,t)$ that describes a wave on a string must satisfy the wave eqn.



$$\frac{\partial^2 y(x,t)}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2 y(x,t)}{\partial t^2} \quad —(1)$$

where, v is the speed of the wave.

Consider the wave function $y(x,t)$ of wavelength λ and frequency ν moving in +ve x-direction,

$$y(x,t) = A\cos(kx-\omega t) + B\sin(kx-\omega t)$$

where $k = 2\pi/\lambda$ (wave no.)

$\omega = 2\pi\nu$ (angular freq.)

Now, $\frac{\partial^2 y(x,t)}{\partial x^2} = -k^2 A[\cos(kx-\omega t)] - k^2 B\sin(kx-\omega t)$

$\frac{\partial^2 y(x,t)}{\partial t^2} = -\omega^2 A\cos(kx-\omega t) - \omega^2 B\sin(kx-\omega t)$

Substituting back in eq.(1) gives,

$$-k^2(A\cos(kx-\omega t) + B\sin(kx-\omega t)) = \frac{1}{v^2}\times(-\omega^2[A\cos(kx-\omega t) + B\sin(kx-\omega t)])$$

$\rightarrow$ we get, $v^2 = \frac{\omega^2}{k^2}$ or, $\boxed{\omega = vk}$

→ All we need is the quantum mechanical version of the wave-equation for particle waves.

From, Planck's and de Broglie's hypothesis we know that,

$$E = h\nu = \left(\frac{h}{2\pi}\right)(2\pi\nu) = \hbar\omega$$

and
$$p = \frac{h}{\lambda} = \left(\frac{h}{2\pi}\right)\left(\frac{2\pi}{\lambda}\right) = \hbar k$$

For free particle, $E = \dfrac{p^2}{2m}$

$$\Rightarrow \boxed{\hbar\omega = \frac{\hbar^2 k^2}{2m}}$$

— this relation is different than the waves on string (where, $\omega \propto k$)

— Therefore the quantum mechanical wave-eqn. for a (1-dim) free particle becomes,

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

→ this eqn. is known as, one-dimensional Schrödinger eqn. for a free-particle.

— The solution of eqn. (2) gives the free particle wave eqn.,

$$\psi(x,t) = A e^{i(kx-\omega t)}$$

Further ψ must be ~~sig~~ single-valued since the probability can have only one value at a particular time.

☑ <u>Important characteristics of wave function</u> :—

(i) ψ must be finite, continuous and single valued everywhere.

(ii) $\frac{\partial \psi}{\partial x}$, $\frac{\partial \psi}{\partial y}$, $\frac{\partial \psi}{\partial z}$ must be finite and continuous.

(iii) ψ must be normalisable.

☑ Time-dependent Schrödinger wave eqn. :—

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x)\,\psi(x,t) = i\hbar\frac{\partial\psi(x,t)}{\partial t} \quad —(1)$$

Solution :— $\psi(x,t) = A e^{-i(px-Et)/\hbar}$

⟶ is a solution of this ~~eqn~~ eqn. for a free particle, $V(x)=0$.

☑ Time-independent Schrödinger Eqn. :—

Guess solution, $\Psi(x,t) = \psi(x)\, e^{-iEt/\hbar}$

Let us substitute the ~~above~~ solution in eq (1).

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} e^{-iEt/\hbar} + V(x)\,\psi(x)\, e^{-iEt/\hbar}$$

$$= i\hbar\left(-\frac{iE}{\hbar}\right) e^{-iEt/\hbar}\,\psi(x)$$

$$= E\,\psi(x)\, e^{-iEt/\hbar}$$

We see that the factor $(e^{-iEt/\hbar})$ cancels on both sides, we obtain,

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

$$\left\{ \text{Hamiltonian : Total Energy} \quad H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) \right\}$$

$$\therefore\ H\psi(x) = E\,\psi(x)$$

Re-arranging we get,

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

→ which is the time-independent Schrödinger eqn.

<u>Note</u>: The quantity E, identified as the energy of the particle, is actually a free-parameter in this eqn.

☒ <u>Stationary States</u>:-

$$\Psi(x,t) = \psi(x)\, e^{-iEt/\hbar}$$

→ this is the time-dependent wave function for a state of definite energy.

→ A state of definite energy is commonly called a "<u>stationary state</u>".

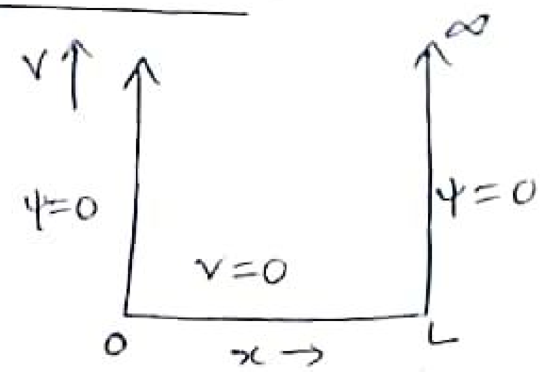
$$|\Psi(x,t)|^2 = \Psi^*(x,t)\,\Psi(x,t)$$
$$= [\psi^*(x)\,e^{iEt/\hbar}][\psi(x)\,e^{-iEt/\hbar}]$$
$$= \psi^*(x)\,\psi(x) = |\psi(x)|^2$$

→ $|\psi(x)|^2$ does not depend on time, shows that the same must be true for the probability distribution function $|\Psi(x,t)|^2$.

But, Stationary state does not mean a stationary particle.

Particle in an one-dimensional box :—

Infinite Potential Well



Let us consider a particle confined to the region $0<x<L$. It can move freely within the region $0<x<L$ but subject to forces at $x=0$ & $x=l$

1-dim potential box
$$\left.\begin{aligned} V &= 0, \quad \text{in the region } 0<x<L \\ &= \infty, \quad \text{at } x=0,\ x=L \end{aligned}\right\} \quad \text{—(1)}$$

The Schrödinger eqn. takes the form (inside the box, $V=0$),

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

$$\Rightarrow \frac{d^2\psi(x)}{dx^2} + \frac{2mE}{\hbar^2}\psi(x) = 0$$

$$\Rightarrow \frac{d^2\psi(x)}{dx^2} + \frac{8\pi^2 m}{h^2}E\,\psi(x) = 0 \qquad \text{—(2)}$$

Let, $\frac{8\pi^2 m}{h^2}E = k^2$ then eq. (2) takes the form,

$$\boxed{\frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0} \qquad \text{—(3)}$$

The general solution to this eqn. is,

$$\psi(x) = A\sin kx + B\cos kx$$

where A and B are constants. The values of these constants can be obtained by applying the boundary conditions of the problem.

The particle is enclosed between two rigid walls and ψ^2 is the probability of finding the particle at any instant. The particle cannot penetrate the walls, hence

$\psi(x) = 0$ at $x = 0$ and $x = L$

At $x = 0$,

$$\psi(0) = 0 = A \sin 0 + B \cos 0 = B$$

$$\Rightarrow \boxed{B = 0}$$

At $x = L$,

$$\psi(L) = 0 = A \sin kL$$

$\Rightarrow$ Either $A = 0$ or $\sin kL = 0$

But $A \neq 0$ because if $A = 0$ the entire wave function will vanish as $B = 0$.

Therefore, $\sin kL = 0$

or, $kL = n\pi$ (or, $k = \frac{n\pi}{L}$)

or, $k^2 = \frac{n^2\pi^2}{L^2}$

$$\Rightarrow \frac{8\cancel{\pi^2} m}{h^2} E_n = \frac{n^2 \cancel{\pi^2}}{L^2}$$

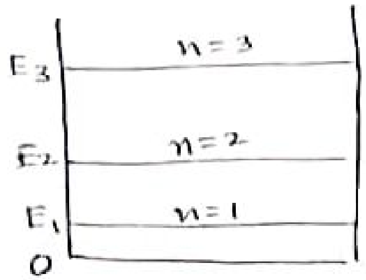
$$\Rightarrow \boxed{E_n = \frac{n^2 h^2}{8 m L^2}} \quad \text{—(4)}$$

$(n = 1, 2, 3, ---)$

Now, the wave function becomes,

$$\boxed{\psi(x) = A \sin \frac{n\pi x}{L}} \quad —(5)$$

Also we conclude that inside an infinite potential well, the particles can have only discrete set of values of energy, i.e, energy of the particle is quantized.



To find the value of the constant A, we use the normalisation condition,

$$\int_0^L |\psi(x)|^2 dx = 1$$

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

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

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

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

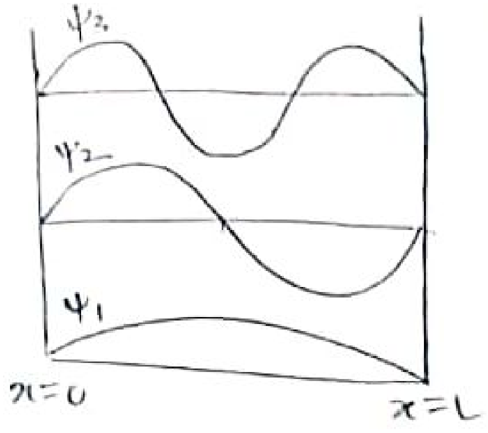
$$\Rightarrow \frac{A^2}{2} L = 1 \quad \text{or,} \quad A^2 = 2/L$$

$$\text{or,} \quad \boxed{A = \sqrt{2/L}}$$

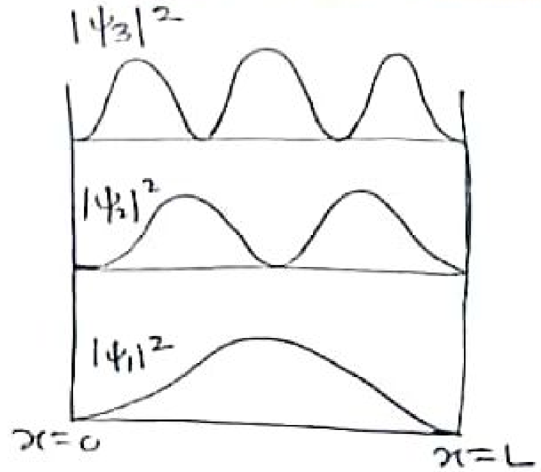
Thus, we obtain,

$$\boxed{\psi(x) = \sqrt{2/L} \sin \frac{n\pi x}{L}} \quad —(6)$$

⟶ this is the normalised wave function of the particle.



Wave function



Probability distribution

Classical mechanics predicts the same probability for the particle being anywhere in the well. Quantum mechanics, on the other hand, predicts that the probability is different at different points. Further, at a particular point, the probability of finding the particle is different for different energy states.

For example, a particle in the lowest energy state ($n=1$) is more likely to be in the middle of the box, while in the next state ($n=2$) it is never there since, $|\psi_2|^2$ is zero there.

Problems :-

1. The position and momentum of a 1.0 keV electron are simultaneously measured. If the position is located within 1 Å, what is the percentage of uncertaint in momentum?

Sol :-

$$\Delta x = 1\,\text{Å} = 10^{-10}\,m$$

$$E = 1\,keV = 1000 \times 1.6 \times 10^{-19}\,J = 1.6 \times 10^{-16}\,J$$

According to Heisenberg uncertainty principle,

$$\Delta x \, \Delta p = \frac{\hbar}{2}$$

Now, $p = \sqrt{2mE} = \sqrt{2 \times 9.1 \times 10^{-31} \times 1.6 \times 10^{-16}}$

$$= 1.71 \times 10^{-23}\ kg\ m/sec.$$

and $\Delta p = \dfrac{h}{2\pi(2\Delta x)} = 5.27 \times 10^{-25}\ kg\ m/sec.$

Percentage of uncertainty in momentum,

$$100 \times \frac{\Delta p}{p} = \frac{5.27 \times 10^{-25}}{1.71 \times 10^{-23}} \times 100 = 3.1\%$$

2. The position and momentum of 0.5 keV electron are simultaneously determined. If its position is located within 0.2 nm, what is the percentage uncertainty in its momentum?

Sol :- (use the same techniane as the previous problem).

$$E = 0.5 \times 1000 \times 1.6 \times 10^{-19}\,J = 0.8 \times 10^{-16}\,J$$

$$\Delta p = \frac{h}{4\pi \Delta x} = \frac{h}{4\pi} \frac{1}{0.2 \times 10^{-9}} = 2.635 \times 10^{-25}$$

kg m/sec.

$$p = \sqrt{2 \times 9.1 \times 10^{-31} \times 0.8 \times 10^{-16}} = 12.06 \times 10^{-24} \text{ kg m/sec}$$

Thus, $\frac{\Delta p}{p} \times 100 = 2.18\%$

3. Find the energy of an electron moving in one dimension in an infinite potential box of width 1.0 Å. Given $m = 9.1 \times 10^{-31}$ kg, $h = 6.62 \times 10^{-34}$ J.sec

Sol:- $L = 1.0 \times 10^{-10}$ m

Energy of the particle,

$$E_n = \frac{n^2 h^2}{8 m L^2} = \frac{n^2 (6.62 \times 10^{-34})^2}{8 \times 9.1 \times 10^{-31} \times (10^{-10})^2}$$

$$= 0.602 \times 10^{-17} n^2 \text{ J}$$

For, $n = 1$, $E_1 = 6.02 \times 10^{-18}$ J

$n = 2$, $E_2 = 4 \times 6.02 \times 10^{-18}$ J

$= 2.41 \times 10^{-18}$ J

4. Calculate the energy difference between the ground state and the first excited state for an electron in a box of length 1.0 Å.

Soln :- $E_n = \frac{n^2 h^2}{8 m L^2}$

$$E_2 - E_1 = \frac{h^2}{8 m L^2} (2^2 - 1^2)$$

$$= 1.81 \times 10^{-17} \text{ J}$$

(5.) An electron in an one-dimensional infinite potential well, ~~go~~ goes from $n = 4$ to $n = 2$ level. The frequency of the emitted photon is $3.43 \times 10^{+14}$ Hz. Find the width of the box.

Soln :— Energy difference between Level $n=4$ and $n=2$ is,

$$E_4 - E_2 = \frac{h^2}{8mL^2}(4^2 - 2^2)$$

$$= \frac{12h^2}{8mL^2}$$

Energy of the emitted photon is '$h\nu$'.

$$\therefore h\nu = \frac{12h^2}{8mL^2}$$

$$\Rightarrow L^2 = \frac{12h}{8m\nu} = \frac{3h}{2m\nu}$$

$$\Rightarrow L = \sqrt{\frac{3h}{2m\nu}} = 17.84 \times 10^{-10} \, m$$

$$= 17.84 \, Å.$$

(6) The wave function of a particle confined in a box of length 'l' is, $\psi(x) = \sqrt{2/l} \sin\frac{\pi x}{l}$, $0 \le x \le l$

Calculate the probability of finding the particle in the region $0 < x < l/2$.

Soln :— The probability of finding the particle is given by,

$$P = \int_0^{l/2} |\psi(x)|^2 dx$$

$$= \frac{2}{l}\int_0^{l/2} \sin^2\left(\frac{\pi x}{l}\right) dx$$

$$= \frac{2}{l}\int_0^{l/2} \frac{1}{2}\left(1 - \cos\frac{2\pi x}{l}\right) dx$$

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

$$= \frac{1}{l}\left[\frac{l}{2} - \frac{l}{2\pi}\underbrace{\sin\frac{2\pi l}{2l}}_{0}\right] = \frac{1}{2}$$