Unit 3 : Fundamentals Of Atomic Physics.

Black Body Radiation:-

A black body is an ideal object that can absorb almost all possible frequency of radiation incident on its surface. A pin hole with a hollow cavity coated with its inner surface coated by carbon black acts as black body practically. When it is heated in a fixed absolute temperature, it emits radiation spectrum of continuous frequency known as black body radiation. On increasing the temperature, the black body will begin to radiate almost all radiation that was absorbed, hence black body is also known to be a perfect absorber and perfect emitter.

Energy spectrum emitted by black body radiation depends on the frequency of that radiation emitted. The experimental result of black body radiation is as shown in figure.

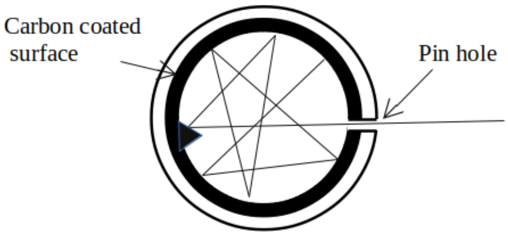


Fig : Pin hole act as Black hole

The characteristics of black body spectrum is

1. The intensity of emitted radiation is continuous with frequency.
2. The intensity of radiation becomes maximum at a particular frequency for particular absolute temperature.
3. The value of maximum frequency of emitted energy spectrum increases with increase in absolute temperature of black body.

In order to explain such experimental result of black body radiation spectrum, Max Plank in 1890 A. D. assumed that the atoms or molecules present in inner surface of black body is composed with simple harmonic oscillator i.e. such atoms or molecules oscillate about their mean position.

Once black body is exposed to radiation these atoms or molecules absorb corresponding energy and atoms are in excited state. On heating, the excited atom come back to their ground sate by emitting absorbed energy as earlier in discrete form as packet form of energy known as quanta. The energy of each quanta is hf, where f is corresponding frequency of atomic vibration.

Accordingly,

$$\Delta E = E_2 - E_1$$

or, $E = n\,hf$ where, $h = 6.62 \times 10^{-34}$ Js (Plank's constant)

$n = 0,1,2,\ldots\ldots$ (integer)

Further, From classical electromagnetic theory, the energy emitted from black body radiation at particular absolute temperature T, from Stefan's law is

$$E \propto T^4$$

or, $E = \sigma T^4$ where $\sigma = 5.67 \times 10^{-8}$ watt/m^2 K^4 (Stefan's Constant)

and Plank's derived the empirical formula for the intensity of radiation spectra emitted of particular frequency from black body in order to explain the experimental results given by,

$$I(f) = \frac{2\pi h f^3}{c^2}\frac{1}{e^{\frac{hf}{K_B T}}-1}$$ where $K_B = 1.38 \times 10^{-23}$ J/K (Boltzmann Constant)

In this way, Plank successfully use the concept of quantum mechanical idea of quantization of energy in order to explain the black body radiation and this idea was found quite strong agreement with experimental result.

Bohr's Atomic Model (for Hydrogen atom):-

In 1911, Neil Bohr gave quantum mechanical model of H-atom in order to address the limitation observed in Rutherford's atomic model regarding issue of stability of atom and about the atomic line spectrum. This model is also named planetary model of the atom and is based on following postulates.

1. Stationary orbit: In an atom, electron revolve around the positive central nucleus electron in fixed orbit called stationary orbit. The centripetal force required for rotation of electron is provided by the attractive electrostatics force between electron and nucleus. i.e.

$$\frac{mv^2}{r} = \frac{Ze.(e)}{4\pi\epsilon_0 r^2}$$

where, ε_0= 8.85 X 10^{-12} $C^2/N\ m^2$ is permittivity of free space.

or, $\frac{mv^2}{r} = \frac{e^2}{4\pi\epsilon_0 r^2}$ for H-atom Z=1

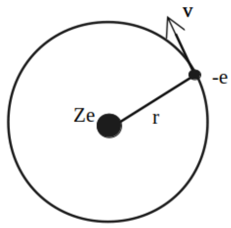


Fig: Electron revolving around a nucleus in an atom.

2. Angular momentum quantization: The electrons revolves in a particular orbit at which its angular momentum is equal to integral multiple of $\frac{h}{2\pi}$. i.e.

$$mvr = \frac{nh}{2\pi}$$

This is also called Bohr's quantization condition.

3. Atomic spectrum : An atom can emit or absorb radiation in a form of discrete energy photons only when an electron jumps from a higher to lower energy orbit or from lower to higher orbit respectively.

hf = E_2-E_1 This is also called Bohr's frequency condition.

or, f = (E_2-E_1) / h

where, h= 6.62 X 10^{-34} Js (Plank's constant) and f is frequency of radiation emitted.

Radius of nth orbit :-

Let us consider a H-atom in which an electron having charge -e revolves around the nucleus of charge +e in a nth circular orbit of radius 'r_n' with 'v_n' orbital velocity. The necessary centripetal force for an electron to be in a circular motion is provided by the electrostatic force of attraction between electron and nucleus. i.e.

$$\frac{mv_n^2}{r_n} = \frac{e^2}{4\pi\epsilon_0 r_n^2}$$

where, ε_0= 8.85 X 10^{-12} $C^2/N\ m^2$ is permittivity of free space.

or, $mv_n^2 = \frac{e^2}{4\pi\epsilon_0 r_n}$ ………… 1

Further, from Bohr's quantization condition,

$$mv_n r_n = \frac{nh}{2\pi}$$

or, $v_n = \frac{nh}{2\pi m r_n}$ ………….. 2

using eqn 2 in 1,we get

$$m(\frac{nh}{2\pi m r_n})^2 = \frac{e^2}{4\pi\epsilon_0 r_n}$$

or, $\frac{mn^2h^2}{4\pi^2 m^2 r_n^2} = \frac{e^2}{4\pi\epsilon_0 r_n}$

or, $r_n = \frac{n^2h^2\epsilon_0}{\pi me^2}$ ………..3 where n=1, 2, 3, ………… is principle quantum number.

With h= 6.62 $X10^{-34}$ JS ; ε_0= 8.85 X 10^{-12} $C^2/N\ m^2$; m= 9.1 $X10^{-31}$ kg ; e= 1.6 X 10^{-19} C

or,$r_n = n^2X0.529X10^{-10}$

or,$r_n = n^2X0.529A^0$ for first orbit n=1 and $r_1 = 0.529A^0$

Thus, $r_n \alpha n^2$

Note: For the radius of hydrogen like species He^+ , Li^{++}, Be^{+++} . As these atom have one electron like hydrogen but the charge of their nucleus is +Ze, where Z is their atomic number, So that in this case, radius of n^{th} orbit of such atom becomes;

$$r_n = \frac{n^2h^2\epsilon_0}{\pi Zme^2}$$

or,$r_n = \frac{n^2}{Z}X0.529A^0$

Speed of electron in n^{th} orbit of hydrogen atom:-

From Bohr's quantization condition, electron at n^{th} orbit is;

$$mv_nr_n = \frac{nh}{2\pi}$$

or,$v_n = \frac{nh}{2\pi mr_n}$

using value of radius of orbit , we get

$$v_n = \frac{nh}{2\pi m(\frac{n^2h^2\epsilon_0}{\pi me^2})} \quad \text{[from eqn 3.]}$$

or, $v_n = \frac{e^2}{2nh\epsilon_0}$ ……………….. 4

or, $v_n = \frac{e^2}{2ch\epsilon_0}\frac{c}{n}$

or, $v_n = \alpha\frac{c}{n}$ where, $\alpha = \frac{e^2}{2ch\epsilon_0}$ is called fine structure constant.

With h= 6.62 $X10^{-34}$ JS ; ε_0= 8.85 X 10^{-12} $C^2/N\ m^2$; e= 1.6 X 10^{-19} C and c=3x 10^8 m/s (speed of light in vacuum).

$$\alpha = \frac{e^2}{2ch\epsilon_0} = \frac{1}{137}$$

Therefore,

$v_n = \frac{1}{137}\frac{c}{n}$ for velocity of electron at first orbit n=1; v_1 = 2.19X 10^6 m/s

Energy of electron in n^{th} orbit of hydrogen atom:-

An electron revolving in an orbit of H-atom has both kinetic energy and electrostatic potential energy.

The velocity of electron in n^{th} energy orbit is $v_n = \frac{e^2}{2nh\epsilon_0}$

Then the kinetic energy of the electron revolving in a n^{th} circular orbit of radius r is

$$K.E = \frac{1}{2}mv_n^2$$

or, $K.E = \frac{1}{2}\frac{e^2}{4\pi\epsilon_0r_n}$ (from eqn 1.)

or, $K.E = \frac{e^2}{8\pi\epsilon_0r_n}$ ………………. 5

Similarly, the potential energy of electron in given orbit is define as the total work done in bringing it from infinite to given orbit. So the P.E of electron of charge -e revolving round the nucleus of charge +e in an orbit of radius r is;

$$P.E = \frac{-e^2}{4\pi\epsilon_0 r_n} \text{ .... } 6$$

So, the total energy of electron in n^{th} orbit of radius r is;

$$E = K.E + P.E$$

$$\text{or,} E_n = \frac{e^2}{8\pi\epsilon_0 r_n} + \frac{-e^2}{4\pi\epsilon_0 r_n}$$

$$\text{or,} E_n = \frac{-e^2}{8\pi\epsilon_0 r_n}$$

using the value of radius of orbit from eqn 3.
we get;

$$E_n = \frac{-e^2}{8\pi\epsilon_0(\frac{n^2h^2\epsilon_0}{\pi m e^2})}$$

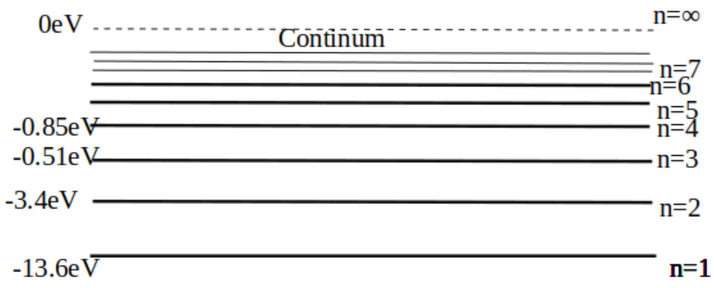


Fig: Energy levels diagram of Hydrogen atom.

or, $$E_n = \frac{-me^4}{8\epsilon_0^2 n^2 h^2} \text{ .... } 7$$

putting h= 6.62 X10^{-34} J/S ; ε_0= 8.85 X 10^{-12} $C^2/N\,m^2$; m= 9.1 X10^{-31} kg ; e= 1.6 X 10^{-19} C

$$E_n = \frac{-13.6}{n^2} eV \text{ .... } 8$$

For energy of electron at first energy level n=1; $E_1 = -13.6eV$

1. As energy of electron in its orbit is inversely proportional to n^2 , the energy of electronic orbit increases with atomic number and maximum at infinity (0eV).
2. The negative energy refers to electron is bounded to nucleus in an atom by attractive potential energy.
3. The energy spacing between energy levels decreases at higher energy levels and continuum at infinity.

Line Spectra of the H-atom:-

Let, us consider an electron jumps in H-atom from higher energy orbit n_2 to lower energy level n_1 and E_2 and E_1 are the corresponding energy level. The difference of energy with these orbit is emitted as a photon of frequency 'f' whose energy is given by

$$\Delta E = E_2 - E_1$$

$$\text{or,} hf = \frac{-me^4}{8\epsilon_0^2 n_2^2 h^2} - (\frac{-me^4}{8\epsilon_0^2 n_1^2 h^2})$$

$$\text{or,} hf = \frac{me^4}{8\epsilon_0^2 n_1^2 h^2} - \frac{me^4}{8\epsilon_0^2 n_2^2 h^2}$$

$$\text{or,} f = \frac{me^4}{8\epsilon_0^2 h^3}(\frac{1}{n_1^2} - \frac{1}{n_2^2})$$

$$\text{or,} \frac{c}{\lambda} = \frac{me^4}{8\epsilon_0^2 h^3}(\frac{1}{n_1^2} - \frac{1}{n_2^2})$$

$$\text{or,} \frac{1}{\lambda} = \frac{me^4}{8c\epsilon_0^2 h^3}(\frac{1}{n_1^2} - \frac{1}{n_2^2})$$

or, $\bar{\upsilon} = \frac{me^4}{8c\epsilon_0^2 h^3}(\frac{1}{n_1^2} - \frac{1}{n_2^2})$

where, $R_H = \frac{me^4}{8c\epsilon_0^2 h^3} = 1.097X10^7 m^{-1}$ is called Rydberg's Constant and $\bar{\upsilon} = \frac{1}{\lambda}$ is wave number i.e. number of wavelength present per unit length.

Or, $\bar{\upsilon} = \frac{1}{\lambda} = R_H(\frac{1}{n_1^2} - \frac{1}{n_2^2})$ ……………9

Spectral Series of H-atom:-

When an electron in a H-atom jumps from higher energy level to lower energy level, the difference of energies of two energy level is emitted as radiation of particular wavelength called spectral line. The wave number of spectral line obtained for transition of electron from higher n_2 energy level to lower n_1 energy level is

$\bar{\upsilon} = \frac{1}{\lambda} = R_H(\frac{1}{n_1^2} - \frac{1}{n_2^2})$ …………. 1

where, $R_H = \frac{me^4}{8c\epsilon_0^2 h^3} = 1.097X10^7 m^{-1}$ is called Rydberg's Constant.

In a H-atom, Spectral lines of different wavelengths are obtained for transition of electron between two different energy levels which are as follow;

1. Lyman Series: This series is obtained when electron jumps from any higher energy level to first energy level i.e. from n_2 =2, 3, 4……..∞ to n_1 = 1. The corresponding radiation from this series lies in UV region in electromagnetic series.

$\bar{\upsilon} = \frac{1}{\lambda} = R_H(1 - \frac{1}{n_2^2})$

2. Balmer Series:

This series is obtained when electron jumps from any higher energy level to second energy level i.e. from n_2 =3, 4 ,5……….∞ to n_1 = 2. The wavelength of corresponding radiation from this series lies in visible region in electromagnetic series.

$\bar{\upsilon} = \frac{1}{\lambda} = R_H(\frac{1}{2^2} - \frac{1}{n_2^2})$

The transition of electron from n_2 = 3 to n_1 = 2 is called first Balmer line or α-line (H_α) and from n_2 = 4 to n_1 = 2 is called second Balmer line or β-line (H_β).

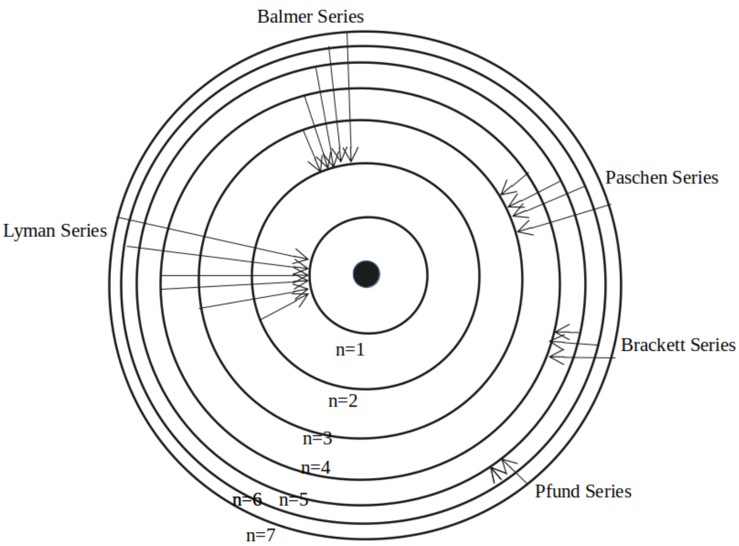


Fig: Spectral Series of Hydrogen atom.

3. Paschen Series:

This series is obtained when electron jumps from any higher energy level to third energy level i.e. from n_2 =4 ,5 ,6....……..∞ to n_1 = 3. The wavelength of corresponding radiation from this series lies in infrared (IR) region in electromagnetic series.

$\bar{\upsilon} = \frac{1}{\lambda} = R_H(\frac{1}{3^2} - \frac{1}{n_2^2})$

4. Brackett Series:

This series is obtained when electron jumps from any higher energy level to fourth energy level i.e. from n_2 =5 ,6 ,7....……..∞ to n_1 = 4. The wavelength of corresponding radiation from this series lies in infrared (IR) region in electromagnetic series.

$$\bar{\upsilon} = \frac{1}{\lambda} = R_H(\frac{1}{4^2} - \frac{1}{n_2^2})$$

5. P-fund Series:

This series is obtained when electron jumps from any higher energy level to fifth energy level i.e. from n_2 =6 ,7, 8....……..∞ to n_1 = 5. The wavelength of corresponding radiation from this series lies in infrared (IR) region in electromagnetic series.

$$\bar{\upsilon} = \frac{1}{\lambda} = R_H(\frac{1}{5^2} - \frac{1}{n_2^2})$$

Transition of electron in H-atom:-

There is two possibilities for the transition of electron between any two energy levels and based on that there is two types of spectrum obtained in case of H-atom.

1. Emission Spectrum: When an electron jumps from higher energy level to lower energy level it emits radiation equivalent to energy difference between two energies level. Thus obtained radiation spectrum is called emission spectrum. Basically, it is of five kinds in H-atom.
2. Absorption Spectrum:As electron jumps from lower energy level to higher energy level it absorbs energy of photons equivalent to energy difference between two energies level. Thus, obtained radiation is called absorption spectrum. This spectrum consists of brighter background with some dark lines corresponding to the frequencies absorbed by the electron. This pattern of dark lines is called absorption spectrum.

Excitation energy/potential :

Electron in particular energy level about nucleus of atom is bounded by attractive potential energy. The first energy level in H-atom is called ground state while others than first is excited energy state.

The potential energy acquired by any electron in any higher excited state from its ground state is called excitation energy and the corresponding potential is called excitation potential.

Excitation energy = $E_n - E_1$

where n= 2, 3, 4, …….. for higher energy level except infinity and 1.

Excitation potential eV= $E_n - E_1$

or, V = $(E_n - E_1)$ /e

Ionization energy/Potential:

The minimum potential energy required to jump electron from its ground state energy level to infinite energy level such that electron is no more bound to nucleus of atom and never return back to it, is called ionization potential energy and corresponding potential is called ionization potential.

At infinity electron have zero energy so, for H-atom its ionization energy is 13.6 eV. i.e.

I.E = E_∞ - E_1

or, I.E = 0- (-13.6 eV) = 13.6 eV.

Numerically, the ground state energy is equal to the ionization energy.

Critical energy/potential:

The minimum energy acquired by an electron to move at least first excitation state from any energy level i.e. from n_1 to n_2 or n_3 to n_4 and on so on is called critical energy and corresponding potential is called critical potential.

Experimental Determination of Critical potential-Frank-Hertz experiment:

In 1914 A.D, Frank and Hertz experiment successfully verified the evidence of existence of discrete nature of energy level in an atom. They perform an experiment for the first time to verify the quantization of atomic energy levels and determine experimentally the value of critical potential of atom popularly known to be Frank-Hertz experiment.

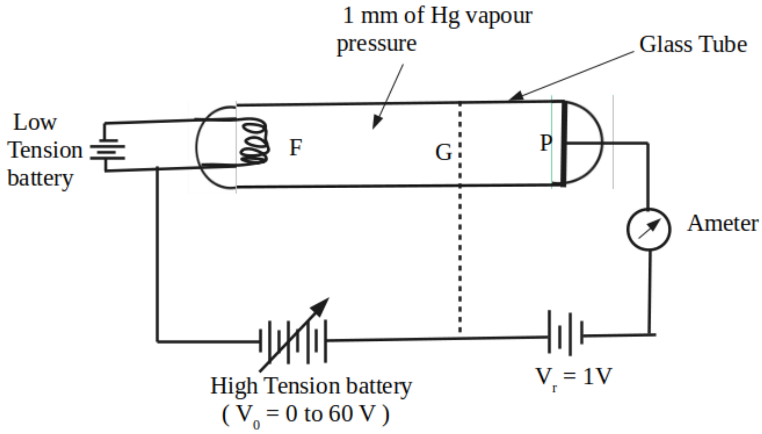


Fig: Experimental Set up for Frank-Hertz Experiment.

The experiment includes a cylindrical glass tube filled with Hg-vapour at very low pressure about 1mm pressure. A low tension battery is used across a heating filament wire 'F' that heated the wire and produce an electron inside tube. A variable potentiometer (V_0) having a range of 0-60V is used as a accelerating potential and a grid (G) which is further connected to the retarding potential (V_r) ranges upto 1 V for screening of electron inside the tube. Finally, to record the plate current an ammeter is connected in series with high potentiometer in the circuit as shown in figure.

As soon as the p.d i.e. accelerating potential is applied across filament wire 'F' and plate 'p', the electrons produced in filament wire due to heating effect ejected out and accelerated towards plate 'P'. Thus, accelerated electron inside tube are able to reach the plate if and only if they have enough energy greater than 1eV otherwise grid 'G' will screen/stop them. On increasing the accelerating potential, there is linear increase in plate current just below 4.9V. At 4.9V , it is observed that plate current drop suddenly and again starts to rise beyond 4.9V linearly up to 9.8V. Further, at 9.8V it fall sharply and again the nature gets repeated as shown in graph.

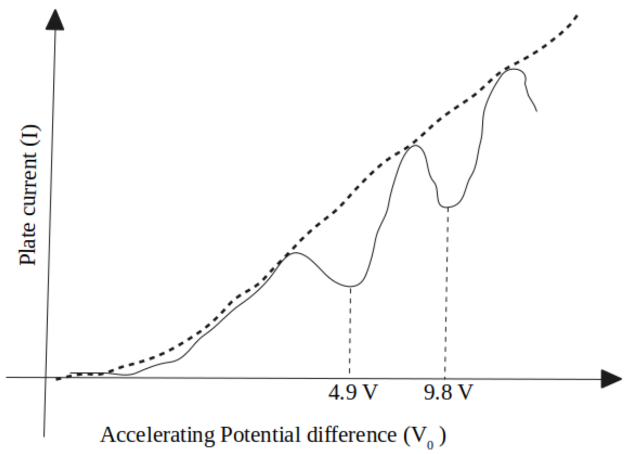


Fig: Graph plot between voltage and plate current in Frank-Hertz experiment.

Explanation of Graph:-

A graph plot between a plate current vs accelerating potential obtained from an Frank and Hertz experiment is as shown in figure. A dashed line represent for current in tube with increasing potential across electrode in absence of Hg vapour inside tube i.e. when tube is vaccum.

The solid curve for the Hg-vapour. A graph consists of number of rise and fall at particular potential value. On increasing the potential inside tube an electron gets accelerated and encounter inelastic collision with Hg-atom such that they losses their energy to Hg-atom and turning them to their excited state. At a potential of about 4.9V Hg-atom The first dip in current at 4.9 V is due to loss of energy by electron to Hg atom on collision. So, this energy 4.9eV is absorbed by Hg-atom and goes to its excited state and as a result there is sharp first fall in plate current was observed. The plate current is not zero because statistically, some of electrons may each the plate escaping from collision.

A second deep in plate current was observed at about 9.8V which is describe due to two successive inelastic collision with Hg-atom. So, Hg-atom get excited from its first excited energy state to next state. Further, thus exited Hg-atom emits the radiation of particular wavelength which can be measured by using the spectroscopic technique and was measured to be λ=2536 A^0.

Hence,the energy emitted by such Hg atom;

$$E = hf = h\frac{c}{\lambda}$$

$$\text{or,}E = \frac{6.626X10^{-34}X3X10^{8}}{2536X10^{-10}} = 7.843X10^{-19}J$$

$$\text{or, } E = \frac{7.843X10^{-19}}{1.6X10^{-19}} = 4.9eV$$

Thus, the energy lost by electron during in inelastic collision with Hg-atom is reobtained as a quantum of radiation energy of wavelength $\lambda = \frac{hc}{E}$. In this way,Frank and Hertz experiment verify the existence of discrete nature of energy in atomic and sub-atomic level.

The energy diagram obtained from experiment for different discrete energy state in Hg-atom is as shown in figure.

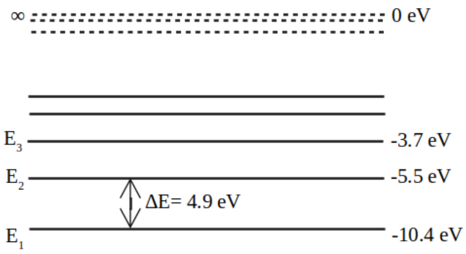


Fig: Discreet Energy level diagram of Hg-atom.

Note:

Limitation of Frank and Hertz experimental

1. It is not able to distinguish between excitation and ionization potentials.
2. Experiment is not not suitable for more electronegativity atoms like oxygen, Fluorine as these atoms high higer attractive force for electron.
3. The actual value of critical potential is slightly less than observed value.

Dual nature of Radiation :-

The phenomenon of interference, diffraction and polarization of light can only be explained on the basis of wave theory of light i.e. light behaves as wave nature while some phenomenon like photoelectric effect, explain Compton effect and absorption of waves by atom can only successfully explain on the basis of quantum theory i.e. light possess packet of energy and behaves like particle. Thus, these phenomenon clearly shows a radiation has dual nature, this is to say light behaves as a wave as well as a particle.

De-Broglie Wave Theory or hypothesis (Matter wave dual nature):-

In 1924 A.D de-Broglie derive a relation of matter wavelength (wave associated with matter) in terms of momentum of particle using concept of dual character of electromagnetic radiation. He used the concept of quantization of energy of light and particle nature of energy.

According, to Plank's theory on black body radiation; energy of radiation of particular frequency is

$$E = hf \text{ ……………… } 1$$

and Further, according to Einstein's mass energy theory; energy equivalent to particle having 'm' mass is

$$E = mc^2 \text{ ……………… } 2$$

So, from 1 and 2

$$hf = mc^2$$

$$h\frac{c}{\lambda} = mc^2$$

$$\text{or, } \frac{h}{\lambda} = mc$$

$$\text{or, } \frac{h}{\lambda} = p$$

$$\text{or, } \lambda = \frac{h}{p}$$

where, h= plank's constant

p = mc is momentum of photon or p= mv for momentum of particle.

Hence, this wave associated with moving particle is called De-Broglie wave or matter wave whose corresponding wavelength is called De-Broglie wavelength or matter wavelength.

De-Broglie wave theory or hypothesis states that " whenever small mass particle moves with very high speed nearly about speed of light, then it is associated with significant value of wave and hence such particle can behaves both as a particle and mass."

De-Broglie's wavelength of an electron:

For an electron with mass 'm' and charge 'e' is moving with 'v' velocity. Then , K.E of electron $(E_K) = \frac{1}{2}mv^2$

$$\text{or, } v = \sqrt{\frac{2E_K}{m}} \text{ …………………. } 1$$

So, De-Borglie wave length of electron is $\lambda = \frac{h}{mv}$………….. 2

from eqn 1 and 2. $\lambda = \frac{h}{m\sqrt{\frac{2E_K}{m}}}$

$$\text{or, } \lambda = \frac{h}{\sqrt{2mE_K}} \text{…………….. } 3$$

This is the De-broglie wave length in term of kinetic energy of particle.

Further, for an electron be accelerated by applying 'V' volts potential in order to have 'v' velocity then ; K.E of electron (E_K)= electric energy

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

$$\text{or, } v = \sqrt{\frac{2eV}{m}} \text{………….. } 4$$

from eqn 2 and 4.

$$\lambda = \frac{h}{m\sqrt{\frac{2eV}{m}}}$$

$$\text{or, } \lambda = \frac{h}{\sqrt{2emV}} \text{ ……………. } 5$$

This is the De-broglie wave length in term of accelerating potential.

Experimental Verification of De-Broglie Hypothesis:

In 1927 A.D Davission and Germer perform an experiment in order to verify the existence of matter wave i.e. De-Broglie wave hypothesis. An experimental set up consists of a filament 'F' which is heated with a low tension battery and thus produced electrons are accelerated towards the nickel crystal surface for its diffraction with the help of variable potentiometer 'V'. A detector is connected with galvanometer which measures the amount of diffracted electron in term of its intensity.

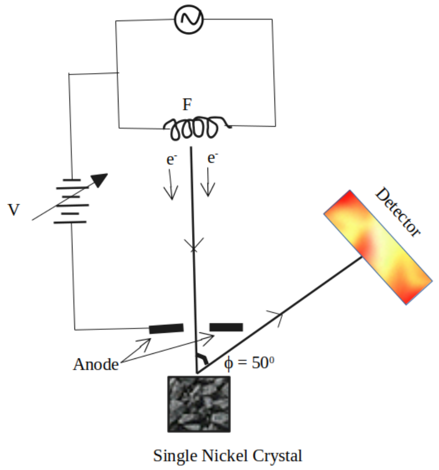


Fig: experimental set up used for Davisson-Germer experiment.

When we plot a graph, for intensity of diffracted electron and accelerating potential we obtained the graph as shown in fig. In this graph, for a specific angle of diffraction $\Phi=50^0$, there is maximum intensity of diffraction electron beam at at potential 54V. If so, the wavelength related to electron that is accelerated by V potential is

$$\lambda = \frac{h}{\sqrt{2emV}} = 1.67A^0 \text{ .... } 1$$

If the electron behaves like a completely a particle nature, we did not expect such variation in intensity of diffracted beam of electrons but the experiment shows a maximum intensity at a particular accelerating potential.

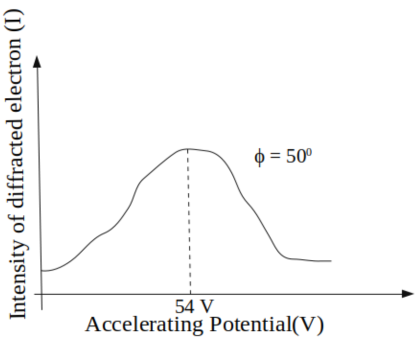


Fig: Graph plot between intensity of electron diffracted Vs accelerating potential.

Now, if we use a X-ray which is wave completely wave in nature, its diffraction on Nickel's crystal surface with crystal lattice spacing (d) equal to 0.91 $A^{0.}$ Then from Bragg's law of diffraction we have;

$$2d \sin\theta_n = n\,\lambda \text{ .... } 2$$

from figure; $\theta_1+\phi+\theta_1= 180^0$

or, $\theta_1 = 65^0$

So, for first order diffraction n=1; and with d=0.91 A^0 and $\theta_1= 65^0$. From eqn 2 we get,

$$\lambda = 1.66\ A^0$$

This is what we have is comparable to the wavelength of electron as obtained from equation 1 and is nearly equal to wavelength of X-ray used for same type of diffraction. Hence, this clearly verified that electron behaves like wave nature and there is existence of matter wave in atomic dimensional level.

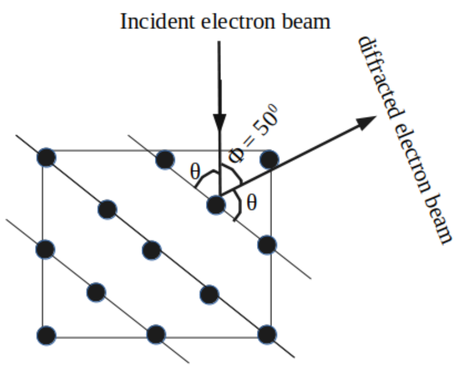


Fig: Atomic plane in Single Nickle Crystal.

Heisenberg's Uncertainty Principle:-

Heisenberg's Uncertainty principle states that It is impossible to determine precisely and simultaneously the values of canonical conjugate variables i.e position and momentum, energy and time , angular momentum and angular displacement to a required degree of accuracy. An error or uncertainty in measurement occurs during measurement of canonical variables, for Δx and Δp be the uncertainty in measurement in position and momentum of an electron in atom respectively. Then, the product of uncertainty is relate by

$$\Delta x \, .\Delta p \geq \hbar \qquad \text{where } \hbar = h/2\pi \text{ is reduced Plank's constant.}$$

Similarly, $\Delta E \, .\Delta t \geq \hbar$ and

$$\Delta L \, .\Delta \Theta \geq \hbar$$

Hence, according to Heisenberg it is obtained that when the uncertainty in measurement in one variable is minimize then this results to large uncertainty in measurement of other.

Application of Heisenberg's Uncertainty principle:

1. This principle is use to verify the existence of proton and neutron inside the nucleus of atom and the non-existence of an electron inside the nucleus.
2. It helps in calculation the size of an atom and binding energy of an electron in an atom.
3. This principle is useful to determine the ground state energy of linear harmonic oscillator (zero point energy).
4. It is applicable to show the stability of atom.
5. It is use to calculate strength of nuclear force.

Proof of Non existence of electron inside the nucleus:

The size of nucleus (radius) is of order 1 fermi unit i.e. 10^{-15} m. Let us consider an electron lies inside the nucleus then the possible maximum uncertainty for position of electron inside nucleus is

$$\Delta x = \text{diameter of nucleus}$$

$$\text{or, } \Delta x = 2X10^{-15} \text{ m}$$

We have;

$$\Delta x \, .\Delta p = \hbar$$

$$\text{or, } m\Delta v = \frac{\hbar}{2X10^{-15}}$$

$$\text{or, } \Delta v = \frac{\hbar}{2X10^{-15} X\, m}$$

$$\text{or, } \Delta v = \frac{1.05X10^{-34}}{2X10^{-15} X\, 9.1X10^{-31}}$$

$$\text{or, } \Delta v = 5.67X10^{10}\, m/s$$

Thus, the uncertainty in speed of electron inside the nucleus is obtained to be greater than speed of light which is not possible as the maximum attainable speed is that of light velocity. This contradicts our assumption and hence proved that electron can not lies inside the nucleus of an atom.

Matter wave equation:-

According to De-Broglie a moving particle is associated with wave and a mater consists of large number of particles. If we consider the wave associate with matter as a mechanical wave, this arises a different complex situation and violets the general assumptions of physical laws. In order to remove such difficulty, Schrodinger provided the concept of wave packet in order to describe the dynamics of particle and matter instead of simple plane wave. A wave packet is a wave which is constructed by superposition of large number of plane wave and highly localized. To obtained a wave packet, different plane waves with slightly different in amplitude, frequency and wavelength are mixed together. So, wave packet have group velocity rather than a single wave velocity train. To represent such matter wave, the matter wave equation can be written as;

$$\psi(x, y) = \iint_0^{\infty} A\,(w, k)\sin(\omega t - kx)dkd\omega$$

where, A is amplitude of wave packet that is function of wavelength and frequency of wave; $\nu = \frac{\omega}{2\pi}$ and $\lambda = \frac{2\pi}{k}$

Phase velocity:

A matter wave is represented by wave packet obtained by linear superposition of number of planes waves that are having slightly different amplitudes and frequencies and thus, the velocity of individual wave train that forms the wave packet is called phase velocity. A phase veolcity is representing the velocity of particle.

$$v_p = f.\lambda = 2\pi f.\frac{\lambda}{2\pi} = \frac{2\pi f.}{\frac{2\pi}{\lambda}} = \frac{\omega}{k}$$

Group velocity:

The velocity of matter wave in which large numbers of waves are mixing together and traveling with a constant speed that guides the waves is called group velocity of matter wave. A group velocity is representing the velocity of wave packet (matter wave).

$$v_g = \frac{d\omega}{dk}$$

Let, us consider two matter wave equation having nearly equal amplitude and of slightly different frequency and wavelength as

$\psi_1 = A\sin(\omega t - kx)$ …………… 1

$\psi_2 = A\sin\{(\omega + \Delta\omega)t - (k + \Delta k)x\}$ …………….. 2

here, $\omega \gg \Delta\omega$ and $k \gg \Delta k$

Now; the new matter wave after the superposition of two waves is,

$$\psi = \psi_1 + \psi_2$$

or, $\psi = ASin(\omega t - kx) + A\sin\{(\omega + \Delta\omega)t - (k + \Delta k)x\}$

or, $\psi = 2A\sin\frac{(2\omega t + \Delta\omega t - 2kx - \Delta kx)}{2}\cos\frac{\{-(\Delta\omega t - \Delta kx)\}}{2}$

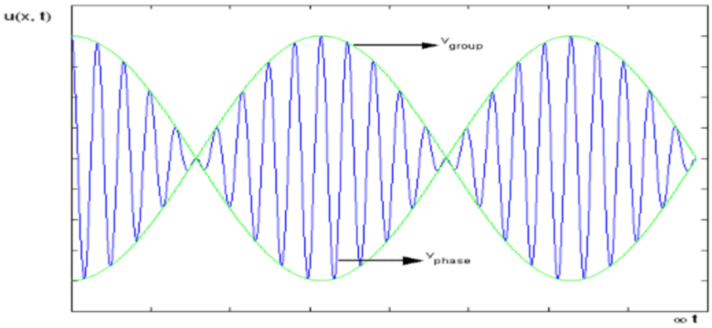
or, $\psi = 2A\sin\frac{2(\omega t - kx)}{2}\cos\frac{\{(\Delta\omega t - \Delta kx)\}}{2}$

or, $\psi = 2A\cos\frac{\{(\Delta\omega t - \Delta kx)\}}{2}\sin(\omega t - kx)$

or, $\psi = A'\sin(\omega t - kx)$ ……..... 3 where, $A' = 2A\cos\frac{\{(\Delta\omega t - \Delta kx)\}}{2}$ is the resultant amplitude of wave that guide the resultant wave.

This shows that resulting wave of two waves is also a traveling wave after superposition with same frequency and wavelength except its amplitude is modulated and periodically varying and describe for a group of particles.

Further, here $A' = 2A\cos(\frac{\Delta\omega t}{2} - \frac{\Delta kx}{2})$ also represent a wave with larger wavelength and smaller frequency that envelopes the resultant wave after superposition as shown in figure.



The velocity of the wave inside the envelops is same as the velocity of individual wave whereas as each envelop includes a group of wave or wave packet and the velocity of this envelop wave (i.e. velocity of wave packet) is term as group velocity and is given as

$$v_g = \frac{d\omega}{dk} \ldots\ldots\ldots\ldots\ldots\ldots 4$$

From De -Broglie wave hypothesis; wave associated with moving particle is

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

or, $p = \frac{h}{\lambda}$

or, $p = \frac{h}{2\pi}\frac{2\pi}{\lambda}$

or, $p = \hbar k$ where, $k = \frac{2\pi}{\lambda}$ is momentum wave vector of wave.

or, $dp = \hbar dk$

$$dk = \frac{dp}{\hbar} \ldots\ldots\ldots\ldots\ldots.. 5$$

Further, energy of wave is, $E = h\nu$

or, $E = \frac{h}{2\pi} 2\pi\nu$

or, $E = \hbar\omega$ where, $\omega = 2\pi\nu$is angular speed of wave.

or, $dE = \hbar d\omega$

or,$d\omega = \frac{dE}{\hbar} \ldots\ldots\ldots\ldots\ldots 6$

From eqns 4, 5 and 6; we get

$$v_g = \frac{\frac{dE}{\hbar}}{\frac{dp}{\hbar}} = \frac{dE}{dp} = d\frac{p^2/_{2m}}{dp} = \frac{1}{2m}\frac{dp^2}{dp} = \frac{1}{2m}2p = \frac{p}{m} = v_{particle}$$

Thus, this shows that the group velocity i.e. wave packet velocity represents the velocity of particle.

Relation between group velocity and phase velocity:

We know; the phase velocity of wave is;

$$v_p = \frac{\omega}{k} \ldots\ldots\ldots\ldots\ldots.. 1$$

and the group velocity of wave as $v_g = \frac{d\omega}{dk} \ldots\ldots\ldots 2$

from 1 and 2 ;

$$v_g = \frac{dv_p k}{dk}$$

or,$v_g = v_p\frac{dk}{dk} + k\frac{dv_p}{dk}$

or,$v_g = v_p + k\frac{dv_p}{dk} \ldots\ldots\ldots\ldots\ldots.. 3$

Now, further we know; $k = \frac{2\pi}{\lambda}$

$$\text{or,}\frac{dk}{d\lambda} = 2\pi\frac{d\lambda^{-1}}{d\lambda}$$

$$\text{or,}\frac{dk}{d\lambda} = -2\pi\frac{1}{\lambda^2}$$

$$\text{or,}dk = -2\pi\frac{1}{\lambda^2}d\lambda$$

then equation 3 becomes;

$$v_g = v_p + k\frac{dv_p}{-2\pi\frac{1}{\lambda^2}d\lambda}$$

$$\text{or,}v_g = v_p - \frac{2\pi}{\lambda}\frac{\lambda^2}{2\pi}\frac{dv_p}{d\lambda}$$

$$\text{or,}v_g = v_p - \lambda\frac{dv_p}{d\lambda} \ldots\ldots\ldots\ldots\ldots\ 4$$

This is the required relationship between group velocity and particle velocity.

Cases I: For dispersive medium i.e. medium in which velocity of wave is function of wavelength of wave. i.e $\frac{dv_p}{d\lambda} \neq 0$

So,

$v_p - v_g = \lambda\frac{dv_p}{d\lambda} = positive$ and phase velocity is greater than group velocity in this case this is to say there is phase difference between phase velocity and particle velocity.

Cases II: For non-dispersive medium i.e. medium in which velocity of wave is not function of wavelength of wave. Different waves with different wavelength have same velocity. i.e $\frac{dv_p}{d\lambda} = 0$ So, $v_p = v_g$ and phase velocity is equal to group velocity in this case