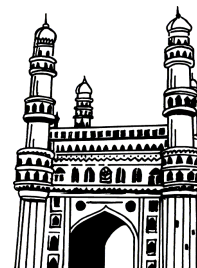


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PHYSICS PAPER - V

STUDY MANUAL

Important Questions	V - VII
Unit - I	1 - 46
Unit - II	47 - 98
Unit - III	99 - 128
Unit - IV	129 - 170

SOLVED MODEL PAPERS

Model Paper - I	171 - 172
Model Paper - II	173 - 174
Model Paper - III	175 - 176

SYLLABUS

UNIT - I

SPECTROSCOPY

Atomic Spectra: Introduction - Drawbacks of Bohr's atomic model - Sommerfeld's elliptical orbits - relativistic correction (no derivation). Stern & Gerlach experiment, Vector atom model and quantum numbers associated with it. L-S and j-j coupling schemes. Spectral terms, selection rules, intensity rules - spectra of alkali atoms, doublet fine structure, Zeeman Effect, Paschen-Back Effect and Stark Effect (basic idea).

Molecular Spectroscopy: Types of molecular spectra, pure rotational energies and spectrum of diatomic molecule. Determination of inter nuclear distance. Vibrational energies and spectrum of diatomic molecule. Raman effect, classical theory of Raman effect. Experimental arrangement for Raman effect and its applications.

UNIT - II

QUANTUM MECHANICS

Inadequacy of classical Physics

Spectral radiation - Planck's law (only discussion). Photoelectric effect - Einstein's photoelectric equation. Compton's effect - experimental verification.

Matter waves & Uncertainty principle

de Broglie's hypothesis wavelength of matter waves, properties of matter waves. Phase and group velocities. Davisson and Germer experiment. Double slit experiment. Standing de Broglie waves of electron in Bohr orbits. Heisenberg's uncertainty principle for position and momentum (x and p_x), Energy and time (E and t). Gamma ray microscope. Diffraction by a single slit. Position of electron in a Bohr orbit. Complementary principle of Bohr.

Schrodinger Wave Equation

Schrodinger time independent and time dependent wave equations. Wave function properties Significance. Basic postulates of quantum mechanics. Operators, eigen functions and eigen values, expectation values.

UNIT - III

NUCLEAR PHYSICS

Nuclear Structure : Basic properties of nucleus - size, charge, mass, spin, magnetic dipole moment and electric quadrupole moment. Binding energy of nucleus, deuteron binding energy, p-p, n-n and n-p scattering (concepts, nuclear forces. Nuclear models - liquid drop model, shell model.

Alpha and Beta Decays : Range of alpha particles, Geiger - Nuttall law. Gamow's theory of alpha decay, Geiger, Nuttall law from Gamow's theory. Beta spectrum - neutrino hypothesis,

Particle Detectors : GM counter, proportional counter, scintillation counter.

UNIT - IV

SOLID STATE PHYSICS & CRYSTALLOGRAPHY

Crystal Structure : Crystalline nature of matter. Crystal lattice, Unit Cell, Elements of symmetry. Crystal systems, Bravais lattices. Miller indices. Simple crystal structures (S.C., BCC, FCC, CsCl, NaCl, diamond and Zinc Blende)

X-ray Diffraction: Diffraction of X-rays by crystals, Bragg's law, Experimental techniques - Laue's method and powder method.

Bonding in Crystals: Types of bonding in crystals - characteristics of crystals with different bondings. Lattice energy of ionic crystals-determination of Madelung constant for NaCl crystal. Calculation of Born Coefficient and repulsive exponent. Born-Haber cycle.

Contents

UNIT - I

Topic	Page No.
1.1 Drawbacks of Bohr's Theory	2
1.2 Sommerfeld Elliptical Orbits - Relativistic Correction	2
1.2.1 Sommerfeld Relativistic Correction	3
1.3 Stern and Gerlach Experiment	4
1.4 Drawbacks of Bohr and Sommerfeld Atomic Model & Concept of Vector Model	6
1.4.1 Concept of Vector Atom Model	7
1.5 Quantum Numbers Associated with Vector Atom Model	8
1.6 Coupling Schemes	10
1.7 Spectral Terms	12
1.8 Selection Rules & Intensity Rules	13
1.8.1 Selection Rules	13
1.8.2 Intensity Rules	13
1.9 Alkali Atoms Spectral Terms	14
1.10 Doublet Finite	15
1.11 Zeeman Effect	20
1.12 Paschen - Back Effect	21
1.13 Stark Effect	22
1.14 Spectroscopy	23
1.14.1 Types of Molecular Spectra	23
1.15 Pure Rotational Energies and Spectrum of Diatomic Molecule	24
1.16 Determination of Inter Nuclear Distance	27
1.17 Vibrational Energies and Spectrum of Diatomic Molecules	27
1.18 Raman Effect & Experimental Study Raman Effect	31
1.18.1 Experimental Setup to Study Raman Effect	32
1.18.2 Applications	33
➤ Problems	34 - 37
➤ Short Question and Answers	38 - 43
➤ Choose the Correct Answers	44 - 45
➤ Fill in the Blanks	46 - 46

Topic	Page No.
UNIT - II	
2.1 Classical Physics	48
2.1.1 Inadequacy of Classical Physics	48
2.2 Spectral Radiation	48
2.3 Planck's Radiation	50
2.4 Experimental Study of Photo - Electric Effect	50
2.4.1 Einstien's Photoelectric Equation	52
2.5 Compton's Effect - Experimental Verification	54
2.6 Matter Waves & Uncertainty Principle	56
2.6.1 de Broglie's Hypothesis Wavelength of Matter Waves	58
2.6.2 Properties of Matter Waves	60
2.6.3 Phase and Group Velocities	60
2.7 Davisson and Germer Experiment	62
2.8 Double Slit Experiment	64
2.9 Standing de-Broglie Waves of Electron in Bohr Orbits	64
2.10 Heisenberg's uncertainty Principle for Position and Momentum (x and px) Energy and time (E and t).	66
2.11 Gamma Ray Microscope	67
2.12 Diffraction by a Single Slit	68
2.12.1 Consequence of Uncertainty Relation (Particle in a Box)	69
2.13 Position of Electron in a Bohr Orbit	70
2.14 Complementary Principle of Bohr	71
2.15 Applications of Uncertainty Principle	71
2.16 Schrodinger Time Independent and Time dependent Wave Equations	74
2.17 Wave Function Properties	77
2.18 Physical Significance of Wave Function	78
2.19 Basic Postulates of Quantum Mechanics	78
2.20 Operators	79
2.21 Eigen Values and Eigen Functions	80
2.22 Expectation Values	81
➤ Problems	82 - 90
➤ Short Question and Answers	91 - 95
➤ Choose the Correct Answers	96 - 97
➤ Fill in the Blanks	98 - 98

Topic	Page No.
UNIT - III	
3.1 Basic Properties of Nucleus	100
3.2 Binding Energy of Nucleus	102
3.3 Binding Energy of Deuteron and Calculate Binding Energy of Deuteron	104
3.4 Proton - Proton Scattering (– Scattering)	104
3.5 Neutron - Proton Scattering (Scattering)	105
3.6 Proton - Neutron Theory of Nuclear Composition	105
3.7 Nuclear Models	106
3.7.1 Liquid Drop Model	106
3.7.2 Shell Model	109
3.8 Range of α -particles	110
3.9 Geiger - Nuttall Law	110
3.9.1 Gamow's Theory of α - Decay	111
3.10 Geiger - Nuttall Law from Gamow's Theory	115
3.10.1 Beta - Ray Continuous and Discrete Spectrum	115
3.10.2 Neutrino Hypothesis of β - Decay	116
3.11 Geiger - Muller Counter	117
3.12 Proportional Counter	118
3.13 Scintillation Counter	119
➤ Problems	121 - 122
➤ Short Question and Answers	123 - 126
➤ Choose the Correct Answers	127 - 127
➤ Fill in the Blanks	128 - 128
UNIT - IV	
4.1 Crystalline Nature of Matter	130
4.1.1 Lattice Translation	130
4.2 Unit Cells	130
4.3 Elements of Symmetry	131
4.4 The Seven Crystal Systems	133
4.4.1 Bravais Space Lattices	135
4.5 Miller Indices	135
4.5.1 Lattice points per unit cell	136

Topic	Page No.
4.6 Some Simple Crystal Structures	136
4.6.1 Simple cubic structure	136
4.6.2 Body centred structure(BCC)	139
4.6.3 Face centred crystal structure	140
4.6.4 Structure of CsCl	142
4.6.5 Sodium chloride structure	143
4.6.6 Diamond Structure	144
4.6.7 Zinc Blende structure	146
4.7 X-ray Diffraction	147
4.7.1 Diffraction of x-ray by crystal	147
4.7.2 Bragg's law	147
4.8 Experimental Technique	148
4.8.1 Crystallography by laue's method	148
4.8.2 Crystallography by Powder Method	150
4.9 Types of Bonding Crystals	151
4.9.1 Characteristics of crystal with different bonding	152
4.9.2 Lattice energy of ionic crystals	153
4.10 Determination of Madelung Constant for NaCl Crystal	154
4.11 Calculation of Born of Coefficient and Repulsive Exponent	156
4.12 Born Haber Cycle	158
➤ Problems	160 - 162
➤ Short Question and Answers	163 - 168
➤ Choose the Correct Answers	169 - 169
➤ Fill in the Blanks	170 - 170

Important Questions

UNIT - I

1. Describe the theory of Stern and Gerlach experiment. Why it is necessary to use a beam of neutral atoms.

Ans :

Refer Unit-I, Q.No. 4.

2. Explain vector atom model ?

Ans :

Refer Unit-I, Q.No. 6.

3. Discuss the L-S and J-J coupling schemes associated with an atom ?

Ans :

Refer Unit-I, Q.No. 8.

4. What is Paschen - Back Effect?

Ans :

Refer Unit-I, Q.No. 16.

5. Give the elementary theory of the origin of the vibrational spectrum of a molecule ?

Ans :

Refer Unit-I, Q.No. 21.

6. What is raman effect ? Explain classical theory of raman effect ?

Ans :

Refer Unit-I, Q.No. 22.

UNIT - II

1. Describe the distribution of energy in the spectrum black body radiation?

Ans :

Refer Unit-II, Q.No. 3.

2. Explain experimental study of photo - electric effect?

Ans :

Refer Unit-II, Q.No. 5.

3. Discuss in brief about Compton effect?

Ans :

Refer Unit-II, Q.No. 7.

4. Obtain an expression for wave velocity and group velocity.

Ans :

Refer Unit-II, Q.No. 13.

5. Describe Davisson Germer Experiment to demonstrate the wave character of electrons?

Ans :

Refer Unit-II, Q.No. 14.

6. Give the experimental illustrations of Heisenberg uncertainty principle.

Ans :

Refer Unit-II, Q.No. 18.

UNIT - III

1. Explain binding energy of nucleus and calculate binding energy of nucleus.

Ans :

Refer Unit-III, Q.No. 2.

2. What are the similarities between liquid drop and a nucleus?

Ans :

Refer Unit-III, Q.No. 8.

3. Discuss in detail Gamow's theory of α - Decay?

Ans :

Refer Unit-III, Q.No. 12.

4. Describe Geiger - Nuttall Law from Gamow's Theory. Explain β -ray spectrum.

Ans :

Refer Unit-III, Q.No. 13.

5. Describe in detail the construction and working of a Geiger - Muller Counter.

Ans :

Refer Unit-III, Q.No. 15.

6. Explain the working of proportional counter.

Ans :

Refer Unit-III, Q.No. 16.

7. Describe the construction and working of scintillation counter.

Ans :

Refer Unit-III, Q.No. 17.

UNIT - IV

1. Mention the seven crystal systems.

Ans :

Refer Unit-IV, Q.No. 6.

2. Explain about miller indices.

Ans :

Refer Unit-IV, Q.No. 8.

3. Explain simple crystal structures.

Ans :

Refer Unit-IV, Q.No. 10.

4. Explain body centred structure.

Ans :

Refer Unit-IV, Q.No. 11.

5. Define Face centred crystal structure.

Ans :

Refer Unit-IV, Q.No. 12.

6. State & Explain Bragg's law.

Ans :

Refer Unit-IV, Q.No. 18.

7. What is madelung constant? Explain it with respect to sodium chloride lattice.

Ans :

Refer Unit-IV, Q.No. 28.

UNIT - I

SPECTROSCOPY

Atomic Spectra: Introduction - Drawbacks of Bohr's atomic model - Sommerfeld's elliptical orbits - relativistic correction (no derivation). Stern & Gerlach experiment, Vector atom model and quantum numbers associated with it. L-S and j-j coupling schemes. Spectral terms, selection rules, intensity rules - spectra of alkali atoms, doublet fine structure, Zeeman Effect, Paschen-Back Effect and Stark Effect (basic idea).

Molecular Spectroscopy: Types of molecular spectra, pure rotational energies and spectrum of diatomic molecule. Determination of inter nuclear distance. Vibrational energies and spectrum of diatomic molecule. Raman effect, classical theory of Raman effect. Experimental arrangement for Raman effect and its applications.

ATOMIC SPECTRA

Introduction

In the nineteenth century it was clear to the scientists that the chemical elements consist of atom. Although, no one has so far seen individual atoms, yet there is no doubt for its existence. Electron, one of the fundamental constituent particles, was first of all invented by J.J. Thomson

To account for the experimentally observed spectroscopic data at that time, several theories have been proposed from time to time regarding the atomic structure which are known as atomic models. The various models are as follows :

1. Thomson's Plum Pudding Model
2. Rutherford's Nuclear Model
3. Bohr's Model
4. Sommerfeld's Relativistic Model
5. Vector Model
6. Wave Mechanical Model

1.1 DRAWBACKS OF BOHR'S THEORY

Q1. Mention the drawback's of Bohr's theory?

Ans :

Bohr's theory was able to explain successfully a number of experimental observed facts and has correctly productly the spectral lines of neutral hydrogen atom and singly ionized helium atom, etc. in terms of only principal quantum number n . However, the theory fails to explain the following facts :

- (i) The theory could not account the spectra of atoms more complex than hydrogen.
- (ii) The theory does not give any information regarding the distribution and arrangement of electrons in atom.
- (iii) It does not explain the experimentally observed variations in intensity of the spectral lines of a element.
- (iv) This theory cannot be used to calculated about transforms from one level to another such as the rate at which they occur or the selection rules which apply to them.
- (v) This theory cannot be used for the quantitative explanation of chemical bonding.

1.2 SOMMERFELD ELLIPTICAL ORBITS - RELATIVISTIC CORRECTION

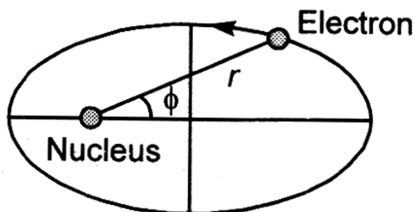
Q2. Explain sommerfeld elliptical orbit theory ?

Ans :

Sommerfeld in 1921 modified Bohr's model by introducing the idea of notion of electron in elliptical orbits and taking into consideration the variation of mass with velocity. The improved model is known as sommerfeld relativistic model.

Elliptical Orbits :

According to Sommerfeld, the electron moving around the nucleus under an inverse - square force. In the elliptical orbit the position of the electron at any time may be fixed by two coordinates r and ϕ where r is the radius vector and ϕ is the angle which the radius vector makes with the major axis of the ellipse, i.e., azimuthal angle. Now consider an electron of mass m and linear tangential velocity of the electron can be resolved into two components - one along radius vector called the radial velocity and other perpendicular to radius vector called the transverse velocity. Corresponding to these velocities the Sommerfeld assumed that the same generalised condition which has been postulated for circular orbit also holds in elliptical orbit, i.e.,



$$\oint P_r dr = n_r h$$

$$\oint P_\phi d\phi = n_\phi h$$

where P_r and P_ϕ are the components of linear momentum p of the electron along the radial direction and transverse direction respectively, n_r and n_ϕ are integers. More specifically n_r is called the radial quantum number and n_ϕ as angular or azimuthal quantum, ϕ indicator that the integration is to be carried out over one cycle of the motion.

1.2.1 Sommerfeld Relativistic Correction

Q3. Discuss the Sommerfeld relativistic correction.

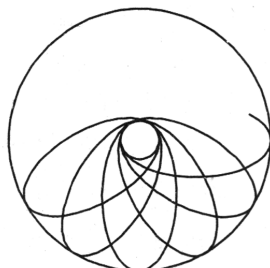
Ans :

Sommerfeld pointed out that the velocity of the electron in the innermost Bohr's orbit is 0.007 of the velocity of light hence the variation of mass of the electron with velocity should be taken into consideration. The velocity of the electron moving in an elliptical orbit varies at different parts of the orbit. It is maximum when the electron is nearest to the nucleus and minimum when it is farthest from the nucleus.

This implies that effective mass of electron will be different at different parts of its orbit. Consequently, the curvature of elliptical path is not exactly the same in two positions and hence the ellipse is not a complete one. Sommerfeld has electron has two momenta one along radius vector called as radial momentum and other perpendicular to radial quantum numbers and n_ϕ as angular or azimuthal quantum number. In order to quantize the elliptical orbits, Sommerfeld introduced the two quantum numbers n_r and n_ϕ and because they stand for one periodic system. Hence $n_r + n_\phi = n$. n_r , quantum number, n is known as principal quantum number, n_r is radial number.

For the normal state of the hydrogen atom, the principal quantum number $n = 1$ corresponding to $n = 1$, there are two possibilities, i.e., $n_r = 0$, $n_\phi = 1$ ($n = n_r + n_\phi$) and $n_r = 1$, $n_\phi = 0$. When $n_\phi = 0$ (semiminor axis is zero), the ellipse converted into a straight line and the electrons have to pass through the nucleus twice during every period. This type of motion is not possible hence n_ϕ is one.

Thus, corresponding to $n = 1$, $n\phi$ is one and the first orbit is a circle identical to Bohr's orbit. With $n = 2$, $n\phi$ may have values 1 and 2. Thus, corresponding to $n = 2$, two orbits are possible, one is $n = 2$, $n\phi = 2$, a circle and other $n = 2$, $n\phi = 1$ an ellipse. Similarly for $n = 3$, $n\phi = 3$, three orbits are possible - one circle corresponding to $n = 3$, $n\phi = 3$ and two ellipses. Similarly for $n = 3$, $n\phi = 3$, three orbits are possible - one circle corresponding to $n = 3$, $n\phi = 3$ and two ellipses with $n = 3$, $n\phi = 1$ and $n\phi = 2$.



Made such calculations and has shown that the parts of the electron is not a closed ellipse but a complicated curve known as rosette - a processing ellipse whose major exist processes slowly in the plane of the ellipse about an axis through one of the foci as.

The expression of energy of an electron in a hydrogen like atom for a particular state characterised by quantum number n and $n\phi$, after relativistic correction can be shown to be

$$E_n = - \frac{mz^2 e^4}{8\epsilon_0^2 C^2 h^2} \times \left[1 + \frac{a^2 z^2}{m} \left[\frac{1}{n\phi} - \frac{3}{4n} \right] \right]$$

Where

$$a = \frac{e^2}{2\epsilon_0 ch} \cong \frac{1}{317}$$

a is called as sommerfeld fine structure constant.

1.3 STERN AND GERLECH EXPERIMENT

Q4. Describe the theory of Stern and Gerlach experiment. Why it is necessary to use a beam of neutral atoms.

Ans :

(Imp.)

In Stern and Gerlach experiment a team of silver atom is passed throug an inhomogenous magnetic field. The silver atoms beam is produced by heating silver is a small electric oven o fig. and passing the beam through slots S_1 and S_2 .

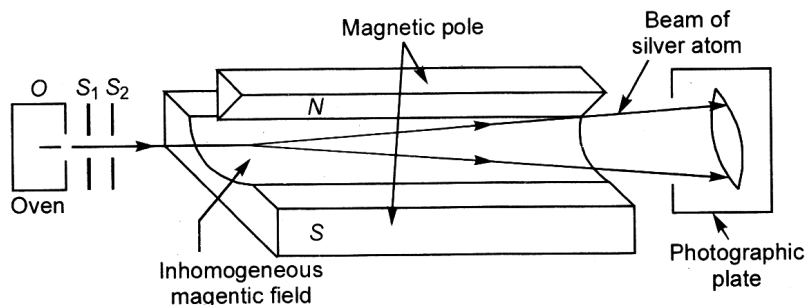


Fig. : Stern - Gerlach Experiment

The inhomogeneous magnetic field is produced having one of the pole pieces of the magnetic flat with a cylindrical groove and the other in the form of a knife edge, parallel to the groove as shown in the figure. Thus the magnetic field is of much greater intensity near the knife edge than anywhere else in the gap i.e., the intensity of the magnetic field increases as we go from the centre towards the upper knife edge pole and decreases as we go below towards the lower pole fig. A photographic plate p records the configuration of the beam after its passage. Through the field to avoid the deflection of silver atoms by gas molecules, the whole arrangement is enclosed in a highly evacuated glass vessel.

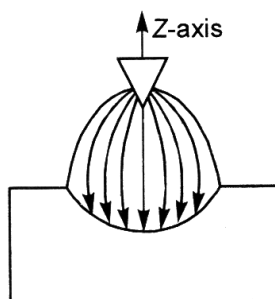
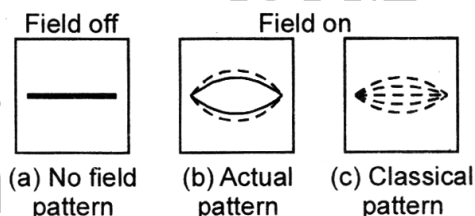


Fig. : Side view of magnet with lines of force

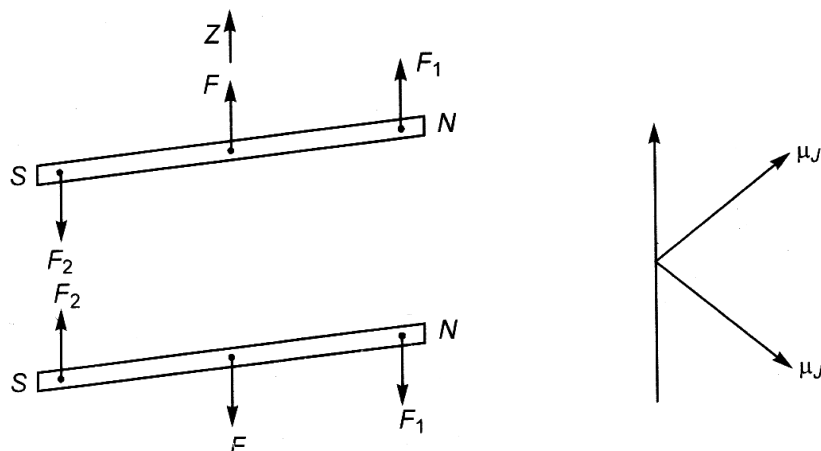
In the absence of magnetic field, a trace of the form of a narrow strip is obtained as shown in fig. in the presence of the inhomogeneous magnetic field the strip splits up into two components as shown in fig. According to the classical shape of the strip in inhomogeneous field is shown in figure.



The splitting of silver beam into two components in inhomogeneous field verifies the existence of electron spin and the postulate of space quantisation as shown below :

When all silver atoms passing a magnetic μ_J pass through the inhomogeneous magnetic field, they experience different amounts of force in vertical direction depending on their orientation. This is due to the fact that when a bar magnet is placed in inhomogeneous magnetic field (let its north pole experiences a greater force the south pole). Then the magnet experiences a resultant force $F_1 - F_2$ fig. The magnitude and direction of the force F depends on the magnitudes of F_1 and F_2 i.e., orientation of the axis of magnet relative to the magnetic field.

This force causes a deflection of the silver atoms to varying degrees in a vertical direction, if, the magnetic moment μ_J can have all possible orientations (according to the classical view), then the beam of silver atoms, consisting of millions of atoms having all possible orientations of μ_J will be spread out into a broad continuous band on emerging from the magnetic field. In this way it should produce a broad continuous path on the photographic plate. Experimentally only two narrow strips are obtained on the photographic plate. Therefore, the predictions of classical physics are not correct in this case. The two narrow strips shown that μ_J cannot have all possible orientations, but only two possible orientations as shown in figure. We know that μ_J is proportional to angular momentum J and hence the direction of J relative to well defined direction should have only two values. According to the quantisation rules, the magnitude of J is given by



$$J = \sqrt{j(j+1)} \cdot \frac{h}{2\pi}$$

There are $(2j + 1)$ possible orientation of J

The stern - Gerlach experiment shown that $(2j + 1) = 2$

(or)

$$j = \frac{1}{2}$$

Thus $J = \frac{\sqrt{3}}{2} \cdot \frac{h}{2\pi}$

It is known that the angular momentum J of silver atoms is entirely due to spin of its valence electrons. Thus we conclude that the electron has a spin angular momentum.

$$S = \sqrt{S(S+1)} \cdot \frac{h}{2\pi}, \text{ where } S = \frac{1}{2}$$

Thus Stern and Gerlach found that the initial beam split into two distinct parts, corresponding to two opposite spin orientation in magnetic field that are permitted by space quantisation.

1.4 DRAWBACKS OF BOHR AND SOMMERFELD ATOMIC MODEL & CONCEPT OF VECTOR MODEL

Q5. What are the drawbacks of Bohr and Sommerfeld atomic model ? Explain concept of vector model ?

Ans :

This model is an extension of Bohr - Sommerfeld atoms model. Following are the drawbacks of Bohr and sommerfeld atomic models :

- (i) Original Bohr's theory was incapable of explaining the fine structure of the spectral lines even in the simplest hydrogen atom.
- (ii) In case of complex atoms, Bohr's theory fails to calculate the energy of the system and frequencies of radiation emitted.

- (iii) Sommerfeld modification, though gave a theoretical back ground of the splitting of individual spectral lines of hydrogen, still in could not predict the correct number of observed fine structure of these lines.
 - (iv) Both the models could not explain the distribution and arrangement of electrons in atoms.
 - (v) Both the models do not throw any light on the intensities of the spectral lines.
 - (vi) Both the models could not explain the anomalous zerman effect and stark effect.
- To overcome all these objections a new model known as vector atom model was proposed.

1.4.1 Concept of Vector Atom Model

Q6. Explain vector atom model ?

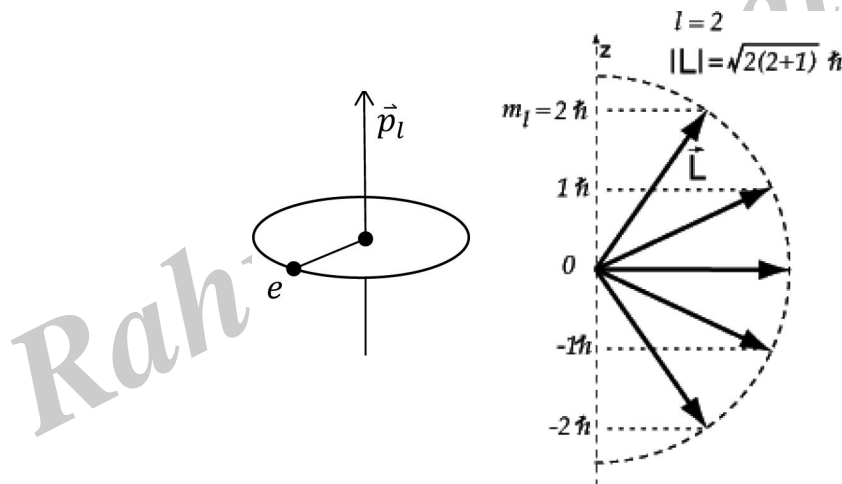
Ans :

(Imp.)

The main contributors for this model are Bohr, Sommerfeld, Uhlenbeck, Goudsmith, Pauli, Stern and Gerlach.

The two main features of vector atom model are :

1. Spatial Quantization
2. Electron Spin



1. Space Quantization

According to spatial quantization, the orientation of the electron orbits in space is quantized. The plane of the orbit in space or the direction of orbital angular momentum can taken only certain selected orientations with respect to a preferred direction which could be an external magnetic field (B). ($B \rightarrow 0$),

The magnitude of orbital angular momentum of the electron is given by

$$L = p_l = l \frac{h}{2\pi} = l\hbar.$$

where

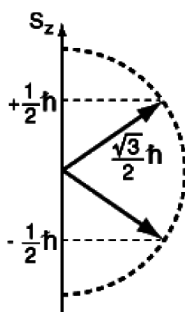
l is the orbital quantum number. The associated magnetic moment is called the orbital magnetic moment μ_l . For a given value of principal quantum number n , l can take n values from 0 to $(n - 1)$. Thus for $n = 3$, $l = 0, 1, 2$. For a given value of l , an orbit in space can have $(2l + 1)$ orientations in space with respect to external magnetic field. Then according to the space quantization rule, only those orientation of

$\bar{p}_i \cdot \hat{p}_i \cos \phi = m_l \frac{h}{2\pi} = m_l \hbar$ where ϕ is the angle between \bar{p}_i and the external field direction in space, m_l is the magnetic quantum number for orbital motion and can have the possible values of $0, \pm 1, \pm 2, \pm 3, \dots \dots \pm l$ i.e., m_l can have $(2l + 1)$ values.

For example, in case of $l = 2$, $m_l = \pm 2, \pm 1, 0, -1, -2$.

2. Spinning Electron Hypothesis

According to electron spin hypothesis proposed by Uhlenbeck and Goudsmit, an electron in addition to orbital motion has a spin motion. The spin motion is quantized. The magnitude of the spin angular



momentum is $p_s = s \frac{h}{2\pi} = s \hbar$ where s is the spin quantum number. The value of $s = 1/2$. The associated magnetic moment is called the spin magnetic moment μ_s . The spin angular momentum has two orientations with respect to external magnetic field i.e., either parallel or antiparallel to field.

1.5 QUANTUM NUMBERS ASSOCIATED WITH VECTOR ATOM MODEL

Q7. Explain quantum numbers associated with vector atom model ?

Ans :

Quantum numbers associated with the vector model of the atom

In vector atom model, for each of the component parts like orbital and spin motion, orbital and spin angular momentum, a quantum number is assigned. They are the set of integers or half integers characterizing the energy states of an electron in an atom. Each electron in an atom is described by four different quantum numbers. They are n, l, s and j . In a strong magnetic field three more quantum numbers arise. They are m_l, m_s and m_j .

1. Principal Quantum Number (n)

It specifies the energy of an electron and the size of the orbital. It can take only integral values i.e. $n = 1, 2, 3, \dots, \infty$. All orbitals that have the same value of n are said to be in the same shell (level). For a hydrogen atom with $n = 1$, the electron is in its ground state; if the electron is in the $n = 2$ orbital, it is in an excited state. The total number of orbitals for a given n value is n^2 .

2. Orbital Quantum Number (l)

It specifies the shape of an orbital with a particular principal quantum number. It takes integral values between 0 and $n - 1$ i.e., $l = 0, 1, 2, 3, \dots, n - 1$. This quantum number divides the shells into smaller groups of orbitals called subshells (sublevels). Usually, a letter code is used to identify l

to avoid confusion with n . For $l = 0, 1, 2, 3, \dots$, the letters are s, p, d, f ... respectively. The orbital angular momentum is quantized and is given by $p_l = l \frac{h}{2\pi} = l\hbar$. According to wave mechanics $L = p_l = \sqrt{l(l+1)} \hbar$.

3. Spin Quantum Number (s) :

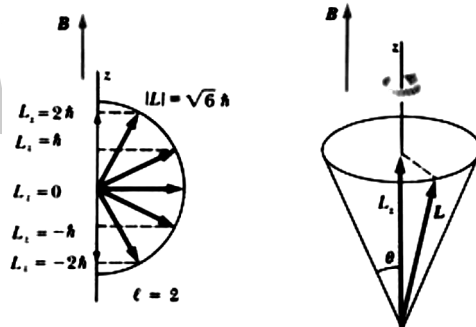
It has a magnitude of $\frac{1}{2}$. An electron can spin in only one of two directions (sometimes called up or down). The spin angular momentum is quantized and is given by $p_s = s \frac{h}{2\pi} = s\hbar$. According to wave mechanics $p_s = \sqrt{s(s+1)} \hbar$.

4. Total Angular Quantum Number (j)

It is the resultant of orbital and the spin motion and is given by $j = l + s = l \pm 1/2$. It is $l + s$ when s is parallel to l and $l - s$ when s is antiparallel to l . The total angular momentum is quantized and is given by $p_j = j \frac{h}{2\pi} = j\hbar$. According to wave mechanics $p_j = \sqrt{j(j+1)} \hbar$.

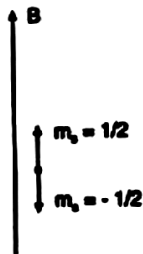
5. Magnetic Quantum Number (m_l)

It specifies the orientation in space of an orbital of a given energy (n) and shape (l). It is the projection of the orbital vector l on the external field direction, i.e., L_z . It is an integer and can have any of the $(2l + 1)$ values from $-l$ to $+l$. This quantum number divides the subshell into individual orbitals which hold the electrons; there are $2l + 1$ orbitals in each subshell. Thus the s subshell has only one orbital, the p subshell has three orbitals, and so on. If $l = 2$, then $m_l = -2, -1, 0, 1, +2$ as shown.



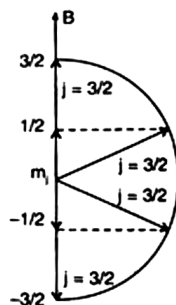
6. Magnetic Spin Quantum Number (m_s)

It specifies the orientation of the spin axis of an electron. It is the projection of the spin vector s on the external field direction. It can have $2s + 1$ from $-s$ to $+s$ excluding zero, m_s can have only two values $+\frac{1}{2}$ or $-\frac{1}{2}$.



7. Magnetic Total Angular Momentum Quantum Number (m_j)

It is the projection of the total angular momentum vector j on the external field direction. It can have $2j + 1$ from $-j$ to $+j$ excluding zero.



1.6 COUPLING SCHEMES

Q8. Discuss the L-S and J-J coupling schemes associated with an atom ?

(OR)

Explain L-S and J-J coupling schemes ?

Ans :

(Imp.)

Generally two types of coupling known as Russell - Saunders or L-S coupling and J-J coupling occurs which are described below :

(i) **L-S coupling** : This type of coupling occurs most frequently and hence is known as normal coupling.

In this coupling orbital angular momentum vectors l of the electrons combine to form a resultant vector L & all the spin angular Momentum vectors S like wise combine to form a resultant vector S .

Now the vectors L & S combine to form a vector J

We can represent the coupling as

$$L = (l^1 + l^2 + l^3, \dots)$$

$$S = (s^1 + s^2 + s^3, \dots)$$

$$J = L + S$$

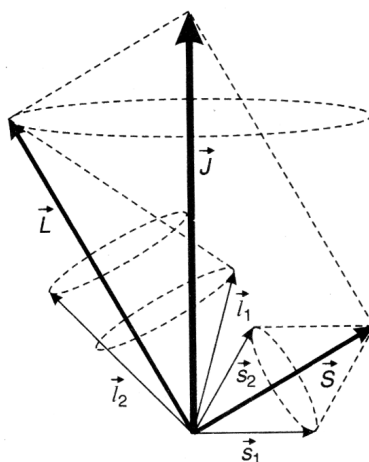


Fig. : Showing L-S Coupling

- Here L is always an integer zero i.e., 0, 1, 2, 3 etc. The value S depends on the number of Electrons & the direction of their Spin vectors.
- In case of two Electrons if the spins are parallel the value is one and when the Spins are antiparallel the value of S is Zero.
- Thus, S is an integer for an Even number of Electrons & half integer for an odd number of Electrons.

Two electrons	Three electrons	Four electrons
$S = 1$ 0	$3/2$ $1/2$	2 1 0

Now $J = \text{Integer (0, 1, 2, 3, etc) where } S \text{ is integer}$
(i.e., for odd electron system)

$$J = \text{Half integer } \left(\frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \dots \text{ etc.} \right)$$

where

S is half integer

(i.e., for odd electron system)

J must always be positive & never negative because it represents the total angular momentum.

- (ii) **J-J Coupling:** The interaction between the spin & orbital vectors in each electron is stronger than the interaction between Either the spin vectors or orbital vectors of different Electrons. In such case j - j coupling is most suitable than $L - S$ coupling.

- In $j - j$ coupling, Each Electron is considered separately & its total angular momentum j is obtained by the relation

$$j = l + S$$

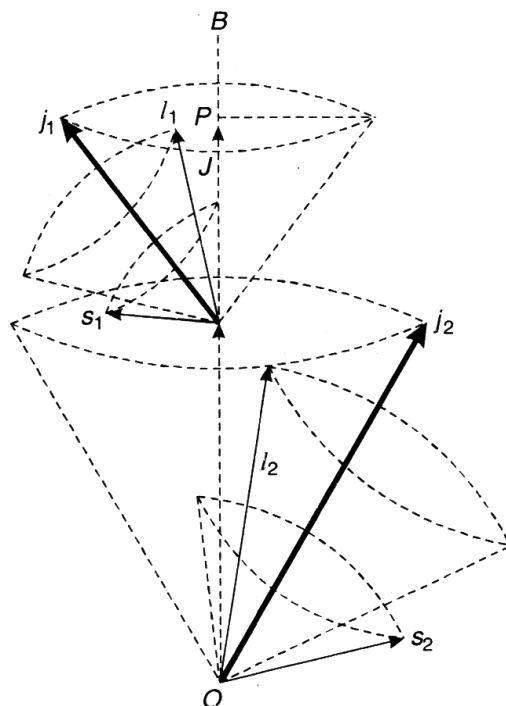
- Then the total angular momentum J of the atom would be vector sum of all the individual j vectors of the electrons.

$$j_1 = (l_1 + S_1), j_2 = (l_2 + S_2), j_3 = (l_3 + S_3), \dots$$

$$J = (j_1 + j_2 + j_3) + \dots$$

$$= \Sigma j.$$

- Pure $j - j$ coupling is seldom found. In most of known cases l - s coupling is effective.



1.7 SPECTRAL TERMS

Q9. Explain the spectral terms ?

Ans :

To describe the Electronic Configuration, Small letters are used to represent the l values are shows again

l	Notation
0	s
1	p
2	d
3	f
4	g
5	h

To represent the configuration, following two points are considered.

- The value of total quantum number n is written as a prefix to the letter representing its ' l ' values.
- The number of Electrons with the same n & p values is written at the upper right hand side of letter representing their ' l ' value.

1.8 SELECTION RULES & INTENSITY RULES

1.8.1 Selection Rules

Q10. Explain selection rules.

Ans :

We know that in an atom, there are number of energy states. It is observed that all the transitions between different energy states (as spectral lines) do not appear. The spectral lines are governed under certain principles known as selection rules. There are three selection rules as described below :

- (a) **The selection rule for L** : Only those lines are observed for which the value of L changes by ± 1 (i.e., $\Delta L = \pm 1$).
- (b) **The selection rule for J** : Only those spectral lines are observed when the transitions take place between states for which $\Delta J = \pm 1$ or 0. The transition $0 \rightarrow 0$ is not allowed.
- (c) **The selection rule for S** : Only those spectral lines are observed for which the value of S changes by 0 (i.e., $\Delta S = 0$).
- (d) **Selection rules for magnetic quantum numbers** : In the presence of magnetic field, the orbital magnetic quantum number m_l and spin magnetic quantum numbers m_s play an important part in the transition. Their selection rules are

$$\Delta m_l = 0 \text{ or } \pm 1 \text{ and } \Delta m_s = 0$$

In consequence

$$\Delta m_j = 0 \text{ or } \pm 1$$

1.8.2 Intensity Rules

Q11. Explain Intensity Rules.

Ans :

The intensity rules are :

- (i) The intensity of the transition (i.e., a line) is strong for which L and J change in the same sense.
- (ii) The intensity of the transition is weak for which L and J change in opposite sense.
- (iii) The intensity of a line is strong when the transition is in the decreasing sense i.e., from $L \rightarrow (L - 1)$.
- (iv) The intensity of a line is weak the transition is in the increasing sense i.e., from $L \rightarrow (L + 1)$.
- (v) The oppositely directed transition does not occur.

The above rules can be summarized as :

$\Delta L = -1,$	$\Delta J = -1$	Most intense line
$\Delta L = -1,$	$\Delta J = 0$	Less intense
$\Delta L = +1,$	$\Delta J = +1$	Weaker
$\Delta L = +1,$	$\Delta J = 0$	Weaker
$\Delta L = -1,$	$\Delta J = +1$	No transition
$\Delta L = +1,$	$\Delta J = -1$	No transition

1.9 ALKALI ATOMS SPECTRAL TERMS

Q12. Explain the spectra of alkali atoms ?

Ans :

After hydrogen, the next simplified spectra are of 'monovalent' atoms of alkali metals lithium (Li), Sodium (Na), Potassium (K), Rubidium (Rb), Cesium (Cs), etc. These belong to the group first of periodic table. In case of alkali atoms, the modified field shows the net effect of nucleus and the core elements i.e., the atom reduces to hydrogen-like. As the value of n increases, the energy levels in case of alkali metal approaches to that of hydrogen level. However, all alkali levels lie below the corresponding hydrogen level.

As the electron comes closer to the nucleus, it penetrates the atomic tank and the field is changed (Fig.). Due to penetration, the energy of the moving electron.

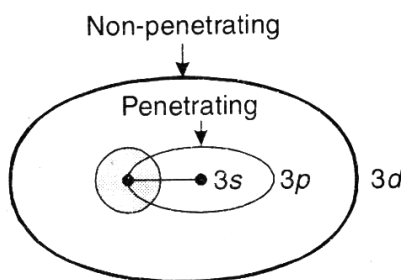


Fig. : Penetration of Orbits

Cannot be expressed by the term $-(R/n^2)$, i.e., by hydrogen-like atom. Now it is more convenient to use a term value in case of alkali spectra defined as

$$T = \frac{R}{n_{\text{eff}}^2} \quad \dots (1)$$

where n_{eff} is the effective quantum number.

The energy is also expressed by the following relation

$$T = \frac{R}{(m + \mu)^2} \quad \dots (2)$$

Where m is currently to n but not equal to n and μ is a fraction less than unity.

The value of μ is constant for a given value of L . Larger is the value of L . Smaller will be the value of μ and vice-versa. For smaller value of μ , the penetration of electron to nucleus core will be small.

The lines in the spectrum of an alkali atom can be grouped into following distinct four series :

1. Principal series (intense lines)
2. Sharp series (fine lines)
3. Diffuse series (comparatively broader lines)
4. Fundamental series (lies in infra-red region)

Let us express the wave numbers of these series in terms of their term values.

1. Principal Series

The series arises from the transitions between various P levels and lowest S level. The lowest S-level has the lowest possible value for the energy. This represents the ground state of the atom. The term values are as follows :

$$T_s = \frac{R}{(1 + \mu_s)^2}$$

Where R is Rydberg constant and μ_s , is the characteristic constant for the sharp series. Similarly, the term value for p dates are

$$T_p = \frac{R}{(m + \mu_p)^2}$$

Where μ_p is the characteristic constant of principal series, m is an integer equal to Or greater than 2. Further, $T_s > T_p$

The wave - number of principal series is given by

$$\bar{\nu}_p = T_s - T_p = \frac{R}{(1 + \mu_s)^2} - \frac{R}{(m + \mu_p)^2} \quad (m \geq 2) \quad \dots (1)$$

2. Sharp Series

This series comes from the transitions from S-levels (exclusive or lowest) of S-levels. The wave - number is given by

$$\bar{\nu}_p = \frac{R}{(2 + \mu_p)^2} - \frac{R}{(m + \mu_s)^2} \quad (m \geq 2) \quad \dots (2)$$

3. Diffuse Series

This series arises from transitions between the various transitions between D levels and lowest P - Level. The wave - number is expressed as

$$\bar{\nu}_D = \frac{R}{(2 + \mu_p)^2} - \frac{R}{(m + \mu_D)^2} \quad (m \geq 3) \quad \dots (3)$$

Where μ_D is the characteristics of diffuse series.

4. Fundamental Series

The fundamental series arises from the transitions from various F levels to the lowest D - level. The wave - number is expressed as

$$\bar{\nu}_F = \frac{R}{(3 + \mu_D)^2} - \frac{R}{(m + \mu_p)^2} \quad (m \geq 4) \quad \dots (4)$$

Where μ_p is the characteristic constant of fundamental series.

1.10 DOUBLET FINITE

Q13. Show how the concept of spinning electron accounts for the doubling of levels in spectrum of alkalis?

Ans :

The lines of optical spectra emitted by alkali atoms show a fine structure splitting. This splitting is small for lighter atoms and increases rapidly with increasing atomic number. All lines of the sharp series are close doublets and similarly, each line of principal series is also a double.

In the analysis of alkali spectra, it has been observed that 5-level is single while others P, D, F, ... are doublet levels. The splitting of the levels is due to the spin of electron. Actually, the spin magnetic moment

of optically active electron interacts with the internal magnetic field created by the motion of electron through the nuclear electric field. The phenomenon is known as spin orbit interaction. Due to this interaction, orbital angular momentum l of the optical electron is coupled with spin angular momentum s to form resultant j .

The quantum number j can take the following two values, i.e.,

$$j = l \pm s = l \pm \frac{1}{2}$$

The splitting of each energy level into two results due to $j = l + \frac{1}{2}$ and $j = l - \frac{1}{2}$ values. There is an expectation for 5-level because for 5-level, $l = 0$.

The complete notation of the levels is shown below :

Level	l	s	Multiplicity ($2s + 1$)	j	Full Notation
S	0	1/2	2	1/2	$^2S_{1/2}$
P	1	1/2	2	3/2, 1/2	$^2P_{3/2}, ^2P_{1/2}$
D	2	1/2	2	5/2, 3/2	$^2D_{5/2}, ^2D_{3/2}$
F	3	1/2	2	7/2, 5/2	$^2F_{7/2}, ^2F_{5/2}$

The relative splitting of levels $2P$, $2D$ and $2F$ for a given n value is illustrated in fig..

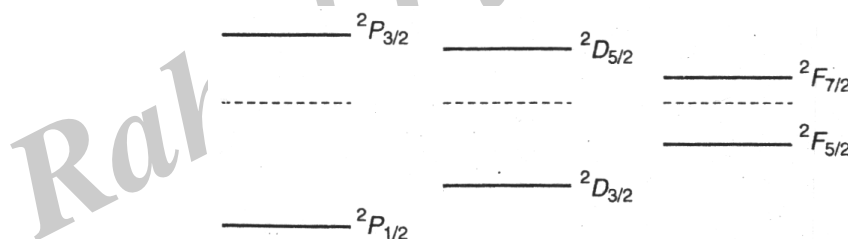


Fig. : Splitting of Alkali Level

The $2P$ levels are splitted as $^2P_{3/2}$ and $^2P_{1/2}$ where $^2P_{1/2}$ being deeper. Similarly, $2D$ and $2F$ levels are splitted as $^2D_{5/2}, ^2D_{3/2}$ and $^2F_{7/2}, ^2F_{5/2}$. It is also obvious that these splitting are much smaller.

The doublets of the sharp series are formed by the following transitions.:

$$n \ ^2S_{1/2} \rightarrow m \ ^2P_{1/2} \text{ and } m \ ^2P_{3/2} \text{ (with } n > m \text{)}$$

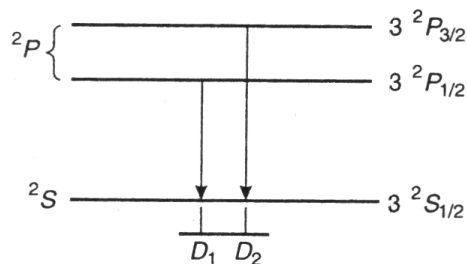
The principal series doublets are due to transitions

$$n \ ^2P_{3/2} \text{ and } n \ ^2P_{1/2} \rightarrow m \ ^2S_{1/2} \text{ (with } n > m \text{)}$$

Here n and m represent the total quantum numbers in vector atom mode.

The two transitions $3 \ ^2P_{1/2} \rightarrow 3 \ ^2S_{1/2}$ and $3 \ ^2P_{3/2} \rightarrow 3 \ ^2S_{1/2}$ are the first members of principal series and are lines of sodium referred to as sodium D lines doublet.

These are shown in fig.



Figure

The lines of the diffuse and fundamental series show a three component structure and are called component doublets. Diffuse lines arising from transition $3^2D_{5/2} \rightarrow 3^2P_{3/2}$, $3^2D_{3/2} \rightarrow 3^2P_{3/2}$, $3^2D_{3/2} \rightarrow 3^2P_{1/2}$ are shown in fig.

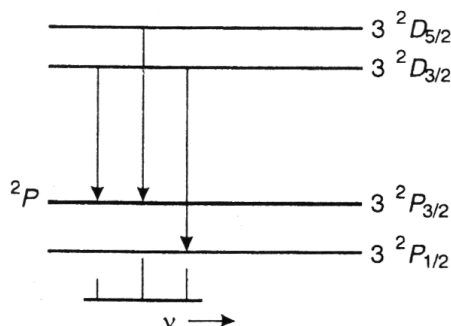
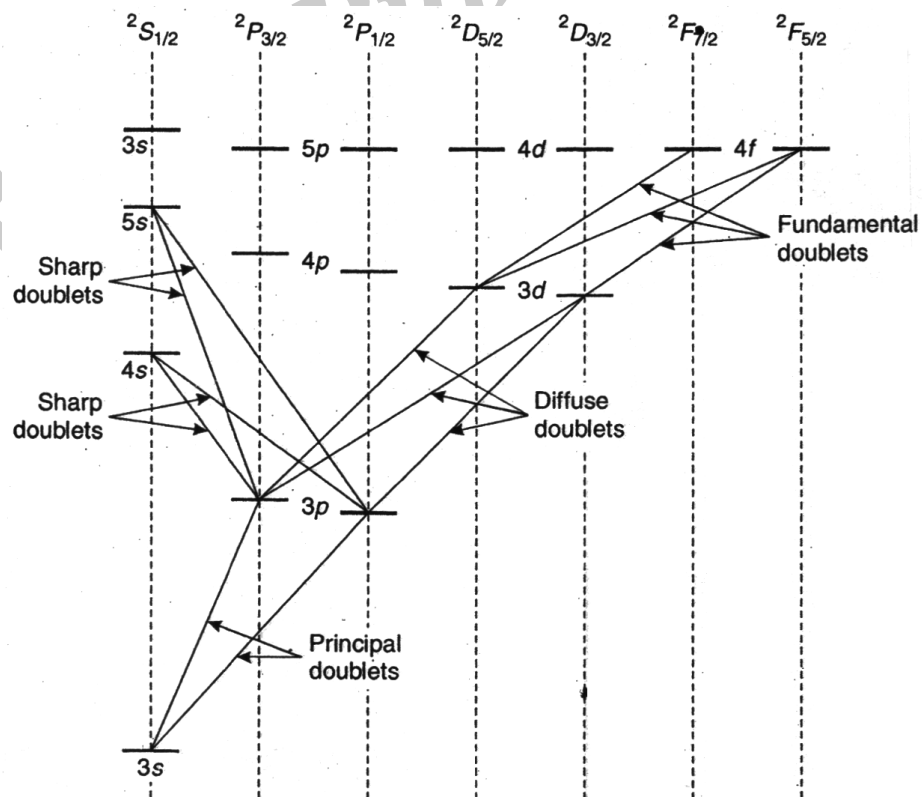


Fig. : Compound Doublets of Diffuse Series

The doublet character of Na spectrum is shown in fig.



Q14. Explain the singlet and triplet fine structures in alkaline earth spectra.*Ans :*

The alkaline earth elements are beryllium (Be), magnesium (Mg), calcium (Ca), strontium (Sr), barium (Ba) and mercury (Hg). They have two electrons in their outermost shell. The spectra of alkaline earth elements resemble the spectra of helium atom.

On excitation either one or both of the two valence electrons can go to higher energy states. Afterwards they give rise to transitions to lower energy states. Due to two electrons, a large number of transitions are possible. Therefore, the spectra of alkaline earths consists of a very large number of lines. The spectrum consists of two types of spectral lines, singlets and triplet.

These lines of each type can be grouped into four chief series, i.e., principal, sharp, diffuse and fundamental.

Let us consider the ground state of two valence electron system. In this case,

$$n = 1, l = 0 \text{ and } s = \frac{1}{2} \text{ for each electron.}$$

For two electrons system

$$L = l_1 + l_2 = 0 \text{ and } S = s_1 + s_2 = 0 \text{ or } 1$$

But Pauli's exclusion principle does not allow $S = 1$ state (parallel spins of two electrons).

Therefore, the term symbol is 1S_0 . So, the ground state of alkaline earth only shows singlet structure.

When the electron is excited, it comes into higher states. We consider the following cases :

1. Consider the first excited state (P state). For this state

$$L = l_1 + l_2 = 1$$

$$S = s_1 + s_2 = 0 \text{ or } 1$$

(i) With $S = 0$, $J = L + S = 1$ and we get singlet state 1P_1 .

(ii) With $S = 1$, $J = 2, 0 [(1 + 1), 1, (1 - 1)]$. In this case, we have $^3P_2, ^3P_1, ^3P_0$.

This is a triplet state.

2. Let us now consider the second excited state (D state). In this case,

$$L = 2, S = 0 \text{ or } 1.$$

Now we get

(i) With $L = 2$ and $S = 0$, $J = 2$ and the state is 1D_2 . This is a singlet state

(ii) With $L = 2$ and $S = 1$, $J = (3, 2, 1)$

The states are $^3D_3, ^3D_2$ and 3D_1 .

This is a triplet state

Hence, we have two sets of energy states. One set is singlet and is observed when spins are anti-parallel and the other set is of triplet states when spins are parallel.

Taking into account the fine structure of triplets, the following points are observed:

- (i) all members of sharp series are composed of three lines and approach a triplet limit
- (ii) all members of principal series are composed of three lines with decreasing separation and have a single limit
- (iii) all the members of diffuse and fundamental series contain six lines, three strong lines and three satellites with triplet limit.

In Hg-spectrum, the following main series are observed :

(a) Singlet system

$$\text{Principal series } \begin{cases} m \ ^1P_1 \rightarrow 1 \ ^1S_0 \text{ with } m \geq 2 \\ m \ ^1P_1 \rightarrow 2 \ ^1S_0 \text{ with } m \geq 3 \end{cases}$$

$$\text{Sharp series } m \ ^1S_0 \rightarrow 2 \ ^1S_1 \text{ with } m \geq 2$$

$$\text{Diffuse series } m \ ^1D_2 \rightarrow 2 \ ^1P_1 \text{ with } m \geq 3$$

(b) Triplet System

$$\text{Principal series } m \ ^3P_{0,1,2} \rightarrow 2 \ ^3S_1 \text{ with } m \geq 3$$

$$\text{Sharp series } m \ ^3S_1 \rightarrow 2 \ ^3P_{2,1,0}$$

$$\text{Diffuse series } m \ ^3D_{1,2,3} \rightarrow 2 \ ^3P_1 \text{ with } m \geq 3$$

Here m means the ground state of the atom and not the number of orbit, m = 2, first excited state and so on.

The diffuse triplets of mercury spectrum is shown in fig..

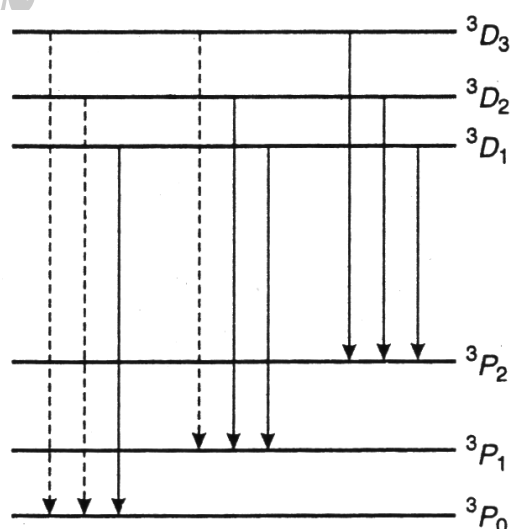


Fig. : Triplet system in Hg spectrum

The diffuse triplet of mercury is more complicated as it is obtained by combination of two triplet levels. Out of nine possible transitions, only six are allowed as shown in fig.

1.11 ZEEMAN EFFECT

Q15. What is zeeman effect? Describe the experimental arrangement to study the zeeman effect.

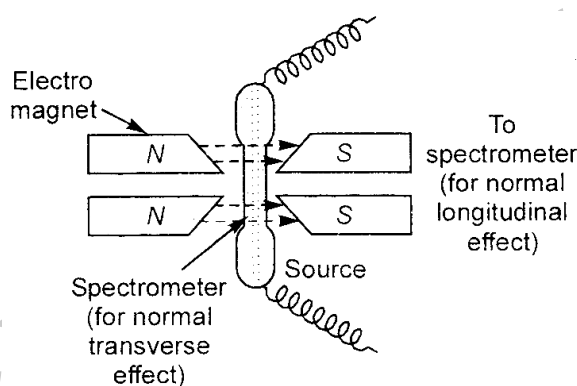
Ans :

Zeeman repeated Faraday's experiment with improved apparatus and observed the splitting of spectral lines. The splitting of spectral lines is known as Zeeman Effect.

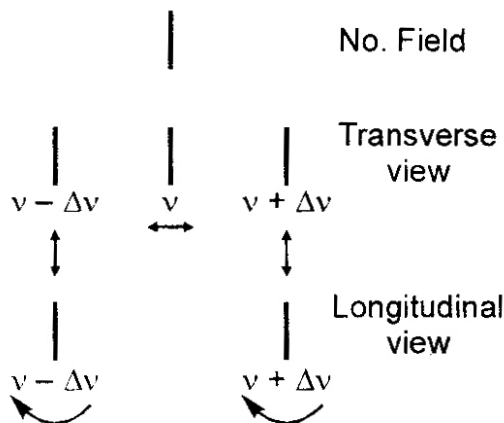
In 1896, Prof Zeeman discovered that when a source of radiation, giving line spectrum is placed in a magnetic field. The spectral lines are split up into a number of component lines, symmetrically distributed about the original line. Doublets, triplets and even more complex systems are observed. This is known as zeeman effect. If the magnetic field is very strong, each spectral line split up into two components in the longitudinal view and in three components in transverse view. This is known as normal Zeeman Effect. When the magnetic field is comparatively weak. Each line split into more than three components this is known as Anomalous Zeeman effect.

Experimental Arrangement

The experimental arrangement for observing normal zeeman effect is shown in figure (31). The source of radiation such as sodium flame as a mercury are is placed between



The pole pieces of a powerful electromagnet. The electromagnet has conical pole pieces and holes are drilled along the length so that light from the source can pass through it. Thus, the spectrum can be observed along the direction of the magnetic field. The spectral lines are observed with high resolving power spectroscope. The spectral lines may also be observed in a direction perpendicular to the magnetic field.



In the normal zeeman effect, when the light is viewed perpendicular to the direction of magnetic field. (Normal transverse zeeman effect). Three components are observed one in the same position as the original line having original frequency ν and two components being on either side of the central line and equally separated from it having frequencies $\nu + \Delta\nu$ and $\nu - \Delta\nu$. It is found that the central or original line is linearly polarised, parallel to the magnetic field whereas the component lines on either side are linearly polarised at right angles to the magnetic field as shown in the figure. (35). Here it should be remembered that the original spectrum line in the absence of magnetic field being unpolarised. When the light is viewed along the direction of magnetic field. (Normal longitudinal zeeman effect), there come two additional lines with frequencies $\nu + \Delta\nu$ and $\nu - \Delta\nu$ are observed while the central line having frequency ν is missing. These two lines are circularly polarised one being clockwise and the other anticlockwise i.e., these two lines are polarised in opposite directions as shown in fig. by arrows.

1.12 PASCHEN - BACK EFFECT

Q16. What is Paschen - Back Effect?

Ans :

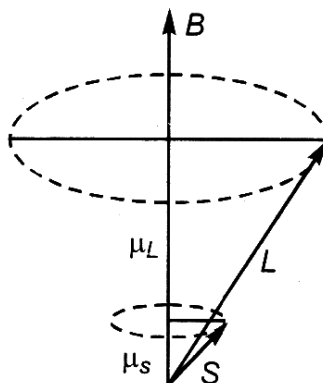
(Imp.)

The alkali metals, like Na, Li, K, etc., show anomalous zeeman effect only in weak fields. Paschen and Back showed that (whatever be the anomalous zeeman pattern of a given line in a magnetic field, the pattern is always approximated as normal zeeman triplet as the field strength is progressively increased). This fact is known as paschen - back effect. Thus the transition phenomenon between the two (anomalous zeeman effect and normal zeeman effect) is known as paschen - back effect.

Explanation of Paschen - Back Effect

When the magnetic field is increased, a stage is reached when the outer precession attains the order of magnitude of the inner one. Now the magnetic coupling between L and S is loosened and we cannot replace the magnetic moment μ of the atom by the parallel component μ_z between μ_L and μ_S when averaged over a period will not be equal to zero. This is the reason of paschen - back effect. If the magnetic field is raised still further the coupling between w and s becomes practically annulled. Now orbit and spin vectors L and S separately precess about the field direction as shown in fig. (34).

We have seen that when the external magnetic field is very strong the coupling between L and S breaks down and they precess separately about the magnetic field B .



The magnitudes of L and S along field direction (z-direction) are

$$L_z = m_l \left[\frac{h}{2\pi} \right] \text{ and } S_z = m_s \left[\frac{h}{2\pi} \right]$$

Here, the orbital quantum number m_l processes $(2l + 1)$ values from $-l$ to l with difference of unity further, the spin quantum number m_s possesses $(2s + 1)$ values from $-s$ to $+s$ with difference of unity.

The angular velocities of precession of L and S about the field directions are given by Larmor's theorem.

Accordingly

$$\omega_L = \frac{\mu_L}{|L|} B = \frac{eB}{2m_o}$$

$$\text{and } \omega_s = \frac{\mu_s}{|S|} B = \frac{2eB}{2m_o}$$

Thus, the change in energy due to magnetic field is

$$\begin{aligned} \Delta E &= \Delta E_L + \Delta E_s \\ &= \omega_L L_z + \omega_s S_z \\ &= \left(\frac{eB}{2m_o} \right) \left(\frac{m_L h}{2\pi} \right) + \left(\frac{2eB}{2m_o} \right) \left(\frac{m_s h}{2\pi} \right) \\ &= \frac{eh}{4\pi m_o} [M_L + 2M_s] B \end{aligned}$$

In terms of wave numbers, the shift is

$$\begin{aligned} \Delta \nu &= \frac{\Delta E}{hc} = \frac{e}{4\pi m_o c} [M_L + 2M_s] B \\ \Delta \nu &= \frac{eB}{4\pi m_o c} \bar{L} \end{aligned}$$

The quantity $(m_L + 2m_s)$ is known as strong field quantum number m_L can take only integral values while m_s can have either integral or half integer values. Thus, $(m_L + 2m_s)$ can have only integral values. As S or m_s can not change during a transition, the only change is due to m_L in the expression $(m_L + 2m_s)$. According to selection rule $m_L = 0$ or ± 1 , hence a given line will split in three components in strong magnetic field as in case of normal zeeman effect.

1.13 STARK EFFECT

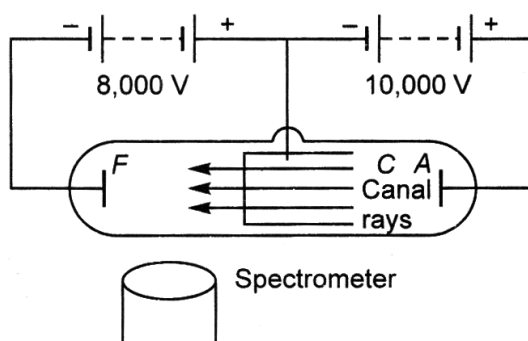
Q17. What is Stark Effect? Describe the experimental arrangement to study Stark Effect.

Ans :

The action of an electric field on the spectrum of hydrogen was discovered by Stark (1913) who observed the splitting of Balmer lines. the splitting of spectral lines due to the action of external electric field is called the Stark effect.

Experimental Study

The experimental arrangement is shown in fig. Stark effect placed on auxiliary electrode .F close behind the cathode cat a distance of few millimeters. The canal rays are produced in an ordinary discharge tube whose cathode is perforated. A. high potential difference is applied between cathode c and electrode F to produce a strong electric field of about 10^7V/M between F and C. The spectrum is studied by a high resolving power spectrometer.



The main features observed in case of Balmer series of hydrogen spectrum are :

1. Every line splits up into a number of sharp components.
2. All hydrogen lines form a symmetrical pattern. The pattern depends markedly on the quantum number n of the term involved. The number of lines and total width of the pattern increases with increase of n . Thus the number of components of H_β lines is greater than those of H_α lines and similarly the number of components of H_γ is greater than those of H_β .
3. The wave number differences are integral multiple of unit which is proportional to ϵ . It is same for all hydrogen lines.
4. Observations perpendicular to the direction of electric field. Show that the components are polarised some parallel to the direction of field strength and other perpendicular to field strength.
5. Upto the electric fields of about 10^7V/M , the resolution increases in proportion to the field strength. In this region, we have linear Stark effect. In case of more intense field. More complicated effects, so called quadratic Stark effect and even of higher orders are observed in addition to linear effect.

1.14 SPECTROSCOPY

1.14.1 Types of Molecular Spectra

Q18. Explain types of molecular spectra ?

Ans :

- The spectra emitted by atoms due to energy in their electronic system is known as atomic spectra. When the element is in the molecular form, the spectra are known as band (or) molecular spectra.
- Molecular spectra generally fall in following three distinct regions.
 1. **Microwave and far infrared region:** The spectrum obtained in this region is called as pure rotational spectrum.

2. **Near infrared region:** The spectrum obtained in this region is called as vibration - rotational spectrum.
3. **Visible (or) ultra] - violet region:** The spectrum obtained in this region is called as electronic spectrum.

1.15 PURE ROTATIONAL ENERGIES AND SPECTRUM OF DIATOMIC MOLECULE

Q19. Give the elementary theory of the origin of pure rotational energies and spectrum of Diatomic molecule?

Ans :

When microwaves radiation is incident on a a molecular, the molecule after absorbing energy rotates about its center of mass. This gives rise to various rotational energy levels.

Rational energies of diatomic molecule

The simplified molecule is a diatomic molecule is a diatomic two atoms, (ray of masses m_1 and m_2 are reproduct at a distances R) are based by alternative forces. To a fixed appropriation, it is assumed that the distance between two nuclei remains constant i.e., the molecular behaviour as a rigid rotator. The molecular rotates about an aim passing through its centre of mass e and perpendicular to the line joining the atoms as shown in fig.

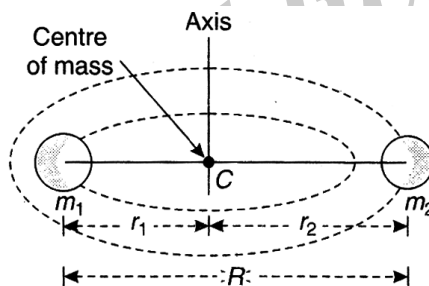


Fig. : Diatomic molecule

As the energy of the molecule depends upon its moments of inertia. Hence find of all, we shall calculates the moment of inertia. The moment of inertia of diatomic module about an aim passing through its centre of mass e and perpendicular to the line joining the two man in given by.

$$I = m_1 v_1^2 + m_2 v_2^2$$

As the system in balanced about its centre of graceful

$$m_1 v_1 = m_2 v_2$$

$$R = (v_1 + v_2)$$

Substituting eqn. (2) and (3) for v_1 and v_2 , we have

$$v_1 = \frac{m_2}{(m_1 + m_2)} R \text{ and } v_2 = \frac{m_1}{(m_1 + m_2)} R$$

Substitute the value in eq. (1), we get

$$I = \frac{m_1 m_2^2}{(m_1 + m_2)} \times R^2 + \frac{m_2 m_1^2}{(m_1 + m_2)^2} \times R^2$$

$$= \frac{m_1 m_2}{(m_1 + m_2)} R^2$$

$$I = MR^2$$

(or)

When $M = \frac{m_1 m_2}{(m_1 + m_2)}$ in the reduced mass of the molecule. Thus, instead of considering the rotation of diatomic molecule. We can equally well consider the rotation of a single mass point of mass m is at a fixed distance, R from the axis of rotation.

The angular momentum L_r of the molecule is given

$$L_r = L_w$$

The orbital angular momentum of the electrons in hydrogen atom can have only these values given by the following

$$L = \{\sqrt{r(r+1)}\} \cdot h \quad (\text{where } h = h/2\pi)$$

The orbital angular momentum of the rotating molecule is also quantified with value

$$L_r = \{\sqrt{J(J+1)}\} \cdot h$$

Where J = rotational quantum number. Then value $J = 0, 1$ classically, the energy of rotation of a is $(1/2) I\omega^2$ and hence the energy levels are separated by

$$E_r = \frac{1}{2} I\omega^2 = \frac{1}{2J} (L_r)^2$$

$$E_r = \frac{J(J+1)h^2}{2I}$$

E_r given the rotational states.

Molecule or Raman

In order to obtain a more accurate value of the energy we have to solve the Schrödinger wave equation for this system. The Schrödinger wave equation is given by

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

But in present case, $m = u$ and $v = 0$ (rigid rotation). Hence

$$\nabla^2 \Psi + \frac{8\pi^2 m}{h^2} E \Psi = 0$$

Solution of eq. (8) is only possible for certain value of E vcalled as eigen values. The eigen values are given by

$$E = \frac{h^2}{8\pi^2 4I^2} J (J + 1) = \frac{h^2}{\pi^2 2} J (J + 1)$$

Where J is a rotational quantum number. it can take value 0, 1, 2, ... Thus, we have a ----- of directs energy levels, with emergine $0, 2h^2 / 8\pi^2 I, 6h^2 / 8\pi^2, \dots$. The various allowed rotational energy levels of a diatomic modular and the spectrum is show in fig.

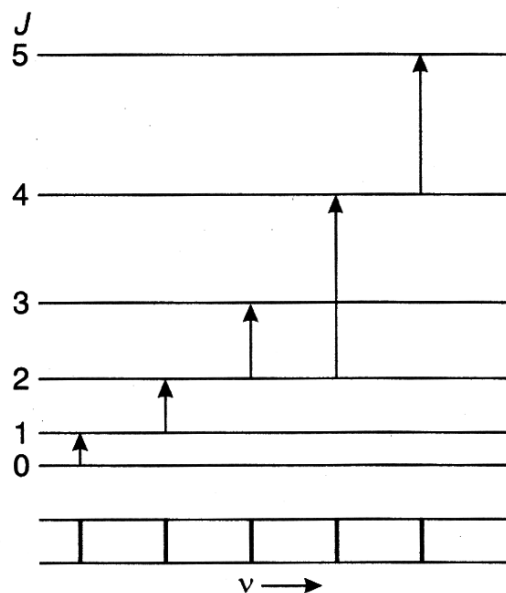


Fig. : Allowed energy levels and spectrum of diatomic module

Spectrum of a Diatomic Molecule

According to quantum theory, the emission of light quantum take plans as a result of transition of the rotator from higher to lower energy state which the absorption of quantum of proper frequency produces a transmission from lower energy state to higher energy state. W.K.T

$$E = \frac{h^2}{8\pi^2 I} J (J + 1)$$

where, $J = 0, 1, 2, \dots$

Now we consider the frequency of transition from a level of energy E_{J_1} to a level of energy E_{J_2} where $(E_{J_1} > E_{J_2})$. The energies of their two states are given as :

$$E_{J_1} = \frac{h^2}{8\pi^2 I} J_1 (J_1 + 1)$$

$$E_{J_2} = \frac{h^2}{8\pi^2 I} J_2 (J_2 + 1)$$

The frequency ν of the rotation is given by

$$\nu = \frac{E_{J_1} - E_{J_2}}{h} = \frac{\Delta E}{h} = \frac{1}{h} \left[\frac{h^2}{8\pi^2 I} \{J_1(J_1 + 1) - J_2(J_2 + 1)\} \right]$$

$$\nu = \frac{h}{8\pi^2 I} [J_1(J_1 + 1) - J_2(J_2 + 1)]$$

Corresponding to different values of J_1 and J_2 , we get different lines in absorption spectrum of the molecule. The set of lines (in emission (or) absorption spectrum) obtained in this way forms the pure rotational spectrum of the molecule.

1.16 DETERMINATION OF INTER NUCLEAR DISTANCE

Q20. How do you use rotational spectrum to determining internuclear distance?

Ans :

The rotational spectra of rigid diatomic molecule consist of equidistant series of line.

When the molecule is raised from J to $J+1$, the absorption is represented by

$$\Delta E = \frac{h^2}{8\pi^2 I} [(J + 1)(J + 2) - J(J + 1)]$$

$$= \frac{h^2}{8\pi^2 I} \times 2(J + 1)$$

The wave number of radiation is given by

$$\bar{\nu} = \frac{\Delta E}{hc} = \frac{2h}{8\pi^2 IC} (J + 1) = 2B(J + 1)$$

where

$$B \text{ is constant equal to } \frac{2h}{8\pi^2 IC}$$

So, the spacing between lines is $2B$. Therefore, from rotational spectra, B can be determined. By knowing the value of B , the moment of inertia and bond length or internuclear distance can be calculated.

1.17 VIBRATIONAL ENERGIES AND SPECTRUM OF DIATOMIC MOLECULES

Q21. Give the elementary theory of the origin of the vibrational spectrum of a molecule?

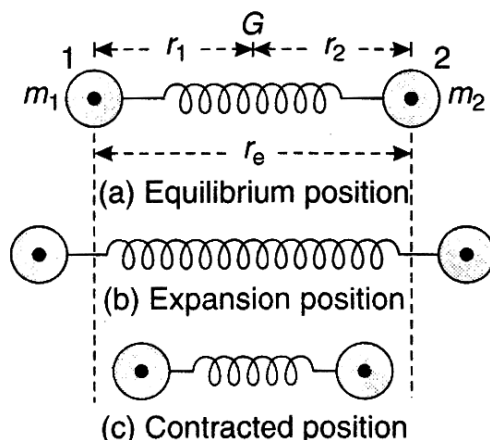
Ans :

(Imp.)

The atoms of the molecule vibrate about the mean position. In this way, their internuclear distance is changed. Further, the adsorption of radiation will also increase the vibrational energy of the molecule. This gives rise to the vibrational spectra. Therefore, the combination of vibrational and rotational effect results the modification in the spectrum. The spectrum is now called as rotational - vibrational spectrum.

(i) Vibration of Diatomic Molecule

Consider a diatomic molecule consisting of nuclei masses m_1 and m_2 separated by equilibrium distance r_e . The nuclei are held together by attractive forces. The molecule is in equilibrium state when the two nuclei are separated by a distance r_e . When the two nuclei are slightly separated, disturbed, they experience restoring forces. Thus, the two vibrating nuclei are equivalent to a linear harmonic oscillator of reduced mass μ .

**Frequency of Vibration**

A vibrating diatomic molecule can be approximated to a linear harmonic oscillator. Its frequency of vibration can be calculated on the classical lines using Newton's Equation of motion. Suppose the bond is distorted from its equilibrium length r_e to a new length r . The restoring forces on each atom of diatomic molecules are

$$m_1 \frac{d^2 r_1}{dt^2} = -K (r_1 - r_e) \quad \dots (1)$$

$$\text{and } m_2 \frac{d^2 r_2}{dt^2} = -K (r_2 - r_e) \quad \dots (2)$$

Where K is known as force constant. This is a measure of the stiffness of the bond. r_1 and r_2 are the positions of atoms 1 and 2 relative to the centre of mass. We know that

$$r_1 = \frac{m_2 r}{m_1 + m_2} \quad \text{and} \quad r_2 = \frac{m_1 r}{m_1 + m_2} \quad \dots (3)$$

Putting the value of r_1 in eq. (1), we get

$$\left(\frac{m_1 m_2}{m_1 + m_2} \right) \frac{d^2 r}{dt^2} = -K (r - r_e) \quad \dots (4)$$

Since, r_e is constant, its differentiation with respect to t will be zero. Therefore,

$$\frac{d^2 r}{dt^2} = \frac{d^2 (r - r_e)}{dt^2} \quad \dots (5)$$

Putting in eq. (4), we get

$$\left(\frac{m_1 m_2}{m_1 + m_2} \right) \frac{d^2 (r - r_e)}{dt^2} = -K (r - r_e) \quad \dots (6)$$

Let

$$r - r_e = n \text{ and } \frac{m_1 m_2}{m_1 + m_2} = \mu \quad (\text{reduced mass})$$

Now eq. (6) becomes

$$\mu = \frac{d^2 n}{dt^2} = -Kn$$

$$\text{or } \frac{d^2 n}{dt^2} + \frac{K}{\mu} n = 0$$

$$\text{or } \frac{d^2 n}{dt^2} + w^2 n = 0 \quad (\text{where } w^2 = K / \mu) \quad \dots (7)$$

This is equation of simple harmonic motion. The frequency of vibration is given by

$$V_v = \frac{1}{2\pi} \sqrt{\frac{K}{\mu}} \quad \dots (8)$$

Energy Levels

Vibrational energies, like other molecular energies are quantized. The permitted vibrational energies for any particular system can be calculated from Schrodinger equation. The eigen values for the energy of a linear harmonic oscillator is given by

$$E_v = \left(v + \frac{1}{2} \right) h \nu_v \quad \dots (9)$$

Where v is vibrational quantum number,

It may have many values 0, 1, 2, 3,

Eq. (9) is also written as

$$E_v = \left(v + \frac{1}{2} \right) hc \bar{\omega} \quad \dots (10)$$

Where $\bar{\omega}$ is the vibrational frequency of vibrating diatomic molecule expressed in wave number.

From eq. (10), it is clear that the minimum energy (even at absolute zero) possessed by the oscillator (i.e., for $v = 0$) is not zero. This is known as zero point energy.

Therefore,

$$\text{Zero point energy} = \frac{1}{2} hc \bar{\omega}$$

Figure shows the vibrational energy levels.

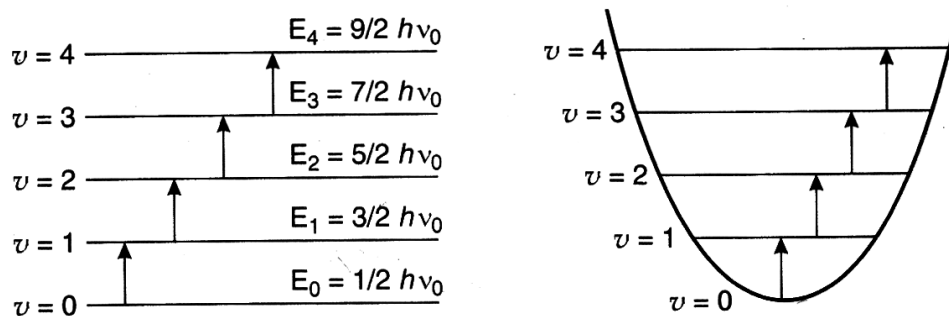


Fig. : Equispaced Discrete Vibrational Levels

Spectrum

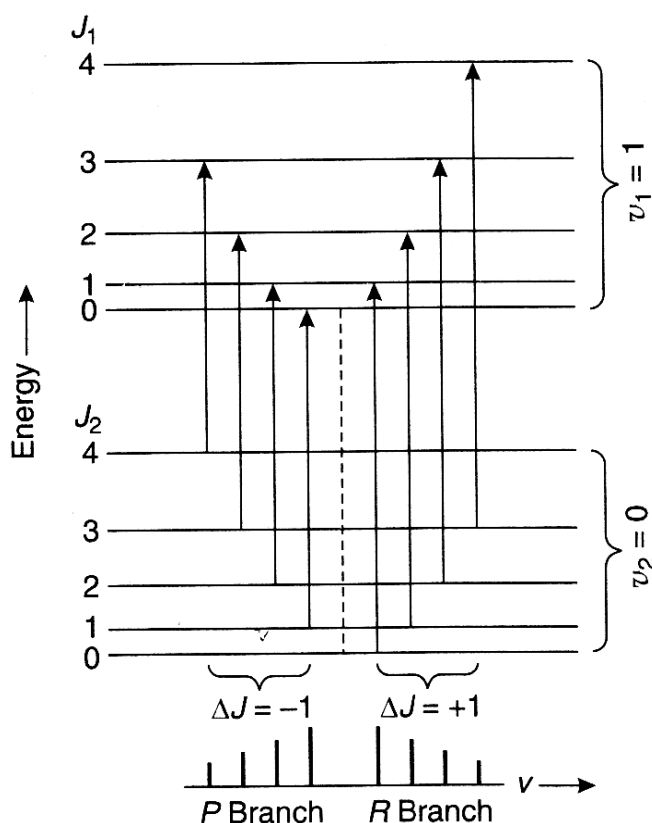


Fig. : Transition between rotational-vibrational energy levels of a diatomic molecule

The selection rule for transition between vibrational states is $\Delta v = \pm 1$ in the harmonic oscillator approximation and $\Delta J = \pm 1$ for the rotational states. The transition corresponding to $\Delta J = 0$ is forbidden.

Fig. (7) shows that $J_2 = 0, 1, 2, 3$ and 4 levels of a diatomic molecule for $v_2 = 0$ and $J_1 = 0, 1, 2, 3$ and 4 levels for $v_1 = 1$. The allowed transitions are also shown.

The $v_2 = 0 \rightarrow v_1 = 0$ transitions fall into two categories, the P branch in which $\Delta J = -1$ (i.e., $J \rightarrow J - 1$) and R branch in which $\Delta J = \pm 1$ (i.e., $J = J + 1$). The frequencies of the spectral lines in each branch is given by

$$\begin{aligned}
 V_p &= E_{1,J-1} - E_{0,J} \\
 &= \frac{1}{2\pi} \sqrt{\left(\frac{K}{\mu}\right)} + [(J-1)F - J(J+1)] \frac{h}{8\pi^2I} \\
 &= \nu_0 - J \frac{h}{4\pi^2I} \quad J = 1, 2, 3 \text{ (P branch)} \\
 &= \nu_0 - J \frac{h}{4\pi^2I} \\
 \text{and } V_R &= E_{1,J+1} - E_{0,J} \\
 &= \frac{1}{2\pi} \sqrt{\left(\frac{K}{\mu}\right)} + [(J+1)(J+2) - J(J+1)] \frac{h}{8\pi^2I} \\
 &= \nu_0 + (J+1) \frac{h}{4\pi^2I} \quad J = 0, 1, 2, 3 \text{ (R branch)}
 \end{aligned}$$

There is no line at $\nu = \nu_0$ because transitions for which $\Delta J = 0$ are forbidden in diatomic molecules. This missing line, or the gap, in the band is called the origin of the band.

1.18 RAMAN EFFECT & EXPERIMENTAL STUDY RAMAN EFFECT

Q22. What is raman effect ? Explain classical theory of raman effect ?

Ans :

(Imp.)

Rayleigh observed that in the spectrum of scattered light, there is change in the intensity scattered light but there is no change in the wavelengths or frequency. This scattering is called as Rayleigh scattering. In 1928, Sri, C.V. Raman observed that the spectrum of scattered light (in addition to the frequency of incident light) consists of frequencies greater and smaller than those of the incident beam. This is known as Raman effect. The spectrum of the scattered light is called Raman spectrum. The new lines are known Raman lines. The lines of greater frequency are called as Stokes lines. The lines are shown in fig. The displacements of the lines, are independent of the frequency of incident light but are functions of the scattering substance.

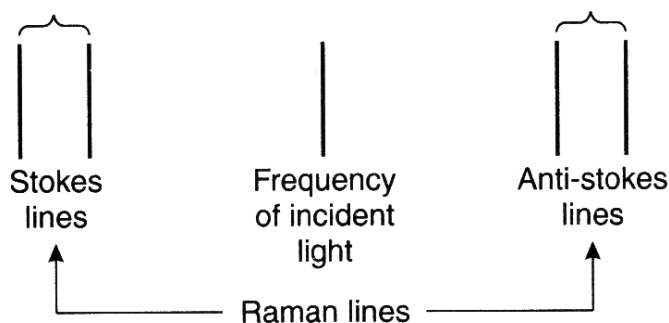


Fig. : Raman Lines

Characteristics of Raman Effect

Following are the characteristics of Raman Effect :

- (i) The frequencies of Raman lines depend on the frequency of incident light.
- (ii) The anti - stokes lines are weaker - than stokes lines.
- (iii) The rotational or vibrational state of the molecule is changed due to scattering of light by it.
- (iv) Raman effect is purely a molecular phenomenon.

Classical Theory of Raman Effect

When an atom or a molecular is placed in an electric field, the electrons and nuclei are displaced. The electrons are attracted towards the positive pole while the nuclei towards the negative pole. Due to the displacement of nuclei and electrons, an induced dipole moment is produced and the molecule is said to be polarised.

Then E be the strength of applied electric field and μ be the magnitude of induced dipole moment.

Now,

$$\mu = \alpha E \quad \dots (1)$$

Where α is polarisability of molecule. The strength E of electric field of electromagnetic wave of frequency ν , then

$$E = E_0 \sin 2\pi\nu t \quad \dots (2)$$

Where E_0 is the equilibrium value of field strength from eq. (1),

$$\mu = \alpha E \sin 2\pi\nu t \quad \dots (3)$$

The atom a molecule oscillates with same frequency ν . By classical theory, this oscillating dipole should scatter (emit) radiation of the identical frequency ν , i.e., of incident frequency, a case of Rayleigh scattering.

1.18.1 Experimental Setup to Study Raman Effect

Q23. Describe an experimental setup to study Raman effect. Give the theory?

Ans :

The Raman effect has been studied by a number of Investigators. The principle involved in their researches is to illuminate the experimental substance with an intense monochromatic source of light and then to photograph the scattered light by means of spectrograph arranged in transverse direction. Here the source of light should be very strong otherwise the Raman lines will be of very low intensity. Now-a-days lasers are used for this purpose.

The experimental arrangement is shown in fig. It consists of

- (i) Source
- (ii) Raman tube and
- (iii) Spectrograph

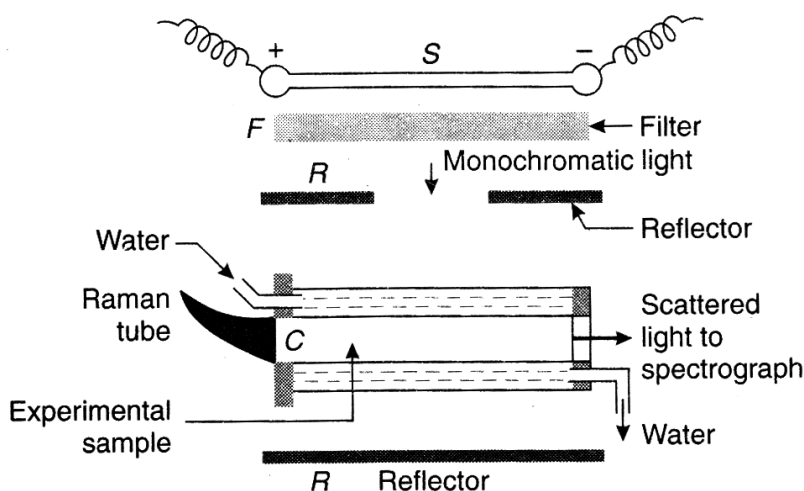


Fig. : Experimental Arrangement for Raman Spectrum

In the figure, S is mercury arc lamp, i.e., a source of light is passed through a filter F, to obtain a monochromatic beam, i.e., light of a single frequency. The light is then allowed to pass through an opening in a metallic reflector which then falls on Raman tube. The Raman tube consists of a glass tube of about 1 or 2cm in diameter and 10 to 15 cm long. One end of the tube has a flat glass surface through which the scattered light emerges. The other end is drawn out into horn shaped and blanchened outside to provide the black background. The tube is surrounded by a water jacket in which cold water is circulated to prevent overheating the sample in Raman tube due to proximity of the exciting arc. The experimental sample is placed inside Raman tube. The scattered beam emerges from the flat end of the Raman tube and is examined by means of spectrograph.

When the sample is a gas, it is enclosed in a tube at a pressure of few cm of mercury. In case of solids, powders are used. Which are mixed either with liquid paraffin or any other solvents.

1.18.2 Applications

Q24. What are the applications of raman effect and Problems?

Ans :

Raman effect has the following applications :

1. To study the molecular structure of crystals and compounds.
2. To know the number of atoms in a molecule, their relative arrangement, relative masses and chemical bonds between them.
3. To study the composition in plastics, mixtures, etc.
4. To decide about single, double or triple bond.
5. To study the spin and statistics of nuclei.
6. To study the binding forces between the atoms or group of atoms in crystals.
7. To study the vibrational and rotational energy levels of homo-nuclear molecules, for example nitrogen, oxygen, etc.

PROBLEMS

1. Prove that for a given principal quantum number n , there are n^2 possible states each of which can accommodate a maximum of 2 electrons.

Sol:

For a given n , the orbital quantum number l has following values $l = 0, 1, 2, \dots, (n - 1)$

For each value of l , the magnetic quantum number m_l has the following values $m_l = +l, + (l - 1), + (l - 2), \dots, 0, -1, -2, \dots, - (l - 2), - (l - 1), -l$.

The total number of possible states is

$$\sum_{(l=0)}^{(n-1)} (2l + 1) = 1 + 3 + 5 + \dots + (2n - 1)$$

It is a A.P. series whose sum is given by

$$n \left[\frac{a + l}{2} \right] = n \left[\frac{1 + (2n - 1)}{2} \right] = n^2$$

\therefore Total number of states is n^2

Now corresponding to two different values of spin, each state can accommodate a maximum of 2 electrons.

2. Indicate the possible (n, l, j) values of electrons in the first three shells of an atom. The symbols have their usual significance.

Sol:

Case I :

First shell, i.e, $n = 1$

In this case $l = 0$ and $j = l \pm s = 0 \pm \frac{1}{2}$ or $j = \frac{1}{2}$ because negative value of j is not permissible.

Hence, possible values of (n, l, j) are $(1, 0, \frac{1}{2})$

Case II :

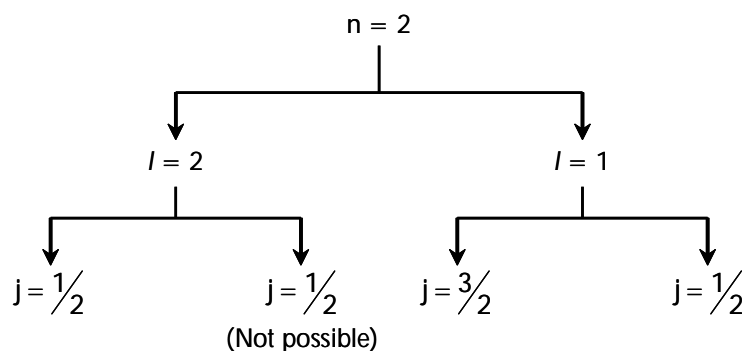
Second shell, i.e., $n = 2$

In this case $l = 0$ and 1

Now $j = (0 \pm \frac{1}{2})$ or $\frac{1}{2}$ and $(1 \pm \frac{1}{2})$ i.e., $\frac{3}{2}, \frac{1}{2}$

$\therefore j = \frac{1}{2}$ and $\frac{3}{2}, \frac{1}{2}$

Hence three states are possible. They are $(2, 0, \frac{1}{2})$, $(2, 1, \frac{3}{2})$ and $(2, 1, \frac{1}{2})$. These states are shown on next page in the form of a diagram.

**Case III :**

Third shell, i.e., $n = 3$

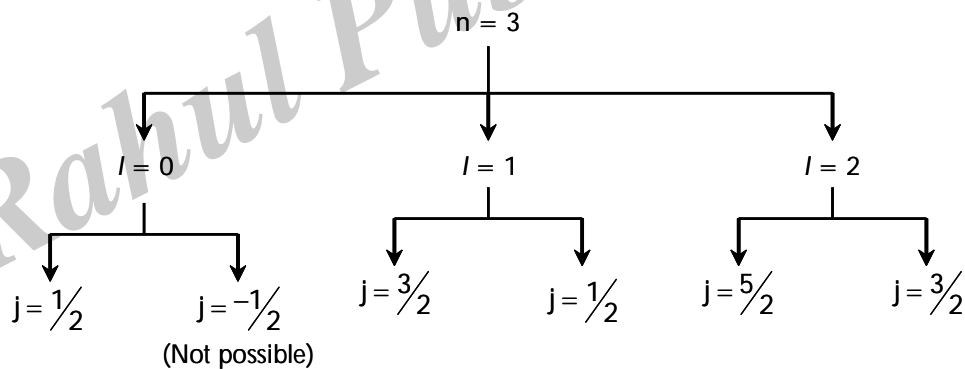
In this case $l = 0, 1, 2$

$$\text{and } j = \left(0 \pm \frac{1}{2}\right), \left(1 \pm \frac{1}{2}\right), \left(2 \pm \frac{1}{2}\right)$$

$$= \frac{1}{2}, \left(\frac{3}{2}, \frac{1}{2}\right), \left(\frac{5}{2}, \frac{3}{2}\right)$$

Following five states are possible

$$\left(3, 0, \frac{1}{2}\right), \left(3, 1, \frac{3}{2}\right), \left(3, 1, \frac{1}{2}\right), \left(3, 2, \frac{5}{2}\right) \text{ and } \left(3, 2, \frac{3}{2}\right)$$



3. Calculate the wavelength separation between the unmodified line of wavelength 6000 \AA and the modified line when a magnetic field of flux density 1 weber / m^2 is applied in normal Zeeman effect.

Sol :

The wavelength separating $d\lambda$ is given by

$$d\lambda = \frac{Be\lambda^2}{4\pi m_0 c}$$

Substituting the given values, we get

$$d\lambda = \frac{(1 \text{ weber/m}^2) (1.6 \times 10^{-19} \text{ coulomb}) (6000 \times 10^{-10} \text{ m})}{4\pi (9.1 \times 10^{-31} \text{ kg}) (3 \times 10^2 \text{ m/sec})}$$

$$= 0.68 \times 10^{-10} \text{ m} = 0.68 \text{ \AA}.$$

4. In the normal zeeman effect the frequency separation between two consecutive spectral lines $8.3 \times 10^8 \text{ Hz}$. Find the magnetic field.

Sol:

The energy separated between two consecutive lines is given by $\Delta E = \mu_B B$ where μ_B in Bohr magneton. Now the corresponding energy separation ΔV is given by

$$\Delta V = \frac{\mu_B B}{h} \text{ or } B = \frac{h\Delta V}{\mu_B}$$

$$B = \frac{(6.6 \times 10^{-34}) (8.3 \times 10^8)}{9.3 \times 10^{-24} \text{ joule/tesla}}$$

5. The red line of cadmium splits up into three components separated by 120 MHz when the source is placed in a magnetic field of flux density 8.6 mT, the light being examined in a direction perpendicular to the magnetic field. Calculate the ratio of charge mass of electron.

Sol:

The change in frequency is given by

$$dv = \frac{e}{4\pi m_o} B \text{ or } \frac{e}{m_o} = \frac{4\pi dv}{B}$$

$$\frac{e}{m_o} = \frac{4 \times 3.14 \times (120 \times 10^6)}{(8.6 \times 10^{-13})}$$

$$= 1.76 \times 10^{11} \text{ coulomb / kg}$$

6. A prominent spectral line of calcium has wavelength of 4226.73 \AA . When calcium atoms are placed in uniform magnetic field of 4 weber / m², the normal zeeman pattern is obtained. Calculate the wavelength of the three components of the normal zeeman pattern and show the wavelength separation are each 0.13 \AA .

Sol:

The wavelength separation $d\lambda$ is given by

$$d\lambda = \frac{eB \lambda^2}{4\pi m_o c}$$

Substituting the values, we get

$$d\lambda = \frac{(1.6 \times 10^{-19}) \times 4 \times (4226.73 \times 10^{-10})^2}{4 \times 3.14 \times (9.1 \times 10^{-31}) \times (3 \times 10^8)} = 0.1268 \times 10^{-10} \text{ m}$$

$$= 0.1268 \text{ \AA} \approx 0.13 \text{ \AA}$$

The three wavelength are :

$$(i) \quad (4226.73 - 0.13) = 4226.6 \text{ \AA}$$

$$(ii) \quad 4226.73 \text{ \AA}$$

$$(iii) \quad (4226.73 + 0.13) = 4226.86 \text{ \AA}$$

7. The zeeman components of a 500 nm spectral line are 0.0116 nm apart when the magnetic field is 1.00T. Find the ratio e/m_e for the electron.

Sol :

The zeeman shift wavelength is given by

$$D\lambda = \frac{Be\lambda^2}{4\pi m_e c}$$

$$\therefore \frac{e}{m_e} = \frac{4\pi c}{B} \left(\frac{D\lambda}{\lambda^2} \right)$$

Here $\lambda = 500 \text{ nm} = 5.00 \times 10^{-7} \text{ m}$, $D\lambda = 0.0116 \text{ nm} = 0.000116 \times 10^{-7} \text{ m}$,

$B = 1.00 \text{ tesla} = 1.00 \text{ N / A-m}$

Hence

$$\begin{aligned} \frac{e}{m_e} &= \frac{4 \times 3.14 \times (3.0 \times 10^8)}{1.00} \left[\frac{0.000116 \times 10^{-7}}{(5.00 \times 10^{-7})^2} \right] \\ &= 1.75 \times 10^{11} \text{ C/kg} \end{aligned}$$

Short Question and Answers

1. Mention the drawback's of Bohr's theory?

Ans :

Bohr's theory was able to explain successfully a number of experimental observed facts and has correctly productly the spectral lines of neutral hydrogen atom and singly ionized helium atom, etc. in terms of only principal quantum number n. However, the theory fails to explain the following facts :

- (i) The theory could not account the spectra of atoms more complex than hydrogen.
- (ii) The theory does not give any information regarding the distribution and arrangement of electrons in atom.
- (iii) It does not explain the experimentally observed variations in intensity of the spectral lines of a element.
- (iv) This theory cannot be used to calculated about transforms from one level to another such as the rate at which they occur or the selection rules which apply to them.
- (v) This theory cannot be used for the quantitative explanation of chemical bonding.

2. What are the drawbacks of Bohr and Sommerfeld atomic model ? Explain concept of vector model ?

Ans :

This model is an extension of Bohr - Sommerfeld atoms model. Following are the drawbacks of Bohr and sommerfeld atomic models :

- (i) Original Bohr's theory was incapable of explaining the fine structure of the spectral lines even in the simplest hydrogen a form.
- (ii) In case of complex atoms, Bohr's theory fails to calculate the energy of the system and frequencies of radiation emitted.
- (iii) Sommerfeld modification, though gave a theoretical back ground of the splitting of individual spectral lines of hydrogen, still in could not predict the correct number of observed fine structure of these lines.
- (iv) Both the models could not explain the distribution and arrangement of electrons in atoms.
- (v) Both the models do not throw any light on the intensities of the spectral lines.
- (vi) Both the models could not explain the anomalous zerman effect and stark effect.

To overcome all these objections a new model known as vector atom model was proposed.

3. Discuss the L-S and J-J coupling schemes associated with an atom ?

Ans :

This type of coupling occurs most frequently and hence is known as normal coupling.

In this coupling orbital angular momentum vectors l of the electrons combine to from a resultant vector L & all the spin angular Momentum vectors S like wise combine to form a resultant vector S .

Now the vectors L & S combine to form a vector J

We can represent the coupling as

$$L = (l^1 + l^2 + l^3, \dots)$$

$$S = (s^1 + s^2 + s^3, \dots)$$

$$J = L + S$$

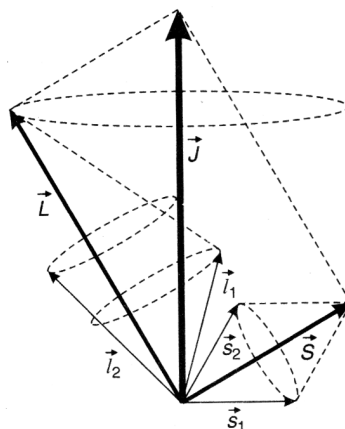


Fig. : Showing L-S Coupling

- Here L is always an integer zero i.e., 0, 1, 2, 3 etc. The value S depends on the number of Electrons & the direction of their Spin vectors.
- In case of two Electrons if the spins are parallel the value is one and when the Spins are antiparallel the value of S is Zero.
- Thus, S is an integer for an Even number of Electrons & half integer for an odd number of Electrons.

Two electrons	Three electrons	Four electrons
$s_2 \uparrow$ $s_1 \uparrow$ $s_1 \downarrow$ $s_2 \uparrow$	$s_3 \uparrow$ $s_2 \uparrow$ $s_1 \uparrow$ $s_2 \uparrow$ $s_3 \downarrow$ $s_1 \downarrow$	$s_4 \uparrow$ $s_3 \uparrow$ $s_2 \uparrow$ $s_1 \uparrow$ $s_3 \uparrow$ $s_2 \downarrow$ $s_4 \downarrow$ $s_1 \downarrow$ $s_2 \uparrow$ $s_3 \downarrow$ $s_1 \downarrow$
S = 1 0	3/2 1/2	2 1 0

Now $J = \text{Integer (0, 1, 2, 3, etc)}$ where S is integer
(i.e., for odd electron system)

$$J = \text{Half integer } \left(\frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \dots \text{ etc.} \right)$$

where

S is half integer

(i.e., for odd electron system)

J must always be positive & never negative because it represents the total angular momentum.

4. Explain L-S and J-J coupling schemes ?

Ans :

The interaction between the spin & orbital vectors in each electron is stronger than the interaction between Either the spin vectors or orbital vectors of different Electrons. In such case j-j coupling is most suitable than L - S coupling.

- In j - j coupling, Each Electron is considered separately & its total angular momentum j is obtained by the relation

$$j = l + s$$

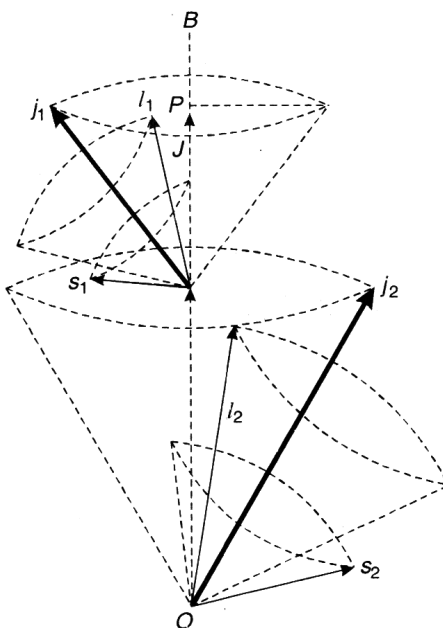
- Then the total angular momentum J of the atom would be vector sum of all the individual j vectors of the electrons.

$$j_1 = (l_1 + s_1), j_2 = (l_2 + s_2), j_3 = (l_3 + s_3), \dots$$

$$J = (j_1 + j_2 + j_3) + \dots$$

$$= \sum j.$$

- Pure j - j coupling is seldom found. In most of known cases l-s coupling is effective.



5. Explain the spectral terms ?

Ans :

To describe the Electronic Configuration, Small letters are used to represent the l values are shown again

l	Notation
0	s
1	p
2	d
3	f
4	g
5	h

To represent the configuration, following two points are considered.

- i) The value of total quantum number n is written as a prefix to the letter representing its 'l' values.
- ii) The number of Electrons with the same n & p values is written at the upper right hand side of letter representing their l value.

6. Explain selection rules.

Ans :

We know that in an atom, there are number of energy states. It is observed that all the transitions between different energy states (as spectral lines) do not appear. The spectral lines are governed under certain principles known as selection rules. There are three selection rules as described below :

- (a) **The selection rule for L :** Only those lines are observed for which the value of L changes by ± 1 (i.e., $\Delta L = \pm 1$).
- (b) **The selection rule for J :** Only those spectral lines are observed when the transitions take place between states for which $\Delta J = \pm 1$ or 0 . The transition $0 \rightarrow 0$ is not allowed.
- (c) **The selection rule for S :** Only those spectral lines are observed for which the value of S changes by 0 (i.e., $\Delta S = 0$).
- (d) **Selection rules for magnetic quantum numbers :** In the presence of magnetic field, the orbital magnetic quantum number m_l and spin magnetic quantum numbers m_s play an important part in the transition. Their selection rules are

$$\Delta m_l = 0 \text{ or } \pm 1 \text{ and } \Delta m_s = 0$$

In consequence

$$\Delta m_j = 0 \text{ or } \pm 1$$

7. Explain Intensity Rules.

Ans :

The intensity rules are :

- (i) The intensity of the transition (i.e., a line) is strong for which L and J change in the same sense.
- (ii) The intensity of the transition is weak for which L and J change in opposite sense.
- (iii) The intensity of a line is strong when the transition is in the decreasing sense i.e., from $L \rightarrow (L - 1)$.
- (iv) The intensity of a line is weak the transition is in the increasing sense i.e., from $L \rightarrow (L + 1)$.
- (v) The oppositely directed transition does not occur.

The above rules can be summarized as :

$\Delta L = -1,$	$\Delta J = -1$	Most intense line
$\Delta L = -1,$	$\Delta J = 0$	Less intense
$\Delta L = +1,$	$\Delta J = +1$	Weaker
$\Delta L = +1,$	$\Delta J = 0$	Weaker
$\Delta L = -1,$	$\Delta J = +1$	No transition
$\Delta L = +1,$	$\Delta J = -1$	No transition

8. What is zeeman effect?*Ans :*

Zeeman repeated Faraday's experiment with improved apparatus and observed the splitting of spectral lines. The splitting of spectral lines is known as Zeeman Effect.

In 1896, Prof Zeeman discovered that when a source of radiation, giving line spectrum is placed in a magnetic field. The spectral lines are split up into a number of component lines, symmetrically distributed about the original line. Doublets, triplets and even more complex systems are observed. This is known as zeeman effect. If the magnetic field is very strong, each spectral line split up into two components in the longitudinal view and in three components in transverse view. This is known as normal Zeeman Effect. When the magnetic field is comparatively weak. Each line split into more than three components this is known as Anomalous Zeeman effect.

9. What is Paschen - Back Effect?*Ans :*

The alkali metals, like Na, Li, K, etc., show anomalous zeeman effect only in weak fields. Paschen and Back showed that (whatever be the anomalous zeeman pattern of a given line in a magnetic field, the pattern is always approximated as normal zeeman triplet as the field strength is - Progressively increased). This fact is known as paschen - back effect. Thus the transition phenomenon between the two (anomalous zeeman effect and normal zeeman effect) is known as paschen - back effect.

10. What is Stark Effect?*Ans :*

The action of an electric field on the spectrum of hydrogen was discovered by Stark (1913) who observed the splitting of Balmer lines. The splitting of spectral lines due to the action of external electric field is called the Stark effect.

11. How do you use rotational spectrum to determine internuclear distance?*Ans :*

The rotational spectra of rigid diatomic molecule consist of equidistant series of lines.

When the molecule is raised from J to $J+1$, the absorption is represented by

$$\begin{aligned}\Delta E &= \frac{h^2}{8\pi^2 I} [(J+1)(J+2) - J(J+1)] \\ &= \frac{h^2}{8\pi^2 I} \times 2(J+1)\end{aligned}$$

The wave number of radiation is given by

$$\bar{\nu} = \frac{\Delta E}{hc} = \frac{2h}{8\pi^2 IC} (J+1) = 2B(J+1)$$

where

$$B \text{ is constant equal to } \frac{2h}{8\pi^2 IC}$$

So, the spacing between lines is $2B$. Therefore, from rotational spectra, B can be determined. By knowing the value of B , the moment of inertia and bond length or internuclear distance can be calculated.

12. What is raman effect ?

Ans :

Rayleigh observed that in the spectrum of scattered light, there is change in the intensity scattered light but there is no change in the wavelengths or frequency. This scattering is called as Rayleigh scattering. In 1928, Sri, C.V. Raman observed that the spectrum of scattered light (in addition to the frequency of incident light) consists of frequencies greater and smaller than those of the incident beam. This is known as Raman effect.

13. Define Classical Theory of Raman Effect.

Ans :

When an atom or a molecule is placed in an electric field, the electrons and nuclei are displaced. The electrons are attracted towards the positive pole while the nuclei towards the negative pole. Due to the displacement of nuclei and electrons, an induced dipole moment is produced and the molecule is said to be polarised.

Then E be the strength of applied electric field and μ be the magnitude of induced dipole moment.

Now,

$$\mu = \alpha E \quad \dots (1)$$

Where α is polarisability of molecule. The strength E of electric field of electromagnetic wave of frequency ν , then

$$E = E_0 \sin 2\pi \nu t \quad \dots (2)$$

Where E_0 is the equilibrium value of field strength from eq. (1),

$$\mu = \alpha E \sin 2\pi \nu t \quad \dots (3)$$

The atom or a molecule oscillates with same frequency ν . By classical theory, this oscillating dipole should scatter (emit) radiation of the identical frequency ν , i.e., of incident frequency, a case of Rayleigh scattering.

14. What are the applications of raman effect and Problems?

Ans :

Raman effect has the following applications :

- (i) To study the molecular structure of crystals and compounds.
- (ii) To know the number of atoms in a molecule, their relative arrangement, relative masses and chemical bonds between them.
- (iii) To study the composition in plastics, mixtures, etc.
- (iv) To decide about single, double or triple bond.
- (v) To study the spin and statistics of nuclei.
- (vi) To study the binding forces between the atoms or group of atoms in crystals.
- (vii) To study the vibrational and rotational energy levels of homo-nuclear molecules, for example nitrogen, oxygen, etc.

Choose the Correct Answers

1. Specifically n_r is called the ____ [a]
(a) radial quantum number (b) spin quantum number
(c) both (a) and (b) (d) none of the above
2. Velocity of electron perpendicular to radius vector known as [a]
(a) azimuthal momentum (b) radial momentum
(c) both (a) and (b) (d) none of the above
3. $\frac{n_\phi}{n} =$ [c]
(a) b (b) $\frac{a}{b}$
(c) $\frac{b}{a}$ (d) a
4. The angular momentum of the atom, will now be due to ____ motion and ____ motion of the e^- [b]
(a) orbital, antispin (b) orbital, spin
(c) sperical, spin (d) none of the above
5. According the quantisation rules, the magnitude of J is given by [a]
(a) $J = \sqrt{j(j+1)} \frac{h}{2\pi}$ (b) $J = \sqrt{(j+1)} \frac{h}{2\pi}$
(c) $J = \sqrt{J} \frac{h}{2\pi}$ (d) none of the above
6. $pI = M$, where $M =$ ____ [c]
(a) magnetic field (b) magnetic flux
(c) magnetic moment (d) none of the above
7. The nucleus of hydrogen atom is given by [b]
(a) $E_n = \frac{13.6}{n^2} \text{ eV}$ (b) $E_n = \frac{-13.6}{n^2} \text{ eV}$
(c) $E_n = 0$ (d) $E_n = \pm 1$
8. According to sommerfeld model the electron moves around the nucleus in ____ orbit [c]
(a) Spherical (b) Circular
(c) Elliptical (d) None of the above

9. According to Bohr model velocity of revolving electron. [b]

(a) $v = \frac{e^2}{2nh}$

(b) $v = \frac{e^2}{2nh \epsilon_0}$

(c) $v = \frac{e}{2hn}$

(d) $v = \frac{e}{2nh \epsilon_0}$

10. Symbolically, we can represent the coupling as [c]

(a) $J = L - S$

(b) $J = \frac{L}{S}$

(c) $J = L + S$

(d) $J = L^2 - S^2$

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Fill in the Blanks

1. The value of Rydberg constant _____.
2. Motion of electron in elliptical orbits and taking into consideration the variation of mass with _____.
3. In vector atom model, based on quantum theory, the orbits are assumed to be quantized in _____ and _____.
4. Ag is _____ element.
5. _____ is known as angular momentum J of silver atoms is due to its spin of its valence electrons.
6. $\alpha_y = \frac{F_y}{m}$ when m is the mass of _____.
7. L-S coupling is also known as _____.
8. Complex motion of the electron subjected to an additional force is called _____.
9. The quantity ($m_L + 2m_S$) is known as _____ quantum number.
10. By analysis of alkali spectra, it has been observed that S-vel is _____, while other P.D.F. are _____ levels.

ANSWERS

1. $10.97 \times 10^6 \text{ m}^{-1}$
2. velocity
3. magnitude, direction
4. monovalent
5. $J = \frac{\sqrt{3}}{2} \frac{h}{2\pi}$
6. atomic magnet
7. normal coupling
8. Larmor precession
9. strong field
10. single, doublet

UNIT - II

QUANTUM MECHANICS

Inadequacy of classical Physics

Spectral radiation - Planck's law (only discussion). Photoelectric effect - Einstein's photoelectric equation. Compton's effect - experimental verification.

Matter waves & Uncertainty principle

de Broglie's hypothesis wavelength of matter waves, properties of matter waves. Phase and group velocities. Davisson and Germer experiment. Double slit experiment. Standing de Broglie waves of electron in Bohr orbits. Heisenberg's uncertainty principle for position and momentum (x and p_x), Energy and time (E and t). Gamma ray microscope. Diffraction by a single slit. Position of electron in a Bohr orbit. Complementary principle of Bohr.

Schrodinger Wave Equation

Schrodinger time independent and time dependent wave equations. Wave function properties Significance. Basic postulates of quantum mechanics. Operators, eigen functions and eigen values, expectation values.

QUANTUM MECHANICS

2.1 CLASSICAL PHYSICS

Q1. Explain about classical physics.

Ans :

Classical physics is basically based on three Newton's Law of motion -

- (i) law of inertia,
- (ii) law of force and
- (iii) law of action and reaction.

According to classical mechanics, it is possible to determine exactly the quantities like position, velocity, momentum, acceleration, etc., which characterise the state of the systems at any instant.

2.1.1 Inadequacy of Classical Physics

Q2. Discuss the inadequacy of classical physics ?

Ans :

The reasons of failure of classical physics are :

1. Classical mechanics successfully explained the motion of the objects which are either observable directly or can be made observable by instruments like microscope. When the classical concepts were applied to the particles of atomic dimensions like electrons, they failed to describe the actual behaviour. Thus, the classical concepts cannot be applied to atomic phenomenon, e.g., motion of an electron in an atom.
2. The energy of the electron should decrease continuously and it should come closer and closer until it collapses with nucleus. This shows the instability of the atom. This statement is contradictory to the observed fact of the stability of atom. Thus, classical mechanics failed to explain the stability of the atom.
3. Classical mechanics failed to explain the spectrum of hydrogen atom.
4. It could not explain observed spectrum of black body.
5. It could not explain the observed variation of specific heat of metals and gases.
6. The classical mechanics failed to explain photo - electric effect, Compton effect, Raman effect etc.

2.2 SPECTRAL RADIATION

Q3. Describe the distribution of energy in the spectrum black body radiation?

Ans :

(Imp.)

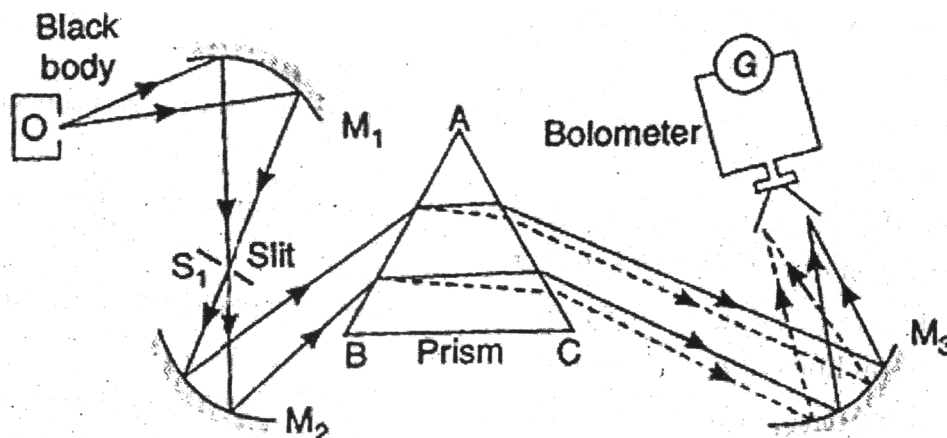
According to Stefan's law, total amount of radiant energy by a black body per unit area per second due to all wavelengths is directly proportional to the fourth power of absolute temperature.

i.e. $E \propto T^4$ (or) $E = \sigma T^4$

Where

$$\sigma = \text{Stefan's constant} = 5.67 \times 10^{-8} \text{ Wm}^{-2} \text{ K}^{-4}$$

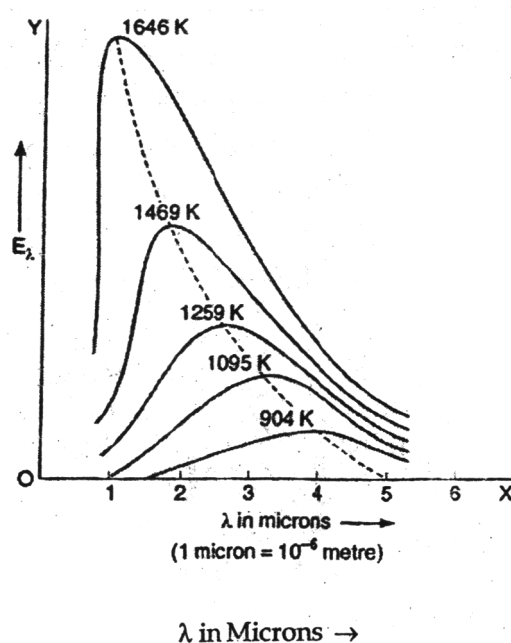
This law gives the total energy radiated by a black body and does not throw any light on energy distribution. The distribution of energy in black body radiation for different wavelengths and at various temperature was determined by Lummer and pringsheim in 1899.



The radiation from a black body O was focussed on a slit S by a concave mirror M. The slit S is placed at the focus of another concave mirror M_2 so that radiation after reflection from mirror M_2 becomes parallel. The parallel beam of radiation is allowed to incident on a flint glass prism ABC. The prism produces the spectrum of radiations. The emergent dispersed beam is incident on concave mirror M_3 . The radiations are detected by means of bolometer, fitted with galvanometer G. The deflection in the galvanometer gives the intensity of radiation E_λ .

This is the quantity $E_\lambda d\lambda$ is the energy, for wavelengths lying between $\lambda + d\lambda$ emitted per second per unit surface areas of black body. The wavelengths at different parts of the spectrum was calculated by prism dispersion formula.

Instead of rotating bolometer, the mirror M_3 was rotated about a vertical axis and different maxima were detected by bolometer. The same is repeated with same wavelengths at different temperatures. The curve is as shown in figure.



The total energy of radiation at any temperature is given by the area between the curve corresponding to that temperature and the horizontal axis. The increase in area is found in accordance with the Stefan's law.

$$E = \int_0^{\infty} E_{\lambda} d\lambda = \sigma T^4$$

The wave length corresponding to the maximum energy represented by the peak of the curve shifts towards shorter wave lengths as the temperature increases. This is called Wien's displacement law. According to this law

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

2.3 PLANCK'S RADIATION

Q4. Explain and derive Planck's Radiation formula ?

Ans :

Planck in 1900 suggested that the correct results can be obtained if the energy of the oscillating can be obtained if the energy of the oscillating electrons is taken as discrete rather than continuous.

- A chamber containing black body radiation also contains simple harmonic oscillators of molecular dimensions which can vibrate with all possible frequencies.
- The frequency of radiation emitted by an oscillator is the same as the frequency of its vibration.
- An oscillator cannot emit energy in a continuous manner, it can emit energy in the multiples of a small unit called quantum (photon). If an oscillator is vibrating with a frequency ν , it can only radiate in quanta of magnitude $h\nu$, i.e., the oscillator can have only discrete energy values E_n given by

$$E_n = nh\nu = n\varepsilon$$

where $h\nu = \varepsilon$

Here n is an integer and h is Planck's constant

$(6.625 \times 10^{-34} \text{ joules} \cdot \text{sec})$

- The oscillators can emit or absorb radiation energy in packets of $h\nu$.

If N be the total number of Planck's oscillators and E be their total energy, then the average energy per Planck's oscillators and given by

$$\bar{\varepsilon} = \frac{E}{N}$$

2.4 EXPERIMENTAL STUDY OF PHOTO - ELECTRIC EFFECT

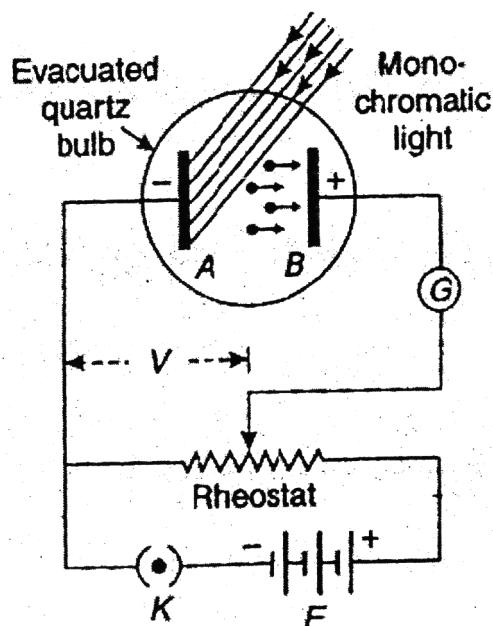
Q5. Explain experimental study of photo - electric effect?

Ans :

(Imp.)

A simple experimental arrangement to study the photoelectric effect is shown in fig. The apparatus consists of two photosensitive surfaces A and B enclosed in an evacuated quartz bulb. The plate A is connected to the negative terminal of a potential divider while the plate B is connected to the positive terminal through a galvanometer G or a micro ammeter.

In the absence of any light, there is no flow of current and hence there is no deflection in the galvanometer or micro ammeter. But when monochromatic light is allowed to fall on plate A, current starts flowing in the circuit which is indicated by galvanometer. The current is known as photo - current. This shows that when light falls on the metallic surface, electrons are ejected.

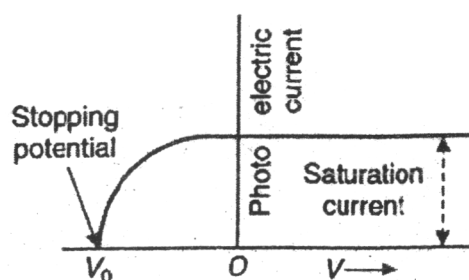


The number of electrons emitted and their kinetic energy depend upon the following factors.

1. The potential difference between the two electrodes i.e. between plates A and B.
2. The intensity of incident radiation
3. The frequency of incident radiation
4. The photometal used

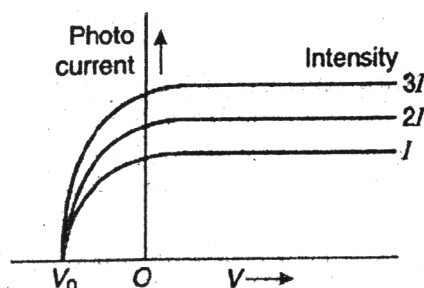
The effect of potential difference:

- When the positive potential of plate B is increased, photoelectric current also increases. All the photoelectrons are emitted from plate A and the photoelectric current reaches a certain maximum value called saturation current.
- If the potential difference is kept zero, the photo electric current still flows in same direction.
- When the negative potential is applied, the photo current continues to flow and if the negative potential is increased the photocurrent decreases and finally becomes zero. (V_0)

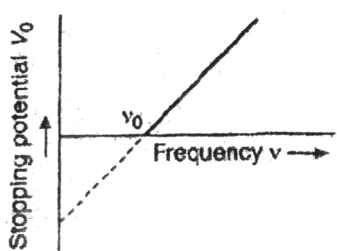


Effect of Intensity of Incident Radiation:

- The stopping potential is independent of the intensity of incident radiation.
- As the intensity of the incident radiation is increased, the photocurrent also increases i.e. the saturation current is proportional to intensity of incident radiation.

**Effect of frequency of Incident Radiation:**

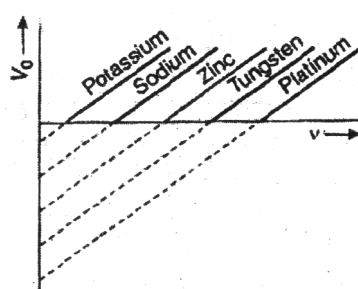
- The graph shows that at the frequency ν_0 the stopping potential is zero. The frequency ν_0 is known as threshold frequency and corresponding wavelength is called threshold wavelength.



- The threshold frequency is defined as minimum frequency (ν_0) of incident radiation, which can cause photoelectric emission.

Effect of Photometal

- All the lines in the graph have same slope, but their interactions with frequency axis is different.
- The threshold frequency depends on the nature of photometal.

**2.4.1 Einstien's Photoelectric Equation**

Q6. State and explain einstein photo electric equations.

Ans :

Einstien proposed an explanation of photo - electric effect as early as 1905. According to Einstein's explanation in photo - electric effect one photon is completely absorbed by one electron, which thereby gains the quantum of energy and may be emitted from the metal. The photon's energy is used in the following two parts :

- (i) A part of its energy is used to free the electron from the atom and away from the metal surface. This energy is known as photoelectric work function of the metal. This is denoted by W_0 .
- (ii) The other part is used in giving kinetic energy $\left(\frac{1}{2}mv^2\right)$ to the electron.

Thus,

$$h\nu = W_0 + \frac{1}{2}mv^2 \quad \dots (1)$$

Where v is the velocity of emitted electron, eq (1) is known as Einstein's photoelectric equation.

When the photon's energy is of such a value that it can only liberate the electron from metal, then the kinetic energy of the electron will be zero eq. (1) now reduces to

$$h\nu_0 = W_0$$

Where

ν_0 is called the threshold frequency.

Threshold frequency is defined as the minimum frequency which can cause photo - electric omission. The value of λ_0 is given by

$$c = \nu_0 \lambda_0 \quad \dots (2)$$

$$\text{or } \lambda_0 = \frac{c}{\nu_0} = \frac{ch}{W_0} \quad [\because W_0 = h\nu_0]$$

$$\begin{aligned} \lambda_0 &= \frac{3 \times 10^8 \times 6.625 \times 10^{-34}}{W_0} \\ &= \frac{19.875 \times 10^{-26}}{W_0} \text{ meter} \end{aligned}$$

There W_0 is expressed in joules. If W_0 is expressed in electron volts (eV), then

$$\begin{aligned} \lambda_0 &= \frac{19.875 \times 10^{-26}}{1.602 \times 10^{-19} W_0} \\ &= \frac{12.4 \times 10^{-7}}{W_0} \text{ meter} \\ \lambda_0 &= \frac{12400}{W_0} \text{ \AA} \quad \dots (3) \end{aligned}$$

From eq. (3), the value of photo - electric work function is given by

$$W_0 = \frac{12400}{\lambda_0} \text{ (eV) where } \lambda_0 \text{ is in } \text{\AA}$$

Substituting the value of $W_0 = hv_0$ in eq. (1), we have

$$hv = hv_0 + \frac{1}{2} mv^2 \quad \dots (4)$$

$$\text{or } \frac{1}{2} mv^2 = (hv - hv_0) = h(v - v_0)$$

This is another form of Einstein's photo - electric equation

The Einstein's photo - electric equation predicts all the experimental results. From eq. (1), we have

$$\frac{1}{2} mv^2 = hv - W_0$$

For a particular emitters, work function W_0 is constant and hence

$$\text{K.E.} = \frac{1}{2} mv^2 \propto hv \quad \dots (5)$$

$$\text{or } v^2 \propto v \quad \dots (5)$$

Thus, the increase in frequency v of incidents light cause increase in velocity of photo - electrons provided intensity light is constant.

An increase in the intensity of radiation is equivalent to an increase in the number of photon's falling on the emitting surface.

In this way the intensity of emitted electrons is directly proportional to the intensity of incident radiation

From eq. (5), we have

$$\frac{1}{2} mv^2 = hv - h\nu_0$$

If ν_0 be the stopping potential, then

$$eV_0 = hv - h\nu_0 \quad \dots (6)$$

$$\text{or } V_0 = \frac{hv}{e} - \frac{h\nu_0}{e} \quad \dots (7)$$

As h and e are constant V_0 is also constant for a given photo cathode, eq (7) shows that graph between stopping potential V_0 and frequency V would be a straight line of slope $\frac{h}{e}$.

2.5 COMPTON'S EFFECT - EXPERIMENTAL VERIFICATION

Q7. Discuss in brief about compton effect?

Ans :

(Imp.)

Compton Effect

According to Compton, the phenomenon of scattering is due to an elastic collision between two particles, the photon of incident radiation and the electron of scatterer. The observed change in frequency or wavelength of the scattered radiation is known as Compton effect.

The experimental demonstration of the Compton effect is shown in figure

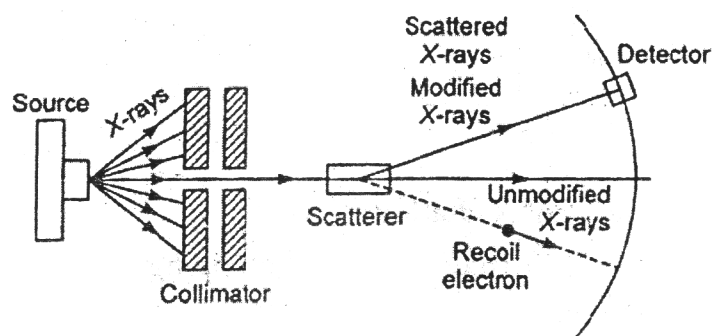
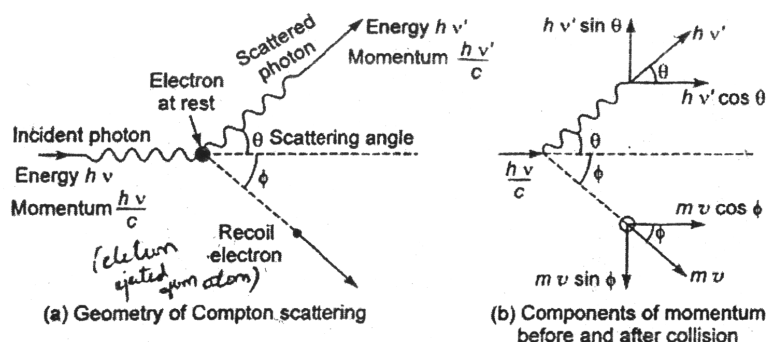


Fig. : Experimental arrangement for the study of Compton effect

A beam of monochromatic x-rays of known wave length are directed to a target. The scattered X-rays at various angles ' ϕ ' (observed on x-rays spectrometer) determine their wavelengths.

The scattering of Photon and the vector diagram of compton effect is shown in figure (3)



The amount of energy lost by the photon during collision is same as the kinetic energy gained by the electron.

Loss in photon energy = gain in electron energy.

According to the principle of conservation of energy

$$h\nu + m_0c^2 = h\nu' + mc^2 \quad \dots (1)$$

where

h - planck's constant

ν - frequency of incident photon

ν' - frequency of scattered photon

But energy of a particle in terms of momentum is given by

$$E = pv$$

$$\Rightarrow P = \frac{E}{c} = \frac{h\nu}{c} \quad [\because E = h\nu]$$

Where (p - photon momentum, c -velocity of light)

In figure, if one direction is chosen for original photon, the perpendicular to it results in electron and the other as scattered photon.

The initial and final momentum of original photon direction is same, i.e. Initial momentum = final momentum

$$\Rightarrow \frac{hv}{c} + 0 \cdot \cos\theta = \frac{hv^1}{c} \cos\phi + p \cos\theta \quad \dots (2)$$

$$\Rightarrow \frac{hv}{c} = \frac{hv^1}{c} \cos\theta + p \cos\theta \quad \dots (3)$$

$$\Rightarrow pc \cos\theta = hv - hv^1 \cos\phi \quad \dots (4)$$

$$\Rightarrow pc \sin\theta = hv^1 \sin\phi \quad \dots (5)$$

Where,

squaring equations (4) and (5) then adding

$$\begin{aligned} p^2 c^2 &= (hv - hv^1 \cos\theta)^2 + (hv^1 \sin\theta)^2 \\ &= h^2 v^2 - 2h^2 v v^1 \cos\theta + h^2 v^{1^2} \cos^2 \theta + h^2 v^{1^2} \sin^2 \theta \\ &= h^2 [v^2 + v^{1^2} - 2v v^1 \cos\theta] \end{aligned} \quad \dots (6)$$

From equation (1)

$$mc^2 = h(v - v^1) + m_0 c^2$$

Squaring on both sides

$$m^2 c^4 = h^2 (v^2 - 2v v^1 + v^{1^2}) + 2h (v - v^1) m_0 c^2 + m_0^2 c^4 \quad \dots (7)$$

Subtracting equation (6) from equation (7)

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

$$\Rightarrow \frac{m_0^2 c^4}{(c^2 - v^2)} (c^2 - v^2) = -2h^2 v v^1 (1 - \cos\theta) + 2h (v - v^1) m_0 c^2 + m_0^2 c^4 \quad \left[\because m = \frac{m_0}{\sqrt{1 - \frac{v^2}{c^2}}} \right]$$

2.6 MATTER WAVES & UNCERTAINTY PRINCIPLE

Q8. Given an account of velocity of de-Broglie wave.

Ans :

The velocity of matter wave depends on the velocity of matter particle i.e. it is not constant while the velocity of electromagnetic wave is constant.

The velocity of matter wave (de - Broglie wave velocity) is greater than the velocity of light.

A particle in motion with associated with matter wave has two different velocities represented by v and w related to the propagation of the wave represented by w .

We know that $E = h\nu$ and $E = mc^2$

$$h\nu = mc^2 \text{ (or) } \nu = \frac{mc^2}{h}$$

Tire wave velocity (w) is given by

$$w = \nu \times \lambda \quad \left\{ \because \lambda = \frac{h}{mc} \right\}$$

$$w = \frac{mc^2}{h} \times \frac{h}{mv} \text{ (or) } w = \frac{c^2}{v}$$

As particle velocity v ca nnot exceed c (velocity of light) hence w is greater than velocity of light.

Heisenberg Uncertainty Principle

Q9. State and explain Heisenberg uncertainty principle.

Ans :

According to Heisenberg uncetainity principle, it is impossible to measure both the position and momentum of a particle simultaneously to any desired degree of accuracy.

- "The order of magnitude of the uncertainties in the knowledge of two variable must be atleast planck's constant h ".

$$\Delta x = v_x \Delta t \quad \dots (3)$$

From equations (2) and (3), we get

$$\Delta x \cdot \Delta p_x = \Delta t \cdot \Delta E \quad \dots (4)$$

We know that $\Delta x \Delta p_x \geq \frac{h}{4\pi}$

$$\Delta x \cdot \Delta p_x \geq \frac{h}{4\pi} \quad \dots (5)$$

Q10. Relation between group velocity a nd wave velocity.

Ans :

The phase velocity of a wave is given by $V_p = \frac{\omega}{k}$ and group velocity $V_g = \frac{d\omega}{dk}$

$$\omega = v_p k \text{ (or) } d\omega = dv_p k + v_p dk \Rightarrow \frac{d\omega}{dk} = v_p + k \frac{dv_p}{dk}$$

from the above equations, we can write

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

$$\text{or } v_g = v_p + k \frac{dv_p}{d\lambda} \times \frac{d\lambda}{dk}$$

$$\text{Since } k = \frac{2\pi}{\lambda} \text{ hence } \frac{d\lambda}{dk} = -\frac{2\pi}{k^2}$$

2.6.1 de Broglie's Hypothesis Wavelength of Matter Waves

Q11. Explain de-broglie hypothesis of matter wave Derive an expression for de-Broglie wavelength?

Ans :

Light has dual nature i.e. it possesses both particle and wave properties. In some phenomena corpuscular nature while in others wave nature is predominate. The wave and particle donot appear together.

- The correspondance between wave and particle' are not confined only to electromagnetic radiation, but also valid for material particles i.e. like radiation, matter also has dual characteristics.
- A moving particle has always got a wave associated with it and the particle is controlled by waves.
- According to de-Broglie's hypothesis, a moving particle is associated with a wave which is known as de-Broglie wave. The wavelength of the matter wave is given by

$$\lambda = \frac{h}{mv} = \frac{h}{p} \quad \dots (1)$$

Where

$m \rightarrow$ mass of the material particle

$v \rightarrow$ velocity of particle

$p \rightarrow$ Momentum of the particle

Expression for de-broglie wavelength

Consider planck's theory of radiation, the energy of the photon is given by

$$E = hv = \frac{hc}{\lambda} \quad \dots (1) \quad \left\{ v = \frac{C}{\lambda} \right\}$$

Where

$c \rightarrow$ velocity of light in vaccum

$\lambda \rightarrow$ wavelength

According to Einstein energy - mass relation $E = mc^2$... (2)

From eqn's (1) and (2) $mc^2 = \frac{hc}{\lambda}$

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

$$\lambda = \frac{h}{mc} \quad \dots (3)$$

(where $mc = p$ momentum of photon)

If we consider particle with mass m and velocity v i.e. momentum mv , then

the wavelength associated with the particle is given by $\lambda = \frac{h}{mc} = \frac{h}{p}$... (4)

- (a) If E is the kinetic energy of the material particle, then

$$E = \frac{1}{2} mv^2 = \frac{1}{2} \frac{m^2 v^2}{m} = \frac{p^2}{2m}$$

$$F = \sqrt{2mE}$$

$$\therefore \text{de-broglie wavelength } \lambda = \frac{h}{\sqrt{2mE}} \quad \dots (5)$$

- (b) When a charged particle carrying a charge q is accelerated by a potential difference V volts, then its kinetic energy E is given by $E = qV$ de-Broglie wavelength associated with this particle

$$\text{is given by } \lambda = \frac{h}{\sqrt{2mqV}} \quad \dots (6)$$

- (c) When a particle is in thermal equilibrium at a temperature T , Then $E = \frac{3}{2} kT$

(Where k is Boltzmann constant $k = 1.38 \times 10^{-23} \text{ J / K}$)

The De-Broglie wavelength of particle at temperature T is given

$$\text{by } \lambda = \frac{h}{\sqrt{2m\left(\frac{3}{2}kT\right)}}$$

$$\lambda = \frac{h}{\sqrt{3kmT}}$$

De-Broglie wavelength associated with electron

Consider an electron of rest mass m_0 and charge e which is accelerated by a potential V volt from rest to velocity v , then

$$\frac{1}{2} m_0 v^2 = eV \quad (\text{or}) \quad v = \sqrt{\frac{2eV}{m_0}}$$

$$\text{Now } \lambda = \frac{h}{m_0 v} = \frac{h\sqrt{m_0}}{m_0 \sqrt{2eV}} = \frac{h}{\sqrt{2eVm_0}}$$

Substituting the values of

$$h = 6.625 \times 10^{-34} \text{ J.s}$$

$$e = 1.632 \times 10^{-19} \text{ C}$$

$$m = 9.1 \times 10^{-31} \text{ kg}$$

$$\lambda = \frac{6.625 \times 10^{-34}}{\sqrt{(2 \times 1.632 \times 10^{-19} \text{ V} \times 9.1 \times 10^{-31})}}$$

$$\lambda = \frac{12.26}{\sqrt{V}} \text{ \AA}$$

If $V = 100$ volts, then $\lambda = 1.226 \text{ \AA}$

This shows that the wavelength associated with an electron accelerated to 100 volts is 1.226 \AA .

2.6.2 Properties of Matter Waves

Q12. Define Properties of Matter Waves.

Ans :

Following are the properties of matter waves :

1. Lighter is the particle, greater is the wavelength associated with it.
2. Smaller is the velocity of the particle, greater is the wavelength associated with it.
3. When $v = 0$ then $\lambda = \infty$, i.e., wave becomes indeterminate and if $v = \infty$ then $\lambda = 0$. This shows that matter waves are generated by the motion of particle.

These waves are produced whether the particle are charged particles or they are uncharged ($\lambda = h/mv$ is independent of charge). This fact reveals that these waves are not electromagnetic waves but they are a new kind of waves (electromagnetic waves are produced only by motion of charged particles).

4. The velocity of matter wave depends on the velocity of matter particle i.e., it is not a constant while the velocity of electromagnetic wave is constant.
5. The velocity of matter wave is greater than the velocity of light.

The velocity of matter wave (de-Broglie wave velocity) is greater than the velocity of light. This can be proved as under

A particle in motion with associated matter wave has two different velocities, one referring to the mechanical motion of the particle represented by v and second related to the propagation of the wave represented by w .

We know that $E = hv$ and $E = mc^2$.

$$hv = mc^2 \text{ or } V = \frac{mc^2}{h}$$

The wave velocity (w) is given by

$$w = v \times \lambda = \frac{mc^2}{h} \times \frac{h}{mv} \quad \left[\because \lambda = \frac{h}{mv} \right]$$

$$\text{or } w = \frac{c^2}{v}$$

2.6.3 Phase and Group Velocities

Q13. Obtain an expression for wave velocity and group velocity.

Ans :

(Imp.)

When a monochromatic wave i.e., a wave of single frequency and wavelength travels a medium, its velocity of advancement in the medium is called as wave velocity. Consider a wave whose displacement y is expressed as $y = a \sin(\omega t - kx)$.

Where a is the amplitude, ω is angular frequency ($=2\pi n$) and k ($=2\pi / \lambda$) is the propagation constant of the wave.

The ratio of angular frequency ω to the propagation constant k is defined as wave velocity. This is expressed by v_p . Hence

$$v_p = (\omega/k) \quad \dots (1)$$

For the wave $(\omega t - kx)$ is the phase of wave motion for the planes of constant phase (wavefronts), we have

$$\omega t - kx = \text{constant} \quad \dots (2)$$

Differentiating equation (2) with respect to time t

$$\omega - k \frac{dx}{dt} = 0$$

$$\text{or } \frac{dx}{dt} = \frac{\omega}{k} = v_p$$

Thus the wave velocity is the velocity with which the planes of constant phase advances through the medium.

Group Velocity

When a group of waves of slightly different frequencies travels in the medium, the phase velocities of different components are different. However, the observed velocity is the velocity with which the maximum amplitude of the group advances. This is called group velocity. Thus the group velocity is the velocity with which the energy in the group is transmitted.

Let us consider the case of two wave trains having same amplitude a but slightly different angular frequencies (ω and ω') and phase velocity (u and u'). The waves can be represented as

$$y_1 = a \sin (\omega t - kx) \quad \dots (1)$$

$$\text{and } y_2 = a \sin (\omega' t - k'x) \quad \dots (2)$$

Where k and k' are propagation constants defined as ($2\pi / \lambda$). The resultant wave is given by

$$y = y_1 + y_2 = a \sin (\omega t - kx) + a \sin (\omega' t - k'x)$$

$$= 2a \cos \left[\left(\frac{\omega - \omega'}{2} \right) t - \left(\frac{k - k'}{2} \right) x \right] \times \sin \left[\left(\frac{\omega + \omega'}{2} \right) t - \left(\frac{k + k'}{2} \right) x \right]$$

$$\therefore \sin A + \sin B = 2 \sin \left(\frac{A+B}{2} \right) \cos \left(\frac{A-B}{2} \right)$$

$$y = 2a \cos \left[\left(\frac{d\omega}{2} \right) t - \left(\frac{dk}{2} \right) x \right] \sin (\omega t - kx) \quad \dots (3)$$

Where

$$\frac{\omega + \omega'}{2} = \omega \text{ and } \frac{k + k'}{2} = k \text{ (approx).}$$

Equation (3) represents a wave of angular frequency ω and propagation constant k . The phase velocity v_p of the resultant wave is given by

$$v_p = \frac{\omega}{k}$$

The amplitude given by

$$2a \cos \left[\left(\frac{d\omega}{2} \right) t - \left(\frac{dk}{2} \right) x \right]$$

$$\text{or } 2a \cos \frac{d\omega}{2} \left[t - \frac{dk}{d\omega} x \right] = 2a \cos \frac{d\omega}{2} \left[t - \frac{x}{v_g} \right]$$

Where v_g is known as group velocity. This is given as

$$v_g = \frac{d\omega}{dk} = \frac{\omega - \omega'}{k - k'}$$

2.7 DAVISSON AND GERMER EXPERIMENT

Q14. Describe Davisson Germer Experiment to demonstrate the wave character of electrons?

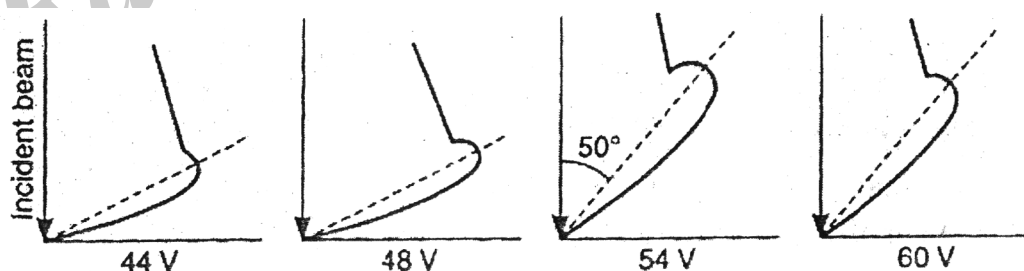
Ans :

(Imp.)

Davisson and Germer were two American physicists who has given first experimental evidence of matter waves.

Experimental Arrangement:

The apparatus consists of an electron gun G where the electrons are produced and obtained in a fine pencil of electronic beam of known velocity. The electron gun consists of a tungsten filament F. heated to dull red so that the electrons are emitted due to the thermionic emission.

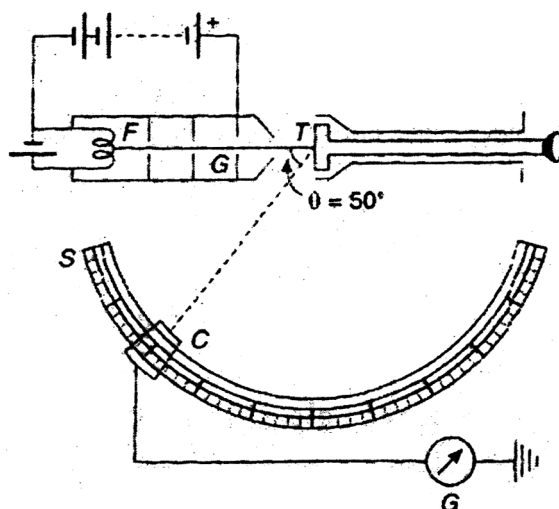


- The electrons are accelerated in the electric field of known potential difference. The electrons are collimated by suitable slits to obtain a fine beam. The beam of electron are directed to fall on a large single crystal of nickel, known as target T. The electrons acts as waves as they are diffracted indifferent directions.
- The angular distribution is measured by an electron detector (Faraday cylinder C) which is connected to a galvanometer.
- The Faraday cylinder can move on a circular graduated scales between 29° to 90° to receive to reflected electrons.

- The Faraday cylinder consists of two walls, which are insulated from each other.
- A retarding potential is maintained between them so that only fast moving electrons coming from electron gun may enter it. The secondary electrons produced by collisions with atoms from nickel target are reflected by Faraday cylinder.

Procedure

- The accelerating potential V is given a low value and the crystal is set at any azimuth (θ). The Faraday cylinder is moved to various positions on the scales and galvanometer current is noted for each position. The galvanometer meter current is noted for each position. The galvanometer current is a measure of intensity of diffracted beam



- A graph is plotted between galvanometer current and angle θ between incident beam and beam entering the cylinder. The observations are repeated for different accelerating potentials.

Observations

It is observed that a bump begins to appear in the curve for 44 volts electrons.

- With increasing potential, the bump moves upwards.
- The bump becomes most prominent in the curve for 54 volts electrons at $\theta = 50^\circ$

(iii) At higher potentials, the bumps gradually disappear.

The bump in its most prominent state verifies the existence of electron waves. According to De-Broglie, the wavelength associated with electron accelerated through a potential V is given by

$$\lambda = \frac{12.26}{\sqrt{V}} \text{ \AA}$$

Hence, the wavelength associated with 54 volt electrons is

$$\lambda = \frac{12.26}{\sqrt{54}} = 1.67 \text{ \AA}$$

2.8 DOUBLE SLIT EXPERIMENT

Q15. Describe the double slit experiment.

Ans :

The interference of electron waves can be exhibited by double slit experiment. The interference pattern so obtained resembles with the pattern obtained in case of visible light. This proves the association of waves with electrons just like photons.

The experimental arrangement is shown in fig.

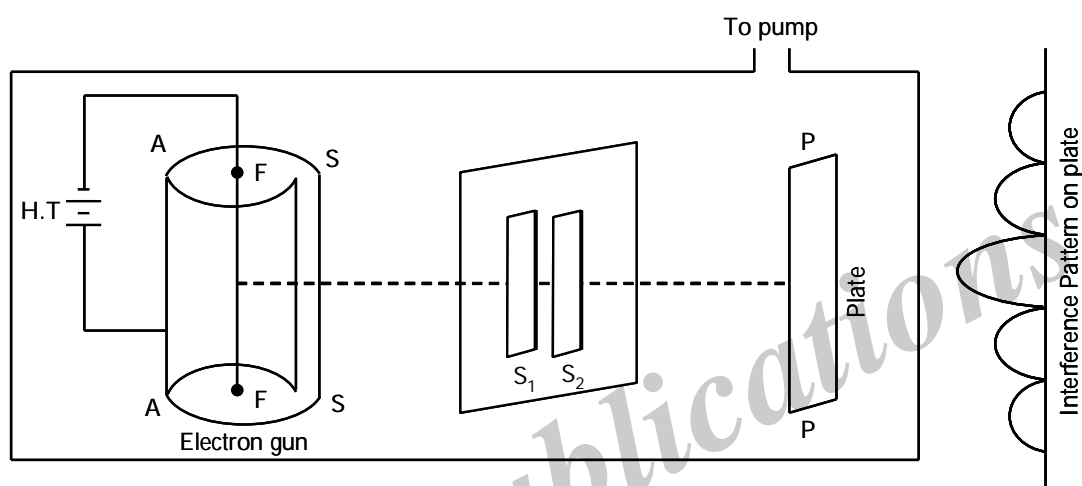


Fig. : Double slit interference pattern with electrons.

In the figure, FF is the filament and cylindrical anode AA acts as electron gun. The function of electron gun is to supply a monoenergetic beam of electrons. The electronic beam passes through a narrow slit SS. An arrangement of two slits S_1 , S_2 (very fine, closely spaced and symmetrically situated with respect to SS) is placed in the path of electronic beam. PP is a photographic plate where the beam produces interference pattern. The whole chamber is evacuated.

The electrons pass through the slit SS and diffracted by S_1 , S_2 . The two slits act as coherent sources and hence the diffracted beams of electrons interfere and produces interference pattern on photographic plate PP. The interference pattern is also shown in the side of figure. The interference pattern shows the existence of waves associated with electrons.

Knowing the separation between S_1 , S_2 and their distance from photographic plate, the value of wavelength associated with electrons can be calculated. The value of wavelength comes out to be the same as obtained by de-Broglie relation. This proves the existence of matter waves associated with material particles.

2.9 STANDING DE-BROGLIE WAVES OF ELECTRON IN BOHR ORBITS

Q16. Derive standing de-Broglie Waves of Electron in Bohr Orbits.

Ans :

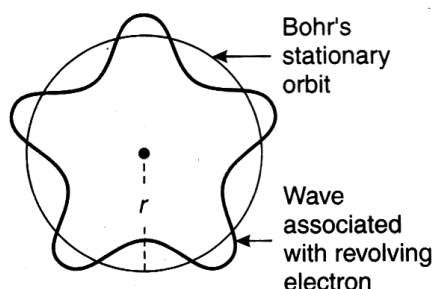
According to de-broglie hypothesis, an electron of mass m in motion with velocity v is associated with a wave whose wavelength λ is given by

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

where

h is Planck's constant ... (1)

de-Broglie, on the basis of his hypothesis proposed an atomic model in which the stationary orbits of the Bohr's model were retained but with the difference that electron in various orbits behaves as wave. This is shown in fig.



He suggested that stationary orbits are those in which orbital circumference ($2\pi r$) an integral multiple of de-Broglie wavelength λ , i.e., stationary orbits for an electron are those which contain the complete waves of electron. This,

$$2\pi r = n\lambda$$

Where

$$n = 1, 2, 3, \dots \quad \dots (2)$$

But

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

$$2\pi r = n \frac{h}{mv}$$

$$\text{or } L = mvr = n \frac{h}{2\pi} \quad \dots (3)$$

mvr is the angular momentum if the electron as particle. The eq. (3) is nothing but the Bohr's postulate, i.e., the total angular momentum of the moving electron is an integral multiple of $\frac{h}{2\pi}$.

Thus, the new concept of de-Broglie confirms the Bohr's postulate

$$\text{or } 2a \cos \frac{d\omega}{2} \left[t - \frac{dk}{d\omega} x \right] = 2a \cos \frac{d\omega}{2} \left[t - \frac{x}{v_g} \right]$$

Where v_g is known as group velocity. This is given as

$$v_g = \frac{d\omega}{dk} = \frac{\omega - \omega'}{k - k'}$$

2.10 HEISENBERG'S UNCERTAINTY PRINCIPLE FOR POSITION AND MOMENTUM (x AND px) ENERGY AND TIME (E AND t).

Q17. Explain Heisenberg's uncertainty Principle for Position and Momentum (x and px) Energy and time (E and t).

Ans :

Uncertainty Principle

It is impossible to know where within the wave packet the particle is and what is its exact momentum. Hence we can measure either the position or the momentum of a particle with any desired degree of accuracy.

According to Heisenberg uncertainty principle, it is impossible to measure both the position and momentum of a particle simultaneously to any desired degree of accuracy. In general, this principle states that "It is impossible to specify precisely and unultaneously the values of both members of particular pairs of physical variables that describe the behaviour of an atomic system. "Qualitatively this principle states" that "the order of magnitude of the uncertainties in the knowledge of two variables must heat least Planck's constant h" Considering the pair of physical variables as position and momentum, we have

$$\Delta p \Delta x \approx h \quad \dots(1)$$

where Δp the uncertainty in determining the momentum and Δx is the uncertainty in determining the position of the particle. Similarly, we have

$$\Delta E \Delta t \approx h \quad \dots(2)$$

$$\Delta J \Delta \theta \approx h \quad \dots(3)$$

where ΔE and Δt are uncertainties in determining the energy and time while ΔJ and $\Delta \theta$ are uncertainties in determining the angular momentum and angle.

The exact statement of uncertainty principle is as follows :

The product of uncertainties in determining the position and momentum of the particle can never be smaller than the order of $\frac{h}{4\pi}$. So. we have

$$\Delta p \Delta x \geq \frac{h}{4\pi}, \Delta E \Delta t \geq \frac{h}{4\pi}, \Delta J \Delta \theta \geq \frac{h}{4\pi}.$$

Time-energy Uncertainty Principle

Although the time-energy uncertainty relation can be obtained by considering a wave packet over limited time interval but the proof is beyond the level of this book. However, we shall consider the time-energy uncertainty with the help of position momentum uncertainty. Consider the case of a free particle with rest mass m_0 moving along A-direction with velocity v_x . The kinetic energy is given by

$$E = \frac{1}{2} m_0 v_x^2 = \frac{p_x^2}{2m_0} \quad \dots(1)$$

If Δp_x and ΔE be the uncertainties in momentum and energy respectively, then differentiating eq. (1), we have

$$\Delta E = \frac{2p_x \Delta p_x}{2m_0}$$

or $p_x \Delta p = m_0 \Delta E$

$$\therefore \Delta p_x = \frac{m_0}{p_x} \Delta E = \frac{1}{v_x} \Delta E \quad \dots(2)$$

2.11 GAMMA RAY MICROSCOPE

Q18. Give the experimental illustrations of Heisenberg uncertainty principle.

Ans :

(Imp.)

According to Heisenberg uncertainty principle, it is impossible to measure both the position and momentum of a particle simultaneously to any desired degree of accuracy

Experimental Illustration

- Determination of the position of a particle by Gamma ray Microscope:** Consider the case of the measurement of the position of a particle say electron in the field of microscope. The resolving power i.e. the smallest distance between the two points that can be just resolved by the microscope is given by

$$\Delta x = \frac{\lambda}{2 \sin \theta} \quad \dots (1)$$

Where

$\lambda \rightarrow$ wavelength of light used

$\theta \rightarrow$ semi vertical angle of of light

$\Delta x \rightarrow$ uncertainty in determining the position of the particle.

In order to observe the electron. It is necessary that atleast one photon must strike the electron and scatter inside the microscope. When a photon of initial momentum $p = h / \lambda$, after

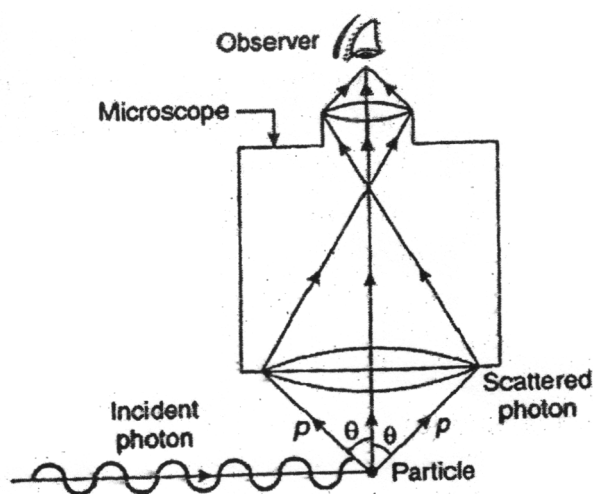
After scattering enters the field of view of microscope, it may be anywhere, within angle 2θ . Thus its x component of momentum i.e. p_x may lie between $p \sin \theta$ and $-p \sin \theta$

As the momentum is conserved in the collision, the uncertainty in the 'x' component of momentum is given by

$$\begin{aligned} \Delta p_s &= p \sin \theta - (-p \sin \theta) \\ &= 2p \sin \theta \\ &= 2 \frac{h}{\lambda} \sin \theta \rightarrow (2) \end{aligned} \quad \dots (2)$$

From equations (1) and (2), we have

$$\begin{aligned} \Delta x \Delta p_x &\approx \frac{\lambda}{2 \sin \theta} \times \frac{2h}{\lambda} \sin \theta \\ \text{i.e., } \Delta x \cdot \Delta p_x &\approx h \rightarrow (3) \end{aligned} \quad \dots (3)$$



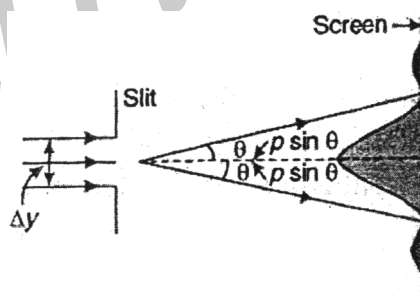
This shows that the product of uncertainties in position and momentum is of the order of Planck's constant

2.12 DIFFRACTION BY A SINGLE SLIT

Q19. Explain diffraction by a single slit.

Ans :

Suppose a narrow beam of electrons passes through a single narrow slit and produces a diffraction pattern on the screen as shown in fig:



The first minimum of the pattern is obtained by putting $n = 1$ in the equation describing the behaviour of diffraction pattern due to a single slit

(i.e., $d \sin \theta = n\lambda$) hence

$$\Delta y \sin \theta = \lambda \quad \dots (4)$$

Where Δy is the width of the slit

θ is the angle of deviation corresponding to first minimum

In producing the diffraction pattern on the screen all electrons have passed through the slit but we cannot say definitely at what place of the slit. Hence the uncertainty in determining the position of the electron is equal to the width Δy of the slit.

$$\text{from equation (4) } \Delta y = \frac{\lambda}{\sin \theta} \quad \dots (5)$$

Initially the electrons are moving along the x - axis and hence they have no component of momentum along y - axis. After diffraction at the slit, they are deviated from their initial path to form the pattern and have a component $p \sin \theta$. As y component of momentum may lie anywhere between $p \sin \theta$, and $-p \sin \theta$, uncertainty in y - component of momentum is

$$\Delta P_y = 2p \sin \theta = \frac{2h}{\lambda} \sin \theta \quad \left[\because p = \frac{h}{\lambda} \right] \quad \dots (6)$$

from equation (5) and (6)

$$\Delta y \cdot \Delta p_y \approx \frac{\lambda}{\sin \theta} \times \frac{2h \sin \theta}{\lambda} \approx 2h$$

$$(\text{or}) \Delta y \cdot \Delta p_y \approx h \quad \dots (7)$$

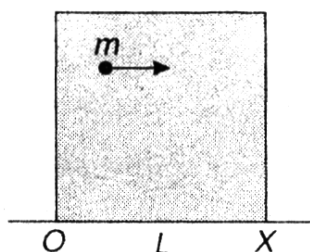
The relation shows that the product of uncertainties in position and momentum is of the order of planck's constant.

2.12.1 Consequence of Uncertainty Relation (Particle in a Box)

Q20. Explain uncertainty relation (Particle in a Box).

Ans :

Consider a particle of mass m moving in one dimensional box of length l . In A-direction as shown in fig. The minimum uncertainty in the position x of the particle will be $\Delta x = L$. Here L is the width of the box.



According to uncertainty principle,

$$\Delta x \cdot \Delta p \approx h$$

$$\text{or} \quad \Delta p \approx \frac{h}{\Delta x} \approx \frac{h}{L}$$

Approximately, the above expression can be written as

$$p \sim \Delta p \approx \frac{h}{2L}$$

$$\text{Now, Energy } E = \frac{p^2}{2m} \approx \frac{h^2}{8mL^2}$$

$$\text{or} \quad E \approx \frac{\pi^2 h^2}{2mL^2}$$

2.13 POSITION OF ELECTRON IN A BOHR ORBIT

Q21. Derive position of electron in Bohr Orbit.

Ans. :

In calculating the radius of Bohr's first orbit: If Δx and Δp are the uncertainties in position and momentum of the electron in the first orbit, then according to uncertainty principle, we have

$$\Delta x \cdot \Delta p \geq \frac{h}{4\pi}$$

$$\Delta p \geq \frac{h}{4\pi \Delta x} \quad \dots(1)$$

The uncertainty in the kinetic energy ΔT of the electron may be written as

$$\Delta T = \frac{1}{2} m (\Delta v)^2 \geq \frac{m^2 (\Delta v)^2}{2m} \geq \frac{(\Delta p)^2}{2m}$$

$$\Delta T \geq \frac{h^2}{16\pi^2 \cdot 2m \cdot (\Delta x)^2} \quad \dots(2)$$

The uncertainty in the potential energy ΔV of the same electron is given by

$$\Delta T \geq \frac{-Ze^2}{\Delta x} \quad \dots(3)$$

The uncertainty in the total energy ΔE is given by

$$\Delta E \geq \Delta T \geq \Delta V \geq \frac{h^2}{16\pi^2 \cdot 2m \cdot (\Delta x)^2} + \frac{-Ze^2}{\Delta x} \quad \dots(4)$$

The uncertainty in the energy will be minimum, if

$$\frac{d(\Delta E)}{d(\Delta x)} = 0 \text{ and } \frac{d^2(\Delta E)}{d^2(\Delta x)} \text{ is positive}$$

$$\text{Now, } \frac{d(\Delta E)}{d(\Delta x)} \geq \frac{-2h^2}{16\pi^2 \cdot 2m \cdot (\Delta x)^3} + \frac{Ze^2}{(\Delta x)^2} = 0$$

$$\text{or } \frac{h^2}{16\pi^2 \cdot m \cdot (\Delta x)^3} \approx \frac{Ze^2}{(\Delta x)^2}$$

$$\text{or } \Delta x \approx \frac{h^2}{16\pi^2 m Ze^2} \quad \dots(5)$$

If we calculate the value of $\frac{d^2(DE)}{d(\Delta x)^2}$, this comes out to be positive and hence Δx

given by eq.(5) represents a minimum. This shows that in order to have minimum energy, the electron must be at least Δx away from the nucleus. We know that the energy at the electron is minimum in the first orbit. Therefore, the radius of the first orbit is given by

$$r \approx \Delta x \approx \frac{h^2}{16\pi^2 mZe^2} \quad \dots(6)$$

or $r \approx \frac{h^2}{4mZe^2}$ using $h = \frac{h}{2\pi}$

2.14 COMPLEMENTARY PRINCIPLE OF BOHR

Q22. Define complementary Principle of Bohr.

Ans :

The most important consequence of uncertainty principle is that it is impossible to determine the wave and particle properties at the same time in a single experiment.

According to complementary principle, the wave and particle nature of matter and light are complementary rather than contradictory, i.e., both aspects are necessary to have a complete picture of the system. Both these aspects have never been shown in a single experiment.

Let us consider an experimental arrangement in which light is diffracted by a double slit and is detected on a screen that consists of many adjacent photoelectric cells. The photoelectric cells respond to photons having particle properties. However, if we plot the number of photons, each cell counts in a certain period of time against the location of cell, a wave-like pattern (like the interference of a pair of coherent wave trains) is obtained. It follows that only experiment which can be devised displays either the particle-like characteristics or wave-like characteristics of the system, in moreover the wave and particle pictures give complementary description of the same pattern.

2.15 APPLICATIONS OF UNCERTAINTY PRINCIPLE

Q23. Explain and derive Applications of Uncertainty Principle.

Ans :

Non-existence of electrons and existence of protons and neutrons in nucleus

The radius of the nucleus of any atom is of the order of 10^{-14} m. If an electron is confined inside the nucleus, then uncertainty in the position Δx of the electron is equal to the diameter of the nucleus.

i.e., $\Delta x \approx 2 \times 10^{-14}$ m. Using the Heisenberg's uncertainty relation, the uncertainty in momentum of electron is given by

$$\Delta p_x \geq \frac{h}{2\pi \Delta x} \geq \frac{1.055 \times 10^{-34}}{2 \times 10^{-14}} \text{ kg ms}^{-1} \quad (\because \Delta x \geq 2 \times 10^{-14})$$

where $\frac{h}{2\pi} = 1.055 \times 10^{-34}$

$\therefore \Delta p_x \geq 0.527 \times 10^{-20} \text{ N-s}$

It means that the momentum component p_x and hence the magnitude of total momentum $|\vec{p}|$ of the electron in the nucleus must be at least of the order of magnitude.

Uncertainty Principle

Since the mass of the electron is $9.1 \times 10^{-31} \text{ kg}$, the order of magnitude of momentum ($0.527 \times 10^{-20} \text{ kg ms}^{-1}$) is relativistic. Using the relativistic formula for the energy E of the electron, we have

$$E^2 = p^2 c^2 + m_0^2 c^4$$

As the rest energy $m_0 c^2$ of the electron is of the order of 0.511 MeV, which is smaller than the value of first term, hence it can be neglected. Thus,

$$E^2 = p^2 c^2 \quad \text{or} \quad E = pc$$

$$E \approx (0.527 \times 10^{-20}) \times (3 \times 10^8) \text{ joule}$$

$$\approx (0.527 \times 10^{-20}) (3 \times 10^8)$$

$$\approx 10 \text{ MeV}$$

This means that if the electrons exist inside the nucleus their energy must be of the order at 10 MeV. However, we know that the electrons emitted by radioactive nuclei doing beta decay have energies only 3 to 4 MeV. Hence, in general electrons exist in the nucleus.

For protons and neutrons, $m_0 \approx 1.67 \times 10^{-27} \text{ kg}$. This is a non-relativistic problem as $|\vec{d}| \approx |\vec{p}| / m_0 \approx 10^6 \text{ ms}^{-1}$. The kinetic energy E in this case is given by

$$E = \frac{p^2}{2m_0} = \frac{(0.527 \times 10^{-20})^2}{2 \times 1.67 \times 10^{-27}} \text{ joule}$$

$$\approx \frac{(0.527 \times 10^{-20})^2}{2 \times 1.67 \times 10^{-27} \times 1.6 \times 10^{-19}} \text{ eV} = 52 \text{ keV}$$

Since the energy is smaller than the energies carried by these particles emitted in nuclear reactions, these particles can exist inside the nuclei.

Binding energy of an electron in atom

In an atom the electron is under the influence of electrostatic potential of the positively charged nucleus. It is confined to the linear dimensions equal to the diameter of electronic orbit. The uncertainty in the position Δx of the electron is of the order of R where R is the radius of the orbit. The corresponding uncertainty in momentum component Δp_x is given by

$$\Delta p_x \geq \frac{h}{4\pi \cdot 2R}$$

This expression shows that the momentum of an electron in atomic orbit is at least

This is non-relativistic momentum for an electron. The kinetic energy K is given by

$$K = \frac{p^2}{2m_0} \approx \left(\frac{h}{4\pi R} \right)^2 \frac{1}{2m_0} \approx \frac{h^2}{32\pi^2 m_0 R^2}$$

The potential energy of an electron in the field of nucleus with atomic number Z is

$$V = \frac{-Ze^2}{4\pi\epsilon_0 R}$$

The total energy of the electron in its orbit is

$$E = K + V = \frac{h^2}{32\pi^2 m_0 R^2} - \frac{Ze^2}{4\pi\epsilon_0 R}$$

$$\approx \frac{(1.055 \times 10^{-34})^2}{8 \times 9.1 \times 10^{-31} \times R^2} - \frac{Z(1.6 \times 10^{-19})^2}{4 \times 3.14 \times 8.85 \times 10^{-12} \times R}$$

where $\frac{h}{2\pi} = 1.055 \times 10^{-34}$

$$\therefore E \approx \frac{10^{-20}}{R^2} - \frac{15 \times 10^{-10} Z}{R} \text{ eV}$$

Taking $R \approx 10^{-10} \text{ m}$, we have

$$E \approx (0 - 15 Z) \text{ eV} \approx (-15 Z) \text{ eV}$$

As we know that the binding energies of outermost electrons in H and He are -13.6 and 24.6 eV respectively, hence the value of binding energy derived on the basis of uncertainty principle is acceptable in view of magnitudes.

Radiation of light from an excited atom

We know that the a range time period that an atom takes to come to its unexcited from the excited state is of the order of 10^{-8} seconds. Thus, the uncertainty in the energy is given by

$$\Delta E \geq \frac{h}{4\pi \cdot \Delta t} \geq \frac{6.6 \times 10^{-34}}{4 \times 3.14 \times 10^{-8}} \approx 10^{-26} \text{ joule}$$

Thus, the uncertainty in the frequency of light is

$$\Delta \nu = \frac{\Delta E}{h} \geq \frac{10^{-26} \times 4 \times 3.14}{6.6 \times 10^{-34}} \approx 10^7 \text{ hertz}$$

$$4\Delta$$

2.16 SCHRODINGER TIME INDEPENDENT AND TIME DEPENDENT WAVE EQUATIONS

Q24. Derive Schrodinger time independent equation for matter waves ?

Ans :

(Imp.)

Schrodinger time independent wave equation

According to de - Broglie theory, a particle of mass m is always associated with a wave whose wavelength is given by $\lambda = \frac{h}{mv}$. If the particle has wave properties, it is expected that there should be some sort of wave equation which describes the behaviour of the particle consider a system of stationary waves associated with a particle. Let x, y, z be the coordinates of the particle and Ψ , the wave displacement for the de-broglie at any time t Ψ is called as wave function. It is assumed that Ψ is finite angle valued and periodic function. The classical differential equation of a wave motion is given by

$$\frac{\partial^2 \Psi}{\partial t^2} = v^2 \left(\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} \right) = v^2 \nabla^2 \Psi \quad \dots (1)$$

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \quad [\nabla^2 \text{ being Laplacian operator}]$$

Where v is the wave velocity

The solution of eq. (1) is given by

$$\Psi = \Psi_0 \sin \omega t = \Psi_0 \sin 2\pi \nu t \quad \dots (2)$$

Where ν is the frequency of the stationary wave associated with the particle.

Differentiating eq. (2) twice, we get

$$\frac{\partial \Psi}{\partial t} = \Psi_0 (2\pi \nu) \cos 2\pi \nu t$$

$$\frac{\partial^2 \Psi}{\partial t^2} = -\Psi_0 (2\pi \nu)^2 \sin 2\pi \nu t$$

$$\frac{\partial^2 \Psi}{\partial t^2} = -4\pi^2 \nu^2 \Psi = \frac{4\pi^2 \nu^2}{\lambda^2} \Psi \quad \dots (3)$$

Substituting the value of $\left[\frac{\partial^2 \Psi}{\partial t^2} \right]$ from eq. (3) in eq. (1)

$$v^2 \nabla^2 \Psi = \frac{4\pi^2 \nu^2}{\lambda^2} \Psi$$

$$\text{or } \nabla^2 \Psi + \frac{4\pi^2 \nu^2}{\lambda^2} \Psi = 0$$

Now from de - Broglie relation

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

$$\therefore \nabla^2 \Psi + \frac{4\pi^2}{h^2} m^2 v^2 \Psi = 0 \quad \dots (5)$$

If E and V be the total and potential energies of the particle respectively, then its kinetic energy $\frac{1}{2}mv^2$ is given by

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

$$\text{or} \quad m^2 v^2 = 2m (E - V) \quad \dots (6)$$

From equ. (5) and (6) we have

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

$$\nabla^2 \Psi + \frac{8\pi^2 m}{h^2} (E - V) \Psi = 0 \quad \dots (7)$$

Equ. (7) is known as Schroedinger time - independent wave equation

Substituting $h = \frac{h}{2\pi}$ in eq. (7) the Schroedinger wave equation can be written as

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

Equ. (8) can also be expressed in following way

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

$$\text{or} \quad \frac{h^2}{2m} \nabla^2 \Psi - v\Psi = E\Psi$$

$$\text{or} \quad \left[\frac{h^2}{2m} \nabla^2 + v \right] \Psi = E\Psi$$

$$\text{or} \quad \boxed{\hat{H}\Psi = E\Psi}$$

Where $\hat{H} = \left[\frac{-h^2}{2m} \nabla^2 + v \right] \Psi$ and H is known as Hamiltonian operator

For a free particle $V = 0$, hence the Schroedinger wave equation for a free particle can be expressed as

$$\nabla^2 \Psi + \frac{2mE}{h^2} \Psi = 0 \quad \dots (10)$$

Q25. Derive Schroedinger time dependent equations for matter waves ?*Ans :***(Imp.)**

The Schroedinger time - dependent wave equation may be obtained from Schroedinger time - independent wave equation by eliminating E.

In order to derive time - dependent wave equation, Schroedinger introduced a numerical function Ψ which is a variable quantity associated with the moving particle. This is complex function of space coordinates of the particle and time. The function Ψ is called as wave function as it characterises de - Broglie waves associated with particle.

The differential equation representing a one - dimensional wave motion is

$$\frac{\partial^2 \Psi}{\partial t^2} = v^2 \nabla^2 \Psi \quad \dots (1)$$

Considering Ψ to be a complex function of space coordinates of the particle and time the general solution of eq. (1) is given by

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

$$\text{or} \quad \Psi = \Psi_0 e^{-i\omega t} \quad \dots (2)$$

Differentiating eq. (2) with respect to time t, we have

$$\begin{aligned} \frac{\partial \Psi}{\partial t} &= \Psi_0 (-i\omega) e^{-i\omega t} \\ &= \Psi_0 (-i2\pi\nu) e^{-i\omega t} = 2\pi i\nu \Psi \\ &= -2\pi i (E/h) \Psi \quad (\because E = h\nu \text{ (or) } \nu = E/h) \\ &= \frac{-iE}{h} \Psi \\ E \Psi &= ih \frac{\partial \Psi}{\partial t} \quad \dots (3) \end{aligned}$$

Substituting the value of $E \Psi$ in Schroedinger time - independent wave equation to get

$$\begin{aligned} \nabla^2 \Psi + \frac{2m}{h^2} \left[ih \frac{\partial \Psi}{\partial t} - v\Psi \right] &= 0 \\ \nabla^2 \Psi &= \frac{2m}{h^2} \left[ih \frac{\partial \Psi}{\partial t} - v\Psi \right] \\ \frac{-h^2}{2m} \nabla^2 \Psi + v\Psi &= ih \frac{\partial \Psi}{\partial t} \quad \dots (4) \end{aligned}$$

This equation is known as Schrodinger time - dependent wave equation Eq. (4) can be written as

$$\left[\frac{-h^2}{2m} \nabla^2 + v \right] \Psi = ih \frac{\partial \Psi}{\partial t}$$

$$\hat{H}\Psi = \hat{E}\Psi \quad \dots (5)$$

Where

$$\hat{H} = \left[\frac{-\hbar^2}{2m} \nabla^2 + v \right] = \text{Hamiltonian operator}$$

and $\hat{E} = i\hbar \frac{\partial}{\partial t} = \text{Energy operator}$

Eq. (5) describes the motion of a nonrelativistic material particle

2.17 WAVE FUNCTION PROPERTIES

Q26. Explain wave function properties ?

Ans :

The wave function Ψ must fulfil the following requirements

(i) It must be finite everywhere

If Ψ is infinite at a particular point, then it would mean an infinitely large probability of finding the particle at that point. This is not possible. Hence Ψ must have a finite or zero value at any point.

(ii) It must be single valued

Let us consider that Ψ has more than one value at any point. It means that there is more than one value of probability of finding the particle at that point. This is obviously ridiculous.

(iii) It must be continuous

For Schrodinger equation $\frac{d^2\Psi}{dx^2}$ must be finite everywhere. This is possible only when $\frac{d\Psi}{dx}$ has no discontinuity at any boundary where potential changes. This implies that Ψ too must be continuous across a boundary.

Important Points

1. Since a physical system must exist somewhere, the probability of its finding must be 1, i.e.,

$$\int_{-\infty}^{+\infty} |\Psi|^2 dx dy dz = 1$$

This is known as normalization condition

2. The probability of finding the system between x_1 and x_2 is given by

$$\rho = \int_{x_1}^{x_2} |\Psi|^2 dx$$

3. The probability per unit volume of a system being in the state Ψ is called probability density i.e., $\rho = |\Psi|^2 dx$

$$\int \rho dV = \int |\Psi|^2 dV = 1$$

2.18 PHYSICAL SIGNIFICANCE OF WAVE FUNCTION

Q27. Define physical significance of wave function.

Ans :

It is observed that in some cases, Ψ is appreciably different from zero within some finite region known as wave packet. It is natural to ask, "where is the particle in relation to wave packet?" To explain it, Max Born suggested a new idea about the physical significance of Ψ which is generally accepted now-a-days. According to Max Born $\Psi\Psi^*$ $|\Psi|^2$ gives the probability of finding the particle in the state Ψ , i.e., Ψ^2 is a measure of probability density. The probability of finding a particle in volume $dT = dx dy dz$ is given by $|\Psi|^2 dx dy dz$. For the total probability of finding the particle somewhere is, of course, unity, i.e., particle is certainly to be found somewhere in space

$$\iiint |\Psi|^2 dx dy dz = 1$$

Satisfying above requirement is said to be normalized.

2.19 BASIC POSTULATES OF QUANTUM MECHANICS

Q28. Define basic postulates of quantum mechanics ?

Ans :

The particulars of the quantum mechanics may be stated as follows :

Postulate 1 :

Where function to describe physical system

There is an associated wave function Ψ with system and any state of system is described as fully as possible by this wave function. This is state function of the system.

For a wave function Ψ to describe any physical system, the following boundary conditions must be satisfied :

- (i) $\Psi(x)$ as well as $d\Psi(x)$ must be finite for all values of x . Let $\Psi(x)$ be finite at the any point in the space. The probability of finding. The system at the that point, i.e., $|\Psi(x)|^2$ is infinite. This shows that the particle is completely localized.
- (ii) $\Psi(x)$ as well as $d\Psi(x) / dx$ must be continuous for all values of x in the region expect where the finite. For $d\Psi(x) / dx$ to be infinite, $\Psi(x)$ must be continuous because derivative, of a discontinuous function is always infinite. The discontinuous value of the function i.e., the infinite values of $d\Psi(x) / dx$ will lead to the infinite value of the system which is not possible.
- (iii) $\Psi(x)$ as well as $d\Psi(x) / dx$ must be single - valued for all x in the region. Let $\Psi(x)$ has a multi valued at some point. Then the probability of finding the system between x and $x + dx$ is $|\Psi(x)|^2 dx$ and will be multi-valued.
- (iv) In addition to the above condition, the wave - function $\Psi(x)$ must satisfy the Born conditions. According to earn condition, the probability of finding a particle in volume element $dx dy dz$ is given by $|\Psi(x)|^2 dx dy dz$ or $\Psi\Psi^* dx dy dz$. If the particle is somewhere in the space, then the probability will be equal do unity, i.e.,

$$\int \Psi\Psi^* dx dy dz = 1$$

All space

This is called normalization condition

When, there are n - particles in the space then

$$\int \Psi \Psi^* dx dy dz = n$$

All space

Where Ψ is now unnormalized wave function. The normalized wave function will be $\frac{\Psi}{\sqrt{n}}$. The quantity $(\sqrt{n}) = e$. Is called the normalization constant.

Postulate 2 :

Operators for observable quantities.

With every dynamical variable, there is associated an operator. An operator is anything which is capable of doing something to a function or any mathematical operation as multiplication x , differentiation d/dy integration \int can be expressed by contain symbols known as operator. When any operator say \hat{O} operates on a wave function Ψ and the result is expressed as

$$\hat{O} \Psi = a\Psi,$$

Then the observable quantity a is known as eigen value of the operator \hat{O} for the function Ψ known as eigen function. The table given below shows some quantum mechanical operators corresponding to different classical observable quantities.

2.20 OPERATORS

Q29. State the operators ?

Ans :

S.No.	Classical Quantity	Equivalent Quantum Mechanical Operator
1.	Certain coordinates of particle in space (x, y, z)	$\bar{x}, \bar{y}, \bar{z}$
2.	Position of particle (r)	\bar{r}
3.	Momentum (p)	$\frac{h}{i} \nabla$
	x - component of momentum (P_x)	$\frac{h}{i} \frac{\partial}{\partial x}$
	y - component of momentum (P_y)	$\frac{h}{i} \frac{\partial}{\partial y}$
	z - component of momentum (P_z)	$\frac{h}{i} \frac{\partial}{\partial z}$

4.	Kinetic energy	$-\frac{h^2}{2m} \nabla^2$
	x - component of K.E	$(-h^2 / 2m) \frac{\partial^2}{\partial x^2}$
	y - component of K.E	$(-h^2 / 2m) \frac{\partial^2}{\partial y^2}$
	z - component of K.E	$(-h^2 / 2m) \frac{\partial^2}{\partial z^2}$
5.	Velocity (v)	$\frac{h}{im} \nabla$
	x - component of velocity (v_x)	$\frac{h}{im} \frac{\partial}{\partial x}$
	y - component of velocity (v_y)	$\frac{h}{im} \frac{\partial}{\partial y}$
	z - component of velocity (v_z)	$\frac{h}{im} \frac{\partial}{\partial z}$

2.21 EIGEN VALUES AND EIGEN FUNCTIONS

Q30. Discuss Eigen values and Eigen functions of a particle enclosed box.

Ans :

(Imp.)

There is a class of function (known as well behaviour function)

Ψ which when operated by an operator \hat{O} are merely multiplied by some constant say λ , i.e.,

$$\hat{O} \Psi(x) = \lambda \Psi(x)$$

Then we say that the number λ is an eigen value of the operator \hat{O} and the operate and $\Psi(x)$ is an eigen function of \hat{O} in operator form, Schrodinger, wave equation can be written as

$$H = \frac{h^2}{2m} \nabla^2 + V \text{ and } E = \int \frac{\partial}{\partial t}$$

Where

Schrodinger study - state eq (1) be solved only for certain values of energy E . The values of energy E_n , for which Schrodinger steady state equation can be solved are called eigen values and corresponding wave functions Ψ_n are called eigen functions.

According to Max Born, $\Psi\Psi$ gives the probability of finding a particle. It is also essential to calculate the average or expectation values of dynamical quantity by the wave function. The expected or the average value of a dynamic quantity is the mathematical expectation for the result of a single measured, taken on the independent system.

Let $f(\gamma)$ be any function for an observable quantity associated with a moving particle. The expectation value of $f(\gamma)$ is given by

$$\langle f(\gamma) \rangle = \frac{\iiint \Psi^* f(\gamma) \Psi \, dx \, dy \, dz}{\iiint \Psi^* \Psi \, dx \, dy \, dz} \quad \dots (1)$$

where the integration is taken over the entire space

In case, the function is normalised wave function, then

$$\langle f(\gamma) \rangle = \iiint \Psi^* f(\gamma) \Psi \, dx \, dy \, dz \quad \dots (2)$$

$$\left[\because \iiint \Psi^* \Psi \, dx \, dy \, dz = 1 \right]$$

If the probability of moving particle of de - Broglie wave is Ψ^2 , then its position of sometime t is expressed by $f(\gamma)$

2.22 EXPECTATION VALUES

Q31. Write short note on Expectation Values.

Ans :

The expectations value of position is

$$\langle f(\gamma) \rangle = \int \Psi^2 f(\gamma) \, dx \, dy \, dz$$

The expectation value of a quantity in terms of position coordinate is written as

$$\left. \begin{aligned} \langle x \rangle &= \int \Psi^* x \Psi \, dx \text{ or } \langle x \rangle = \int \Psi^2 x \, dx \\ \langle y \rangle &= \int \Psi^* y \Psi \, dy \text{ or } \langle y \rangle = \int \Psi^2 y \, dy \\ \langle z \rangle &= \int \Psi^* z \Psi \, dz \text{ or } \langle z \rangle = \int \Psi^2 z \, dz \end{aligned} \right\}$$

For momentum p ,

$$\begin{aligned} \langle p \rangle &= \iiint \Psi^* p \Psi \, dx \, dy \, dz \\ &= \iiint \Psi^* (-i\hbar \vec{\nabla}) \Psi \, dx \, dy \, dz \\ &= -i\hbar \iiint \Psi^* \vec{\nabla} \Psi \, dx \, dy \, dz \end{aligned}$$

PROBLEMS

1. If the uncertainty in position of an electron is 4×10^{-10} m, calculate the uncertainty in its momentum.

Sol :

We know that

$$\Delta x \cdot \Delta p_x \approx h$$

$$\begin{aligned} \Delta p_x &\approx \frac{h}{\Delta x} \approx \frac{6.6 \times 10^{-34}}{4 \times 10^{-10}} \\ &= 1.65 \times 10^{-24} \text{ kg m/sec.} \end{aligned}$$

2. An electron has a speed of 600 m/s with an accuracy of 0.005%. Calculate the certainty with which we can locate the position of the electron. Given

$$h = 6.6 \times 10^{-34} \text{ joule-sec, } m = 9.1 \times 10^{-31} \text{ kg.}$$

Sol :

The momentum of electron = mv

$$= 9.1 \times 10^{-31} \times 600 \text{ kg m/s}$$

$$\Delta p_x = \left(\frac{0.005}{100} \right) mv = 5 \times 10^{-5} \times 9.1 \times 10^{-31} \times 600 \text{ kg m/s}$$

$$\begin{aligned} \Delta x &= \frac{h}{\Delta p_x} \approx \frac{6.6 \times 10^{-34}}{5 \times 10^{-5} \times 9.1 \times 10^{-31} \times 600} \\ &\approx 0.02254 \text{ m.} \end{aligned}$$

3. Show that if the uncertainty' in the location of a particle is equal to us de-Brogle wavelength, the uncertainty in its velocity is equal to its velocity.

Sol :

According to uncertainty principle,

$$\Delta p \cdot \Delta x = h$$

$$\Delta(mv) \Delta x = h \text{ or } \Delta v \cdot \Delta x = h/m$$

Given that $\Delta x = \lambda$

$$\Delta v = \frac{h}{m\lambda} = \frac{h}{m(h/mv)} \quad (\because \lambda = h/mv)$$

$$\Delta v = v = \text{velocity of the particle.}$$

4. A microscope using photons is employed to locate an electrons in an atom to within a distance of 0.1 \AA . What is the uncertainty in the momentum of the electron located in this way? What is the uncertainty in velocity? Rest mass of electron = $9.1 \times 10^{-31} \text{ kg}$.

Sol :

According to uncertainty principle,

$$\Delta p = \frac{h}{\Delta x} = \frac{6.63 \times 10^{-34} \text{ J-s}}{(0.1 \times 10^{-10} \text{ m})}$$

$$= 6.63 \times 10^{-23} \text{ kg-m/sec.}$$

The uncertainty in the velocity of the electron is

$$\Delta v = \frac{\Delta p}{m_0} = \frac{6.63 \times 10^{-23} \text{ kg.m / sec}}{9.1 \times 10^{-31} \text{ kg}}$$

$$= 7.28 \times 10^7 \text{ m/sec.}$$

5. Compare the uncertainties in the velocities of an electron and a proton confined to 1 nm box. Their masses are 9.10×10^{-31} and 1.67×10^{-27} kg respectively.

Sol:

Let $(\Delta v)_e$ and $(\Delta v)_p$ be the uncertainties in velocities of electron and a proton respectively. Then

$$(\Delta v)_e = \frac{\Delta p}{m_e} \quad \text{and} \quad (\Delta v)_p = \frac{\Delta p}{m_p}$$

$$\frac{(\Delta v)_e}{(\Delta v)_p} = \frac{m_p}{m_e} = \frac{1.67 \times 10^{-27} \text{ kg}}{9.10 \times 10^{-31} \text{ kg}} = 18.35.$$

6. Calculate the smallest possible uncertainty in the position of an electron moving with velocity 3×10^7 m/sec.

Sol:

Let $(\Delta x)_{\min}$ be the minimum uncertainty in the position of the electron i.e., $(\Delta p)_{\max}$, the maximum uncertainty in the momentum of the electron. Then

$$(\Delta x)_{\min} (\Delta p)_{\max} = h/2\pi$$

But $(\Delta p)_{\max} = \text{momentum of the electron}$

Now,
$$p = mv = \frac{m_0 v}{\sqrt{1 - (v^2/c^2)}}$$

$$(\Delta x)_{\min} \times \frac{m_0 v}{\sqrt{1 - v^2/c^2}} = \frac{h}{2\pi}$$

or
$$(\Delta x)_{\min} \approx \frac{h\sqrt{1 - v^2/c^2}}{2\pi m_0 v}$$

Substituting the values, we get

7. An electron is confined to a box of length 10^{-9} m. Calculate the minimum uncertainty in its velocity. Given mass of electron $m = 9 \times 10^{-31}$ kg and given constant $h = 6.6 \times 10^{-34}$ J-s.

Sol :

We know that

$$\Delta x = \Delta p_x = h$$

If Δx is maximum, Δp_x must be minimum

$$\text{i.e., } (\Delta x)_{\max} \cdot (\Delta p_x)_{\min} \approx h$$

$$\text{According to problem, } (\Delta x)_{\max} = 10^{-9} \text{ m}$$

$$\begin{aligned} (\Delta p)_{\min} &= \frac{h}{(\Delta x)_{\max}} = \frac{6.6 \times 10^{-34}}{10^{-9}} \\ &= 6.6 \times 10^{-25} \text{ kg} \cdot \text{m/s} \end{aligned}$$

Again,

$$(\Delta p)_{\min} = m (\Delta v_x)_{\min}$$

$$\begin{aligned} (\Delta v_x)_{\min} &= \frac{(\Delta p_x)_{\min}}{m} = \frac{6.6 \times 10^{-25}}{9 \times 10^{-31}} \\ &= 7.3 \times 10^5 \text{ m/s.} \end{aligned}$$

8. Using the uncertainty relation $\Delta E \cdot \Delta t \approx \frac{h}{2\pi}$, calculate the time required for the atomic system to retain the excitation energy for a line of wavelength 6000 \AA and width 10^{-4} \AA

Sol :

Here, the width of spectral line

$$\begin{aligned} d\lambda &= 10^{-4} \text{ \AA} \\ &= 10^{-4} \times 10^{-10} = 10^{-14} \text{ m} \end{aligned}$$

$$\lambda = 6000 \text{ \AA} = 6 \times 10^{-7} \text{ m}$$

We know that

$$E = hv = \frac{hc}{\lambda}$$

$$\text{or } \Delta E = \frac{hc}{\lambda^2} \Delta \lambda$$

Using uncertainty relation $\Delta E = (h/2\pi)$, we obtain

$$\Delta t = \frac{h}{2\pi \Delta E} = \frac{h}{2\pi \left(\frac{hc}{\lambda^2} \right) \Delta \lambda} = \frac{\lambda^2}{2\pi c \Delta \lambda}$$

9. The spacing between the principal planes of NaCl crystal is 2.82 \AA . It is found that the first order Bragg reflection occurs at an angle of 10° . What is the wavelength of X-rays?

Sol:

According to Bragg's law,

$$2d \sin \theta = n\lambda$$

$$\lambda = \frac{2d \sin \theta}{n}$$

Given that

$$n = 1, d = 2.82 \times 10^{-10} \text{ m and } \sin \theta = \sin 10^\circ = 0.1736$$

$$\begin{aligned} \lambda &= \frac{2 \times (2.82 \times 10^{-10}) \times 0.1736}{1} \\ &= 0.9793 \times 10^{-10} \text{ m} \\ &= 0.9793 \text{ \AA} \end{aligned}$$

10. Calculate the wavelength of an X-ray beam incident at 12° for the first order reflection from a calcite crystal, if the grating constant of the crystal is 3.035 \AA . ($\sin 12^\circ = 0.2079$).

Sol:

We know that

$$\lambda = \frac{2d \sin \theta}{n}$$

Here,

$$n = 1, d = 3.035 \text{ \AA} = 3.035 \times 10^{-10} \text{ m and } \sin \theta = \sin 12^\circ$$

$$\begin{aligned} \lambda &= \frac{2 \times (3.035 \times 10^{-10}) \times \sin 12^\circ}{1} \\ &= 1.262 \times 10^{-10} \text{ m} \\ &= 1.262 \text{ \AA} \end{aligned}$$

11. When a nickel target is used in an X-ray tube, two shortest wavelengths emitted are found with Bragg crystal respectively to be diffracted at angle 15.1° and 17.1° respectively. Find their wavelength. Assume the crystal spacing to be 2.81 \AA .

Sol:

According to Bragg's equation, $2d \sin \theta = n\lambda$. Consider diffraction maximum to be of first order, i.e., $n = 1$

$$\therefore \lambda = 2d \sin \theta$$

$$(i) \lambda_1 = 2 \times (2.81 \text{ \AA}) \times \sin 15.1^\circ = 1.468 \text{ \AA}$$

$$(ii) \lambda_2 = 2 \times (2.81 \text{ \AA}) \times \sin 17.1^\circ = 1.652 \text{ \AA}$$

12. X-rays of wavelength 1.54 \AA are diffracted by a crystal with the first maximum occurring at 11° . What is the separation between the lattice planes.

Sol.:

We know that, $2d \sin \theta = n\lambda$

For first order diffraction,

$$n = 1$$

$$d = \frac{\lambda}{2 \sin \theta}$$

Here,

$$\lambda = 1.54 \text{ \AA} \text{ and } \theta = 11^\circ$$

$$\begin{aligned} d &= \frac{1.54 \text{ \AA}}{2 \sin 11^\circ} \\ &= 4.035 \text{ \AA} \end{aligned}$$

13. The line A of X-ray beam gives a first order reflection maximum at a glancing angle of 30° to the smooth face of a crystal. Line B of $\lambda = 0.92 \text{ \AA}$ gives a third order reflection maximum at an angle of 60° from the face of the same crystal. Find the wavelength of line A.

Sol.:

According to Bragg's law,

$$2d \sin \theta = n\lambda$$

$$\text{For line A, } 2d \sin 30^\circ = 1 \times \lambda_A$$

$$\text{For line B, } 2d \sin 60^\circ = 3 \times \lambda_B$$

$$\frac{\lambda_A}{3\lambda_B} = \frac{\sin 30^\circ}{\sin 60^\circ}$$

$$\text{or } \lambda_A = 3\lambda_B \frac{\sin 30^\circ}{\sin 60^\circ}$$

$$\text{or } \lambda_A = 3 \times 0.92 \times \frac{\sin 30^\circ}{\sin 60^\circ}$$

$$= 1.68 \text{ \AA}$$

14. The first order Bragg maximum of electron diffraction in a nickel crystal ($d = 0.4086 \text{ \AA}$) occurred at a glancing angle of 65° . Calculate the de-Broglie wavelength of the electrons and their velocity.

Sol.:

According to Bragg's law,

$$2d \sin \theta = n\lambda$$

$$\begin{aligned}\lambda &= \frac{2d \sin \theta}{n} = \frac{2 \times (0.4086 \times 10^{-10}) \times \sin 65^\circ}{1} \\ &= \frac{2 \times (0.4086 \times 10^{-10}) \times (0.9063)}{1} \\ &= 0.7501 \times 10^{-10} \text{ metre.}\end{aligned}$$

15. Calculate the energy of a photon of sodium light of wavelength $5893 \times 10^{-10} \text{ m}$ in (a) joules and (b) in electron volt. Take $h = 6.62 \times 10^{-34} \text{ J}_3$ and $c = 3 \times 10^8 \text{ m/sec}$.

Sol:

- (a) We know that

$$E = hv = hc/\lambda \text{ joules}$$

$$\begin{aligned}E &= \frac{(6.62 \times 10^{-34}) \times (3 \times 10^8)}{5893 \times 10^{-10}} \\ &= 3.370 \times 10^{-19} \text{ joules}\end{aligned}$$

- (b) As $1 \text{ eV} = 1.6 \times 10^{-19} \text{ joules}$

$$\begin{aligned}E &= \frac{3.370 \times 10^{-19}}{1.6 \times 10^{-19}} \text{ eV} \\ &= 2.10 \text{ eV}\end{aligned}$$

16. What is the threshold wavelength for nickel whose work - function is 4.84 eV ?

Sol:

$$\text{Work function} = 4.84 \text{ eV}$$

$$= 4.84 \times (1.6 \times 10^{-19}) \text{ joule}$$

$$\text{The work function } W_0 = hv_0 = hc / \lambda_0$$

Where

$$\begin{aligned}\lambda_0 &= \frac{hc}{W_0} = \frac{(6.624 \times 10^{-34}) (3 \times 10^8)}{4.84 \times (1.6 \times 10^{-19})} \\ &= 2.566 \times 10^{-7} \text{ meter} \\ &= 2566 \text{ \AA}\end{aligned}$$

17. Calculate the work function of sodium if its threshold wavelength is 5040 \AA

Sol:

We know that

$$W_0 = \frac{hc}{\lambda_0}$$

$$W_0 = \frac{(6.624 \times 10^{-34}) \times (3 \times 10^8)}{5040 \times 10^{-10}}$$

$$= 3.928 \times 10^{-19} \text{ joule.}$$

18. The work function of sodium is 2.46 eV and its threshold wavelength is 5040 \AA . Calculate the value of Plank's constant.

Sol:

$$W_0 = \frac{hc}{\lambda_0} \text{ or } h = W_0 \lambda_0 / c$$

$$h = \frac{(2.46 \times 1.6 \times 10^{-19} \text{ J}) (5040 \times 10^{-10} \text{ m})}{(3 \times 10^8 \text{ m/sec})}$$

$$= 6.612 \times 10^{-34} \text{ joule - sec.}$$

19. The photo - electric work function of potassium surface is 2.2 eV. When ultra - violet light of wavelength 3200 \AA falls on potassium surface. Calculate the energy of the most energetic photon emitted. What is the threshold frequency for potassium.

Sol:

According to Finstein's photo - electric equation,

$$h\nu = W_0 + K_{\max}$$

$$K_{\max} = h\nu - W_0 = (hc / \lambda) - W_0$$

$$K_{\max} = \frac{(6.62 \times 10^{-34}) (3 \times 10^8)}{3200 \times 10^{-10}} = 2.2 \times (1.6 \times 10^{-19})$$

$$= (6.21 \times 10^{-19} - 2.2 \times 1.6 \times 10^{-19}) \text{ joule}$$

$$= 1.6 \times 10^{-19} (3.386 - 2.2) = 1.686 \times (1.6 \times 10^{-19}) \text{ joule}$$

$$= 1.686 \text{ eV.}$$

The work function W_0 and threshold frequency ν_0 are relation as

$$W_0 = h\nu_0 \text{ or } \nu_0 = \frac{W_0}{h}$$

$$\nu_0 = \frac{2.2 \times (1.6 \times 10^{-19})}{6.62 \times 10^{-34}}$$

$$= 5.309 \times 10^{-4} \text{ Hz.}$$

20. Complete the value of planck's constant h if photoelectron ejected from the surface of a certain metal by light of frequency by light of frequency $4.6 \times 10^{15} \text{ Hz}$ are fully stopped by a reverse potential of 16.5 V.

Sol:

We know that

$$eV_0 = h(\nu - \nu_0)$$

Substituting the two given values, we have

$$6.6 \text{ e} = h(2.2 \times 10^{19} - \nu_0)$$

$$\text{and } 16.5 \text{ e} = h(4.6 \times 10^{15} - \nu_0)$$

Substituting eqn. (1) from (2), we get

$$h = \frac{9.9 \times 1.602 \times 10^{-19}}{2.4 \times 10^{15}}$$

$$= 6.6 \times 10^{-34} \text{ J.s}$$

21. In Compton scattering the incident photons have wavelength $8.0 \times 10^{-10} \text{ m}$. Calculate the wavelength of scattered radiation if they are viewed at an angle of 60° to the direction of incidence.

Sol:

In Compton scattering, we have

$$\lambda' - \lambda = \frac{2h}{m_0 c} \sin^2 \left[\frac{\theta}{2} \right]$$

$$\text{Here, } \lambda = 8.0 \times 10^{-10} \text{ m, } \theta = 60^\circ$$

$$\therefore \lambda' = 8.0 \times 10^{-10} + \frac{2 \times 6.6 \times 10^{-34}}{9.1 \times 10^{-31} \times 3 \times 10^8} \sin^2 30^\circ$$

$$= 8.0 \times 10^{-10} + \frac{2 \times 6.6 \times 10^{-34}}{9.1 \times 10^{-31} \times 3 \times 10^8} \times \frac{1}{4}$$

$$= 8.0 \times 10^{-10} + 0.012 \times 10^{-10}$$

$$= 8.012 \times 10^{-10} \text{ m} = 8.012 \text{ \AA}$$

22. A photon recoils back after striking an electron at rest. What is the change in the wavelength of the photon.

*Sol:*The Compton shift $\Delta\lambda$ is given by

$$\Delta\lambda = \lambda' - \lambda = \frac{2h}{m_0 c} \sin^2 \left[\frac{\theta}{2} \right]$$

Substituting the values, we get

$$\Delta\lambda = \frac{2 \times 6.624 \times 10^{-34}}{(9.1 \times 10^{-31})(3 \times 10^8)} \sin^2 \left[\frac{180^\circ}{2} \right]$$

$$= \frac{2 \times 6.624 \times 10^{-34}}{(9.1 \times 10^{-31})(3 \times 10^8)} \sin^2 90^\circ$$

$$= 0.048 \times 10^{-10} \text{ metre} = 0.048 \text{ \AA}$$

23. X-rays of wavelength 1 \AA are scattered at such an angle that the recoil electron has the maximum K.E. Calculate the wavelength of the scattered ray.

Sol:

$$\text{We know that } \Delta\lambda = \frac{2h}{m_e c} \sin^2 \left[\frac{\theta}{2} \right]$$

The Compton shift is maximum when $\theta = 180^\circ$

$$\therefore (\Delta\lambda)_{\max} = \frac{2h}{m_e c} = 0.048 \text{ \AA}$$

The incident wavelength $\lambda = 1 \text{ \AA}$

$$\text{Hence, } \lambda = \lambda + \Delta\lambda = 1 \text{ \AA} + 0.048 \text{ \AA} = 1.048 \text{ \AA}$$

Short Question & Answers

1. Discuss the inadequacy of classical physics ?

Ans :

The reasons of failure of classical physics are :

- (i) Classical mechanics successfully explained the motion of the objects which are either observable directly or can be made observable by instruments like microscope. When the classical concepts were applied to the particles of atomic dimensions like electrons, they failed to describe the actual behaviour. Thus, the classical concepts cannot be applied to atomic phenomenon, e.g., motion of an electron in an atom.
- (ii) The energy of the electron should decrease continuously and it should come closer and closer until it collapses with nucleus. This shows the instability of the atom. This statement is contradictory to the observed fact of the stability of atom. Thus, classical mechanics failed to explain the stability of the atom.
- (iii) Classical mechanics failed to explain the spectrum of hydrogen atom.
- (iv) It could not explain observed spectrum of black body.
- (v) It could not explain the observed variation of specific heat of metals and gases.
- (vi) The classical mechanics failed to explain photo - electric effect, Compton effect, Raman effect etc.

2. Explain and derive Planck's Radiation formula ?

Ans :

Planck in 1900 suggested that the correct results can be obtained if the energy of the oscillating can be obtained if the energy of the oscillating electrons is taken as discrete rather than continuous.

- (i) A chamber containing black body radiation also contains simple harmonic oscillators of molecular dimensions which can vibrate with all possible frequencies.
- (ii) The frequency of radiation emitted by an oscillator is the same as the frequency of its vibration.
- (iii) An oscillator cannot emit energy in a continuous manner, it can emit energy in the multiples of a small unit called quantum (photon). If an oscillator is vibrating with a frequency ν , it can only radiate in quanta of magnitude $h\nu$, i.e., the oscillator can have only discrete energy values E_n given by

$$E_n = nh\nu = n\varepsilon$$

where $h\nu = \varepsilon$

Here n is an integer and h is Planck's constant

$(6.625 \times 10^{-34} \text{ joules} \cdot \text{sec})$

- (iv) The oscillators can emit or absorb radiation energy in packets of $h\nu$.

If N be the total number of Planck's oscillators and E be their total energy, then the average energy per Planck's oscillators and given by

$$\bar{\varepsilon} = \frac{E}{N}$$

3. Define Compton Effect*Ans :*

According to Compton, the phenomenon of scattering is due to an elastic collision between two particles, the photon of incident radiation and the electron of scatterer. The observed change in frequency or wavelength of the scattered radiation is known as Compton effect.

4. State and explain Heisenberg uncertainty principle.*Ans :*

According to Heisenberg uncertainty principle, it is impossible to measure both the position and momentum of a particle simultaneously to any desired degree of accuracy.

- "The order of magnitude of the uncertainties in the knowledge of two variable must be atleast planck's constant h ".

$$\Delta x = v_x \Delta t \quad \dots (3)$$

From equations (2) and (3), we get

$$\Delta x \cdot \Delta p_x = \Delta t \cdot \Delta E \quad \dots (4)$$

We know that $\Delta x \Delta p_x \geq \frac{h}{4\pi}$

$$\Delta x \cdot \Delta p_x \geq \frac{h}{4\pi} \quad \dots (5)$$

5. Relation between group velocity and wave velocity.*Ans :*

The phase velocity of a wave is given by $V_p = \frac{\omega}{k}$ and group velocity $V_g = \frac{d\omega}{dk}$

$$\omega = v_p k \text{ (or) } d\omega = dv_p k + v_p dk \Rightarrow \frac{d\omega}{dk} = v_p + k \frac{dv_p}{dk}$$

from the above equations, we can write

$$V_g = v_p + k \frac{dv_p}{dk}$$

$$\text{or } V_g = v_p + k \frac{dv_p}{d\lambda} \times \frac{d\lambda}{dk}$$

$$\text{Since } k = \frac{2\pi}{\lambda} \text{ hence } \frac{d\lambda}{dk} = -\frac{2\pi}{k^2}$$

6. Define Properties of Matter Waves.*Ans :*

Following are the properties of matter waves :

- (i) Lighter is the particle, greater is the wavelength associated with it.
- (ii) Smaller is the velocity of the particle, greater is the wavelength associated with it.

- (iii) When $v = 0$ then $\lambda = \infty$, i.e., wave becomes indeterminate and if $v = \infty$ then $\lambda = 0$. This shows that matter waves are generated by the motion of particle.

These waves are produced whether the particle are charged particles or they are uncharged ($\lambda = h/mv$ is independent of charge). This fact reveals that these waves are not electromagnetic waves but they are a new kind of waves (electromagnetic waves are produced only by motion of charged particles).

- (iv) The velocity of matter wave depends on the velocity of matter particle i.e., it is not a constant while the velocity of electromagnetic wave is constant.
- (v) The velocity of matter wave is greater than the velocity of light.

The velocity of matter wave (de-Broglie wave velocity) is greater than the velocity of light. This can be proved as under

A particle in motion with associated matter wave has two different velocities, one referring to the mechanical motion of the particle represented by v and second related to the propagation of the wave represented by w .

We know that $E = hv$ and $E = mc^2$.

$$hv = mc^2 \text{ or } v = \frac{mc^2}{h}$$

The wave velocity (w) is given by

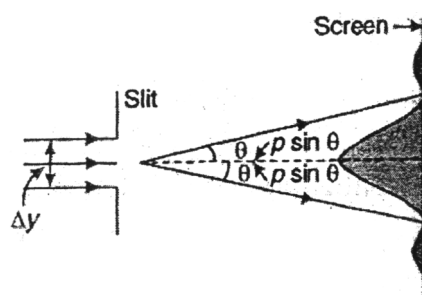
$$w = v \times \lambda = \frac{mc^2}{h} \times \frac{h}{mv} \quad \left[\because \lambda = \frac{h}{mv} \right]$$

$$\text{or } w = \frac{c^2}{v}$$

7. Explain diffraction by a single slit.

Ans :

Suppose a narrow beam of electrons passes through a single narrow slit and produces a diffraction pattern on the screen as shows in fig:



The first minimum of the pattern is obtained by putting $n = 1$ in the equation describing the behaviour of diffraction pattern due to a single slit

(i.e., $d \sin \theta = n\lambda$) hence

$$\Delta y \sin \theta = \lambda \quad \dots (4)$$

Where Δy is the width of the slit

θ is the angle of deviation corresponding to first minimum

In producing the diffraction pattern on the screen all electrons have-passed through the slit but we cannot say definitely at what place of the slit. Hence the uncertainty in determining the position of the electron is equal to the width Δy of the slit.

$$\text{from equation (4) } \Delta y = \frac{\lambda}{\sin\theta} \quad \dots (5)$$

Initially the electrons are moving along the x - axis and hence they have no component of momentum along y - axis. After diffraction at the slit, they are deviated from their initial path to form the pattern and have a component $p \sin\theta$. As y component of momentum may lie any where between $p \sin\theta$, and $-p \sin\theta$, uncertainty in y - component of momentum is

$$\Delta P_y = 2p \sin\theta = \frac{2h}{\lambda} \sin\theta \quad \left[\because p = \frac{h}{\lambda} \right] \quad \dots (6)$$

from equation (5) and (6)

$$\Delta y \cdot \Delta p_y \approx \frac{\lambda}{\sin\theta} \times \frac{2h \sin\theta}{\lambda} \approx 2h$$

$$(\text{or}) \Delta y \cdot \Delta p_y \approx h \quad \dots (7)$$

The relation shows that the product of uncertainties in position and momentum is of the order of planck's constant.

8. Define complementary Principle of Bohr.

Ans :

The most important consequence of uncertainty principle is that it is impossible to determine the wave and particle properties at the same time in a single experiment.

According to complementary principle, the wave and particle nature of matter and light are complementary rather than contradictory, i.e., both aspects are necessary to have a complete picture of the system. Both these aspects have never been shown in a single experiment.

Let us consider an experimental arrangement in which light is diffracted by a double slit and is detected on a screen that consists of many adjacent photoelectric cells. The photoelectric cells respond to photons having particle properties. However, if we plot the number of photons, each cell counts in a certain period of time against the location of cell, a wave-like pattern (like the interference of a pair of coherent wave trains) is obtained. It follows that only experiment which can be devised displays either the particle-like characteristics or wave-like characteristics of the system, in moreover the wave and particle pictures give complementary description of the same pattern.

9. Define physical significance of wave function.

Ans :

It is observed that in some cases, Ψ is appreciably different from zero within some finite region known as wave packet. It is natural to ask, "where is the particle in relation to wave packet?" To explain it, Max Born suggested a new idea about the physical significance of Ψ which is generally accepted now-a-days. According to Max Born $\Psi\Psi^* = |\Psi|^2$ gives the probability of finding the particle in the state Ψ , i.e., Ψ^2

is a measure of probability density. The probability of finding a particle in volume $dT = dx dy dz$ is given by $|\Psi|^2 dx dy dz$. For the total probability of finding the particle somewhere is, of course, unity, i.e., particle is certainly to be found somewhere in space

$$\iiint |\Psi|^2 dx dy dz = 1$$

Satisfying above requirement is said to be normalized.

10. Write short note on Expectation Values.

Ans :

The expectations value of position is

$$\langle f(\gamma) \rangle = \int \Psi^2 f(\gamma) dx dy dz$$

The expectation value of a quantity in terms of position coordinate is written as

$$\left. \begin{aligned} \langle x \rangle &= \int \Psi^* x \Psi dx \text{ or } \langle x \rangle = \int \Psi^2 x dz \\ \langle y \rangle &= \int \Psi^* y \Psi dx \text{ or } \langle y \rangle = \int \Psi^2 y dy \\ \langle z \rangle &= \int \Psi^* z \Psi dz \text{ or } \langle z \rangle = \int \Psi^2 z dz \end{aligned} \right\}$$

For momentum p ,

$$\begin{aligned} \langle p \rangle &= \iiint \Psi^* p \Psi dx dy dz \\ &= \iiint \Psi^* (-i\hbar \vec{\nabla}) \Psi dx dy dz \\ &= -i\hbar \iiint \Psi^* \vec{\nabla} \Psi dx dy dz \end{aligned}$$

Choose the Correct Answers

1. The potential energy of the electron with charge -e in the field of nucleus charge is [b]

(a) $V = \frac{-e}{4\pi\epsilon_0 r}$

(b) $V = \frac{-e^2}{4\pi\epsilon_0 r}$

(c) $V = \frac{e}{4\pi\epsilon_0 r}$

(d) $V = \frac{-e}{4\pi\epsilon_0 r}$
2. Schrodinger time dependent wave equation is [b]

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

(b) $\left(\frac{\hbar^2}{2m}\nabla^2 + V\right)\psi = i\hbar\frac{\partial\psi}{\partial t}$

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

(d) $\left(-\frac{\hbar^2}{2m}\nabla^2 - V\right)\psi = i\hbar\frac{\partial\psi}{\partial t}$
3. Expression for wave velocity [c]

(a) wk

(b) k/w

(c) w/k

(d) $\frac{dw}{dk}$
4. Expression for Hamiltonian operator [b]

(a) $\frac{-\hbar^2}{2m}\nabla^2 - V$

(b) $\frac{-\hbar^2}{2m}\nabla^2 - V$

(c) $\frac{-\hbar^2}{2m}\nabla^2 + V$

(d) $\frac{-\hbar^2}{2m}\nabla^2 + V$
5. Relation between group velocity and wave velocity. [c]

(a) $V_g = V_p + \lambda\frac{dV_p}{d\lambda}$

(b) $V_g = -V_p + \lambda\frac{dV_p}{d\lambda}$

(c) $V_g = V_p - \lambda\frac{dV_p}{d\lambda}$

(d) $V_g = V_p - \lambda^2\frac{dV_p}{d\lambda}$
6. Expression for de-broglie wavelength in terms of energy. [b]

(a) $\lambda = \frac{h}{\sqrt{4mE}}$

(b) $\lambda = \frac{h}{\sqrt{2mE}}$

(c) $\lambda = \frac{h}{\sqrt{mE}}$

(d) $\lambda = \frac{h}{\sqrt{6mE}}$

7. Wave length associated with 54 volt electron is [a]
(a) 1.67 Å (b) 1.6 Å
(c) 1.5 Å (d) 1.4 Å
8. Heisenberg uncertainty principle for energy and time. [d]
(a) $\Delta E \cdot \Delta t = \frac{h}{4\pi}$ (b) $\Delta E \cdot \Delta t > \frac{h}{4\pi}$
(c) $\Delta E \cdot \Delta t = \frac{h}{2\pi}$ (d) $\Delta E \cdot \Delta t > \frac{h}{4\pi}$
9. According to phenomena diffraction by slit width of the slit [b]
(a) $\Delta d = \lambda \sin \theta$ (b) $\Delta y = \frac{\lambda}{\sin \theta}$
(c) $\Delta y = \lambda \cos \theta$ (d) $\Delta y = \frac{\lambda}{\cos \theta}$
10. In order exist in the nucleus the electron must have the energy of the order [a]
(a) 10 MeV (b) 9 MeV
(c) 6 MeV (d) 1 MeV

Fill in the Blanks

1. According to de-Broglie wavelength for matter waves is $\lambda =$ _____.
2. _____ is the experiment for confirmation of matter waves.
3. Uncertainty relation for energy and time _____.
4. According to Gamma ray microscope uncertainty in position and momentum inversely proportional to _____.
5. Ψ is finite, _____ and _____ function.
6. Expression for wave velocity $V_p =$ _____.
7. Relationship between group velocity and wave velocity $v_g =$ _____.
8. The value of zero point energy _____.
9. The propagation constant 'k' is inversely proportional to _____.
10. The expression for classical frequency is given by _____.

ANSWERS

1. h/mv
2. Davisson and Germer
3. $\Delta E \cdot \Delta T \approx h$
4. $\sin \theta$
5. single value, Periodic
6. ω/k
7. $v_g = v_p - \lambda \frac{dv_p}{d\lambda}$
8. $\frac{1}{2} h \gamma$
9. l
10. $\nu = \frac{1}{2\pi} \sqrt{\frac{k}{m}}$

UNIT - III

Nuclear Physics

Nuclear Structure : Basic properties of nucleus - size, charge, mass, spin, magnetic dipole moment and electric quadrupole moment. Binding energy of nucleus, deuteron binding energy, p-p, n-n and n-p scattering (concepts, nuclear forces. Nuclear models - liquid drop model, shell model.

Alpha and Beta Decays : Range of alpha particles, Geiger - Nuttal law. Gammow's theory of alpha decay, Geiger, Nuttal law from Gammow's theory. Beta spectrum - neutrino hypothesis,

Particle Detectors : GM counter, proportional counter, scintillation counter.

3.1 BASIC PROPERTIES OF NUCLEUS

Q1. Explain the properties of nucleus with reference to size, charge, mass, density, spin, magnetic dipole moment.

Ans :

Basic Properties of Nucleus

Some of the important properties of atomic nucleus are given below:

(a) Nuclear Size

The mean radius of an atomic nucleus is of the order of 10^{-14}m to 10^{-15}m while that of the atom is about 10^{-10}m . Thus radius of the nucleus is about 10,000 times smaller than the atomic radius.

The empirical formula for the nuclear radius R is

$$R = R_0 A^{1/3}$$

Where A is the mass number

$$R_0 = 1.3 \times 10^{-19} \text{ m} = 1.3\text{fm}; \{1\text{fm} = 10^{-15}\text{m}\}$$

Nuclei are so small that the fermi (fm) is an appropriate unit of length.

(b) Nuclear Charge

The charge of the nucleus is due to the protons contained in it. Each proton has a positive charge of 1.6×10^{-19} coulomb. The nuclear charge is Ze , where Z is the atomic number of the nucleus.

(c) Nuclear Mass

The mass of nucleus is the sum of the masses of the neutrons and protons contained in it. Then the mass of the nucleus should be $Zm_p + Nm_n$

Where m_p and m_n are the masses of proton and neutron respectively.

The real nuclear mass is less than the sum of masses of individual nucleons.

This difference in masses is called the mass defect.

(d) Nuclear Density

The nuclear density ρ_N can be calculated from

$$\rho_N = \frac{\text{Nuclear Mass}}{\text{Nuclear volume}}$$

$$\text{Nuclear Mass} = Am_n$$

Where A = mass number

$$m_n = \text{mass of the nucleon} = 1.67 \times 10^{-27} \text{ Kg}$$

$$\text{Nuclear volume} = \frac{4}{3} \pi R^3 = \frac{4}{3} \pi (R_0 A^{1/3})^3$$

$$= \frac{4}{3} \pi (R_0^3 A)$$

$$\therefore \rho_N = \frac{Am_n}{\frac{4}{3}\pi R_0^3 A} = \frac{m_n}{\frac{4}{3}\pi R_0^3}$$

$$= \frac{1.67 \times 10^{-27}}{\frac{4}{3}\pi (1.3 \times 10^{-15})^3}$$

$$\rho_N = 1.816 \times 10^{17} \text{ kg m}^{-3}$$

This shows that the nuclear density is independent of mass number (A).

$$\text{Number of nucleons per c.c.} = \frac{\text{Nuclear density}}{\text{Nucleon mass}}$$

$$= \frac{10^{17} \text{ kg / m}^3}{1.67 \times 10^{-27} \text{ kg}} = 10^{44} \text{ nucleons / c.c.}$$

Thus nucleus is a very tightly bound system of particles with a large potential energy.

(e) Nuclear Spin

Both proton and neutron like electron have a n intrinsic angular momentum known as its spin. The magnitude of spin angular minimum is $\frac{1}{2}h$. In addition, the nucleons posses orbital angular momentum due to their motion about the centre of nucleus. The resultant angular momentum of the nucleus is obtained by adding spin (s) and orbital angular momenta (L) of all nucleons within the nucleus. This total angular momentum of the nucleus is known as nuclear spin denoted by

$$I = L + S$$

According to wave mechanics we have $I = h \sqrt{I(I+1)}$

The value of I depends on the type of interaction between the nucleons.

(f) Nuclear Magnetic Dipole Moment (μ)

We know that a charged particle moving in a closed path produces a magnetic field. The magnetic field, at a large distance, may be considered as due to magnetic dipole located at the current loop. The spinning electron has an associated magnetic dipole moment of 1 (one) Bohr magneton .

$$\text{i.e., } \mu_e = \frac{eh}{2m_e}$$

Proton has a positive elementary charge e. Due to its spin, it has magnetic dipole moment μ_N . According to Dirac's theory.

$$\mu_p = \frac{eh}{2m_p}$$

Where m_p is the mass of proton

Here μ_N is called nuclear magneton.

$$\mu_N = 5.050 \times 10^{-27} \frac{\text{J}}{\text{T}}$$

Since $m_p = 1836 m_e$ nuclear magneton is only $\frac{1}{1836}$ of a Bohr magnetism.

Since neutron donot have any charge. It is believed that neutron donot have any magnetic moment up to a long time. According to Yukawa's theory, neutron transforms to proton and a negative n meson for a fraction of time. The two particles are changed and have magnetic moments. But mass of neutron is very small and magnetic moment will be very large when compared to proton. Therefore net magnetic moment appearing on neutron will be negative.

(g) Electric Quadrupole Moment (Q)

An electric dipole moment is zero for atoms and nuclei in stationary states.

The electric quadrupole moment is defined as $Q = \left(\frac{1}{e}\right) \int (3z^2 - r^2) \rho \, dt$

Where dt = volume element, r = radius, ρ is the charge density in the nucleus.

It is also given by $Q = \frac{2}{5} Ze\{b^2 - a^2\}$

Considering the symmetry as ellipsoid of revolution, let the diameter along the axis be $2a$ and the diameter in a perpendicular be $2b$ as shown in figure.

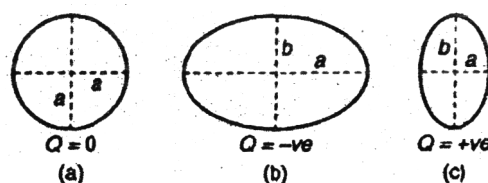


Fig. : Shapes of the nucleus and electric quadrupole - moments Q

Shape of the nucleus & electric quadrupole moment

It is obvious from the expression that

- i) $Q = 0$ for spherically shaped nucleus.
- ii) $Q = +ve$ for ellipsoid (oblate distribution) $a > b$
- iii) $Q = +ve$ for ellipsoid (prolate distribution) $a < b$.

The dimension of the quadrupole moment is that of an area. In nuclear physics it is measured, in barns ($1 \text{ bam} = 10^{-28} \text{ m}^2$).

3.2 BINDING ENERGY OF NUCLEUS

Q2. Explain binding energy of nucleus and calculate binding energy of nucleus.

Ans :

(Imp.)

Binding Energy

The neutrons and protons within a nucleus are held together by strong attractive forces among the nucleons. In order to break a nucleus into its constituents, certain amount of energy is required against the attractive forces. This energy is known as binding energy of the nucleus.

The binding energy is defined as the energy required to decompose a nucleus into its constituent particles.

It has been observed that mass of the nucleus is always different from the sum of the masses of its constituents. The difference in measured mass M and the mass number A is called as mass defect.

$$\therefore \text{mass defect } \Delta w = (M - A)$$

When two nucleons (protons and neutrons) are bound together to form a nucleus, a certain mass (Δw) disappears. This mass Δw is converted into an amount of energy $\Delta E = (\Delta w)c^2$. This energy is called as the binding energy of the nucleus. In order to break the nucleus into its constituent particles, the same amount of energy is required for this purpose.

Binding Energy of nucleus

If M is the mass of a nucleus having Z protons and N neutrons, then

$$B.E = [(Zm_p + Nm_n) - M] c^2 \quad \dots (1)$$

Where m_p and m_n are masses of proton and neutron respectively, When binding energy $B.E < 0$, the nucleus is unstable.

If A is the mass number (number of protons and neutrons) in the nucleus.

$$B.E = [Zm_p + (A - Z)m_n - M] c^2 \quad \dots (2)$$

Adding and subtracting Zm_e on right hand side

$$B.E = [Z(m_p + m_e) + (A - Z)m_n - \{M + Zm_e\}] c^2 \quad \dots (3)$$

Where m is the mass of electron.

Now, $(m_p + m_e) = m_H$ (mass of hydrogen atom)

and $[M (\text{nucleus}) + Zm_e] = M_A$ (atomic mass)

$$\begin{aligned} B.E &= [Zm_H + (A - Z)m_n - M_A] c^2 \\ &= [Zm_H + Am_n - Zm_n - M_A] c^2 \\ &= [Am_n - Z(m_n - m_H) - M_A] c^2 \end{aligned} \quad \dots (4)$$

Dividing both sides by mass number A , we get average binding energy per nucleon

$$\frac{B.E}{A} = \left[m_n - \frac{Z}{A}(m_n - m_H) - \frac{M_A}{A} \right] c^2 \quad \dots (5)$$

Binding Energy per nucleon

The binding energy per nucleon as a function of mass number is shown in figure. It is observed from.

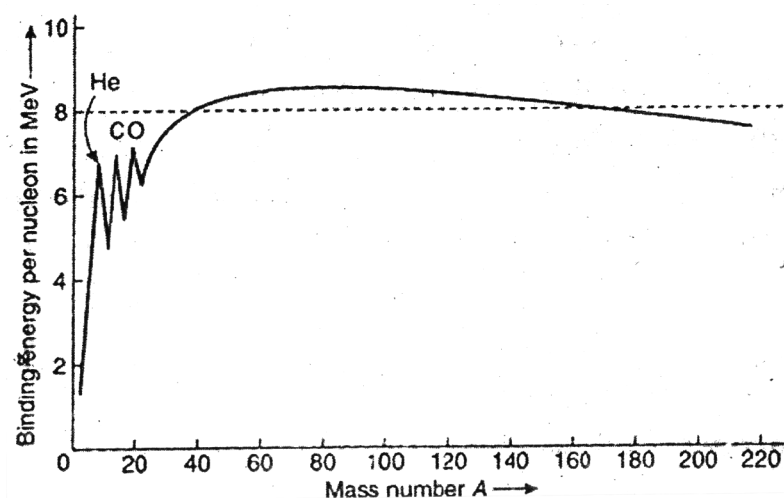


Fig. : Binding energy per nucleon as a function of A.

The graph, that binding energy per nucleon (except for He^4 , C^{12} , and O^{16}) rises first sharply and reaches a maximum value 8.8 MeV in the neighbourhood of $A = 50$. The curve falls very slowly after $A = 50$ and reaches at 8.4 MeV at about $A = 140$. For higher (mass number, the energy) decreases to about 7.6 MeV. It should also be pointed out here that the packing, fraction curve is also minimum at about $A = 50$, predicting that nuclei near $A = 50$ are most stable.

Q3. Explain the structure of nucleus.

Ans :

The atomic nucleus was discovered in 1911 by Rutherford experiments. According to the experiment conducted on scattering of α particles, an atom consists a very small nucleus ($\approx 10^{-14}$ m in diameter) surrounded by orbiting electrons. The proton and neutron are considered to be two different charge states of the same particle which is called as nucleon.

A constituent particle of nucleus is known as a nuclide. The atoms are represented by ${}_Z\text{X}^A$ where Z , the atomic number, indicates the number of protons. A , the mass number, indicates the total number of protons and neutrons and X is the chemical symbol of the atom N is the Number of neutrons .

$$N = A - Z$$

As an example, the chlorine nucleus ${}_{17}\text{Cl}^{35}$ has $Z = 17$ protons,

$$A = 35 \text{ nucleons and}$$

$$N = 35 - 17$$

$$= 18 \text{ neutrons}$$

3.3 BINDING ENERGY OF DEUTERON AND CALCULATE BINDING ENERGY OF DEUTERON

Q4. Calculate binding energy of deuteron (H^2).

Ans :

A deuteron nucleus is formed by a proton and a neutron.

The mass of proton = 1.007270 amu

The mass of neutron = 1.008665 amu

\therefore The total mass of proton and neutron in free state

$$= 1.007270 + 1.008665 = 2.01594 \text{ amu}$$

actual mass of deuteron nucleus = 2.013555 amu

3.4 PROTON - PROTON SCATTERING (– SCATTERING)

Q5. Explain p – p scattering. What is its significance?

Ans :

This scattering is only the way to get direct evidence on proton - proton interaction force inside the nucleus. This scattering is caused not only by the nuclear forces but also by coulomb force. As the two particles are identical, they obey pauli exclusion principle. Therefore, the wave function describing the two protons must change sign on the interchange of two particles. Hence, a symmetric space wave function can be associated with anti - symmetric spin wave function. Similarly, an anti - symmetric space function may be constructed with a symmetric spin wave function. It is important to mention here that more information regarding the shape and exchange character of potential can be obtained from high energy

p – p scattering. When the energy is increased, the coulomb potential plays a smaller and smaller part in the scattering. Therefore a comparison of n – p and p – p interaction may be possible at high energies.

The experimental study of p – p scattering is more accurate than p – p scattering due to the following reason :

- (i) Protons are easily available over a wide range of energies.
- (ii) Protons can be produced in a well collimated beam.
- (iii) Protons can be made more mono - energetic.
- (iv) Protons can be detected by their ionizing properties.

3.5 NEUTRON - PROTON SCATTERING (SCATTERING)

Q6. Explain n - p scattering ?

Ans :

Let us consider a deuteron nucleus which is a bound system. There must be attractive forces between neutrons and protons. Further intermission regarding the inter-nucleon force can be obtained by the scattering of free neutrons by protons. For this purpose a parallel beam of neutrons is allowed to incident on a target containing hydrogen atoms. The number of neutrons deflected through various angle is determined as a function of neutron energy. As neutrons have no charge, they will not be deflected by coulomb field. Therefore, the scattering will directly reflect upon the operation of the nuclear forces. The interactions which may be involved are

- (i) Scattering and (ii) Radioactive capture which has low probability
- (i) For neutron energies greater than 1 eV, the proton can be assumed free. This sets the lower limit to the neutron energy.
- (ii) For neutron energy less than 10_M eV, only the associated 'S' wave overlaps with the nuclear potential and is scattered.

It is important to mention here that n – p scattering is affected by the chemical bounding and depends on relative spin orientations of the neutron and proton.

3.6 PROTON - NEUTRON THEORY OF NUCLEAR COMPOSITION

Q7. Explain p-n scattering. What is its, significance?

Ans :

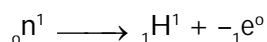
According to Heisenberg hypothesis, the nuclei are composed of protons and neutrons. The total number of protons and neutrons in nucleus gives its mass number A. The number of protons in the nucleus is equal to atomic number z and the number of neutrons is equal to (A – Z).

The total charge, i (i.e., to)* of the nucleus is due to protons only. To neutralize the positive charge of the nucleus, i.e., to make the atom electrically neutral, the number of extranuclear electrons is z.

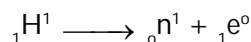
As the number of protons increases, the electrostatic repulsive force also increases but the additional short range attractive nuclear forces [(c_n – n) and (n – p)] components the growing potential repulsion.

The β - ray emission of radiative elements, which gives a strong experimental support to proton - electron theory (nucleus consists of protons and electrons) can also be accounted in this theory in the following way :

The electron does not exist in the nucleus, but it is formed just at the instant of emission. It is produced due to the transformation of a neutron into a proton by the following equation



likewise, the positron emission is due to the conversion of a proton into a neutron as shown by the equation.



This, proton and neutron are mutually convertible. They are regarded as two alternative states of a single heavy nuclear particle named as nucleon.

3.7 NUCLEAR MODELS

3.7.1 Liquid Drop Model

Q8. What are the similarities between liquid drop and a nucleus?

(OR)

Discuss the liquid drop model of nucleus.

Ans :

(Imp.)

This model was proposed by Neils Bohr who observed that there are certain similarities between an atomic nucleus and a liquid drop. In this model the forces acting in the nucleus are assumed to be analogous to the molecular forces in a droplet of a liquid. Hence this model is named as liquid drop model.

- i) The nucleus is supposed to have spherical shape in the stable state and a liquid drop is also spherical due to the surface tension forces.
- ii) A force due to surface tension acts on the surface of the liquid drop. Similarly there is a potential barrier at the surface of the nucleus.
- iii) The density of liquid is independent of surface area / volume. Similarly density of nuclides is almost constant.
- iv) In the liquid, the molecules / atoms have nearest neighbour interaction only. Similarly the nucleons will also have nearest neighbour interaction.
- v) Molecules / atoms in the liquid are attracted by short range tensional forces, similarly, nucleons in the nucleus are attracted by short range forces.
- vi) Liquids exhibits the phenomenon of evaporation, which is compared with radioactivity property of nuclides.
- vii) Upon oscillation, the liquid drop breaks into components. Similarly the nuclides will also undergo the process of nuclear fission.
- viii) The energy necessary to evaporate the drop is proportional to the mass number A. This is similar to the binding energy of the nucleus which is proportional to A.

These concepts are used to find the mass of the nucleus. This formula is known as semiempirical mass formula.

Semi - Empirical Mass Formula

In 1935, Ven Weizsacker expressed the atomic mass of a nuclide in terms of the series of binding energy correction terms with the main mass contribution from proton and neutron. The modified expression of the mass is known as semiempirical mass formula. The mass of neutral atom can be expressed as

$${}_Z M^A = ZM_p + NM_n - E_b \quad \dots (1)$$

Where

${}_Z M^A$ = Atomic mass of the nuclide

Z - number of protons,

M_p - Mass of the proton

N = Number of neutrons

M = Mass of the neutrons

E_b = Binding energy expressed in mass units.

The value of E_b is calculated empirically as made up of a number of correction given by

$$E_b = E_v + E_s + E_c + E_r + E_p \quad \dots (2)$$

Where E_v , E_s , E_c , E_r and E_p are volume energy correction, surface energy, coulomb energy, a symmetry energy and pairing energy respectively,

(i) Volume Energy correction E_v

It has been experimentally verified that the binding energy per nucleon is approximately constant over a wide range of mass number. The total binding energy of nucleus is proportional to the total number of nucleons A in it i.e.

$$E_b \propto A \text{ or } E_v = a_v A \quad \dots (3)$$

Where a_v is an undetermined constant. Here subscript v is used to show that the contribution to the binding energy comes from the entire volume of the nucleus.

(ii) Surface Energy E_s

Nucleus of an atom has some nucleons on its surface.

As a molecule at the surface of a liquid is attracted less strongly in comparison to a molecule in the interior.

Similarly, the nucleons on the surface of nucleus are bound less tightly. This gives rise to a slight reduction in the total binding energy of the nucleus. So it has a negative contribution.

The number of nucleons on the surface are proportional to surface area of the nucleus and therefore to r^2 . We know that $r = r_0 A^{1/3}$ where r_0 is a constant. So, the number of nucleons on the surface are proportional to $A^{2/3}$. Hence

$$E_s = -a_s A^{2/3} \quad \dots (4)$$

Where a_s is a constant.

(iii) Coulomb Energy E_c

Coulomb's repulsive forces are produced due to the mutual repulsion of protons which are positively charged particles of the nucleus. Due to these repulsive forces, the binding energy is decreased. Assuming that the nuclear charge Ze is uniformly distributed throughout the nuclear volume the electrostatic potential energy is given by $3/5 \cdot (Z^2 e^2 / r)$

The Coulomb repulsion is proportional to electrostatic potential energy,

Hence coulomb repulsion of binding energy E_c is written as $E_c = a_c^1 \cdot \frac{3}{5} \frac{Z^2 e^2}{r}$

But $r = r_0 A^{1/3}$

$$E_c = a_c^1 \cdot \frac{3}{5} \frac{Z^2 e^2}{A^{1/3}} = -a_e \frac{Z^2}{A^{1/3}}$$

More accurate calculations show that

$$E_c = a_c \frac{Z(Z-1)}{A^{1/3}} \quad \dots (5)$$

Considering the sum of volume, surface and coulomb energies, the total binding energy E_b of nucleus is given by

$$E_b = E_v + E_s + E_c$$

$$\text{or } E_b = a_v A - a_s A^{2/3} - a_c \frac{Z(Z-1)}{A^{1/3}} \quad \dots (6)$$

Thus, binding energy per nucleon

$$\frac{E_b}{A} = a_v = \frac{a_s}{A^{1/3}} - a_c \frac{Z(Z-1)}{A^{4/3}} \quad \dots (7)$$

Let us consider the contribution of asymmetry energy and pairing energy. The contributions are as follows.

(iv) Asymmetry Energy E_r

The nuclei are most stable when nucleus contains equal number of protons and neutrons, i.e. the condition of stability is $N = Z$. This is called symmetry effect. As the value of A increases, the number of neutrons increases and alternately the binding energy decreases. This decrement is known as asymmetric energy correction.

The binding energy of the nucleus is given by

$$E_r = -a_r \frac{(A - 2Z)^2}{A} \quad \dots (8)$$

Where a_r is a constant

Pairing Energy

The nuclei containing even number of protons and even number of neutrons are most stable. On the other hand, nuclei containing odd number of protons and odd number of neutrons are least stable. Moreover, nuclei containing even number odd protons and odd number of neutrons or vice versa have intermediate stability. This pairing effect changes the binding energy as shown below.

Number of protons	Z number of neutrons Z	E_s
even	even	$+a_p A^{-3/4}$
odd	even	0
even	odd	0
odd	odd	$-a_p A^{-3/4}$

Where a_p is constant

$$\text{Pairing energy } E_p = a_p A^{-3/4} \quad \dots (9)$$

The final expression for binding energy of a nucleus with atomic mass number A and atomic number Z is

$$E_b = a_v A - a_s A^{2/3} - a_c \frac{Z(Z-1)}{A^{1/3}} - a_r \frac{(A-2Z)^2}{A} + a_p \left[\frac{1}{\sigma A^{3/4}} \right]$$

This is semi-empirical binding energy formula.

Semi - Empirical Mass Formula

Combining all the above correction terms, the semi-empirical mass formula is given by

$${}_Z M^A = Z M_p + (A - Z) M_n - a_v A + a_s A^{2/3} + a_e \frac{Z(Z-1)}{A^{1/3}} + a_r \frac{(A-2Z)^2}{A} + E_p$$

The formula is not exact expression but a fairly valid for mass number $A > 15$.

Merits

1. The liquid drop model accounts for many of the salient features of nuclear matter, such as the observed binding energies of nuclei and their stability against α and disintegration as well as nuclear fission.
2. The calculation of atomic masses and binding energies can be done with liquid drop model with good accuracy.

Demerits

1. It fails to explain other properties like magic numbers.
2. It fails to explain the measured spins and magnetic moments of nuclei.

3.7.2 Shell Model

Q9. Explain shell model with magic numbers?

Ans :

- In liquid drop model we emphasize the properties of nuclear matter and nothing about single nucleons.
- So, it is great departure from the atomic model who emphasizes on the motion of the electrons in the field provided by the nucleus for. Certain numbers of neutrons or protons are called, magic numbers.
- The nuclei containing protons and neutrons number 2, 8, 20, 50, 82, 156 etc. known as magic numbers or shell numbers are exceptionally stable in base of electronic shell rule of 2, 8, 18 etc. This show that there are definite energy shell in nuclei.
- The magic numbers of the nucleons, can be explain by shell model of the nucleons.
- This model is capable of explaining not only the magic numbers but also many other nuclear properties such as spin magnetic moment and energy levels.

Evidence for the existence of magic numbers:

- "Mayer" suggested in 1948 that the nuclei with magic number of nucleon are especially abundant in nature.
- ${}^4_2\text{He}$, ${}^{16}_8\text{O}$ are particularly stable it can be observed from the binding energy curve. So we can observe magic numbers 2, 8 which indicates stability.
- $z = 28$, the only nucleons of even z have isotropic evidence existing 60% Sr^{88} ($N = 50$), Ba^{138} ($N = 82$)
 Ce^{140} ($N = 82$)
- Sn ($Z = 50$) has ten isotopes more than any other element while Ca ($Z = 20$) has 6 isotopes.
- This indicates that $z = 50$ and $z = 20$ are more than usually stable.
- α -decay energies of α for given z strikes in the discontinuities of $N = 126$.
- This represents the magic character of number 126 for neutrons.
- Schmith theory of magnetic moments for odd A nucleosides shows that ground state of nuclides change from even parity to odd parity or vice-versa.
- The electric quadruple moment of the nuclei which shows the sharp minima at the closed shell numbers which is indicating the nuclei is nearly spherical type.

Merits

1. Shell model describes the arrangement of nucleons in different shells of nucleus
2. The concept of magic numbers can only be explained based on shell model.

Demerits

The quadrapole moment values calculated as per shell model donot tally with the experimental values.

3.8 RANGE OF α -PARTICLES**Q10. Explain Rane Range of α -particles.**

Ans :

The range of α - particles is customarily defined as the distance which these particles travel through air at 76 cm of mercury pressure and 15°C temperature before they lose their energy to the extent that no longer ionise the gas particles. The range of α - particles depend upon the following factors :

- (i) Initial velocity of α - particles
- (ii) Nature of emitting radioactive element
- (iii) Nature and pressure of the gas or nature of absorber.

3.9 GEIGER - NUTTAL LAW**Q11. Write a note on Geiger nuttal law ?**

Ans :

The different α - emitters emit α - particles of different energies and hence of different ranges. It has been observed that α - emitters giving higher energy particles have the shortest half - lives (largest decay constant) and vice-versa.

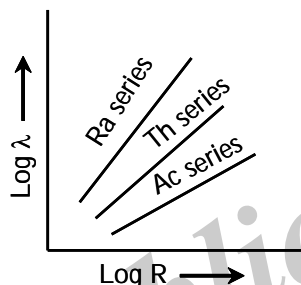
Geiger and Nuttall measured the range of α - particles emitted by several radio active elements and found that there exists a regular relationship between the ranges and the half lives of the elements. The relationship is expressed as

$$\log \lambda = A + B \log R$$

Where R is the range of α - particles emitted by an element, λ is its disintegration constant and A and B are constant. This relation is called Geiger - Nuttall law.

The law is helpful in determining roughly the decay constants of radioactive substance of very short or very long lives.

If a graph is plotted between logarithms of disintegration constant λ and the logarithms of range R for various radioactive substances emitting α - particles in the three series, nearly parallel straight lines are obtained. It is obvious from the figure that the three lines have different intercepts on log R axis. This indicates that A is different for different series while B is same for all series.



3.9.1 Gamow's Theory of α - Decay

Q12. Discuss in detail Gamow's theory of α - Decay?

Ans :

(Imp.)

According to classical theory, an α - particle cannot escape from the nucleus i.e., classical theory fails to explain α - decay. On the other hand, using quantum mechanics, Gamow has shown that there is a finite probability for an α - particle (possessing an energy less than the potential barrier) to penetrate the potential barrier and escape from the nucleus.

Gamow made the following assumptions :

- (i) The α - particle is pre - formed inside the parent nucleus.
- (ii) The α - particle is in constant motion and bounces back and forth from the barriers walls. In each collision with the wall of potential barrier, there is a definite probability of leakage through the barrier.

Let p be the probability of transmission of α - particle in each collision. Suppose λ be frequency with which the α - particle collides with the walls in order to escape from the nucleus.

Now, the decay probability per unit time is given by

$$\lambda = v_p$$

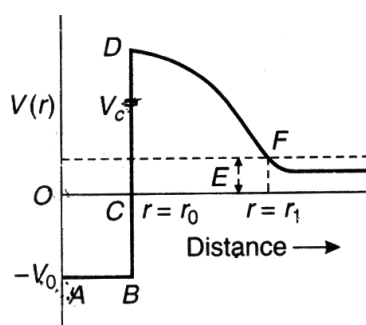
If there be only one α - particle in the nucleus which moves back and forth along the nuclear diameter, then

$$v = \frac{v}{2r_0}$$

Where v is the velocity of α - particle and r_0 be the nucleus radius

$$\therefore \lambda = \left[\frac{v}{2r_0} \right] p$$

Represents qualitatively approximate form of potential energy of α - particle as a function of its distance from the nucleus. The potential that exists around the nucleus is known as potential well. In the figure, $OA = -V_0$ is potential energy at α - particle when it is inside the nucleus, CD is equal to V_c , the electrostatic potential energy of α - particle when it is first outside the range. If the total energy ϵ of α - particle is less than V_c , and the particle is initially outside the nucleus, it is unable to enter the nucleus. The reason being that the particle gets repelled back away from the nucleus. On the other hand, if the particle is inside the nucleus, it is also unable to escape from the nucleus, because it is pulled back into the nucleus. However, quantum mechanically, a moving particle is treated as a wave and there is a definite probability to leak through the barrier (Tunnel effect). The α - particle has a finite probability of being able to cross the potential till.



Using WKB approximation, the probability P can be calculated by the following formula

$$\log_e P = \frac{-2}{h} \int_0^1 \sqrt{2mV(r) - \epsilon} \, dr$$

where m is the mass of the particle and $h = \frac{h}{2\pi}$

$$\text{Further, } V(r) = \frac{2Ze^2}{4\pi\epsilon_0 r}$$

is the electrostatic potential energy of α - particle at a distance r from the nucleus at charge Ze . The charge on α - particle is $2e$.

$$\log_e P = \frac{-2}{h} \int_{r_0}^{r_1} \sqrt{2m \left(\frac{2Ze^2}{4\pi\epsilon_0 r} - \epsilon \right)} \, dr$$

$$\text{At } r = r_1; \epsilon = \frac{2Ze^2}{4\pi\epsilon_0 r_1}$$

$$\therefore \log_e P = \frac{-2}{h} \int_{r_0}^{r_1} \sqrt{2m \left(\frac{\epsilon r_1}{r} - \epsilon \right)} \, dr$$

$$(\text{or}) \log_e P = \frac{-2}{h} (2m\epsilon)^{1/2} \int_{r_0}^{r_1} \left(\frac{r_1}{r} - 1 \right)^{1/2} dr$$

Let us solve the integral

$$\int_{r_0}^{r_1} \left(\frac{r_1}{r} - 1 \right)^{1/2} dr.$$

Let us substitute $r = r_1 \cos^2 \theta$ and $r_0 = r_1 \cos^2 \theta_0$

$$\therefore dr = -2r_1 \cos \theta \sin \theta d\theta$$

$$= \int_{\theta_0}^0 \left(\frac{r_1}{r_1 \cos^2 \theta} - 1 \right)^{1/2} (-2r_1 \cos \theta \sin \theta d\theta)$$

$$= -2r_1 \int_{\theta_0}^0 (1 - \cos^2 \theta)^{1/2} \sin \theta d\theta = -2r_1 \int_{\theta_0}^0 \sin^2 \theta d\theta$$

$$= -2r_1 \int_{\theta_0}^0 \frac{1}{2} (1 - \cos 2\theta) d\theta = -2r_1 \left[\frac{1}{2} \theta - \frac{1}{2} \frac{\sin 2\theta}{2} \right]_{\theta_0}^0$$

$$= -2r_1 \left[-\frac{1}{2} \theta_0 + \frac{1}{4} \sin 2\theta_0 \right] = r_1 [\theta_0 - \sin \theta_0 \cos \theta_0]$$

$$\text{As } \cos^2 \theta_0 = \frac{r_0}{r_1} \text{ hence } \theta_0 = \cos^{-1} \sqrt{\left(\frac{r_0}{r_1} \right)}$$

$$\text{and } \sin \theta_0 = \sqrt{\left(1 - \frac{r_0}{r_1} \right)}$$

$$\therefore \int_{r_0}^{r_1} \left(\frac{r_1}{r} - 1 \right)^{1/2} dr = r_1 \left(\cos^{-1} \sqrt{\left(\frac{r_0}{r_1} \right)} - \sqrt{\left(1 - \frac{r_0}{r_1} \right)} - \sqrt{\left(\frac{r_0}{r_1} \right)} \right)$$

From equation, we get

$$\log_e P = -\frac{2}{h} (2m\epsilon)^{1/2} r_1 \left(\cos^{-1} \sqrt{\left(\frac{r_0}{r_1} \right)} - \sqrt{\left(1 - \frac{r_0}{r_1} \right)} - \sqrt{\left(\frac{r_0}{r_1} \right)} \right)$$

Because the potential barrier is relatively wide ($r > r_0$). Hence

$$\cos^{-1} \left(\frac{r_0}{r_1} \right)^{1/2} = \frac{\pi}{2} - \left(\frac{r_0}{r_1} \right)^{1/2}$$

$$\text{and } \left(1 - \frac{r_0}{r_1} \right)^{1/2} = 1.$$

Substituting these values in eq, we get

$$\begin{aligned}\log_e p &= \frac{2}{h} (2m\epsilon)^{1/2} r_1 \left[\frac{\pi}{2} - \left(\frac{r_0}{r_1}\right)^{1/2} - \left(\frac{r_0}{r_1}\right)^{1/2} \right] \\ &= \frac{-2}{h} (2m\epsilon)^{1/2} r_1 \left\{ \frac{\pi}{2} - 2\left(\frac{r_0}{r_1}\right)^{1/2} \right\}\end{aligned}$$

Here $r_1 = \frac{2Ze^2}{4\pi\epsilon_0\epsilon}$

$$\therefore \log_e p = \frac{-2}{h} (2m\epsilon)^{1/2} \frac{2Ze^2}{4\pi\epsilon_0\epsilon} \left[\frac{4}{2} - 2 \times \left(\frac{r\pi\epsilon_0\epsilon}{2Ze^2} \right)^{1/2} \right]$$

(or)

$$\log_e P = \frac{4e}{h} \left(\frac{m}{\pi\epsilon_0} \right)^{1/2} Z^{1/2} r_0^{1/2} \frac{-e^2}{h\epsilon_0} \left(\frac{m}{2} \right)^{1/2} Z\epsilon^{-1/2}$$

Substituting the values of various constant in eq. We have

$$\log_e P = 2.97 Z^{1/2} r_0^{1/2} - 3.95 Z\epsilon^{-1/2}$$

Here ϵ = kinetic energy in Mev, r_0 = nuclear radius in fermi (1 fermi = 10^{-15}m) and z = atomic number of nuclear - alpha particle.

The decay constant is given by

$$\lambda = v_p = \left(\frac{v}{2r_0} \right) p$$

$$\therefore \log_e \lambda = \log_e \left(\frac{v}{2r_0} \right) + \log_e p$$

$$= \log_e \left(\frac{v}{2r_0} \right) + 2.97 Z^{1/2} r_0^{1/2} - 3.95 Z\epsilon^{-1/2}$$

Represents the α - decay

When base of \log_e is changed to base₁₀, we have

$$\log_{10} \lambda = \log_{10} \left(\frac{v}{2r_0} \right) + 1.29 Z^{1/2} r_0^{1/2} - 1.72 Z\epsilon^{-1/2}$$

3.10 GEIGER - NUTTAL LAW FROM GAMOW'S THEORY

3.10.1 Beta - Ray Continuous and Discrete Spectrum

Q13. Describe Geiger - Nuttall Law from Gamow's Theory. Explain β -ray spectrum.

Ans. :

(Imp.)

Expression is regarded as theoretical form of Geiger - Nuttall Law.

$$\log \lambda = A + B \log R$$

tells that the decay constant varies exponentially with the energy of α - particle. So, the Gamow theory explains qualitatively the essential features of α - decay.

β -ray spectrum.

The head of velocity and energy of β - particle, using a G.M counter the number of electrons per unit time with different velocities is counted.

A graph is then plotted between number of electrons and their energy. The graph is shown in fig. 6

The graph is extensive continuum upon which a few sharp lines are superposed. The graph shows that the β - particles emitted by radioactive substance possess a continuous range of energies.

i.e., β - ray spectrum is continuous

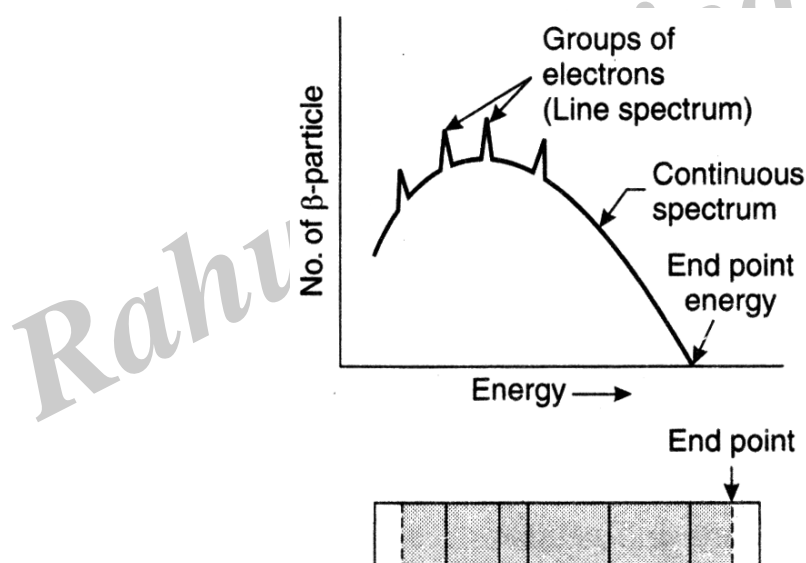


Fig. : β -ray spectrum

1. Continuous Spectrum

The β - particles have a continuous distribution of energy. The continuous spectrum energy ranging from 0 to a certain maximum value. The upper value is called the end point energy and is a characteristic of the emitter.

2. Discrete Spectrum

Some radioactive (susbo)_x substances emit beta particles which produce line spectra (Discrete spectrum) superimposed on the continuous faint background. These are called secondary spectra. Now we shall explain the features of β - ray energy spectra in detail.

Alpha and Beta Decays

Features of β - ray Energy Spectra

There are two distinct types of β - ray spectra viz. continuous spectrum and sharp line spectrum.

The description of disintegration electrons and internal conversion electrons is as follows :

(i) Primary or disintegration Electrons

These electrons are emitted by nucleus itself with varying velocities. These electrons give rise to continuous spectrum. the continuous spectrum has an end point or a cut-off point at the high energy end. This point signifies that there is an upper limit to the velocity or energy of these electrons. The end point energies are different for different sources. Some elements give rise to continuous spectra with single β end point energies where as some others exhibit spectra with two or more point energies.

(ii) Secondary or Internal Conversion Electrons

The sharp lines observed in β - spectrum are due to the process of internal conversion. We know that γ - rays are emitted from the radioactive nucleus with discrete energies. These rays knocked out electrons from K, L, M and N shells of the atom. Thus the secondary electrons are the orbital or extra - nuclear electrons which are knocked off by γ - rays during their escape from nucleus.

These electrons form the line spectrum i.e., sharp peaks on continuous curve.

The process of β - disintegration differs from α disintegration in the following two respects.

- (i) The α - particles are already present in the initial nucleus while β - particles are not present in the initial nucleus β - particles are created at the time of emission.
- (ii) The energy spectrum of α - particles is discrete while the energy spectrum of β - particles is continuous

3.10.2 Neutrino Hypothesis of β - Decay

Q14. Explain neutrino hypothesis of β - Decay.

Ans :

In order to explain the difficulties with β - ray spectra, Pauli in 1930 forwarded a new hypothesis known as Neutron hypothesis. According to this hypothesis, in the process of β - decay, a neutral particle which has negligible mass as compared to electron, charge zero and spin half is emitted along with β - particles. This particle carries a part of available energy and momentum and is called neutrino. Neutrino travels with the velocity of light. In fact, in some respect, it resembles with photon. On the basis of neutrino theory, the conservation of linear and angular momentum in β - decay may be explained.

The β - decay can be represented by the following equation.

Neutron \rightarrow proton + electron + neutrino

$$\begin{array}{rclclcl} \text{O}^{n^1} & \longrightarrow & \text{H}^1 & + & -1e^0 & + & \nu \\ \text{mass} & 1 & \longrightarrow & 1 & + & 0 & + & 0 \\ & 0 & \longrightarrow & +1 & + & -1 & + & 0 \end{array}$$

So both the mass and charge are conserved

The neutrino theory successfully explains the continuous energy spectrum of β - rays. In β - decay the proton remains in the nucleus while both β - particle and the neutrino come out. The both particles are emitted simultaneously. The total energy of these two particles is constant and is equal to the end point energy observed in β - ray spectrum.

3.11 GEIGER - MULLER COUNTER

Q15. Describe in detail the construction and working of a Geiger - Muller Counter.

Ans :

(Imp.)

Description :

The Geiger - Muller counter is just like the proportional counter. It consists of a fine wire (usually tungsten) placed along the axis of a hollow metal-cylinder electrode (Cathode) enclosed in a thin glass tube. The tube contains a mixture of 90% Argon at 10 cm pressure and 10% ethyl alcohol vapour of 1 cm pressure. Different mixtures of gases at different pressure are used in different design. At one end of the tube, a window covered with thin mica sheet (fig. 2) is provided through which the ionizing particles or radiation may enter the tube. A d.c. potential of about 1200 volts is applied between the cathode and the wire which acts as an anode.

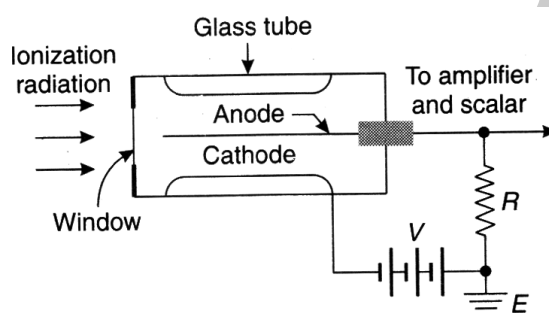


Fig. : G.M. Counter

The value of the voltage is adjusted to be somewhat below the breakdown voltage of the gaseous mixture. A high resistance R is connected in series with battery.

Working

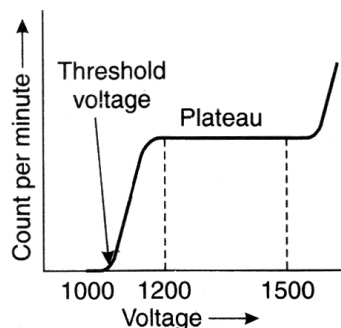
When a charged particle passes through the counter, it ionizes the gas molecules. The central wire attracts the electrons while the cylindrical electrode attracts the positive ion. This causes an ionization current which depends upon the applied voltage. At sufficiently high voltage, the electrons gain high kinetic energy and causes further ionization of argon atoms. Thus, the larger number of secondary electrons are produced by incoming particle due to the following reasons :

- (i) The production of secondary electrons is not continued to the region near the primary electrons but it takes place all along the length of the wire as their number is extremely large ($= 10^8$).
- (ii) The production of secondary electrons at one point affects the production at other points.

The incoming particle serves the purpose of triggering the release of an avalanche of secondary electrons. The electrons quickly reach the anode and cause ionization current. The positive ions move more slowly away from anode and they form a sheath around the anode for a short while. They reduce the potential difference between the electrodes to a very low value because ion sheath depresses electric field near anode. The current therefore stops. In this way brief pulse of current flows through resistance R .

This current creates a potential difference across R. The pulse is amplified and fed to counter circuit. As each incoming particle produces a pulse, hence the number of incoming particles can be counted.

Voltage Characteristics Curve



Quenching

When the positive ions reach the cathode, they detach secondary electrons from the cathode because they have acquired large kinetic energies. These electrons travel to the anode and produce fresh avalanches i.e., unwanted pulse. The self-quenching is obtained by adding a quenching agent like alcohol vapour in the tube. Alcohol has low ionization potential (11.3 eV). The argon ions (having ionization potential 15.7 eV) on their journey to the cathode and practically all neutralized by acquiring an electron from the alcohol molecules. Now only alcohol ions reach the cathode. They acquire electrons from cathode and become neutral alcohol molecules. Through the alcohol molecules still possess kinetic energy yet this is used for dissociation into alcohol atom and not for the production of secondary electrons by colliding with cathode. Thus, the possibility of continuous avalanching is removed.

Counting Rate

The G.M. counter can count about 500 particles per second. The counting rate depends upon (i) dead time, (ii) recovery time and (iii) paralysis time. The slowly moving positive ions take about 100 microseconds to reach the cathode. This time is known as dead time.

If a second particle enters the tube during this time, it will not be recorded as the potential difference across the electrodes is very low. After dead time, the tube takes nearly 100 microseconds before it regains its original working conditions. This time interval is known as recovery time. The sum of dead time and recovery time is known as paralysis time which, of course, is 200 microseconds. The tube responds fully to the second incoming particle after 200 microseconds. Thus, the tube can count nearly 500 particles per second.

Advantages and Disadvantages :

The G.M. counter is very useful for counting β -particles. It can also be used for measuring γ -ray intensities. It cannot be used for counting α -particles due to their low energy as the window cannot be made thin enough to pass them. It cannot give other information as charge, momentum, energy of the particle.

3.12 PROPORTIONAL COUNTER

Q16. Explain the working of proportional counter.

Ans :

(Imp.)

The proportional counter consists of a cylindrical metal chamber with a thin wire situated along its axis and insulated from it. The wire is connected to the positive pole of high tension battery and serves as

collecting electrode. The negative of high tension battery is connected to the chamber as shown in fig. (1). A high resistance R is connected in the battery circuit. The wire in turn is connected to pulse amplifier and counting circuit. The cylindrical tube is also provided with a mica window so that charged particles and ionizing radiations can enter inside it. The chamber is filled with a gas like methane, organ, carbon dioxide

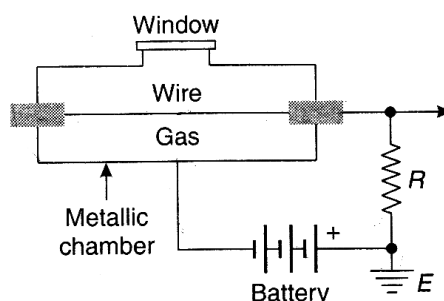


Fig. : Proportional Counter

or a mixture of suitable gases for a particular purpose of suitable atmospheric pressure. The proportional counter functions satisfactorily at voltage 500 to 800 volts or above at pressure of about one atmosphere.

When a charged particle enters in metallic chamber, ionization of gas takes place resulting in an ion pair formation. The positive ions move to the chamber while the negative ion (electrons) move towards the central wire. Now an extremely short electric flow or pulse passes through high resistance R which develops a voltage across it. When the applied voltage is low, many ions recombine before reaching the central wire and hence the current is small. But when the voltage is increased, more and more ions reach the central wire and the current increased. When all the ions are collected by the central electrode, the current reaches the saturation value.

When the voltage is further increased, the ions gain sufficient kinetic energy to produce secondary electrons by collisions with the atoms of the gas. In this case, the current would be very large. For a given applied voltage, the current is proportional to the number of primary ion - pairs produced by incoming charged particles. The counter now works as proportional counter.

Every incoming charged particle produces one voltage pulse across the resistance which is amplified by the amplifier and passed to the counter. The number of particles entering the tube in a given time can thus be counted. As α -particle or a beta particle or γ -ray produces different number of primary ion - pairs, the voltage pulse developed across R will be different in these cases. Thus different incoming particles may be distinguished from each other.

This counter can be used to detect neutrons. In this case the chamber is filled with a small amount of boron Trifluoride (BF_3) molecules. Now α -particle is recorded as usual. The disadvantage of this counter is that the proportionality factor depends on the applied voltage. Therefore, the applied voltage should be maintained at a constant value.

3.13 SCINTILLATION COUNTER

Q17. Describe the construction and working of scintillation counter.

Ans :

(Imp.)

Principle :

We know that one of the properties of ionizing particles (like α -particle) is their ability to produce fluorescence in certain materials. When high energy charged particles pass through active fluorescence

material (called scintillation or phosphor). Some of its atoms are excited. As these excited atoms return to their ground states, photons are emitted. The intensity of the light flash so produced depends on the energy given up by the charged particle. These flashes are converted into amplified electrical pulse by means of a photomultiplier tube. The electrical pulses are then recorded electronically.

Construction and Working

The main parts of a scintillation counter are shown in fig, it consists of scintillation chamber, photomultiplier tube and electronics counter. The scintillation chamber, consists of an aluminium casing in which a suitable scintillation crystal is placed. The aluminium case shields the crystal from all stray light.

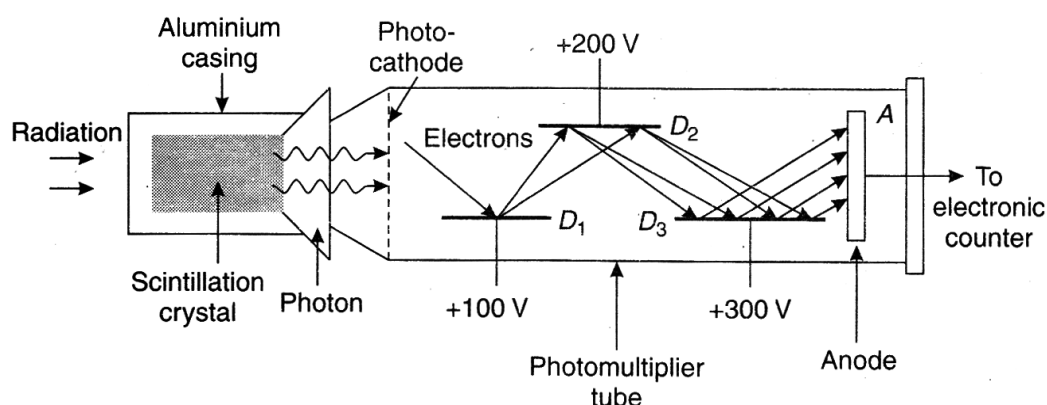


Fig. : Scintillation Counter

The scintillation chamber is fitted at the end of photomultiplier tube, High energy radiation is allowed to incident on the crystal which produces tiny flash of light (photons). The photons from scintillator chamber enter the photo - multiplier tube and strike the photo cathode. Now photo - electrons are emitted due to photo-electric emission. The photo - multiplier tube has several electrodes called dynodes (shown by D_1 , D_2 , D_3 , etc) to which progressively higher potentials are applied. These dynodes in the photo - multiplied tube. Finally a highly amplified electric pulse impinges on the anode acting as a collector of electrons. These pulses are fed into an electronic system where they are counted. The scintillation counter can count 10^{16} particles per second.

The scintillation counter, has many advantages over other detectors. They are :

- (i) high efficiency
- (ii) short time rise and recovery
- (iii) large life of use.

Problems

1. A G.M. counter wire collects 10^8 electrons per discharge. When the counting rate is 500 counts/minute, what will be the average current in the circuit ?

Sol :

Counting rate = 500 counts/min.

The wire collects 10 electrons per discharge

\therefore Total number of electrons collected in one min.

$$n = 500 \times 10^8 = 5 \times 10^{10}$$

Charge/min = $ne = (5 \times 10^{10}) (1.6 \times 10^{-19})$ coul/min.

$$\text{Charge/second} = \frac{(5 \times 10^{10}) \cdot (1.6 \times 10^{-19})}{60} = 1.33 \times 10^{-19} \text{ amp.}$$

Now charge/second gives the average current

$$\text{Average current} = 1.33 \times 10^{-10} \text{ amp.}$$

2. A Geiger Muller counter collects 10^7 electrons/discharge. The average current in the circuit is 1.333×10^{-18} amp. Find the counting rate/min.

Sol :

The number of electrons received in 1 sec. by wire of G.M. counter.

$$\begin{aligned} &= \frac{\text{current}}{\text{charge on electron}} \\ &= \frac{1.333 \times 10^{-18}}{1.6 \times 10^{-19}} = \frac{13.33}{1.6} \end{aligned}$$

No. of discharges in one minute

$$= \frac{13.33}{1.6} \times 60 = 499.8$$

Therefore, counting rate per minute is 500.

3. A G.M. counter has a plateau slope of 3% per 100 volt. If the operating point is at 100 volt, what is the maximum permissible voltage fluctuations, when the counting is not affected by more than 0.1 %?

Sol :

Working voltage of the counts = 100 volt

$$\text{slope} = \frac{\text{Change in count rate}}{\text{Change in working volt}} = \frac{3\%}{100}$$

The count rate limit = 0.1 %

The corresponding change in volt = V

$$\text{The slope} = \frac{0.1\%}{V}$$

The slope is same for the counter

$$\frac{3\%}{100} = \frac{0.1\%}{V}$$

$$V = 3.3 \text{ volt}$$

4. A self - quenched G.M. counter operates at 1000 volts and has a wire of diameter 0.2 mm. The radius of the cathode is 2 cm and the tube has a guaranteed life time of 10^9 counts. What is the max radial field and how long will the counter last if it is used on as average for 30 hr per week at 8000 counts per minute? Assume 50 weeks to a year.

Sol :

The radial field at the centre is given by

$$E_{\max} = \frac{V}{r \log_e(b/a)} \rightarrow \frac{1000}{0.02 \times [2.3 \log_{10}(2 \times 10^{-2} / 10^{-4})]}$$

$$= 1.89 \times 10^6 \text{ V/m}$$

Let the life time of the tube be Nyr. Now the total number of counts recorded will be

$$N \times 50 \times 30 \times 60 \times 3000 = 2.7 \times 10^8 N$$

According to given problem,

$$2.7 \times 10^8 N = 10^9$$

$$N = \frac{10^9}{2.7 \times 10^8}$$

$$= 3.7 \text{ years.}$$

Short Question and Answers

1. Define Nuclear Size and Nuclear Charge.

Ans :

Nuclear Size

The mean radius of an atomic nucleus is of the order of 10^{-14}m to 10^{-15}m while that of the atom is about 10^{-10}m . Thus radius of the nucleus is about 10,000 times smaller than the atomic radius.

The empirical formula for the nuclear radius R is

$$R = R_0 A^{1/3}$$

Where A is the mass number

$$R_0 = 1.3 \times 10^{-19} \text{ m} = 1.3\text{fm}; \{1\text{fm} = 10^{-15}\text{m}\}$$

Nuclei are so small that the fermi (fm) is an appropriate unit of length.

Nuclear Charge

The charge of the nucleus is due to the protons contained in it. Each proton has a positive charge of 1.6×10^{-19} coulomb. The nuclear charge is Ze , where Z is the atomic number of the nucleus.

2. Define Nuclear Mass and Nuclear Density.

Ans :

Nuclear Mass

The mass of nucleus is the sum of the masses of the neutrons and protons contained in it. Then the mass of the nucleus should be $ZM_p + NM_n$

Where m_p and m_n are the masses of proton and neutron respectively.

The real nuclear mass is less than the sum of masses of individual nucleons.

This difference in masses is called the mass defect.

Nuclear Density

The nuclear density ρ_N can be calculated from

$$\rho_N = \frac{\text{Nuclear Mass}}{\text{Nuclear volume}}$$

$$\text{Nuclear Mass} = Am_n$$

Where A = mass number

$$m_n = \text{mass of the nucleon} = 1.67 \times 10^{-27} \text{ Kg}$$

$$\text{Nuclear volume} = \frac{4}{3} \pi R^3 = \frac{4}{3} \pi (R_0 A^{1/3})^3$$

$$= \frac{4}{3} \pi (R_0^3 A)$$

$$\therefore \rho_N = \frac{Am_n}{\frac{4}{3}\pi R_0^3 A} = \frac{m_n}{\frac{4}{3}\pi R_0^3}$$

$$= \frac{1.67 \times 10^{-27}}{\frac{4}{3}\pi (1.3 \times 10^{-15})^3}$$

$$\rho_N = 1.816 \times 10^{17} \text{ kg m}^{-3}$$

This shows that the nuclear density is independent of mass number (A).

$$\text{Number of nucleons per c.c.} = \frac{\text{Nuclear density}}{\text{Nucleon mass}}$$

$$= \frac{10^{17} \text{ kg / m}^3}{1.67 \times 10^{-27} \text{ kg}} = 10^{44} \text{ nucleons / c.c.}$$

Thus nucleus is a very tightly bound system of particles with a large potential energy.

3. Define Nuclear Spin and Nuclear Magnetic Dipole Moment(μ).

Ans :

Nuclear Spin

Both proton and neutron like electron have an intrinsic angular momentum known as its spin. The magnitude of spin angular momentum is $\frac{1}{2}h$. In addition, the nucleons possess orbital angular momentum due to their motion about the centre of nucleus. The resultant angular momentum of the nucleus is obtained by adding spin (s) and orbital angular momenta (L) of all nucleons within the nucleus. This total angular momentum of the nucleus is known as nuclear spin denoted by

$$I = L + S$$

According to wave mechanics we have $I = h \sqrt{I(I+1)}$

The value of I depends on the type of interaction between the nucleons.

Nuclear Magnetic Dipole Moment(μ)

We know that a charged particle moving in a closed path produces a magnetic field. The magnetic field, at a large distance, may be considered as due to magnetic dipole located at the current loop. The spinning electron has an associated magnetic dipole moment of 1 (one) Bohr magneton.

$$\text{i.e., } \mu_e = \frac{eh}{2m_e}$$

Proton has a positive elementary charge e. Due to its spin, it has magnetic dipole moment μ_N . According to Dirac's theory.

$$\mu_p = \frac{eh}{2m_p}$$

Where m_p is the mass of proton

Here μ_N is called nuclear magneton.

$$\mu_N = 5.050 \times 10^{-27} \frac{\text{J}}{\text{T}}$$

Since $m_p = 1836 m_e$ nuclear magneton is only $\frac{1}{1836}$ of a Bohr magnetism.

4. Explain the structure of nucleus.

Ans :

The atomic nucleus was discovered in 1911 by Rutherford experiments. According to the experiment conducted on scattering of a particles, an atom consists a very small nucleus ($\approx 10^{-14}$ m in diameter) surrounded by orbiting electrons. The proton and neutron are considered to be two different charge states of the same particle which is called as nucleon.

A constituent particle of nucleus is known as a nuclide. The atoms are represented by ${}_Z^AX$ where Z, the atomic number, indicates the number of protons. A, the mass number, indicates the total number of protons and neutrons and X is the chemical symbol of the atom N is the Number of neutrons .

$$N = A - Z$$

As an example, the chlorine nucleus ${}_{17}^{35}\text{Cl}$ has $Z = 17$ protons,

$$A = 35 \text{ nucleons and}$$

$$N = 35 - 17$$

$$= 18 \text{ neutrons}$$

5. Calculate binding energy of deuteron (${}_1^2\text{H}$).

Ans :

A deuteron nucleus is formed by a proton and a neutron.

The mass of proton = 1.007270 amu

The mass of neutron = 1.008665 amu

\therefore The total mass of proton and neutron in free state

$$= 1.007270 + 1.008665 = 2.01594 \text{ amu}$$

$$\text{actual mass of deuteron nucleus} = 2.013555 \text{ amu}$$

6. Explain Range of α -particles.

Ans :

The range of α - particles is customarily defined as the distance which these particles travel through air at 76 cm of mercury pressure and 15°C temperature before they lose their energy to the extent that no longer ionise the gas particles. The range of α - particles depend upon the following factors :

- (i) Initial velocity of α - particles
- (ii) Nature of emitting radioactive element
- (iii) Nature and pressure of the gas or nature of absorber.

7. Explain neutrino hypothesis of β - Decay.*Ans :*

In order to explain the difficulties with β - ray spectra, Pauli in 1930 forwarded a new hypothesis known as Neutron hypothesis. According to this hypothesis, in the process of β - decay, a neutral particle which has negligible mass as compared to electron, charge zero and spin half is emitted along with β - particles. This particle carries a part of available energy and momentum and is called neutrino. Neutrino travels with the velocity of light. In fact, in some respect, it resembles with photon. On the basis of neutrino theory, the conservation of linear and angular momentum in β - decay may be explained.

The β - decay can be represented by the following equation.

Neutron \rightarrow proton + electron + neutrino

$$\begin{array}{rclcl} O^{n^1} & \longrightarrow & H^1 & + & -1e^0 + \nu \\ \text{mass} & 1 & \longrightarrow & 1 & + 0 + 0 \\ & 0 & \longrightarrow & +1 & + -1 + 0 \end{array}$$

So both the mass and charge are conserved

8. A Geiger Muller counter collects 10^7 electrons/discharge. The average current in the circuit is 1.333×10^{-18} amp. Find the counting rate/min.*Sol :*

The number of electrons received in 1 sec. by wire of G.M. counter.

$$\begin{aligned} &= \frac{\text{current}}{\text{charge on electron}} \\ &= \frac{1.333 \times 10^{-18}}{1.6 \times 10^{-19}} = \frac{13.33}{1.6} \end{aligned}$$

No. of discharges in one minute

$$= \frac{13.33}{1.6} \times 60 = 499.8$$

Therefore, counting rate per minute is 500.

9. A G.M. counter has a plateau slope of 3% per 100 volt. If the operating point is at 100 volt, what is the maximum permissible voltage fluctuations, when the counting is not affected by more than 0.1 %?*Sol :*

Working voltage of the counts = 100 volt

$$\text{slope} = \frac{\text{Change in count rate}}{\text{Change in working volt}} = \frac{3\%}{100}$$

Choose the Correct Answers

1. The diameter of Nuclear is of the order. [a]
(a) 10^{-10} m (b) 10^{-11} m
(c) 10^{-12} m (d) 10^{-14} m
2. The number of neutrons $N =$ [a]
(a) $A - Z$ (b) $A + Z$
(c) $A \cdot Z$ (d) A / Z
3. The charge of proton in coulomb is [c]
(a) 1.6×10^{-17} (b) 1.6×10^{-18}
(c) 1.6×10^{-19} (d) $1.6 \times 10^{+19}$
4. An electric dipole moment is ____ for atoms [b]
(a) -1 (b) 0
(c) +1 (d) ∞
5. For spherically shaped nucleus, the value of Q is [a]
(a) 0 (b) +ve
(c) -ve (d) None
6. 1 barn = ____ m^2 [d]
(a) 10^{-27} (b) 10^{+27}
(c) 10^{+28} (d) 10^{-28}
7. The mass of nucleus is always ____ than total mass of its constituents [a]
(a) Less (b) Greater
(c) Equal to (d) Not equal to
8. The nuclear forces are attractive when the distance between nucleons is of the order of [b]
(a) $10^{15}m$ (b) $10^{-15}m$
(c) $10^{20}m$ (d) $10^{-20}m$
9. Which among the following are magic numbers [d]
(a) 3 (b) 9
(c) 27 (d) 82
10. Nuclear forces are change [b]
(a) Dependent (b) Independent
(c) Free (d) None

Fill in the Blanks

1. The empirical formula for the nucleous radius is _____.
2. The mass of nucleous is the sun of the masse of the _____ and _____ contained in if
3. The number of nucleons per c.c. is _____.
4. The spinning electron has an associated magnetic dipole moment of _____.
5. The electric dipole moment is defined as _____.
6. Mass defect i.e. loss of mass is converted in energy _____.
7. The minimum energy required to separate a stable nucleus into its constituent protons and neutrons is _____.
8. If the binding energy is _____ the nucleous is more stable.
9. The number of nucleons in each shell is limited by _____.
10. A proton and a neutron with their spins parallel exists forces on each other and bind together to form a stable _____.

ANSWERS

1. $R = R_0 A^{\frac{1}{3}}$
2. Newtron, proton
3. Nuclear density
4. 1 Bohr magneton
5. $\phi = \frac{i}{e} (3z^2 - r^2) \text{ idt}$
6. $E = mc^2$
7. binding energy
8. large
9. Paulis exclusion principle
10. deuteron.

UNIT - IV

SOLID STATE PHYSICS & CRYSTOLOGY

Crystal Structure : Crystalline nature of matter. Crystal lattice, Unit Cell, Elements of symmetry. Crystal systems, Bravais lattices. Miller indices. Simple crystal structures (S.C., BCC, FCC, CsCl, NaCl, diamond and Zinc Blende)

X-ray Diffraction: Diffraction of X -rays by crystals, Bragg's law, Experimental techniques - Laue's method and powder method.

Bonding in Crystals: Types of bonding in crystals - characteristics of crystals with different bondings. Lattice energy of ionic crystals-determination of Madelung constant for NaCl crystal. Calculation of Born Coefficient and repulsive exponent. Born-Haber cycle.

4.1 CRYSTALLINE NATURE OF MATTER

Q1. Explain crystalline and amorphous material.

Ans :

If the atoms (or) molecules in a solid are arranged in some regular fashion, then it is known as crystalline.

When the atoms (or) molecules in a solid are arranged in an irregular fashion, then it is known as amorphous.

In a crystalline solid each atom (or) molecule is fixed at a definite point in space at a definite distance from and in a definite angular orientation to other atoms (or) molecules surrounding it.

Q2. Distinction between crystalline and amorphous solids.

Ans :

1. Crystalline solids have a regular arrangement of particles whereas the amorphous solids have a completely random particle arrangement.
2. Crystalline solids have different physical properties in different directions.
3. The cooling curve for amorphous substance is smooth, while the curve of crystalline substance has breaks, the middle of which corresponds to the process of crystallization.
4. All the bonds in a crystalline solid are equally strong due to their symmetry

For example, as the temperature of glass is gradually raised, it softens and starts flowing without any sharp change from solid state to liquid.

4.1.1 Lattice Translation

Q3. What is Lattice translation vector?

Ans :

The position vector of any lattice point in two dimensional lattice by choosing any other lattice point p as origin is expressed as

Where n_1 and n_2 are integral values, which represent the number of lattice point along PA and PB axes and a and b are called primitives. The position vector T is called the translation vector.

The arrangement of points in three dimensions is expressed by the translation operator T as

$$T = n_1a + n_2b + n_3c$$

where a , b and c are primitives taken along the crystal axes PA, PB and PC

4.2 UNIT CELLS

Q4. Describe a unit cell.

Ans :

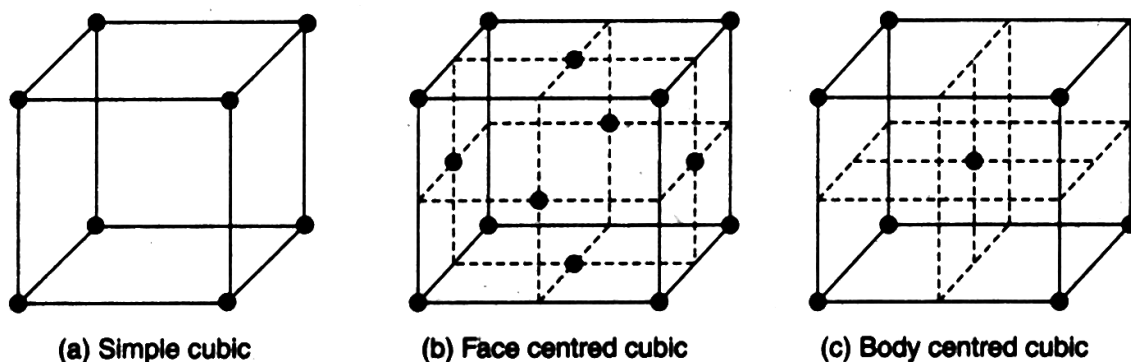
Let us consider a two dimensional crystal in which the atoms are arranged as shown if we consider a parallelogram. ABCD with side $AB = a$ and $AD = b$

ABCD then by rotating this parallelogram by any integral multiples of vectors A and B , the whole crystal lattice may be obtained. This fundamental unit ABCD is called a unit cell is the smallest geometric figure the repetition of which gives the actual crystal structure

The unit cell should be chosen in such a way that it conveys the symmetry of crystal lattice.

A three dimensional unit cell is shown in the unit cell is a parallelepiped formed by the basic vectors a , b , c as concurrent edges and including angles α , β , γ between b & c , c & a and a & b respectively.

In general unit cell may be defined as that volume of a solid from which the entire crystal may be constructed by translational repetition in three dimensions.



4.3 ELEMENTS OF SYMMETRY

Q5. Discuss the elements of symmetry.

Ans :

Following three are the main elements of symmetry :

1. Axes of symmetry
2. Planes of symmetry
3. Centre of symmetry

We shall discuss these one by one

1. Axes of symmetry

This symmetry refers to the axis around through which a crystal is rotated. If the crystal occupies two (or) more identical positions during its rotation through 360° , then the axis of rotation is known as axis of symmetry. For example, consider the rotation of a cube shown in fig. about yy through 90° . In this case the cube has four identical positions in one complete rotation. Therefore, the crystal has four-fold axis of symmetry. In General, if rotation through an angle $(360^\circ/n)$ about an axis brings the crystal figure into an identical position, then the axis is called an n fold axis of symmetry.

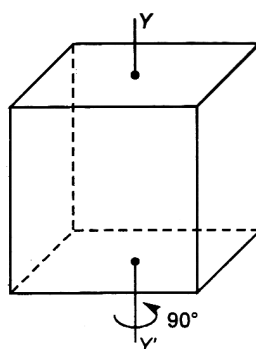


Fig.:Axes of symmetry

2. Planes of symmetry

The planes which cut a crystal into two halves so that each half is a mirror image of the other half, then the plane is known as plane of symmetry fig. shows a plane parallel to the Top and bottom of the cube dividing the cube into mirror image halves. Three such planes can easily be constructed, each parallel to different faces of the cube.

Fig(76). shows a diagonal plane passing through diagonally opposite parallel edge six such diagonal planes of symmetry are possible.

Therefore, for a cube system, there are nine planes of symmetry. In a cubic crystal, there exists only two ways of dividing the crystal into two mirror images.

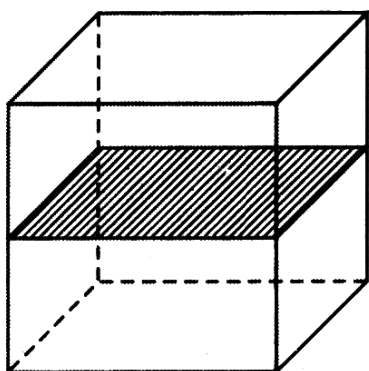


Fig. (a) Plane of symmetry (3 such planes can be constructed)

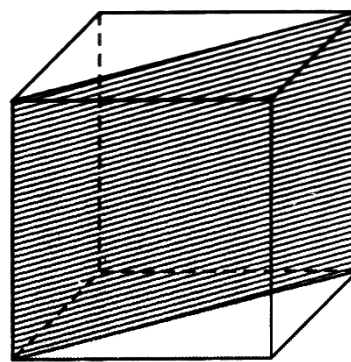


Fig. (b) Diagonal plane of symmetry (Six diagonal planes of symmetry can be constructed)

3. Centre of symmetry

This refers to a point in the crystal fig(8) such that a line drawn from any lattice point in the crystal through this point. When produced equal distance on the opposite side, meets an identical point. This is a translational operation. The cubic system has only one such centre of symmetry

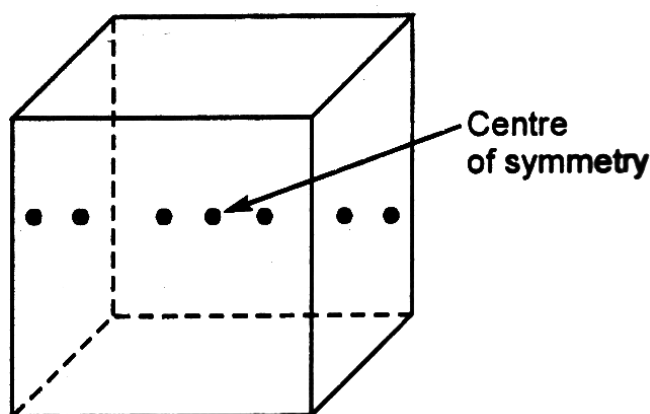


Fig. Centre of symmetry in a cubic system

4.4 THE SEVEN CRYSTAL SYSTEMS

Q6. Mention the seven crystal systems.

Ans :

(Imp.)

On the basis of the lengths and directions of the axes of the systems, all the crystals may be classified into the following seven systems.

(i) Cubic crystal

In this crystal all the three length of the unit cell are equal and are at right angles to each other, i.e., ($a = b = c$ and $\alpha = \beta = \gamma = 90^\circ$). The examples are NaCl, CaF_2 , NaClO_2 , diamond etc.

(ii) Tetragonal crystal

In this crystal the lengths of the unit cell are equal while the third one is longer. The three axes are perpendicular, i.e., ($a = b \neq c$ and $\alpha = \beta = \gamma = 90^\circ$). The examples are NiSO_4 , SnO_2 etc.

(iii) Orthorhombic crystal

In this crystal the lengths of unit cell are different but three axes are perpendicular to each other i.e., ($a \neq b \neq c$ and $\alpha = \beta = \gamma = 90^\circ$). The example are KNO_3 , BaSO_4 , etc.

(iv) Monoclinic crystal

In this crystal the lengths of unit cell are different two axes are at right angles and the third is obliquely inclined, i.e., the axes are perpendicular to each other i.e., ($a \neq b \neq c$ and $\alpha = \beta = 90^\circ \neq \gamma$). The examples are Na_2SO_4 , FeSO_4 etc.

(v) Triclinic crystal

In this crystal the length of unit cell are different and oblique to each other i.e., ($a \neq b \neq c$ and $\alpha \neq \beta \neq \gamma$). The examples are CuSO_4 , $\text{K}_2\text{Cr}_2\text{O}_7$ etc.

(vi) Rhombohedral crystal

In this crystal all the three length of the unit cell are equal in lengths. moreover they are equally inclined to each other at an angle other than 90° i.e., ($a = b = c$ and $\alpha = \beta = \gamma \neq 90^\circ$). The examples are CaSO_4 , Quartz, calcite, etc.

(vii) Hexagonal crystal

In this crystal the three axes of unit cell are equal in one plane at 120° with each other and fourth axis is perpendicular to this plane i.e., ($a = b \neq c$ and $\alpha = \beta = 90^\circ \neq \gamma = 120^\circ$). The examples are SiO_2 , AgI etc.

The seven types of crystal systems are tabulated in the following table.

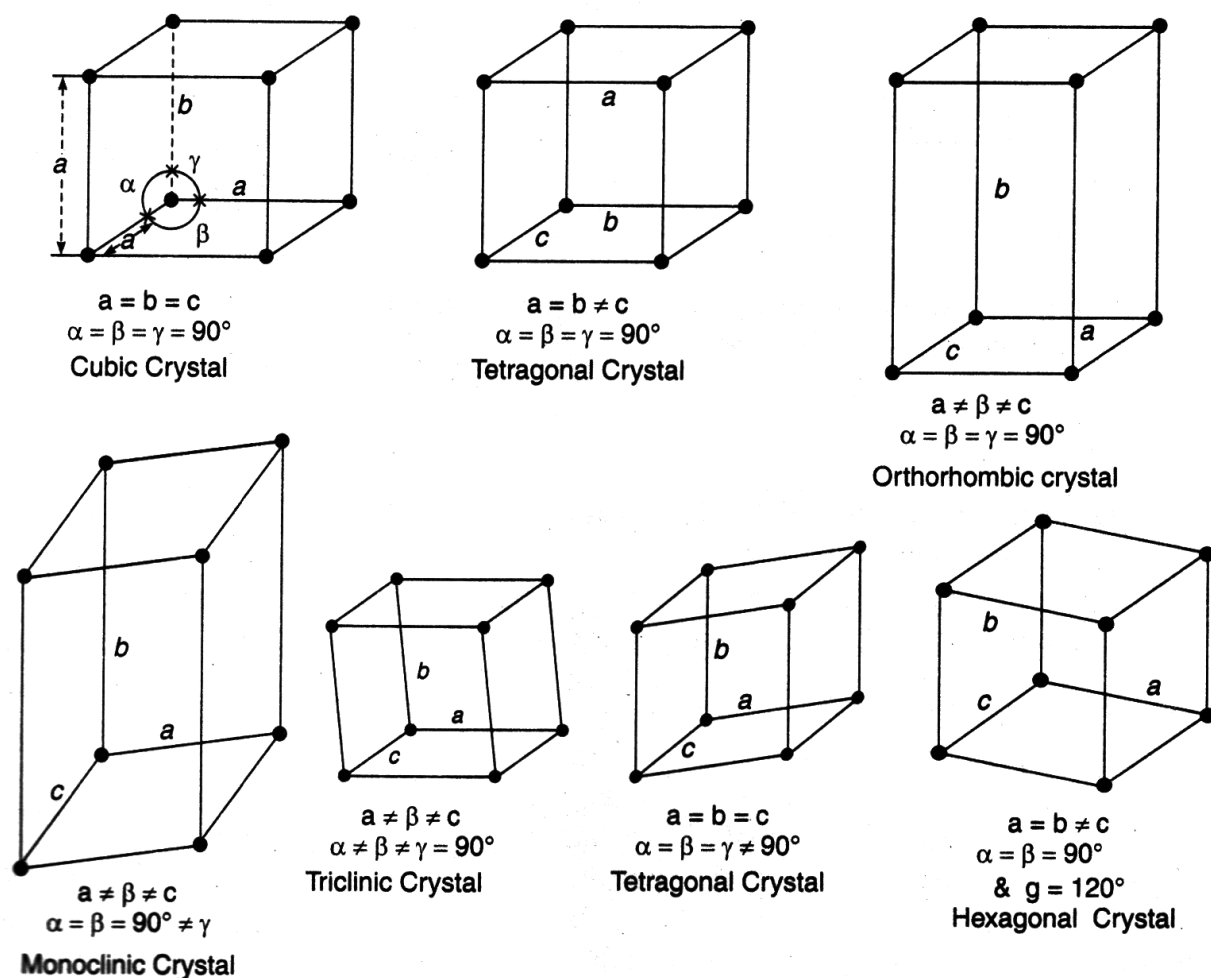


Fig.: Seven crystal systems

S.No.	Name of the crystal system	Relation of lengths of axes unit cell	Relation of angle between axes
1.	Cubic	$a = b = c$	$\alpha = \beta = \gamma = 90^\circ$
2.	Tetragonal	$a = b \neq c$	$\alpha = \beta = \gamma = 90^\circ$
3.	Orthorhombic	$a \neq b \neq c$	$\alpha = \beta = \gamma = 90^\circ$
4.	Monoclinic	$a \neq b \neq c$	$\alpha = \beta = 90^\circ \neq \gamma$
5.	Triclinic	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma \neq 90^\circ$
6.	Rhombohedral (Trigonal)	$a = b = c$	$\alpha = \beta = \gamma \neq 90^\circ$
7.	Hexagonal	$a = b \neq c$	$\alpha = \beta = 90^\circ$ and $\gamma = 120^\circ$

The table shows that the cubic crystals have the largest symmetry while the Triclinic crystal have the least symmetry. It is worth while to mention here that more than half of the elements crystallize into cubic system which is the simplest amongst all.

4.4.1 Bravais Space Lattices

Q7. Explain Bravais space lattices.

Ans :

In 1848 Bravais showed that there are only fourteen ways of arranging points in space so that the environment looks the same from each point. The lattices are called the Bravais lattices named after the discoverer. In case of a cubic system there are three Bravais lattices each of which has the same collection of symmetry elements and the lattice points. The lattices are shown in fig(10) and are referred as.

(i) Simple (or) Primitive cubic or cubic p-type Lattice

There is one Lattice point at each of eight corners of the unit cell. There is no lattice point inside the unit cell (Fig. a).

(ii) Face centred cubic (fcc) or Cubic F Lattice

There is one Lattice point at each of the eight corners and one lattice point at the centres of each of the six faces of the cubic cell. Thus there is an extra point at the centre of each face (fig b).

(iii) Body centred cubic (bcc) or cubic I Lattice

There is one Lattice point at each of the eight corners and one lattice point at the centre of each cell. So there is a lattice point at the centre of each unit cell (fig c).

4.5 MILLER INDICES

Q8. Explain about miller indices.

Ans :

(Imp.)

The planes in a crystal are specified by a set of number called miller indices, derived by miller.

The miller indices are the three smallest integer which have the same ratio as the reciprocals of the intercepts of the plane concerned on the three axes.

The miller index can be determined by adopting the following rules.

1. First, determine the intercepts of plane on the three coordinate axes.
2. Then take the reciprocals of these intercepts.
3. Lastly reduce the reciprocals into whole number obtained after taking LCM of the denominator.

For example, plane ABC has intercepts of 2 axial units on x-axis, 2 axial units on y-axis and 1 axial unit on z-axis.

The numerical parameters of plane ABC are 2, 2, and 1.

Hence its orientation is (2, 2, 1)

According to miller, it is more useful to describe the orientation of the plane by reciprocal of its numerical parameters, rather than by its linear parameters.

The miller indices for ABC are $\left(\frac{1}{2}, \frac{1}{2}, 1\right)$ or (1, 1, 2). The general form for indices of a plane is (h, k, l). The symbol for a family of parallel planes is <hk>

The following information about crystal structure can be obtained from miller indices.

1. The same index number (h, k, l) for different planes indicates that the planes are parallel and equal spaced.
2. Whether plane is parallel to any of the three coordinates axes, its intercept on that axis is as infinity. Hence its miller index for the axis is zero.
3. A bar on miller index indicates that the intercept of a plane of corresponding axis is negative.
4. A set of parallel planes, but not a particular plane are defined by miller indices.
5. A plane passing through the origin is defined in terms of a parallel plane having non-zero intercepts.

4.5.1 Lattice points per unit cell

Q9. What are lattice points per unit cell?

Ans :

(i) Simple cubic lattice

We know that there is one lattice point at each of the eight corners of the unit cell. Moreover, each lattice point forming the simple cubic lattice is a member of 8 surrounding cells.

$$\therefore \text{Number of lattice points in unit cell} = (1/8) \times 8 = 1$$

In this way, there is only one lattice point per unit cell.

(ii) Face centred cubic lattice

In this case, each unit cell consists of eight corner lattice points, each being a member of eight surrounding cells. Moreover, there exists six face lattice points, each being a member of two cells.

Therefore,

$$\text{Total number of corner lattice point concerned with unit cell} = 8 \times (1/8) = 1$$

$$\text{Total number of face centred lattice points concerned with unit cell} = 6 \times (1/2) = 3.$$

$$\text{Hence, total number of lattice points concerned with unit cell} = 1 + 3 = 4$$

(iii) Body centred cubic lattice

In a unit cell, there are eight lattice points at the eight corners and each of them is a member of 8 surrounding cells. Also, there is one lattice point at the centre of the body.

Therefore,

$$\text{Total number of body centre lattice point per unit cell} = 1$$

$$\text{Total number of corner lattice point attached to unit cell} = 8 \times (1/8) = 1$$

$$\text{Hence, total number of lattice points concentrated with unit cell} = 1 + 1 = 2.$$

4.6 SOME SIMPLE CRYSTAL STRUCTURES

4.6.1 Simple cubic structure

Q10. Explain simple crystal structures.

Ans :

(Imp.)

The aim of this article is to consider some simple crystal structures hexagonal closed pack surface, diamond structure zinc blend structure and sodium chloride structure. The cubic system includes the three

Bravais lattice. Simple cubic lattice (SC), the body centered lattice(BCC) and face centred cubic lattice(FCC) all these crystal structures are unique arrangements of atoms, composed of a unit cell periodically repeated in three dimensions.

Simple cubic structure

The unit cell of a simple cubic lattice. There is one lattice point at each of the eight corners of unit cell and no lattice point inside it. We consider the different parameters as follows.

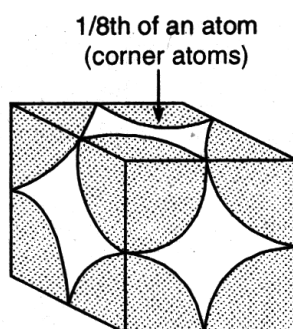


Fig.:

(i) Lattice points per unit cell

We know that there is one lattice point at each of the eight corners of the unit cell.

Moreover, each lattice point forming the simple cubic lattice is a member of 8 surrounding cells.

Therefore the share of each lattice point to the cubic lattice = $\frac{1}{8}$

Number of lattice point in unit cell = $\frac{1}{8} \times 8 = 1$

In this way, there is only one lattice point per unit cell.

(ii) Atomic Radius

The front view of SC lattice

$$2r = a \quad r = \frac{a}{2}$$

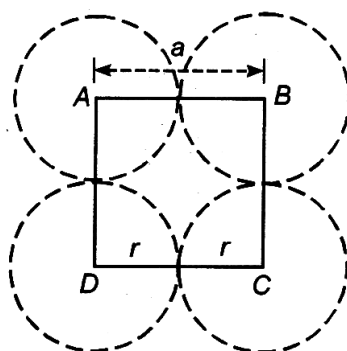


Fig.: Atomic Radius

(iii) Atomic packing fraction

The packing fraction is the ratio of volume occupied by atoms in a unit cell to the total volume of unit cell

Packing fraction

$$= \frac{\text{Volume of all atoms in unit cell}}{\text{Volume of unit cell}}$$

$$= \frac{\text{no. of spheres} \times \text{vol. of each sphere}}{\text{volume of unit cell}}$$

$$= \frac{1 \times \frac{4}{3} \pi r^3}{a^3} = \frac{4 \pi r^3}{3a^3} = \frac{4 \pi (a/2)^3}{3a^3} = \frac{\pi}{6} = 0.52$$

$$= 52\%$$

Thus, the packing fraction is 52% i.e., the structure is loosely packed.

(iv) Co-ordination number

The simple cubic lattice taking any one of the lattice points as origin and the three edges passing through that point as x, y and z axes respectively, the position of the nearest neighbours about origin are

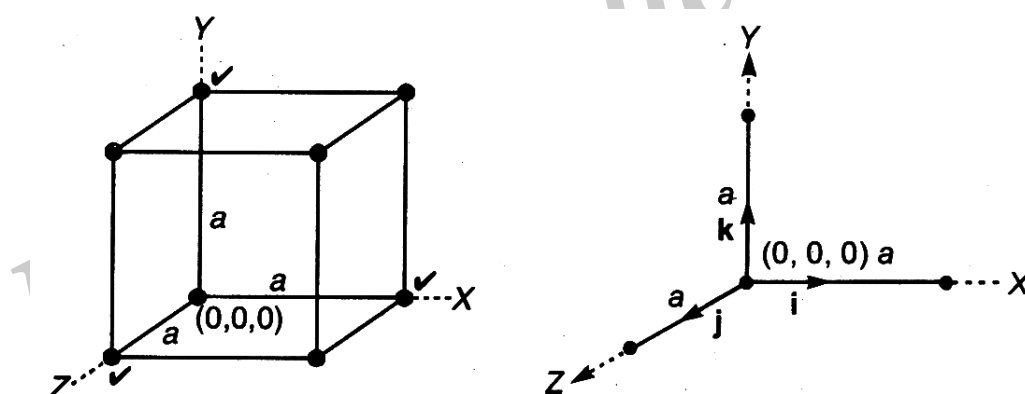


Fig.: Simple cubic lattice

$$\pm ai, \pm aj \text{ and } \pm ak$$

where i, j & k are unit vectors along the three X, Y & Z axes respectively.

We know that in a simple cubic lattice, there is one atom at each of the eight corners of the unit cell. Now, we take an atom at position of the (0, 0, 0) origin. It is observed that this atom is surrounded by six equidistant neighbours. The coordinates of these points are

(+a, 0, 0), (-a, 0, 0) along x-axis

(0, +a, 0), (0, -a, 0) along y-axis

(0, 0, +a) (0, 0, -a) along z-axis

Thus, the coordination number is obviously 6. It is important to mention here that other atoms are not equidistant.

4.6.2 Body centred structure(BCC)

Q11. Explain body centred structure.

Ans :

(Imp.)

There is one lattice point at each of the eight corners and one lattice point at the centre of each cell. The unit cell of body centre cubic lattice. The different parameters are as follows.

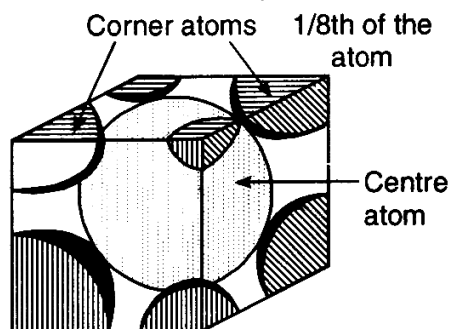


Fig.: Body centred cubic lattice

(i) Lattice point per unit cell

In a unit cell, there are eight lattice points at eight corners and each of them is a member of 8 surrounding cells. Also, there is one lattice point at centre of the body therefore total number of body centred lattice point per unit cell = 1

Total number of corner lattice point attached to unit cell

$$= 8 \times \frac{1}{8} = 1$$

Hence, total number of lattice points concerned with unit cell

$$= 1 + 1 = 2$$

(ii) Atomic radius

For calculation of r in case of BCC

$$AG^2 = AD^2 + DG^2$$

But

$$(DG)^2 = (DC)^2 + (CG)^2 = a^2 + a^2 = 2a^2$$

$$(4r)^2 = a^2 + 2a^2 = 3a^2$$

$$r = \frac{\sqrt{3}}{4} a \quad (\text{or}) \quad a = \frac{4r}{\sqrt{3}}$$

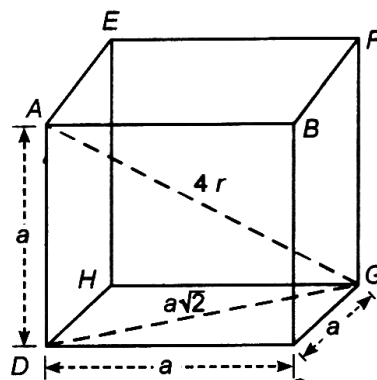


Fig.: Atomic radius

(iii) Atomic packing fraction

$$\text{Packing fraction} = \frac{\text{no. of spheres} \times \text{volume of each sphere}}{\text{volume of each cell}}$$

$$= \frac{2 \times \frac{4}{3} \pi \left(\frac{\sqrt{3}}{4} a \right)^3}{a^3} = \frac{8\pi (\sqrt{3})^3 a^3}{3 \times 64 \times a^3}$$

$$= \frac{\sqrt{3}\pi}{8} = 0.68 = 68\%$$

(iv) Coordination number

In case of body centred cubic lattice there are eight atoms at the eight corners of the unit cell and one atom at the body centre as shown, the body diagonals are also shown in the fig. To compute the coordination number. Let us take the lattice point at the body centre as origin and x, y and z axes being parallel to the edge of unit cell

$$\left(\frac{a}{2}, \frac{a}{2}, \frac{a}{2} \right) \left(-\frac{a}{2}, \frac{a}{2}, \frac{a}{2} \right) \left(\frac{a}{2}, -\frac{a}{2}, \frac{a}{2} \right) \left(\frac{a}{2}, \frac{a}{2}, -\frac{a}{2} \right)$$

$$\left(-\frac{a}{2}, -\frac{a}{2}, \frac{a}{2} \right) \left(-\frac{a}{2}, \frac{a}{2}, -\frac{a}{2} \right) \left(\frac{a}{2}, -\frac{a}{2}, -\frac{a}{2} \right)$$

$$\left(-\frac{a}{2}, -\frac{a}{2}, -\frac{a}{2} \right)$$

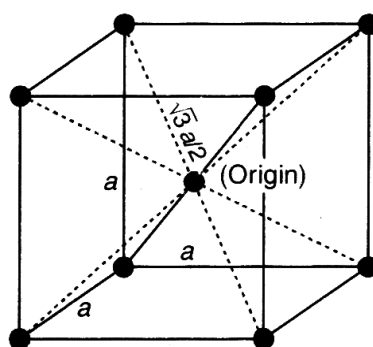


Fig.: Body centred cubic lattice

So, the coordination number is 8

4.6.3 Face centred crystal structure

Q12. Define Face centred crystal structure.

Ans.:

(Imp.)

There is one lattice point at each of eight corners and one lattice point at centre of each of the six faces of the cubic cell. The unit cell is shown, the different parameters.

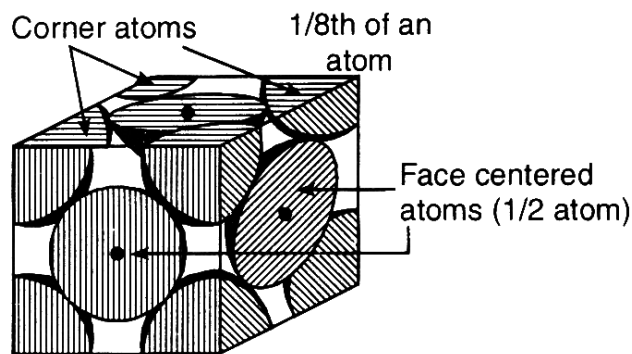


Fig.: Face centred crystal structure

(i) Lattice points per unit cell

In this case, each unit cell consists of eight corner lattice points, each being a member of eight surrounding cells. Moreover there exists six face lattice points, each being a member of two cells

Therefore total number of corner lattice point concerned with unit cell $8 \times \frac{1}{8} = 1$

total no. of face centred lattice points concerned with unit cell $= 6 \times \frac{1}{2} = 3$

Hence, total number of lattice points concerned with unit cell $= 1 + 3 = 4$

(ii) Atomic radius

FCC structure unit cell

$$(DB)^2 = (DC)^2 + (CB)^2$$

$$(4r)^2 = a^2 + a^2 = 2a^2$$

$$r = \frac{\sqrt{2}a}{4} \quad (\text{or}) \quad a = \frac{4r}{\sqrt{2}}$$

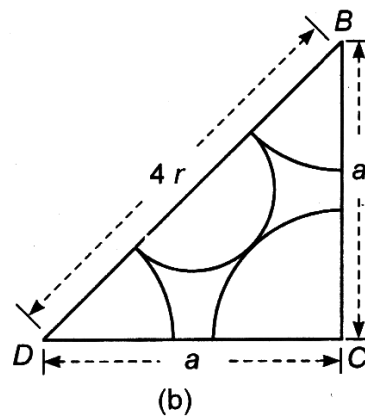
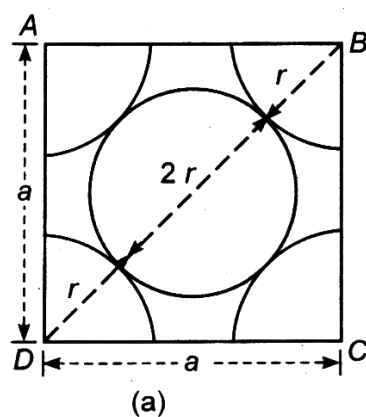


Fig.: (a) Lattice points per unit cell, (b) Atomic radius

(iii) Atomic packing fraction

In case of FCC, we have atomic per unit cell = 4

radius of each sphere = $(\sqrt{2} a / 4)$

∴ Volume of each sphere

$$= \frac{4}{3} \pi r^3 = \frac{4}{3} \pi \left(\frac{\sqrt{2}a}{4} \right)^3 = \frac{\pi a^3 \sqrt{2}}{24}$$

so the maximum fraction of cell filled i.e., packing fraction.

$$= \frac{\text{no. of sphere} \times \text{vol. of each sphere}}{\text{Total volume of each cell}}$$

$$= \frac{4 \times (\pi a^3 \sqrt{2}) / 24}{a^3} = \frac{\pi \sqrt{2}}{6} = 0.74$$

$$= 74\%$$

(vi) Coordination number

The nearest neighbours of any corner atom are the four face centred atoms of surrounding unit cells. The corner atom will have four face centred nearest neighbours in its own plane, 4 in a plane about it and four in a plane below it making the total number of nearest neighbours twelve. Therefore, the total number of nearest neighbours twelve. Therefore, the coordination number of face centred atom is twelve.

Characteristics of three lattices

Characteristics	SC	BCC	FCC
Volume of unit cell	a^3	a^3	a^3
Lattice points per unit cell	1	2	4
Atomic radius	$\frac{a}{2}$	$\frac{\sqrt{3}a}{2}$	$\frac{\sqrt{2}a}{4}$
Nearest neighbour distance $2r$	a	$\frac{\sqrt{3}a}{2}$	$\frac{a}{\sqrt{2}}$
Number of nearest neighbours	6	8	12

4.6.4 Structure of CsCl

Q13. Explain the structure of CsCl.

Ans :

This crystal has simply cubic structure with Cs^+ and Cl^- ions as the basis. The unit cell of Cscl lattice is shown in fig(27). As is obvious from the figure, Cs^+ ions are

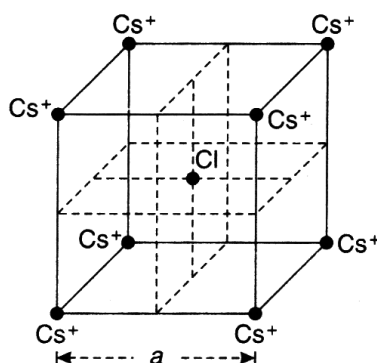


Fig.: Structure of CsCl

This crystal has simple cubic structure with Cs^+ and Cl^- ions as the basis. The unit cell of cell lattice is shown as is obvious from the figure, Cs^+ ions are situated at the corners of the cubic cell and Cl^- ions at the body centre (or) vice versa. So, the crystal may be considered to be a combination of two simple cubic sub-lattice, one of Cs^+ ions and the other of Cl^- ion. Now we consider the coordination number which is defined as the number of nearest neighbours to a given atom in the origin lattice taking at one corner as the origin and x, y and z axes along the three edges passing through that corner, the positions of nearest neighbours are $\pm a\mathbf{i}$, $\pm a\mathbf{j}$, $\pm a\mathbf{k}$ where \mathbf{i} , \mathbf{j} , \mathbf{k} are unit vectors along x , y and z axes respectively. The coordinates of nearest neighbours are $(\pm a, 0, 0)$, $(0, \pm a, 0)$ and $(0, 0, \pm a)$ obviously, their number is 6. Hence, the co-ordination number for same kind of ions is 6 and the nearest neighbour distance is a . Further, there are eight nearest neighbouring ions of opposite kind for an ion of one kind. So, the co-ordination number for opposite kind of ions is 8 and the nearest neighbour distance is $(\sqrt{3} a / 2)$.

4.6.5 Sodium chloride structure

Q14. Explain the sodium chloride structure.

Ans :

The sodium chloride structure is shown in fig. In sodium chloride, sodium atom loses its outer electron and acquired an excess of positive charge while the chlorine atom excess of negative charge. Now due to the electrostatic forces between their excess charges, the two ions attract each other further, due to the strong forces of repulsion as their outer electron shells come into close proximity, the two ions cannot approach each other to within less than a certain distance when attraction and repulsion balance, equilibrium is attained. Now the ions cannot approach further NaCl has a geometrical structure of a simple cube with ions of sodium (Na) and chlorine (Cl) arranged alternatively at the corners of the cube as shown in fig. In terms of the Bravais lattice, NaCl is a face centred cube. The basis consists of Na atom and one Cl atom separated by one-half the body diagonal of unit cube. There are four molecules of NaCl in each unit cube with ions in the positions.

$$\text{Na} : 0, 0, 0, \frac{1}{2}, \frac{1}{2}, 0, \frac{1}{2}, 0, \frac{1}{2}, \frac{1}{2}$$

$$\text{Cl} : \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, 0, 0, \frac{1}{2}, 0, \frac{1}{2}, 0, 0$$

In the crystal each ion is surrounded by six nearest neighbours of the positive kind, i.e., coordination number of six nearest neighbours of the same kind as the reference ion.

Representative crystals having NaCl type arrangement are LiH, KBr, KCl, AgBr, MgO, MnO, BaO, UO etc.

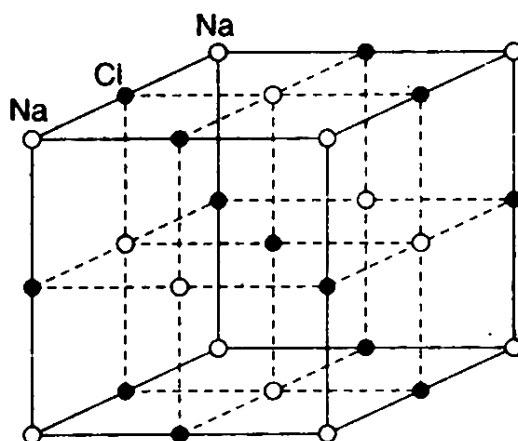


Fig.: Sodium chloride structure

4.6.6 Diamond Structure

Q15. Explain the diamond structure?

Ans :

The diamond structure is a FCC structure with basis of two carbon atoms one located at $(0, 0, 0)$ and other at $(a/4, a/4, a/4)$ associated with each lattice point fig(24a) shows the positions of atoms in the cubic cell of the diamond structure projected on a cubic face. The fraction denote height above the base in unit of a cube edge. The points 0 and $1/2$ are on the FCC lattice while those at $1/4$ and $3/4$ are on a similar lattice displaced along the body diagonal by one fourth of its length. In this way the diamond structure is a combination of two interpenetrating face centred cubic sublattice each atom in this structure has four nearest neighbours, occupying the corner point of a regular tetrahedron (see fig (24b) to which it is bonded by strong covalent bonds. The entire diamond lattice is constructed of such tetrahedral units(fig(24c). The diamond structure is loosely packed since each atom has only 4 nearest neighbours. Carbon, Silicon, Germanium and greytin crystallize in diamond structure. In other words the arrangement inside the unit cells of silicon and germanium is a diamond lattice

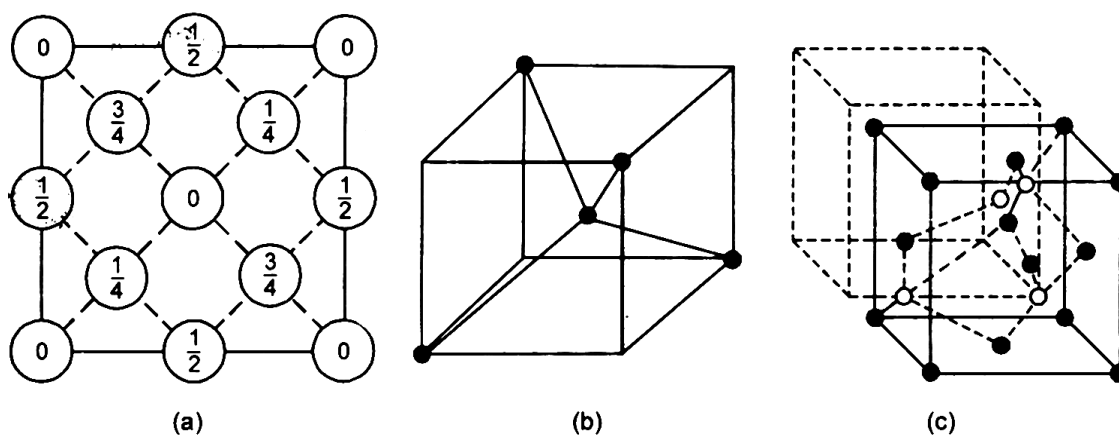


Fig.: Diamond structure

Following are the parameters of diamond cubic structure :

1. Lattice points per unit cell

Referring fig. Points 0 and $1/2$ are on FCC lattice while those at $1/4$ and $3/4$ are on similar FCC lattice displaced along the body diagonal by one fourth of its length.

In diamond cubic unit cell, there are eight corners atoms, six face centred atoms and four more atoms.

Number of atoms and four more atoms to unit cell = $\left(\frac{1}{8}\right) \times 8 = 1$

Number of atoms contributed by face centred atoms to unit cell = $\left(\frac{1}{2}\right) \times 6 = 3$

There are four more atoms inside the structure. Therefore, the number of atoms in diamond cubic unit cell = $1 + 3 = 4 = 8$

2. Atomic Radius

In order to consider the atomic radius. See fig(25) from fig(25)

$$(xy)^2 = (xw)^2 + (wy)^2 + \left(\frac{a}{4}\right)^2 + \left(\frac{a}{4}\right)^2 = \frac{a^2}{8}$$

Similarly, $(xz)^2 = (xy)^2 + (yz)^2$

$$= \frac{a^2}{8} + \left(\frac{a}{4}\right)^2 = \frac{3a^2}{16}$$

$$(2r)^2 = \frac{3a^2}{16} \quad (\text{or}) \quad r^2 = \frac{3a^2}{64}$$

$$r = \frac{\sqrt{3}a}{8}$$

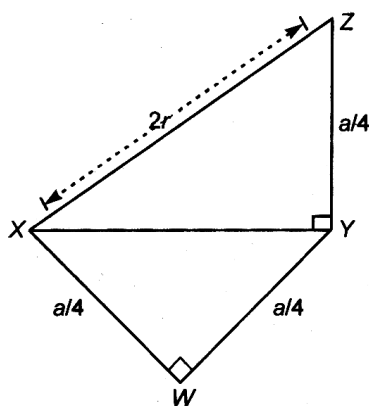


Fig.:

3. Atomic packing fraction

$$\text{Here } v = 8 \times \left(\frac{4}{3} \pi r^3 \right) = 8 \times \frac{4}{3} \pi \left(\frac{\sqrt{3}a}{8} \right)^3$$

$$v = \frac{\sqrt{3}\pi a^3}{16}$$

Situated at the corners of the cubic cell and Cl^- ions at the body centre or vice versa. So, the crystal may be considered to be a combination of two simple cubic sub-lattice one of CS^+ ions and the other of Cl^- ion. Now we consider the co-ordination number which is defined as the number of nearest neighbours to a given atom in the crystal lattice taking the atom at one corner as the origin and x,y and z axes along the three edges passing through that corner the positions of nearest neighbours are $\pm ai, aj, \pm ak$ where i,j,k are unit vectors along x,y and z axes respectively. The co-ordinates of nearest neighbours are $(\pm a, 0, 0), (0, \pm a, 0),$ and $(0, 0, \pm a)$ obviously, their number is 6. Hence the neighbour distance is a same kind of ions is 6 and nearest neighbour distance is a further, there are eight neighbouring ions of opposite kind for an ion of one kind. SO the co-ordination number for opposite kind of ions is 8 and the nearest neighbour distance is $(\sqrt{3} a / 2)$

$$\text{Now } \text{APF} = \frac{v}{V} = \frac{\sqrt{3}\pi a^3}{16 \times a^3} = \frac{\pi\sqrt{3}}{16} = 0.34$$

$$\text{APF} = 34\%$$

Therefore it is a loosely packed structure

4.6.7 Zinc Blende structure

Q16. Explain Zinc blende structure

Ans :

In many compound semi-conductors, atoms are arranged in a basic diamond structure but are different on alternating sites. If the two face centred cubic sub-lattices mentioned in the diamond structure are occupied by different elements, then zinc blende structure results as shown in fig(26). The semi conductors Insb, GaAs and also Zns crystalline in zinc blende structure. In this structure Ga and As are found at alternate locations inside the unit cell.

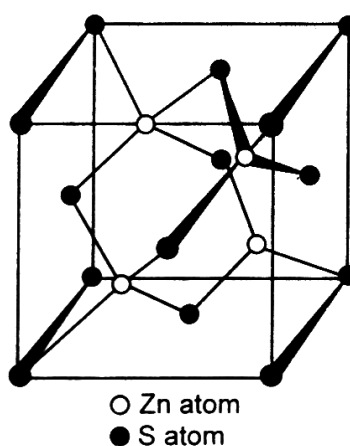


Fig.: Zinc Blende Structure

4.7 X-RAY DIFFRACTION

4.7.1 Diffraction of x-ray by crystal

Q17. Write short note on x-ray diffraction.

Ans :

According to the first theory x-ray were regarded as high speed particles having greater penterating power.

According to the second theory x-rays were treated as electromagnetic waves for extremely high frequency

Frequency of x-rays(F) = $3 \times 10^{16} - 3 \times 10^{10}$ Hz

Wavelength of x-rays(λ) = $0.01 - 10$ nm

$$F \propto \frac{1}{\lambda}$$

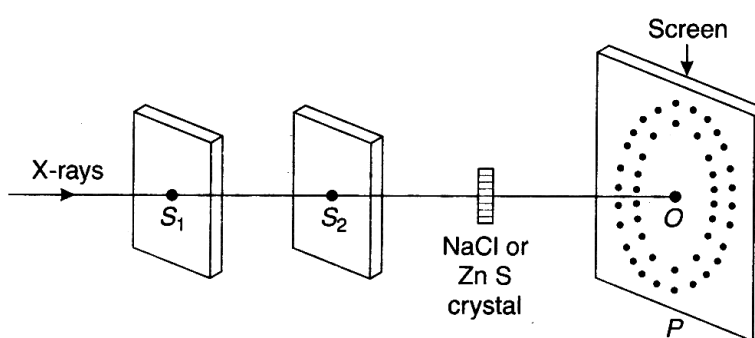


Fig.: Diffraction of x-ray by crystal

4.7.2 Bragg's law

Q18. State & Explain Bragg's law.

Ans :

(Imp.)

Let us consider a set of parallel lattice planes of a crystal separated by a distance d apart. Suppose a narrow beam of x-rays of wavelength λ be incident up on this planes at angle θ . The beam will be reflected in all directions by the atoms of various atomic planes. Because the refractive index of the matter of the crystal is very nearly equal to unity.

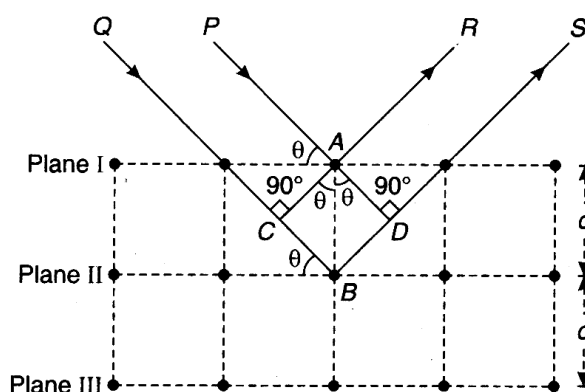


Fig.: Bragg's law

Hence there is practically no bending of the rays entering (or) leaving one crystal. The condition for the reflected waves to be all in phase, as in case (of) optics, is that the path difference between two reflected waves must be an integral multiple of wave length.

Consider a ray PA reflected at atom A in the direction AR from plane 1 and another, ray QB reflected at another atom B in the direction BS. Now from the atom A, draw two perpendicular AC and AD on the incident ray QB and reflected ray BS respectively.

The path difference between these two rays is (CB + BD). The two reflected rays will be in phase or out of phase will depend upon this path difference, when the path difference (CB + BD) is a whole wave length λ , or multiple of whole wave length $n\lambda$, then the two x-ray diffraction rays will reinforce each other and produce an intense spot.

Thus, the condition of reinforcement is

$$CB + BD = n\lambda$$

$$CB = BD = d \sin \theta$$

$$\therefore \boxed{2d \sin \theta = n\lambda}$$

where $n = 1, 2, 3, \dots$ etc., for first order, second order, third order... etc., maxima respectively. The relation is known as Bragg's law.

Different direction in which intense reflection will be produced can be obtained by giving different values to θ i.e.,

$$\text{For 1st maxima, } \sin \theta_1 = \frac{\lambda}{2d}$$

$$\text{For 2nd maxima, } \sin \theta_2 = \frac{2\lambda}{2d}$$

$$\text{For 3rd maxima, } \sin \theta_3 = \frac{3\lambda}{2d} \text{ etc,}$$

4.8 EXPERIMENTAL TECHNIQUE

4.8.1 Crystallography by laue's method

Q19. Explain experimental technique - laue method.

Ans :

The experimental arrangement of laue method is shown in fig. As shown in figure passing through the crystal, the x-rays are diffracted and recorded on a photographic plate. The x-rays before passing through the crystal are limited to a line pencil by a slit system (lead diaphragms). Here the diameter of the pinhole is important because smaller is the diameter, sharper is the interference.

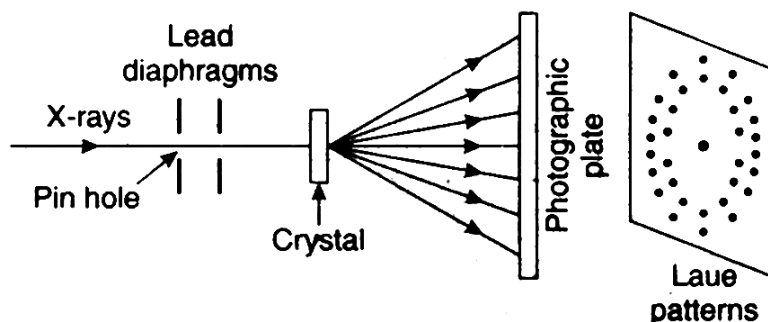


Fig.:

The x-rays which penetrate the crystal are scattered from different atomic diffraction centres. This is possible because there is a whole range of wavelengths in the continuous spectrum and there will be discrete values of λ which satisfy the Bragg condition no matter what may be the orientation of the lattice planes. Here it should be remembered that values of different angles will be different for each set of planes and each set of parallel planes will have its own particular value of the distance. We know that atoms of crystal have an orderly arrangement in all these dimensions in space, hence the diffraction of x-rays will occur from many families of atomic planes at once. Each family picking out the wavelength which it can diffract at angle which it finds itself. The diffraction pattern consists of a central spot and a set of spots arranged in a definite pattern about central spot. The symmetrical pattern of spots known as Laue pattern.

Each spot in the Laue pattern corresponds to an interference maximum for a set of crystal plane satisfying equation $2d \sin \theta = D\lambda$ for a particular wavelength selected from the incident beam. The atomic arrangement in the crystal can therefore, be deduced from a study of the positions and intensities of the Laue spots.

Theory

Imagine a line grating (one dimensional lattice) with atoms on the line as diffracting centres. Let 'a' be the lattice constant, i.e., the constant distance between two successive lattice points. Suppose monochromatic x-rays of wavelength λ are incident on the space lattice. The electrons in the atoms at the lattice points scatter x-rays in all directions coherently. Let θ_0 be the complementary angle of incidence (glancing angle) and θ the complementary angle of diffraction as shown in fig. The path difference between the two diffracted rays is $(AN - BM)$ where AM and BN are perpendiculars dropped on the incident and diffracted rays respectively. The diffracted rays will have maximum intensity if

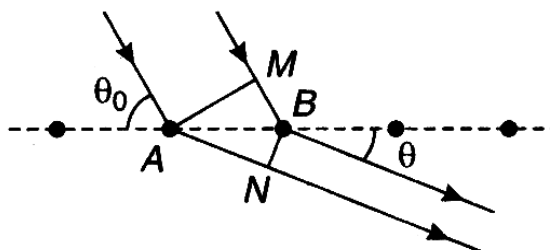


Fig.:

$$AN - BM = n_1 \lambda$$

where n_1 is an integer

From fig, $AN = AB \cos \theta = a \cos \theta$

$$BM = AB \cos \theta_0 = a \cos \theta_0$$

$$a(\cos \theta - \cos \theta_0) = n_1 \lambda \quad \dots(2)$$

is usual to denote $\cos \theta_0$ and $\cos \theta$ by α_0 and α_1 known as directional cosines of the incident and diffracted rays.

Hence

$$a(\alpha - \alpha_0) = n_1 \lambda \quad \dots(3)$$

After being diffracted by the crystal let ray leave the crystal along a path whose direction cosines are α , β and γ . This means that three conditions should be satisfied simultaneously. These conditions are

$$a(\alpha - \alpha_0) = n_1 \lambda$$

$$a(\beta - \beta_0) = n_2 \lambda$$

$$a(\gamma - \gamma_0) = n_3 \lambda$$

where n_1, n_2, n_3 are integers. These are called laue equations.

4.8.2 Crystallography by Powder Method

Q20. Explain experimental technique powder method.

Ans :

The Bragg's spectrometer can be used to diffract x-rays by using a single crystal free from distortion. There are a variety of materials eg., metals, alloys, powder, etc., which are available in micro-crystalline nature.

Actually only few substances are available in the form of a large single crystal. Powder crystal method is a standard technique to study the structure of micro crystals (substances which are available in the form of very small crystals or in powder form). This method gives information regarding the size of crystals, presence of impurities, distortion, preferred orientation on of crystals etc.

The experimental arrangement of powder method is shown in fig. x-rays from x-ray tube are allowed to pass through a filter F which absorbs all wavelengths except one. In this way a monochromatic (single wavelength) beam of x-rays is obtained. The beam is collimated by passing it through two fine slits S_1 and S_2 cut in two lead plates. This fine pencil of x-ray is made to fall on the powdered specimen C. (The specimen in the form of the powdered state is struck on the line wire in the path of x-ray beam). The specimen is located at the centre of drum shaped case the with photographic film at the inner circumference.

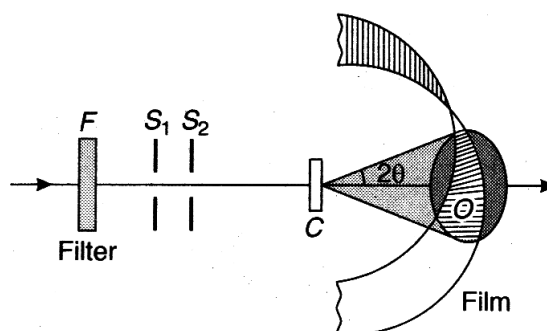


Fig.:

The basic principle underlying this powdered technique is that in the powder, million of micro-crystals have all possible random orientations. Among these very large number of micro-crystals there will always exist some crystal whose lattice planes are so oriented to satisfy the Bragg's relation $n\lambda = 2d \sin\theta$.

The scattered x-rays are incident on the photographic film. The intersections of the different comes of the photographic film are series of concentric circular rings. Radii of these rings (recorded on the film) can be used to find glancing angle. Now the interplanar spacing of crystalline substance can be calculated.

The pattern recorded on the photographic film is shown in fig(9) when the film is laid flat. Due to the narrow width of the film, only parts of circular rings are registered on it. The curvature of arcs reverses when the angle of diffraction exceeds 90° .

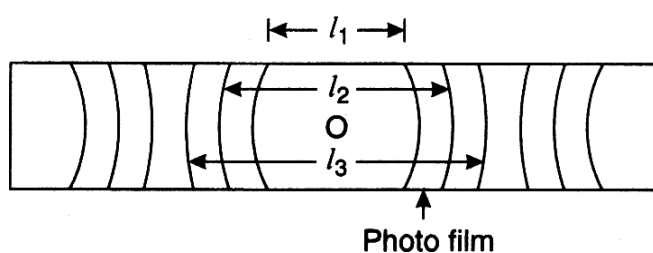


Fig.:

Let l_1, l_2, l_3 etc. be the distances between symmetrical lines on stretched photograph and D , the diameter of cylindrical film, then

$$\frac{L_1}{\pi D} = \frac{4\theta_1}{360} \quad (\text{or}) \quad \theta_1 = \frac{90^\circ}{\pi D} l_1$$

Similarly, $\theta_2 = \frac{90^\circ}{\pi D} l_2$ and $\theta_3 = \frac{90^\circ}{\pi D} l_3$

Using these values of θ in Bragg's formula, interplanar spacing d can be calculated.

4.9 TYPES OF BONDING CRYSTALS

Q21. Explain types of Bonding crystals?

Ans :

A chemical bond is defined as inter - atomic intermolecular or inter-ionic force of attraction which holds the atoms together. On the basis of the nature of forces which bind the crystal lattice together, the crystals can be divided into four categories:

- Ionic Crystals
- Molecular Crystals
- Covalent Crystals
- Metallic Crystals.

The different bindings between them are as follows:

- (a) Ionic Crystal :** These crystals are bound by strong electrostatic attraction between ions of opposite kinds.

Examples are : NaCl, CsCl, KBr, etc.

(b) **Molecular Crystals:** These are also known as inert gas crystals. These crystals are bound by weak Van der Waals forces.

Examples are : Solid CH_4 , etc.

(c) **Covalent Crystals:** These crystals are bound by sharing of electrons between atoms.

Example are : Ge, Si, C (diamond), etc.

(d) **Metallic Crystals:** They are bound by electro-static attraction between the lattice of ion cores and free electron gas.

Example are : Na, Al, Cu, etc.

4.9.1 Characteristics of crystal with different bonding

Q22. Write the characteristics of ionic bonding?

Ans :

The ionic crystals have the following characteristics:

- Ionic compounds are generally crystals in structure.
- Ionic crystals usually crystallize in relatively closed packed structure.
- Ionic crystals are rigid.

Q23. Write the characteristics of ionic bonding.

Ans :

The ionic crystals have the following characteristics:

- Ionic compounds are generally crystals in structure.
- Ionic crystals usually crystallize in relatively closed packed structure.
- Ionic crystals are rigid.
- Due to strong electrostatic binding force, they have high melting and boiling points.
- They are highly soluble in solvents like water and liquid ammonia and insoluble in non-polar solvents.

Q24. Write characteristics of molecular crystals?

Ans :

- The molecular crystals have small binding energy.
- Molecular structure can be both crystalline and non-crystalline.
- They are usually transparent to light.
- They have low melting points because of extremely weak Van der Waals force.
- They are soluble in both polar and non-polar solvents.
- They are good insulators as no valence electrons are available.

Q25. Write characteristics of covalent crystals?

Ans :

Some characteristics of covalent crystals are given below :

- Covalent crystals are usually hard, brittle materials with high binding energies.
- They have high melting and boiling points.

- iii) They generally dissolve in non-polar solvents such as benzene and carbon tetrachloride.
- iv) Basically all the covalent crystals are insulators because ordinarily no electrons are available for conduction. However, some are semi-conductors like germanium.
- v) These crystals are transparent to long wavelength radiation but opaque to shorter wave lengths.

Q26. Write the characteristics of metallic crystals.

Ans :

- i) Metallic crystals have a crystalline structure.
- ii) They have high thermal conductivity due to the presence of free electrons.
- iii) They have high electrical conductivity.
- iv) The metallic bond is comparatively weaker than the ionic and covalent bond. Hence metallic crystals have usually moderate to high melting temperatures.
- v) The metallic crystals are opaque to all electro-magnetic radiations from very low frequency to the middle ultraviolet, where they become transparent. The metallic crystals have high optical reflection and absorption coefficients.

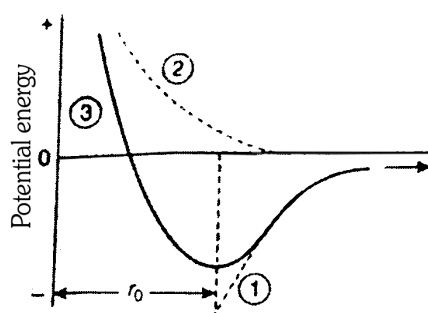
4.9.2 Lattice energy of ionic crystals

Q27. Define lattice energy of a crystal ? Obtain an expression for the lattice energy of ionic molecule?

Ans :

The lattice energy is defined as the energy released in the process when the constituent ions are placed in their respective positions in the crystal lattice or this is the amount of energy which is required to separate the solid ionic crystal into its constituent ions.

Imagine two ions of opposite charge separated by an infinite distance. Let them be allowed to approach each other. There will be electrostatic attraction between the ions which is described by Coulomb's law. In this case the potential energy will be negative because the work is done by the ions. The variation of Coulomb's attractive potential energy with interionic distance is shown by curve (1) in fig.



The two ions are not expected to approach each other sufficiently close to coalesce because there will be repulsive force between them due to electron clouds of the two ions. The situation is shown by curve (2) in fig. In this case the potential energy is positive because the work is done on the ions.

The potential energy of the system is sum of attractive potential energy and repulsive potential energy and this is represented by curve (3). At a certain distance of separation the two forces balance each other. The potential energy is minimum {as shown in curve (3)} and the solid is stable.

The repulsive term is due to short range type of force and it is not effective when the two ions are extremely close to each other. Born proposed that the repulsive potential can be represented by

$$U_R = + \frac{B}{r^n} \quad \dots(1)$$

where r is the distance between the two ions, n is repulsive exponent and B is the repulsive coefficient. Positive sign represents repulsion.

The Coulomb's potential energy is represented by

$$U_C = - A \left(\frac{e^2}{4\pi\epsilon_0 \cdot r} \right) \quad \dots(2)$$

The constant A is called as Madelung constant. The value at A depends upon the crystal structure.

The total energy U_T is given by

$$U_T = U_R + U_C$$

$$U_T = \frac{B}{r^n} - A \left(\frac{e^2}{4\pi\epsilon_0 \cdot r} \right) \quad \dots(3)$$

4.10 DETERMINATION OF MADELUNG CONSTANT FOR NaCl CRYSTAL

Q28. What is madelung constant? Explain it with respect to sodium chloride lattice.

Ans :

(Imp.)

Imagine two ions of opposite charge are allowed to come closer and closer. There will be a coulombain attractive force between them. This force varies inversely as the square of the distance between the two ions. In this way the two ions attract each other when the distance of separation is large and they repel each other for small separation. AT a certain distance of separation the two forces balances each other. Now the potential energy is minimum and the solid is stable.

Madelung Constant for NaCl Crystal

Consider a single Na^+ ion which is situated in sodium chloride lattice as shown in figure (3). Consider a single Na^+ ion situated at the Position A. This is surrounded by

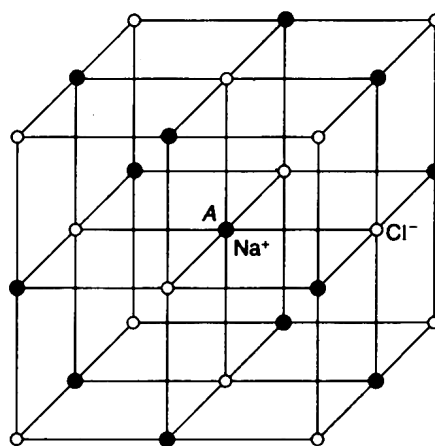


Fig.: Sodium chloride lattice

6Cl^- ions at a distance r_0 , 12Na^+ ions at $\sqrt{2}r_0$, 8Cl^- ions at $\sqrt{3}r_0$ and 6Na^+ ions at a distance $2r_0$ and so on. The attractive potential energy and repulsive potential energy between considered Na^+ ion and other ions are as follow:

Attractive potential energy between Na^+ ion and 6Cl^- ions at a distance r_0 ,

$$U_1 = 6 \left[\frac{e^2}{4\pi\epsilon_0 r_0} \right]$$

Attractive potential energy between Na^+ ion and 8Cl^- ions at a distance $\sqrt{3}r_0$ is given by,

$$U_2 = -8 \left[\frac{e^2}{4\pi\epsilon_0 \sqrt{3}r_0} \right]$$

Repulsive potential energy between Na^+ ion and 12Na^+ ions at a distance $\sqrt{2}r_0$ is given by,

$$U_3 = +12 \left[\frac{e^2}{4\pi\epsilon_0 \sqrt{2}r_0} \right]$$

Repulsive potential energy between Na^+ ion and 6Na^+ ions at a distance $2r_0$ is given by

$$U_4 = +6 \left[\frac{e^2}{4\pi\epsilon_0 2r_0} \right]$$

The sum of all these energies is given by

$$\begin{aligned} &= \frac{e^2}{4\pi\epsilon_0 r_0} \left[-6 - \frac{8}{\sqrt{3}} + \frac{12}{\sqrt{2}} + \frac{6}{2} \dots \right] \\ &= -1.74756 \left[\frac{e^2}{4\pi\epsilon_0 r_0} \right] \end{aligned}$$

For one mole of solid, the lattice energy,

$$= 1.74756 N \left[\frac{e^2}{4\pi\epsilon_0 r_0} \right]$$

Where N is Avogadro's number. Even though there are $2N$ ions, the factor 2 is dropped because the ion should be counted only once.

The constant which multiplies the factor $[-e^2 / r_0]$ is known as Madelung constant. For a NaCl lattice its value is $1.7456 N$.

4.11 CALCULATION OF BORN OF COEFFICIENT AND REPULSIVE EXPONENT

Q29. Give a born calculation of repulsive exponent.

Ans :

According to born, the repulsive energy between two ions due to the short range force is given by,

$$U_R = \frac{B}{r^n} \quad \dots(1)$$

Where B is the repulsive coefficient, r is the distance between two ions and n is the repulsive exponent.

Born obtained the value of repulsive exponent n from the compressibility measurement of crystal.

We know that the compressibility k of a solid is given by,

$$k = -\frac{1}{v} \left[\frac{dv}{dp} \right] \quad \dots(2)$$

According to first law of thermodynamics

$$dQ = dU + dW \quad \dots(3)$$

Where dQ is the quantity of heat given to a system. It is used in two parts: A part is used in increasing the internal energy and the other part is used to perform the external work done dW.

Now,

$$\begin{aligned} dU &= dQ - dW \\ &= dQ - pdV \quad [\because dW = pdV] \end{aligned}$$

($\because dQ = C_v dT$ and at absolute zero, C_v is negligibly small)

$$\therefore \frac{d^2U}{dV^2} = -\frac{dP}{dV} \quad \dots(4)$$

So that compressibility at absolute zero is given by,

$$\frac{1}{k_0} = V_0 \left[\frac{d^2V}{dV^2} \right] \quad \dots(5)$$

For NaCl, $V = 2Nr^3$, where N is the total number of molecule and r is the nearest distance two ions.

$$\text{Now} \quad \frac{dU}{dV} = \frac{dU}{dv} \cdot \frac{dv}{dV} \cdot \frac{dr}{dV}$$

$$\text{and} \quad \frac{d^2U}{dV^2} = \frac{dU}{dr} \cdot \frac{d^2r}{dV^2} + \frac{d^2U}{dr^2} \left[\frac{dr}{dV} \right]^2$$

$$\text{At equilibrium, separation } r = r_0, \quad \frac{dU}{dr} = 0$$

$$\therefore \left[\frac{d^2U}{dV^2} \right]_{r=r_0} = \left[\frac{d^2U}{dr^2} \right]_{r=r_0} \left[\frac{dr}{dV} \right]_{r=r_0}^2 \quad \dots(6)$$

The values of $\left[\frac{dr}{dV} \right]$ and $\left[\frac{d^2U}{dr^2} \right]$ can be obtained by using the relation.

$$V = 2Nr^3$$

$$\therefore \frac{dr}{dV} = \frac{1}{6Nr^2}$$

$$\text{and } \left[\frac{dr}{dV} \right]^2 = \frac{1}{36N^2r^4} \quad \dots(7)$$

At equilibrium separation, $r = r_0$

$$\therefore \left[\frac{dr}{dV} \right]_{r=r_0}^2 = \frac{1}{36N^2r_0^4}$$

For equations (6) and (7), we get

$$\left[\frac{d^2U}{dV^2} \right]_{r=r_0} = \left[\frac{d^2U}{dr^2} \right]_{r=r_0} \left[\frac{1}{36N^2r_0^4} \right]$$

$$\frac{d^2U}{dV^2} = \frac{d^2U}{dr^2} \cdot \frac{1}{36N^2r_0^4}$$

Substituting the value of $\left[\frac{d^2U}{dV^2} \right]$ from equation (8) in equation (5) we get,

$$\frac{1}{K_0} = V_0 \cdot \left[\frac{d^2U}{dr^2} \right] \cdot \left[\frac{1}{36N^2r_0^4} \right] \quad \dots(8)$$

The value of $\left[\frac{d^2U}{dV^2} \right]$ can be obtained as follows. We know that potential energy U for N molecules.

$$\begin{aligned} U &= \frac{NAe^2}{(4\pi\epsilon_0)r} \left[1 - \frac{1}{n} \left(\frac{r_0}{r} \right)^{n-1} \right] \\ &= \frac{NAe^2}{(4\pi\epsilon_0)r} + \frac{NAe^2}{4\pi\epsilon_0 n} \cdot \frac{r_0^{n-1}}{r^n} \end{aligned}$$

$$\text{Now } \frac{dU}{dr} = \frac{NAe^2}{(4\pi\epsilon_0)r^2} - \frac{NAe^2 r_0^{n-1}(n+1)}{(4\pi\epsilon_0)r^{n+2}}$$

$$\therefore \left[\frac{d^2 U}{dr^2} \right]_{r=r_0} = - \frac{2NAe^2}{(4\pi\epsilon_0)r_0^3} + \frac{NAe^2 r_0^{n-1}(n+1)}{(4\pi\epsilon_0)r_0^{n+2}}$$

$$\text{or } \left[\frac{d^2 U}{dr^2} \right]_{r=r_0} = - \frac{NAe^2(n-1)}{4(\pi\epsilon_0)r_0^3} \quad \dots(9)$$

Substituting this value in equation (a), we get

$$\frac{1}{k_0} = 2Nr_0^3 \times \frac{NAe^2(n-1)}{(4\pi\epsilon_0)r_0^3} \times \frac{1}{36N^2r_0^3}$$

$$\text{or } \frac{1}{k_0} = \frac{Ae^2(n-1)}{(4\pi\epsilon_0)18r_0^4} \quad \dots(10)$$

With the help of equation (11) the value of n can be obtained.

$$\text{Now } (n-1) = \frac{18r_0^4}{k_0 Ae^2} (4\pi\epsilon_0)$$

$$\text{or } n = 1 + \frac{18r_0^4}{k_0 Ae^2} (4\pi\epsilon_0)$$

Using this equation the repulsive exponent can be calculated. In case of sodium chloride $n = 9$.

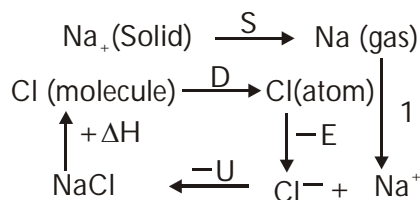
4.12 BORN HABER CYCLE

Q30. Describe Born Harber cycle.

Ans :

(Imp.)

The direct measurement of lattice energy is difficult. Hence Born - Harber cycle is used for this purpose. The Born - Harber cycle for NaCl is represented as follows:



Here S = Heat of sublimation,

D = Dissociation energy

L = Ionisation energy

E = Electron affinity

ΔH = heat of dissociation

U = Lattice energy

They cycle can be explained as follows:

i) Atomization of Na and Chlorine

Initially we start with solid sodium and chlorine molecule. The solid sodium is subjected to the sublimation energy (s) and it is vaporized. To the chlorine molecule, dissociation energy (D) is supplied and as a result it is dissociated into its constituent atoms. Here $D/2$ is the dissociation energy per chlorine atom.

ii) Ionization of Na and Cl

Next ionization energy I is supplied. The outer electron of Na gaseous atom is removed. This electron is added to Cl atom. As the Cl atom has the electron affinity F , an energy E is given out.

iii) Formation of solid

The two ions (Na^+ and Cl^-) are arranged in the lattice and hence the lattice energy U is released.

iv) Back to Square One

We again reach to the starting point by applying an energy (ΔH) known as heat of dissociation.

$$\text{Now} \quad S + \frac{D}{2} + I - E - U - \Delta H = 0$$

$$U = S + \frac{D}{2} + I - E + \Delta H$$

All the quantities on right hand side are known and hence U can be calculated.

Problems

1. A substance with face-centred cubic lattice has density 6250 kg/m^3 and molecular weight 60.2. Calculate the lattice constant a . Given Avogadro's number $6.02 \times 10^{26} (\text{kg mole})^{-1}$.

Sol:

We know that $a = (n M / \rho N)^{1/3}$

Here $n = 4$ = number of molecules per unit cell in fcc lattice

$M = 60.2$, $N = 6.02 \times 10^{26} (\text{kg mole})^{-1}$ and $\rho = 6250 \text{ kg/m}^3$

$$\therefore a = \left[\frac{4 \times 60.2}{6250 \times 6.02 \times 10^{26}} \right]^{1/3} = 4 \times 10^{-10} \text{ m} = 4 \text{ \AA}$$

2. The density of α -ion is 7870 kg/m^3 and its atomic weight is 55.8. Given that α -ion crystallises in the bcc space-lattice. Calculate the value of the lattice constant. Avogadro's number $N = 6.02 \times 10^{26} (\text{kg mole})^{-1}$.

Sol:

$a = (n M / \rho N)^{1/3}$

$n = 2$ = number of molecules per unit cell in bcc lattice

$M = 55.8$, $N = 6.02 \times 10^{26} (\text{kg mole})^{-1}$ and $\rho = 7870 \text{ kg/m}^3$

$$\therefore a = \left(\frac{2 \times 55.8}{7870 \times 6.02 \times 10^{26}} \right)^{1/3} = 2.86 \times 10^{-10} \text{ m} = 2.86 \text{ \AA}$$

3. Copper has a density of 8.96 gm/cm^3 and an atomic weight of 63.5. Calculate the distance between two nearest copper atoms in the bcc structure. The Avogadro's number is 6.02×10^{23} .

Sol:

The lattice constant a for a cubic lattice is given by

$$a = \left[\frac{n M}{\rho N} \right]^{1/3}$$

Here n = number of atoms per unit cell (4), M = atomic weight = 63.5

and ρ = density = 8.96 gm/cm^3

$$\therefore a = \left[\frac{4 \times 63.5}{8.96 \times 6.02 \times 10^{23}} \right]^{1/3} = 3.61 \times 10^{-8} \text{ cm} = 3.61 \text{ \AA}$$

The nearest neighbour distance in fcc lattice is $\frac{a}{\sqrt{2}}$. Hence, the distance between two nearest copper atoms.

$$= \frac{3.61 \text{ \AA}}{\sqrt{2}} = 2.55 \text{ \AA}$$

4. In a crystal a lattice plane cuts intercepts $2a$, $3b$ and $6c$ along the three axes where a , b and c are primitive vectors of the unit cell. Determine the Miller indices of the given plane.

Sol:

$$\text{Here, } p : q : r = 2a : 3b : 6c$$

where a , b and c are primitive vectors of the unit cell.

$$p : q : r = 2 : 3 : 1$$

$$\text{Further } \frac{1}{p} : \frac{1}{q} : \frac{1}{r} = \frac{1}{2} : \frac{1}{3} : \frac{1}{6} = 3 : 2 : 1$$

or

$$h : k : l = 3 : 2 : 1$$

Hence the Miller indices of the plane are (321) .

5. Find the Miller indices of a set of parallel planes which make intercepts in the ratio $4a$ on the X and Y -axes and are parallel to the Z -axis, a , b and c being primitive vectors of the lattice.

Sol:

When the planes are parallel to the Z -axis, their intercept on Z -axis is infinite. Hence

$$p : q : r = 4a : 3b : \infty c$$

or

$$p : q : r = 4 : 3 : \infty$$

or

$$\frac{1}{p} : \frac{1}{q} : \frac{1}{r} = \frac{1}{4} : \frac{1}{3} : \frac{1}{\infty} = 3 : 4 : 0$$

$$h : k : l = 3 : 4 : 0$$

Thus the Miller indices of the given set of planes are (340) .

6. In a simple cubic lattice find the ratio of intercepts on the three axes by $(1, \bar{3}, 2)$ plane.

Sol:

Let a plane cuts intercepts of lengths l_1, l_2, l_3 on the three axes, then

$$l_1, l_2, l_3 = p : q : r \quad \dots(1)$$

If h, k, l be the Miller indices, then

$$h : k : l = \frac{1}{p} : \frac{1}{q} : \frac{1}{r}$$

Here $a = b = c$ and $h = 1, k = -3$ and $l = 2$

$$1 : -3 : 2 = \frac{1}{p} : \frac{1}{q} : \frac{1}{r}$$

$$\therefore p : q : r = \frac{1}{1} : \frac{1}{-3} : \frac{1}{2} = 6 : -2 : 3 \quad \dots(2)$$

From eqs. (1) and (2),

$$l_1 : l_2 : l_3 = 6a : -2a : 3a = 6 : -2 : 3$$

7. In a crystal whose primitives are 1.2\AA , 1.8\AA and 2.0\AA a pla (231) cuts an intercept 1.2\AA on x-axis. Find the corresponding intercepts on the y and Z-axes.

Sol:

Here, we have

$$\begin{aligned} h : k : l &= \frac{1.2}{2} : \frac{1.8}{3} : \frac{2.0}{1} \\ &= 0.6 : 0.6 : 2.0 \end{aligned}$$

Given $h = 1.2\text{\AA}$

$$1.2 : k = 0.6 : 0.6$$

or $k = 1.2\text{\AA}$

Similarly, $1.2 : l = 0.6 : 2.0$

$$\therefore l = \frac{1.2 \times 2.0}{0.6} = 4.0\text{\AA}$$

Short Question and Answers

1. Explain crystalline and amorphous material.

Ans :

If the atoms (or) molecules in a solid are arranged in some regular fashion, then it is known as crystalline.

When the atoms (or) molecules in a solid are arranged in an irregular fashion, then it is known as amorphous.

In a crystalline solid each atom (or) molecule is fixed at a definite point in space at a definite distance from and it in a definite angular orientation to other atoms (or) molecules surrounding it.

2. Distinction between crystalline and amorphous solids.

Ans :

1. Crystalline solids have a regular arrangement of particles whereas the amorphous solids have a completely random particle arrangement.
2. Crystalline solids have different physical properties in different directions.
3. The cooling curve for amorphous substance is smooth, while the curve of crystalline substance has breaks, the middle of which corresponds to the process of crystallization.
4. All the bonds in a crystalline solid are equally strong due to their symmetry

For example, as the temperature of glass is gradually raised, it softens and starts flowing without any sharp change from solid state to liquid.

3. What is Lattice translation vector?

Ans :

The position vector of any lattice point in two dimensional lattice by choosing any other lattice point p as origin is expressed as

Where n_1 and n_2 are integral values, which represent the number of lattice point along PA and PB axes and a and b are called primitives. The position vector T is called the translation vector.

The arrangement of points in three dimensions is expressed by the translation operator T as

$$T = n_1a + n_2b + n_3c$$

where a, b and c are primitives taken along the crystal axes PA, PB and PC

4. Explain Bravais space lattices.

Ans :

In 1848 Bravais showed that there are only fourteen ways of arranging points in space so that the environment looks the same from each point. The lattices are called the Bravais lattices named after the discoverer. In case of a cubic system there are three Bravais lattices each of which has the same collection of symmetry elements and the lattice points. The lattices are shown in fig(10) and are referred as.

(i) Simple (or) Primitive cubic or cubic p-type Lattice

There is one Lattice point at each of eight corners of the unit cell. There is no lattice point inside the unit cell (fig. a).

(ii) Face centred cubic (fcc) or Cubic F Lattice

There is one Lattice point at each of the eight corners and one lattice point at the centres of each of the six faces of the cubic cell. Thus there is an extra point at the centre of each face (fig b).

(iii) Body centred cubic (bcc) or cubic I Lattice

There is one Lattice point at each of the eight corners and one lattice point at the centre of each cell. So there is a lattice point at the centre of each unit cell (fig c).

5. What are lattice points per unit cell?

Ans :

(i) Simple cubic lattice

We know that there is one lattice point at each of the eight corners of the unit cell. Moreover, each lattice point forming the simple cubic lattice is a member of 8 surrounding cells.

$$\therefore \text{Number of lattice points in unit cell} = (1/8) \times 8 = 1$$

In this way, there is only one lattice point per unit cell.

(ii) Face centred cubic lattice

In this case, each unit cell consists of eight corner lattice points, each being a member of eight surrounding cells. Moreover, there exists six face lattice points, each being a member of two cells.

Therefore,

$$\text{Total number of corner lattice point concerned with unit cell} = 8 \times (1/8) = 1$$

$$\text{Total number of face centred lattice points concerned with unit cell} = 6 \times (1/2) = 3.$$

$$\text{Hence, total number of lattice points concerned with unit cell} = 1 + 3 = 4$$

(iii) Body centred cubic lattice

In a unit cell, there are eight lattice points at the eight corners and each of them is a member of 8 surrounding cells. Also, there is one lattice point at the centre of the body.

Therefore,

$$\text{Total number of body centre lattice point per unit cell} = 1$$

$$\text{Total number of corner lattice point attached to unit cell} = 8 \times (1/8) = 1$$

$$\text{Hence, total number of lattice points concentrated with unit cell} = 1 + 1 = 2.$$

6. Explain the structure of CsCl.

Ans :

This crystal has simply cubic structure with Cs^+ and Cl^- ions as the basis. The unit cell of CsCl lattice is shown in fig(27). As is obvious from the figure, Cs^+ ions are

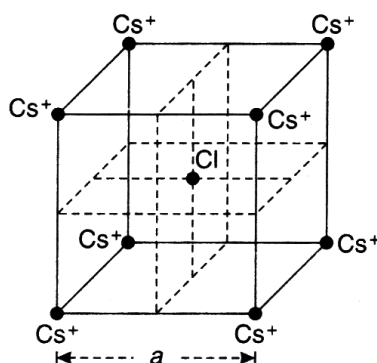


Fig.: Structure of CsCl

This crystal has simple cubic structure with Cs^+ and Cl^- ions as the basis. The unit cell of cell lattice is shown as is obvious from the figure, Cs^+ ions are situated at the corners of the cubic cell and Cl^- ions at the body centre (or) vice versa. So, the crystal may be considered to be a combination of two simple cubic sub-lattice, one of Cs^+ ions and the other of Cl^- ion. Now we consider the coordination number which is defined as the number of nearest neighbours to a given atom in the origin lattice taking at one corner as the origin and x, y and z axes along the three edges passing through that corner, the positions of nearest neighbours are $\pm a\mathbf{i}$, $\pm a\mathbf{j}$, $\pm a\mathbf{k}$ where \mathbf{i} , \mathbf{j} , \mathbf{k} are unit vectors along x , y and z axes respectively. The coordinates of nearest neighbours are $(\pm a, 0, 0)$, $(0, \pm a, 0)$ and $(0, 0, \pm a)$ obviously, their number is 6. Hence, the co-ordination number for same kind of ions is 6 and the nearest neighbour distance is a . Further, there are eight nearest neighbouring ions of opposite kind for an ion of one kind. So, the co-ordination number for opposite kind of ions is 8 and the nearest neighbour distance is $(\sqrt{3} a / 2)$.

7. Explain the sodium chloride structure.

Ans :

The sodium chloride structure is shown in fig. In sodium chloride, sodium atom loses its outer electron and acquires an excess of positive charge while the chlorine atom has an excess of negative charge. Now due to the electrostatic forces between their excess charges, the two ions attract each other further, but due to the strong forces of repulsion as their outer electron shells come into close proximity, the two ions cannot approach each other to within less than a certain distance when attraction and repulsion balance, equilibrium is attained. Now the ions cannot approach further NaCl has a geometrical structure of a simple cube with ions of sodium (Na) and chlorine (Cl) arranged alternatively at the corners of the cube as shown in fig. In terms of the Bravais lattice, NaCl is a face centred cube. The basis consists of Na atom and one Cl atom separated by one-half the body diagonal of unit cube. There are four molecules of NaCl in each unit cube with ions in the positions.

$$\text{Na} : 0, 0, 0, \frac{1}{2}, \frac{1}{2}, 0, \frac{1}{2}, 0, \frac{1}{2}, \frac{1}{2}$$

$$\text{Cl} : \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, 0, 0, \frac{1}{2}, 0, \frac{1}{2}, 0, 0$$

In the crystal each ion is surrounded by six nearest neighbours of the positive kind, i.e., coordination number of six nearest neighbours of the same kind as the reference ion.

Representative crystals having NaCl type arrangement are LiH, KBr, KCl, AgBr, MgO, MnO, BaO, UO etc.

8. Write short note on x-ray diffraction.

Ans :

According to the first theory x-ray were regarded as high speed particles having greater penetrating power.

According to the second theory x-rays were treated as electromagnetic waves for extremely high frequency

Frequency of x-rays(F) = 3×10^{16} – 3×10^{10} Hz

Wavelength of x-rays(λ) = 0.01 – 100 nm

$$F \propto \frac{1}{\lambda}$$

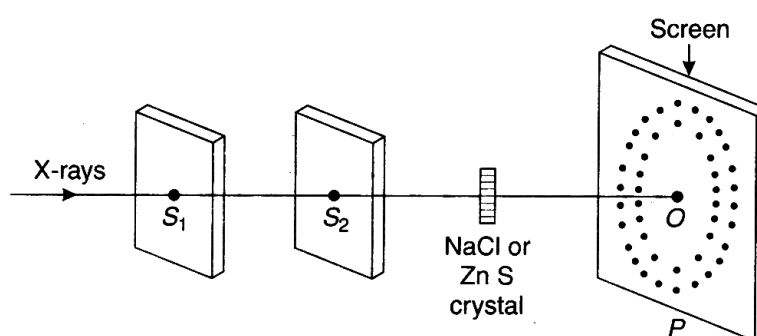


Fig.: Diffraction of x-ray by crystal

9. Explain types of Bonding crystals.

Ans :

A chemical bond is defined as inter - atomic intermolecular or inter-ionic force of attraction which holds the atoms together. On the basis of the nature of forces which bind the crystal lattice together, the crystals can be divided into four categories:

- (a) Ionic Crystals
- (b) Molecular Crystals
- (c) Covalent Crystals
- (d) Metallic Crystals.

The different bindings between them are as follows:

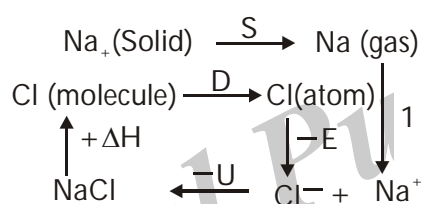
- (a) **Ionic Crystal :** These crystals are bound by strong electrostatic attraction between ions of opposite kinds.
Examples are : NaCl, CsCl, KBr, etc.
- (b) **Molecular Crystals:** These are also known as inert gas crystals. These crystals are bound by weak Van der Waals forces.
Examples are : Solid CH_4 , etc.
- (c) **Covalent Crystals:** These crystals are bound by sharing of electrons between atoms.
Example are : Ge, Si, C (diamond), etc.
- (d) **Metallic Crystals:** They are bound by electro-static attraction between the lattice of ion cores and free electron gas.
Example are : Na, Al, Cu, etc.

10. Write the characteristics of metallic crystals.*Ans :*

- Metallic crystals have a crystalline structure.
- They have high thermal conductivity due to the presence of free electrons.
- They have high electrical conductivity.
- The metallic bond is comparatively weaker than the ionic and covalent bond. Hence metallic crystals have usually moderate to high melting temperatures.
- The metallic crystals are opaque to all elector-magnetic radiations from very low frequency to the middle ultroviolet, where they become transparent. The metallic crystals have high optical reflection and absorpion coefficients.

11. Describe Born Harber cycle.*Ans :*

The direct measurement of lattice energy is difficult. Hence Born - Harber cycle is used for this purpose. The Born - Harber cycle for NaCl is represented as follows:



Here S = Heat of sublimation, D = Dissociation energy
 L = Ionisation energy E = Electron affinity
 ΔH = heat of dissociation U = Lattice energy

12. Find the Miller indices of a set of parallel planes which make intercepts in the ratio 4 a. on the X and Y-axes and are parallel to the Z-axis, a, b and c being primitive vectors of the lattice.*Sol :*

When the planes are parallel to the Z-axis, their intercept on Z-axis is infinite. Hence

$$p a : q b : r c = 4 a : 3 b : \infty c$$

or $p : q : r = 4 : 3 : \infty$

or $\frac{1}{p} : \frac{1}{q} : \frac{1}{r} = \frac{1}{4} : \frac{1}{3} : \frac{1}{\infty} = 3 : 4 : 0$

$$h : k : l = 3 : 4 : 0$$

Thus the Miller indices of the given set of planes are (340).

13. In a crystal whose primitives are 1.2\AA , 1.8\AA and 2.0\AA a plane (231) cuts an intercept 1.2\AA on x-axis. Find the corresponding intercepts on the y and z-axes.

Sol:

Here, we have

$$h : k : l = \frac{1.2}{2} : \frac{1.8}{3} : \frac{2.0}{1} \\ = 0.6 : 0.6 : 2.0$$

Given $h = 1.2\text{\AA}$

$$1.2 : k = 0.6 : 0.6$$

or $k = 1.2\text{\AA}$

Similarly, $1.2 : l = 0.6 : 2.0$

$$\therefore l = \frac{1.2 \times 2.0}{0.6} = 4.0\text{\AA}$$

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Choose the Correct Answers

1. A crystalline solid has _____. [a]
 (a) definite geometric shape (b) flat forces
 (c) sharp edges (d) all of these
2. The elements of geometry are _____. [d]
 (a) plane of symmetry (b) axis of symmetry
 (c) centre of symmetry (d) all of these
3. The diamond structure is a _____ structure. [c]
 (a) BCC (b) SC
 (c) FCC (d) None of these
4. NaCl has a geometrical structure of a _____. [a]
 (a) SC (b) BCC
 (c) FCC (d) None of these
5. Bragg's relation is _____. [d]
 (a) $n\lambda = d \sin\theta$ (b) $n\lambda = 2 \sin\theta$
 (c) $\theta = \lambda \cdot 2d \sin\theta$ (d) $n\lambda = 2d \sin\theta$
6. _____ are also known as invest gas crystals. [b]
 (a) Ionic crystal (b) molecular crystal
 (c) metallic crystal (d) covalent crystal
7. Modeling constant _____. [a]
 (a) $\left(-\frac{e^2}{r_0} \right)$ (b) $\left(\frac{e^2}{r_0} \right)$
 (c) e^2 (d) None of the above
8. Example of ionic crystal _____. [a]
 (a) NaCl (b) CH_4
 (c) Ge (d) Na
9. Atomic radius of SC lattice _____. [b]
 (a) $r = a$ (b) $r = \frac{a}{2}$
 (c) $r = 2a$ (d) $r = \frac{2}{a}$
10. The semiconductors Insb, GaAS and Zns crystalline in _____. [a]
 (a) Zinc blende structure (b) Sodium chloride structure
 (c) CsCl (d) Diamond structure

Fill in the Blanks

1. A set of parallel planes, but not a particular plane are defined by _____.
2. The co-ordination number of body centred cubic lattice is _____.
3. Each point in a crystal lattice is called _____.
4. The _____ can be used to diffract X-rays by using a single crystal free from disturbance.
5. Powder crystal method is standard technique to study the structure of _____.
6. Molecular structure can be both _____ and _____.
7. An energy (ΔH) known as _____.
8. The metallic crystals have high _____ and _____.
9. _____ have high melting and boiling point.
10. Born obtained the value of repulsive exponent n from the _____ measurement of crystal.

ANSWERS

1. Miller indices
2. 8
3. lattice point
4. Bragg's spectrometer
5. Micro crystals
6. crystalline, non-crystalline
7. heat of dissociation
8. optical reflection, absorption coefficients
9. Covalent crystals
10. Compressibility

FACULTY OF SCIENCE
B.Sc. V - Semester(CBCS) Examination
Subject : Physics
Paper-V : MODERN PHYSICS
MODEL PAPER - I

Time : 3 Hours]

[Max. Marks : 80

Part - A (8 × 4 = 32 Marks)

Note : Answer any Eight questions

ANSWERS

- | | |
|--|--------------------|
| 1. Mention the drawback's of Bohr's theory? | (Unit-I, SQA- 1) |
| 2. Discuss the L-S and J-J coupling schemes associated with an atom. | (Unit-I, SQA-3) |
| 3. Explain the spectral terms. | (Unit-I, SQA-5) |
| 4. Discuss the inadequacy of classical physics. | (Unit-II, SQA-1) |
| 5. State and explain Heisenberg uncertainty principle. | (Unit-II, SQA-4) |
| 6. Define physical significance of wave function. | (Unit-II, SQA-9) |
| 7. Define Nuclear Size and Nuclear Charge. | (Unit-III, SQA-1) |
| 8. Explain Range of α -particles. | (Unit-III, SQA-6) |
| 9. A G.M. counter has a plateau slope of 3% per 100 volt. If the operating point is at 100 volt, what is the maximum permissible voltage fluctuations, when the counting is not affected by more than 0.1 %? | (Unit-III, Prob.9) |
| 10. Explain crystalline and amorphous material. | (Unit-IV, SQA-1) |
| 11. Explain Bravais space lattices. | (Unit-IV, SQA-4) |
| 12. Explain types of Bonding crystals. | (Unit-IV, SQA-9) |

Part - B (4 × 12 = 48 Marks)

Note : Answer all the questions

13. (a) Describe the theory of Stern and Gerlach experiment. Why it is necessary to use a beam of neutral atoms. (Unit-I, Q.No.4)
- OR
- (b) What is zeeman effect? Describe the experimental arrangement to study the zeeman effect. (Unit-I, Q.No.15)

14. (a) Explain experimental study of photo-electric effect. **(Unit-II, Q.No.5)**

OR

- (b) Discuss in brief about Compton effect. **(Unit-II, Q.No.7)**

15. (a) Explain the properties of nucleus with reference to size, charge, mass, density, spin, magnetic dipole moment. **(Unit-III, Q.No.1)**

OR

- (b) Explain binding energy of nucleus and calculate binding energy of nucleus. **(Unit-III, Q.No.2)**

16. (a) Explain body centred structure. Explain the diamond structure. **(Unit-IV, Q.No.11,15)**

OR

- (b) Describe Born-Haber cycle. **(Unit-IV, Q.No.30)**

FACULTY OF SCIENCE
B.Sc. V - Semester(CBCS) Examination
Subject : Physics
Paper-V : MODERN PHYSICS
MODEL PAPER - II

Time : 3 Hours]

[Max. Marks : 80

Part - A ($8 \times 4 = 32$ Marks)

Note : Answer any Eight questions

ANSWERS

- | | |
|--|--------------------|
| 1. Explain the spectral terms. | (Unit-I, SQA-5) |
| 2. Explain selection rules. | (Unit-I, SQA- 6) |
| 3. How do you use rotational spectrum to determining internuclear distance? | (Unit-I, SQA- 11) |
| 4. Explain and derive Planck's Radiation formula. | (Unit-II, SQA- 2) |
| 5. Define Compton Effect. | (Unit-II, SQA- 3) |
| 6. Write short note on Expectation Values. | (Unit-II, SQA-10) |
| 7. Define Nuclear Mass and Nuclear Density. | (Unit-III, SQA-2) |
| 8. Define Nuclear Spin and Nuclear Magnetic Dipole Moment(μ). | (Unit-III, SQA-3) |
| 9. Explain the structure of nucleus. | (Unit-III, SQA-4) |
| 10. What is Lattice translation vector? | (Unit-IV, SQA-3) |
| 11. What are lattice points per unit cell? | (Unit-IV, SQA-5) |
| 12. Find the Miller indices of a set of parallel planes which make intercepts in the ratio 4 a. on the X and Y-axes and are parallel to the Z-axis, a, b and c being primitive vectors of the lattice. | (Unit-IV, Prob.12) |

Part - B ($4 \times 12 = 48$ Marks)

Note : Answer all the questions

- | | |
|---|----------------------|
| 13. (a) Discuss the L-S and J-J coupling schemes associated with an atom. | (Unit-I, Q.No.8) |
| OR | |
| (b) What is Paschen - Back Effect? What is Stark Effect? Describe the experimental arrangement to study Stark Effect. | (Unit-I, Q.No.16,17) |

14. (a) Describe Davisson Germer Experiment to demonstrate the wave character of electrons? (Unit-II, Q.No.14)

OR

- (b) Derive Schrodinger time independent equation for matter waves. (Unit-II, Q.No.24)

15. (a) What are the similarities between liquid drop and a nucleus? (Unit-III, Q.No.8)

OR

- (b) Discuss in detail Gamow's theory of α - Decay. (Unit-III, Q.No.12)

16. (a) Define Face centred crystal structure. State & Explain Bragg's law. (Unit-IV, Q.No.12,18)

OR

- (b) Explain experimental technique powder method. (Unit-IV, Q.No.20)

FACULTY OF SCIENCE
B.Sc. V - Semester(CBCS) Examination
Subject : Physics
Paper-V : MODERN PHYSICS
MODEL PAPER - III

Time : 3 Hours]

[Max. Marks : 80

Part - A (8 × 4 = 32 Marks)

Note : Answer any Eight questions

ANSWERS

- | | |
|--|--------------------|
| 1. What is raman effect ? | (Unit-I, SQA-12) |
| 2. What are the applications of raman effect and Problems? | (Unit-I, SQA-14) |
| 3. What is Paschen - Back Effect? | (Unit-I, SQA- 9) |
| 4. Relation between group velocity and wave velocity. | (Unit-II, SQA-5) |
| 5. Define Properties of Matter Waves. | (Unit-II, SQA- 6) |
| 6. Define complementary Principle of Bohr. | (Unit-II, SQA- 8) |
| 7. Explain the structure of nucleus. | (Unit-III, SQA-4) |
| 8. A Geiger Muller counter collects 10^7 electrons/discharge. The average current in the circuit is 1.333×10^{-18} amp. Find the counting rate/min. | (Unit-III, Prob.8) |
| 9. A G.M. counter has a plateau slope of 3% per 100 volt. If the operating point is at 100 volt, what is the maximum permissible voltage fluctuations, when the counting is not affected by more than 0.1 %? | (Unit-III, Prob.9) |
| 10. Distinction between crystalline and amorphous solids. | (Unit-IV, SQA-2) |
| 11. Explain the structure of CsCl. | (Unit-IV, SQA-6) |
| 12. Describe Born Harber cycle. | (Unit-IV, SQA-11) |

Part - B (4 × 12 = 48 Marks)

Note : Answer all the questions

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| 13. (a) Give the elementary theory of the origin of the vibrational spectrum of a molecule ? | (Unit-I, Q.No.22) |
| OR | |
| (b) What is raman effect ? Explain classical theory of raman effect ? | (Unit-I, Q.No.22) |

14. (a) Give the experimental illustrations of Heisenberg uncertainty principle. (Unit-II, Q.No.18)

OR

- (b) Derive Schroedinger time dependent equations for matter waves ? (Unit-II, Q.No.25)

15. (a) Describe in detail the construction and working of a Geiger - Muller Counter. (Unit-III, Q.No.15)

OR

- (b) Explain the working of proportional counter. Describe the construction and working of scintillation Counter. (Unit-III, Q.No.16,17)

16. (a) Define Face centred crystal structure. (Unit-IV, Q.No.12)

OR

- (b) Explain experimental technique - laue method. (Unit-IV, Q.No.19)