

[Drude Lorentz Free electron Theory]

According to Drude Lorentz Theory (known as free electron theory) a metal is supposed to consists of ~~the~~ positive metal ions fixed in lattice whose valence electrons move freely in the boundaries of the metal like gas molecules in a vessel. The Valence of the atoms becomes the conductors of electricity in metal and they are known as conduction electrons.

When an electric field is applied then electrons are accelerated against the direction of applied field. Due to the collision with massive atoms this acceleration does not continue indefinitely. The mutual repulsions of the electrons are neglected in the direction of the applied field. The mean velocity required by the electron gas due to this application of electric field is known as drift velocity and which is superimposed over already existing random motion.

2

Dhmn's law) When an electric field is applied to a solid i.e. a potential difference is maintained between the two ends and the electrons will not be able to move at random as before but they now move along the direction of the applied field. The velocity of the electrons will depend upon the applied field. Higher is the field, greater is the velocity and consequently higher would be the no. of electrons per sec. through unit area i.e. the current passing through the conductor will be higher. This proves theoretically the Ohm's law.

Let —

$E$  = Electric field intensity applied to a conductor

$e$  = charge on electron

$m$  = mass of the electron.

$v$  = velocity  ~~$\alpha T$~~

According to Kinetic Theory

$$\frac{1}{2}mv^2 \propto T$$

$$\frac{1}{2}mv^2 = \frac{3}{2}kT \quad \text{--- (1)}$$

where  $k$  = Boltzmann constant.

Assuming that after each collision with atom, the electron starts with a fresh velocity  $v$  and the time  $t$  between the successive collision which is subjected to the influence of electric field and experiences a force  $Ee$  which imparts an acceleration ' $a$ ' to it.

~~Now~~ we have

$$ma = Ee$$

$$a = \frac{Ee}{m} \quad \text{--- (ii)}$$

If  $\lambda$  be the mean free path of electron, the time  $t$  between two successive collision is given by

$$t = \frac{\lambda}{v} \quad \text{--- (iii)}$$

The average distance travelled by electron in time  $t$

$$\begin{aligned} s &= \frac{1}{2} at^2 \\ &= \frac{1}{2} \left( \frac{Ee}{m} \right) \frac{\lambda^2}{v^2} \quad \text{--- (iv)} \end{aligned}$$

If  $\bar{v}$  is the average velocity of the electron then

$$\bar{v} = \frac{s}{t} = \frac{1}{2} \left( \frac{Ee}{m} \right) \frac{\lambda^2}{v^2} \times \frac{v}{\lambda}$$

$$= \frac{1}{2} \frac{Ee}{m} \times \frac{\lambda^4}{V}$$

$$= \frac{1}{2} \frac{Eev^2}{2 \times \frac{3}{2} kT}$$

$$\therefore V = \frac{Ee\lambda v}{6kT} \quad (\text{v})$$

If  $n$  be the no. of electrons per unit vol. in the conductor and  $s$  be the current density per unit area normal to the current direction then -

$$s = neV$$

$$= ne \frac{Ee\lambda v}{6kT}$$

$$= \frac{nEe^2\lambda v}{6kT}$$

$$\text{or } s = \left( \frac{ne^2\lambda v}{6kT} \right) E \quad (\text{vi})$$

$$\therefore s \propto E \quad (\text{vii})$$

which shows that current is proportional to the applied field, which is known as Ohm's law.

Bragg-Williams Approximation of Ising Model—

Ising model equation is

$$(1) \quad E_I(s_i) = -\epsilon \sum_{\langle i,j \rangle} s_i s_j - \mu H \sum_i s_i \quad (1)$$

for the energy of the system. Here  $I$  (subscript) stands for Ising & the symbol  $\langle i,j \rangle$  denotes a nearest-neighbour pair of spins and  $\mu H$  is the interaction energy associated with an external magnetic field  $H$ .

According to Bragg and Williams, it is assumed that the distribution of spins is at random. Let  $N_A$  be the number of spins for which  $s_i$  is up ( $+1$ ) &  $N_B$  be the no. of spins for which  $s_i$  is down ( $-1$ ). Then  $\frac{N_A}{N}$  &  $\frac{N_B}{N}$  represents the probability of finding a spin  $+1$  or  $-1$  on a given lattice site.

Assuming random arrangement of spins over the whole lattice eqn. (1) written as

$$E_I = -\frac{1}{2} Z N \epsilon \left[ \left( \frac{N_A}{N} \right)^2 + \left( \frac{N_B}{N} \right)^2 - \frac{2 N_A \cdot N_B}{N^2} \right] - \mu H (N_A - N_B) \quad (2)$$

It is assumed that  $N_A \approx N_B$  in the last term, where  $Z$  is the no. of nearest neighbours of a site,  $N = N_A + N_B$  no. of spins. The no.  $N_A/N$  does not require any correlation between the nearest neighbours & it is a measure of the long-range order. It means that, in the entire lattice, a fraction ( $N_A/N$ ) of all the spins are up. Hence, if  $N_A/N$  is known in the neighbourhood of a given spin, then the same average value is likely to occur everywhere on the entire lattice.

If  $\mu$  is the magnetic moment associated with the spin then the total mag. moment is

$$M = \mu (N_A - N_B) \quad (3)$$

$$\text{using } N = N_A + N_B$$

$$M = \mu (N_A - N + N_A)$$

$$\therefore \frac{M}{\mu} = \frac{2N_A}{N} - 1 = m \quad (4)$$

$$\therefore \frac{N_A}{N} = \frac{1}{2} \left( 1 + \frac{m}{\mu} \right) \\ = \frac{1}{2} (1+m) \quad (5)$$

$$\text{Similarly, } \frac{N_B}{N} = \frac{1}{2} (1-m) \quad (6)$$

$$\text{Also, } \frac{2N_A N_B}{N^2} = 2 \cdot \frac{N_A}{N} \cdot \frac{N_B}{N} = 2 \cdot \frac{1}{2}(1+m) \cdot \frac{1}{2}(1-m) \quad (7)$$

$$= \frac{1}{2}(1+m)(1-m) \quad (7)$$

$$\text{From eqn (3)} \frac{M}{MN} = \frac{N_A}{N} - \frac{N_B}{N}$$

$$\text{or, } m = \frac{N_A}{N} - \frac{N_B}{N}$$

$$\therefore N_A - N_B = mN \quad (8)$$

Putting eqn (5), (6), (7) & (8) in eqn. (2)

$$E_1 = -\frac{1}{2}ZN \left[ \frac{1}{4}(1+m)^2 + \frac{1}{4}(1-m)^2 - \frac{1}{2}(1+m)(1-m) \right] - \mu H m N$$

$$= -\frac{1}{2}ZN \left[ \frac{1}{2}(1+m) - \frac{1}{2}(1-m) \right]^2 - \mu H m N$$

$$= -\frac{1}{2}ZN m^2 - \mu H m N \quad (9)$$

Where  $m$  is long-range order parameter ranging as  $-1 \leq m \leq +1$  & represents magnetisation in a ferromagnetic system, dielectric polarisation in a ferromagnetic system etc.

The no. of arrangements of spins over the  $N$  sites is given by the number of ways of choosing  $N_A$  things out of  $N$

$$W = \frac{IN}{I_{N_A} I_{N-B}} = \frac{IN}{I_{N_A} I_{N_B}}$$

Using Stirling's approximation

$$\log_e \underline{N} = N \log N - N$$

$$\log_e W = \log_e \frac{IN}{I_{N_A} I_{N_B}}$$

$$= \log_e \underline{N} - \log_e \underline{N_A} - \log_e \underline{N_B}$$

$$= N \log N - N - N_A \log N_A + N_A - N_B \log N_B + N_B$$

$$= N \log N - N_A \log N_A - N_B \log N_B \quad (\because N = N_A + N_B)$$

$$= -(N_A + N_B) \log \underline{N} - N_A \log N_A - N_B \log N_B$$

$$= -(N_A \log \underline{\frac{N_A}{N}} + N_B \log \underline{\frac{N_B}{N}} - N_A \log N_A - N_B \log N_B)$$

$$= N_A (\log N - \log N_A) + N_B (\log N - \log N_B)$$

$$= -[N_A (\log N_A - \log N) + N_B (\log N_B - \log N)]$$

$$= -[N_A \log \frac{N_A}{N} + N_B \log \frac{N_B}{N}]$$

$$= -N \left[ \frac{N_A}{N} \log \frac{N_A}{N} + \frac{N_B}{N} \log \frac{N_B}{N} \right]$$

$$= -N \left[ \frac{1}{2}(1+m) \log \frac{1}{2}(1+m) + \frac{1}{2}(1-m) \log \frac{1}{2}(1-m) \right] \quad (10)$$

From (5) & (9)

From relation between entropy & Probability

$$S = k \log W$$

$$= -NK \left[ \frac{1}{2} (1+m) \log_2 (1+m) + \frac{1}{2} (1-m) \log_2 (1-m) \right]$$

$$= -NK \left[ \frac{1}{2} (1+m) \log (1+m) + \frac{1}{2} (1-m) \log (1-m) - \log 2 \right] \quad (1)$$

Helmholtz free energy.

$$F = E - TS$$

$$= -\frac{1}{2} Z e^{-\mu m^2} - \mu H m N - NK T \left[ -\log 2 + \frac{1}{2} (1+m) \log (1+m) \right. \\ \left. + \frac{1}{2} (1-m) \log (1-m) \right] \quad (2)$$

The equilibrium value of  $m$  (or  $N_A - N_B$ ) is determined

$$\text{by } \frac{\partial F}{\partial m} = 0$$

$$\text{or } -Z e^{-\mu m} - \mu H - NK T \left[ +\frac{1}{2} + \frac{1}{2} \log (1+m) - \frac{1}{2} - \frac{1}{2} \log (1-m) \right] = 0$$

$$\text{or } Z e^{-\mu m} + \mu H = K T \frac{1}{2} \log \frac{1+m}{1-m} \quad (3)$$

$$\text{or } \log \frac{1+m}{1-m} = 2 \cdot \frac{Z e^{-\mu m} + \mu H}{K T} = 2x \text{ (let)} \quad \text{where } x = \frac{Z e^{-\mu m} + \mu H}{K T}$$

$$\text{or } \frac{1+m}{1-m} = e^{2x}$$

$$\text{or } m = \frac{e^{2x} - 1}{e^{2x} + 1} \quad \text{From eqn(4) } m = \frac{M}{\mu H} \quad (4)$$

$$\text{or } \frac{M}{\mu H} = \tanh x$$

which is well known result of Weiss theory of ferromagnetism.

For  $H=0$ , the spontaneous magnetic moment is

$$M_s = \mu_N \tanh \frac{Z e^{-\mu_s}}{N H K T} \quad \text{From (3) Value of } x$$

$$\text{or } \frac{M_s}{\mu_N} = \tanh \frac{Z e^{-\mu_s}}{N H K T}$$

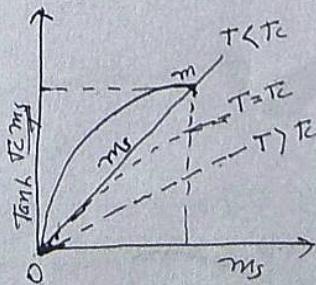
$$\text{or } m_s = \tanh \frac{T_c m_s}{T} \quad (6)$$

where  $m_s = \frac{M_s}{\mu_N}$  &  $T_c = \frac{Z e}{K}$  called Curie temp.

Eqn (6) can be solved to obtain  $m_s$  as function of  $T$  in Bragg-Williams approximation. For this left & right sides are plotted separately as function of  $m_s$ . The intercepts of two curves gives the value of  $m$  at the temp. of intercept. The solution is

(i) for  $T_c/T \leq 1$ ,  $m_s = 0$  &

(ii) for  $T_c/T > 1$ ,  $m_s = m_{s0} - m$ . But



$m_s = 0$  for  $T > T_c$ ) is not acceptable because it corresponds to maximum of function  $F$  (helmholtz free energy) instead of minimum. Thus  $m_s = 0$  for  $T > T_c$  &  $m_s = \pm m$  for  $T < T_c$ . The solution  $m_s = \pm m$  occurs because for  $H = 0$ , there is no difference of spin up & down.

1  
B.Sc III (H)

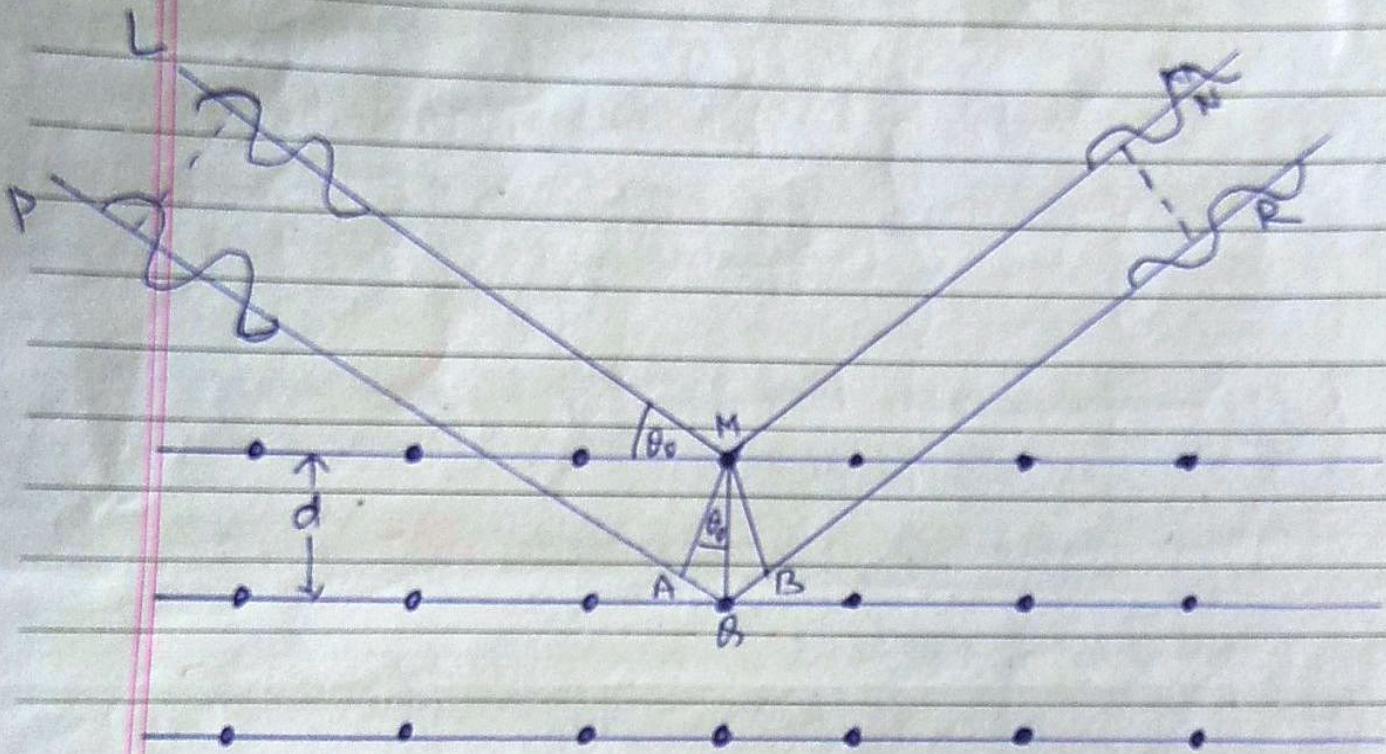
## Bragg's law.

: Dr. Bishwa Mohan Kumar  
Dept. of Physics  
R.K.D. College

W. L. Bragg presented a simple explanation of the observed angles of the diffracted beams from a crystal. Let a series of parallel rows in which the atoms are arranged in a given plane of the crystal. Let parallel beam of X-rays is incident in a direction making a glancing angle  $\theta_0$  with the surface of the planes. Each atom acts as a centre of disturbance and sends a spherical wave-fronts by Huygen construction. As X-rays are much more penetrating than ordinary light, it is necessary to consider the rays reflected not from a single layer but from several layers together.

Let there are two parallel rays LMN and PQR which are reflected by two atoms M and Q in adjacent layers as shown in fig. The atom Q is vertically below M. The length of the path PQR is greater than the length

of the path LMN the path difference is  $(AB + BB)$  and according to the condition of reflection ~~is~~



we have

$$(AB + BB) = n\lambda \quad \text{--- (1)}$$

But from fig

$$AB = BB = d \sin \theta_0$$

$$\therefore d \sin \theta_0 + d \sin \theta_0 = n\lambda$$

$$\therefore AB + BB = d \sin \theta_0 + d \sin \theta_0 = n\lambda \\ = 2d \sin \theta_0 = n\lambda$$

If this path difference is an integral

multiple of the wavelength  $\lambda$ , the reflected beam will interfere constructively giving maximum intensity. Thus strong reflection will be observed in the direction which corresponds to a path difference  $\lambda, 2\lambda, 3\lambda, \dots$  between the rays reflected at consecutive planes, i.e. for strong reflection or reinforcement.

$$2d \sin \theta_0 = n\lambda \quad (1)$$

Where  $n$  is an integer.

Here eqn(1) is the Bragg's eqn. or Bragg's law. From eqn(1) it is clear that for given values of  $n, \lambda$  and  $d$ , there will be strong reflection in a particular direction.

It is now clear that there are only certain directions  $\theta_0$  in which the reflections of a given wavelength  $\lambda$  from all parallel planes add up in phase to give a strong reflected (diffracted) beam. We also conclude accordingly that a beam of monochromatic x-rays incident on a crystal with an arbitrary angle  $\theta_0$  is in general not reflected because  $\sin \theta_0 < 1$ , wavelength  $\lambda \leq 2d$  are essential if the Bragg reflection is to occur. Since  $d = 10^{-8} \text{ cm}$  this condition is equivalent to

It is for this reason that X-rays are most useful for crystal analysis. Just by way of illustration, visible light having a wavelength in the range of  $1 \times 10^{-10}$  m is not Bragg reflected. Instead, the well-known effects of optical refraction and reflection are observed with it.

Thus the Bragg's law is - consequence of the periodicity of the space lattice. The law does not refer to arrangement of the basis of atoms associated with each lattice points. The composition of the basis determines the relative intensity of the various order of n of diffraction from a given set of parallel planes. As stated earlier Bragg reflection can only occur for wavelength  $\lambda \leq 2d$  and due to this fact the visible wavelength can not be used in diffraction.

Bragg's law (in three dimensions):

Let crystal is treated as three dimensional grating. Again let a, b, c are the interplaner separations along three axes and ( $\cos\alpha_0, \cos\beta_0, \cos\gamma_0$ )

and  $(\cos \alpha, \cos \beta, \cos \delta)$  lie direction cosines of incident and scattered radiation respectively. The diffraction conditions for three directions will lie

$$\left. \begin{aligned} a(\cos \alpha - \cos \alpha_0) &= n_1 \lambda \\ b(\cos \beta - \cos \beta_0) &= n_2 \lambda \\ c(\cos \delta - \cos \delta_0) &= n_3 \lambda \end{aligned} \right\} \quad \textcircled{1}$$

Where  $n_1, n_2$  and  $n_3$  are integers.  
For a cubic crystal lattice we have

$a = b = c$ . Hence eqn ① reduce to -

$$\cos \alpha - \cos \alpha_0 = n_1 \lambda / a$$

$$\cos \beta - \cos \beta_0 = n_2 \lambda / a$$

$$\cos \delta - \cos \delta_0 = n_3 \lambda / a$$

Squaring these and then adding them we get

$$\begin{aligned} (\cos \alpha - \cos \alpha_0)^2 + (\cos \beta - \cos \beta_0)^2 + (\cos \delta - \cos \delta_0)^2 \\ = \frac{1}{a^2} (n_1^2 + n_2^2 + n_3^2) \end{aligned}$$

Using  $\cos^2 \alpha + \cos^2 \beta + \cos^2 \delta = 1$  and simplifying we get

$$2a \sin \frac{\theta_0}{2} = \sqrt{(n_1^2 + n_2^2 + n_3^2)} \lambda$$

where  $\theta_0$  is the angle between incident and ~~scattered~~ directions.