



PES
UNIVERSITY

ENGINEERING PHYSICS

Department of Science and Humanities

➤ *Suggested Reading*

1. *Fundamentals of Physics, Resnik and Halliday, Chapter 41*
2. *Concepts of Modern Physics, Arthur Beiser, Chapter 9*
3. *Learning material prepared by the department- Unit III*

➤ *Reference Videos*

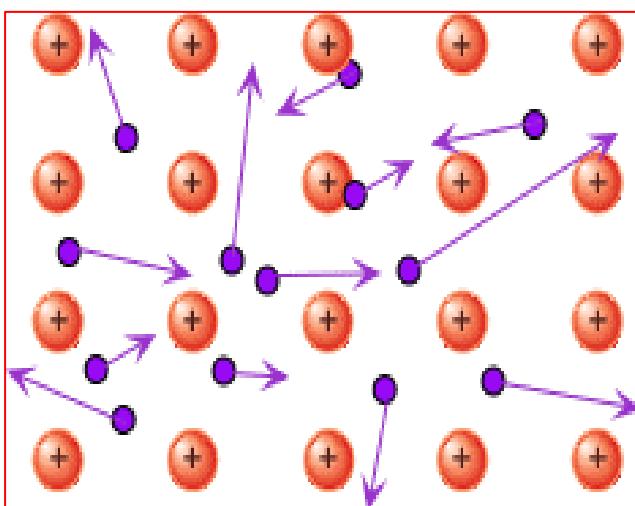
Physics Of Materials-IIT-Madras/lecture-07.html

Class #21

- *Assumptions of classical free electron theory*
- *Expression for electrical conductivity*
- *Matthiessen's rule of total resistivity*
- *Failures of classical free electron theory*

Proposed by Drude and Lorentz (as early as 1904)

- *Valence electrons are treated as conduction electrons*
- *Effect of positive ion cores is considered constant and neglected*
- *Electrostatic repulsion between the electrons is neglected*
- *Valence electrons are considered equivalent to molecules in a gas*
- *Free electron gas – follows Maxwell-Boltzmann statistics*



Metallic specimen: Valence electrons in random motion

1. Thermal velocity

Thermal energy of the free electrons in the absence of the electric field is given by

$$\frac{1}{2} m V_{th}^2 = \frac{3}{2} k_B T$$

Thus, Thermal velocity

$$v_{th} = \sqrt{\frac{3k_B T}{m}}$$

Typical order is 10^5 m/s

Random motion of the electrons do not contribute to a net drift of electrons and hence no current flows

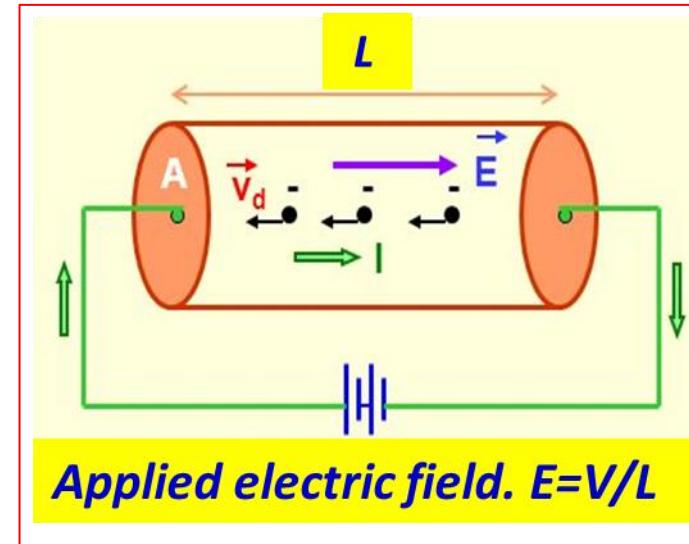
2. Relaxation time and mean free path, $\tau = \frac{\text{mean free path } (\lambda)}{v_{th}}$

(Based on kinetic theory of gas)



3. Drift Velocity: Average velocity in the presence of an electric field

$$v_d = \frac{e\tau E}{m} = \frac{eE}{km}$$



Typical order of V_d for an electric field of 1 V/m is 10^{-4} m/s

➤ Force equation for the electron's drift, $m \frac{dv}{dt} = eE - kmv$

Coefficient of scattering loss (k), $k = \frac{1}{\tau}$

4. Electron mobility or Charge carrier mobility

$$\mu = \frac{e\tau}{m} = \frac{v_d}{E}$$

Mobility: Drift velocity per unit electric field

Expression for current through a conductor

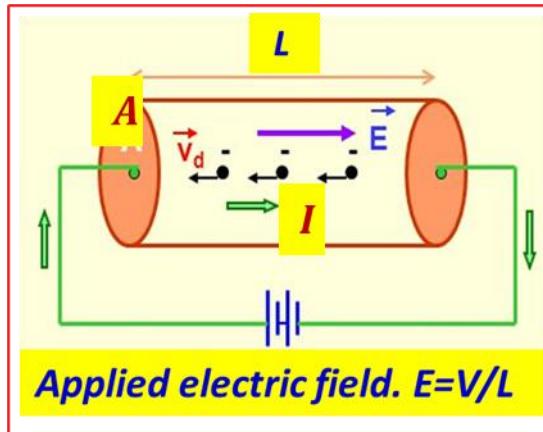
$$I = nev_d A$$

where, $v_d = \frac{e\tau E}{m}$

$$\therefore I = neA \frac{e\tau E}{m}$$

or

$J = \frac{I}{A} = \frac{ne^2\tau}{m} E = \sigma E$ where ' σ ' is a constant for a given metal termed conductivity of the metal



Microscopic form of Ohm's law or Generalized Ohm's law, $J = \sigma E$

$$I\left(\frac{L}{A}\right) = \frac{V}{R}\left(\frac{L}{A}\right)$$

Electrical conductivity, $\sigma = \frac{ne^2\tau}{m} = ne\mu$

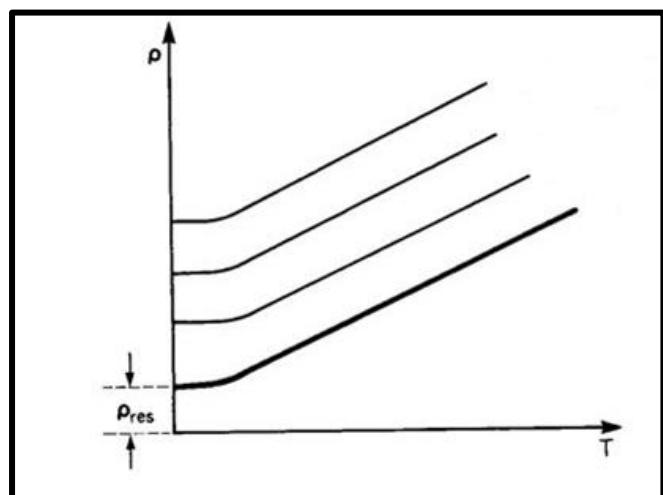
Electrical resistivity, $\rho = \frac{1}{\sigma} = \frac{m}{ne^2\tau} = \frac{1}{ne\mu}$

Electron mobility or Charge carrier mobility $\mu = \frac{e\tau}{m} = \frac{v_d}{E}$

ENGINEERING PHYSICS

Experimental Temperature Dependence of Resistivity : Matthiessen's rule

- Experimentally, resistivity of metals vary linearly with normal operating temperatures (ρ_{sc})
- At low temperatures the resistivity saturate to finite values (ρ_{res})
- Net resistivity, $\rho = \rho_{res} + \rho_{sc}$ or $\frac{m}{ne^2\tau} = \frac{m}{ne^2\tau_{res}} + \frac{m}{ne^2\tau_{sc}}$ ← WKT, Resistivity, $\rho = \frac{1}{\sigma} = \frac{m}{ne^2\tau} = \frac{1}{ne\mu}$
- Known as the Matthiessen's rule of total resistivity



At low temperatures resistivity saturate to finite value

Failed to correlate the experimental results of many phenomena:-

- *Temperature dependence of resistivity*
- *Specific heat of electrons*
- *Dependence of electron concentration on conductivity*

Failure 1: Temperature dependence of resistivity of metals

Resistivity, $\rho = \frac{m}{ne^2\tau}$, **where,** $\tau = \frac{\lambda}{v_{th}}$

As per CFET, considering constant mean free path (λ) the relaxation time dependence only on thermal velocity

That is, $v_{th} = \sqrt{\frac{3k_B T}{m}}$, $v_{th} \propto \sqrt{T}$ or $\tau \propto T^{-\frac{1}{2}}$

As resistivity $\rho \propto \tau^{-1}$, this gives $\rho \propto \sqrt{T}$

But experimental observations showed $\rho \propto T$

Failure 2: Specific heat dependence of electrons in metals

$$\text{Specific heat, } C_{el} = \frac{dU}{dT}$$

For 1 mole of a mono valent metal, the energy of the valence electrons is given by $U = \frac{3}{2} k_B T \cdot N_{avg}$

This gives,

$$C_{el} = \frac{dU}{dT} = \frac{3}{2} k_B \cdot N_{avg} = \frac{3}{2} R \text{ (a constant)}$$

But experimental estimation of the specific heat of electrons is only 1% of this value and is temperature dependent

Failure 3: Dependence of electron concentration on conductivity

As per CFET, $\sigma = \frac{ne^2\tau}{m}$, expected linear dependency on the free electron concentration

But, experimental results show no linear dependence

Example:

Mono-valent Copper has a higher conductivity than trivalent Aluminum

Also, Zinc with higher electronic concentration has lesser conductivity than Aluminum

The concepts which are correct are....

- 1. V_{th} of valence electrons will always be smaller than V_d**
- 2. Valence electrons in metals drift without any loss of energy**
- 3. Resistivity of a metal is directly related to mobility of charge carriers**
- 4. Effective relaxation time is the sum of relaxation time due to scattering and impurities**
- 5. The resistivity in metal due to impurities depend on temperature**

A certain conductor has a free electron concentration of $5.9 \times 10^{28} \text{ m}^{-3}$. What current density in the conductor will correspond to a drift velocity of $1/1.6 \text{ mm s}^{-1}$? Calculate the mobility of charge carriers given conductivity as $6.22 \times 10^7 (\Omega\text{m})^{-1}$.

$$\text{Given, } n = 5.9 \times 10^{28}, V_d = \frac{1}{1.6} \times 10^{-3} \text{ m/s}$$

$$\text{Given, } \sigma = 6.22 \times 10^7 \text{ S/m}$$

$$\begin{aligned}\text{Current Density, } J &= \frac{I}{A} = neV_d \\ &= 5.9 \times 10^6 \text{ A/m}^2\end{aligned}$$

$$\text{Mobility, } \mu = \frac{\sigma}{ne} = 6.59 \times 10^{-3} \text{ m}^2/\text{V.s}$$

Calculate the free electron concentration, mobility and drift velocity of electrons in an Al wire of diameter 0.5mm, length 5m, resistance of 60 milli ohms that carries a current of 15A . Al has 3 free electrons At wt of Al=26.98 and density $2.7 \times 10^3 \text{ kg m}^{-3}$.

$$n = \frac{\text{No. of free electrons per atom} \times \text{Avagadro number} \times \text{Density}}{\text{Atomic wt.}}$$

$$\text{Mobility, } \mu = \frac{1}{\rho n e} = 1.4 \times 10^{-2} \text{ m}^2/\text{V.s}$$

$$\text{Drift velocity, } V_d = \frac{I}{neA} = 2.64 \times 10^{-9} \text{ m/s}$$

Find the relaxation time and mobility of conduction electrons in a metal having 6.5×10^{22} electrons cm^{-3} if the resistivity of the metal is 1.43×10^{-8} ohm m

Given, free electron concentration,
 $n = 6.5 \times 10^{22} / \text{cm}^3 = 6.5 \times 10^{28} / \text{m}^3$

Resistivity, $\rho = 1.43 \times 10^8 \Omega \text{m}$

Resistivity, $\rho = \frac{m}{ne^2\tau}$, where τ is the relaxation time

Mobility, $\mu = \frac{1}{\rho ne}$

Silver has a density of $10.5 \times 10^3 \text{ Kgm}^{-3}$ and atomic weight of 107.9. If conductivity of silver at 27°C is $6.8 \times 10^7 \text{ (ohm-m)}^{-1}$, find the mean free path of electrons as per the classical free electron theory.

$$n = \frac{\text{No. of free electrons per atom} \times \text{Avagadro number} \times \text{Density}}{\text{Atomic wt.}}$$

$$v_{th} = \sqrt{\frac{3k_B T}{m}}$$

$$\text{Electrical conductivity, } \sigma = \frac{ne^2\tau}{m} = ne\mu$$

$$\text{mean free path, } \tau = \frac{\text{mean free path } (\lambda)}{v_{th}}$$

- 1. Define drift velocity, relaxation time and mobility for a free electron in a metal.**

- 2. State the salient features of Drude model and show that the Drude's formula for conductivity can be expressed as, $\sigma = \frac{ne^2\lambda}{(3mkT)^{\frac{1}{2}}}$**

- 3. Briefly discuss the failures of CFET**



PES
UNIVERSITY

THANK YOU

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629



PES
UNIVERSITY

ENGINEERING PHYSICS

Department of Science and Humanities

➤ *Suggested Reading*

1. *Fundamentals of Physics, Resnik and Halliday, Chapter 41*
2. *Concepts of Modern Physics, Arthur Beiser, Chapter 9*
3. *Learning material prepared by the department- Unit III*

➤ *Reference Videos*

[Physics Of Materials-IIT-Madras/lecture-16.html](https://physics.iitm.ac.in/lecture-16.html)

[Physics Of Materials-IIT-Madras/lecture-24.html](https://physics.iitm.ac.in/lecture-24.html)

- *Classical free electron theory was not completely successful and failed to explain many experimental observations*
- *Initial quantum model for the assembly of free electrons in a metal was first advanced through quantum free electron theory*

Proposed by Sommerfeld in 1928

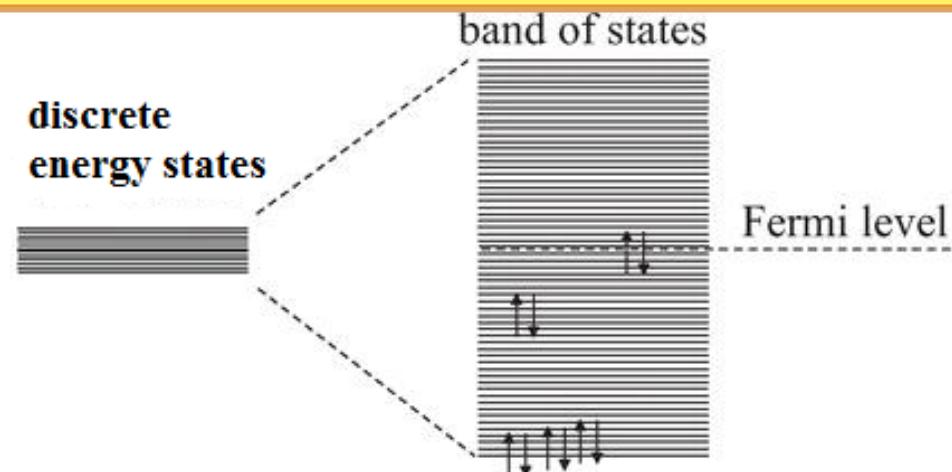
- *Free electron model*
- *Applies quantum mechanical principles to the classical free electron model*
- *Applies Pauli's exclusion principle*
- *Statistical distribution is described by Fermi-Dirac distribution function (electrons as Fermions)*

Quantum model - Suggested modifications to the classical model

- *Valence electrons occupy discrete energy states following Pauli's exclusion principle. Only electrons close to Fermi level participate in conduction process*
- *Occupation probability described by the Fermi Dirac distribution function applicable to fermions*
- *Conduction electrons move in array of positive ions, colliding with ionic centers and other electrons resulting in resistance*
- *The electrostatic interactions, the electron – electron and the electron – ion are negligible*

Quantum model of valence electrons in a metal

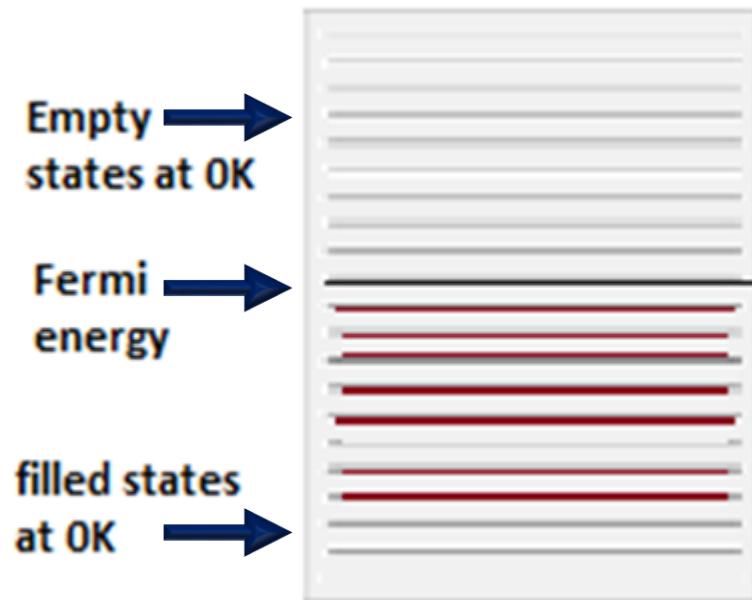
- Valence electrons ($n \approx 10^{28} m^{-3}$) in a metal have discrete energy states following Pauli's exclusion principle
- These energy states split into discrete and closely spaced to accommodate all the valence electrons
- At '0K' such an arrangement leads to a sea of energy levels with a separation as small as $\approx 10^{-20} eV$



Fermi energy- energy corresponding to the highest occupied level at 0K

Fermi Energy

- As per quantum free electron model the upper most occupied energy state at 0K is termed as Fermi energy
- At 0K all the states below the Fermi energy are filled and all the states above are empty



- Occupation probabilities of valence electrons estimated using Fermi Dirac statistics for Fermions
- Particles with spin $\pm \frac{1}{2}$ are classified as Fermions
- Fermi factor $F_d = \frac{1}{\left(e^{\left(\frac{(E-E_F)}{k_B T}\right)} + 1\right)}$ gives the probability of an energy state E to be occupied at a temperature T

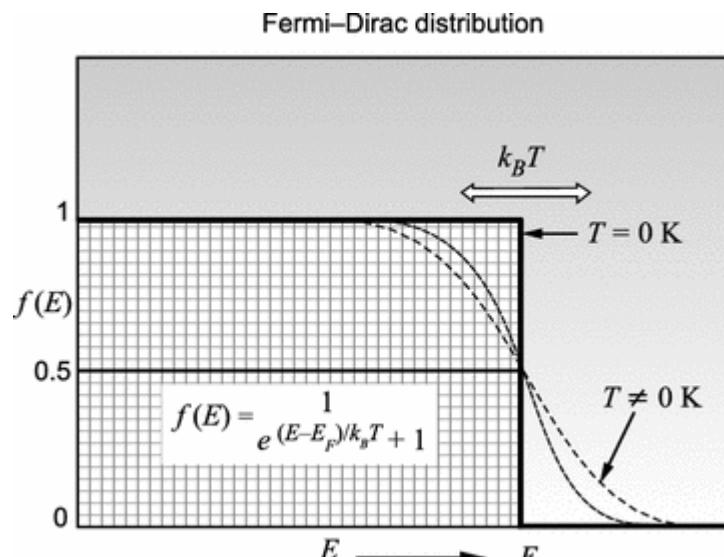


Image courtesy: springer

ENGINEERING PHYSICS

Fermi Factor - Variation with energy at T= 0K

Fermi factor at T=0K gives distinct results for $E < E_f$ and $E > E_f$

- **Case #1 $E < E_f$**

$E-E_f$ is negative, then Fermi factor $F_d = \frac{1}{(e^{-(\frac{\Delta E}{k_B T})} + 1)}$

At 0K this becomes $F_d = \frac{1}{(e^{-(\infty)} + 1)} = 1$

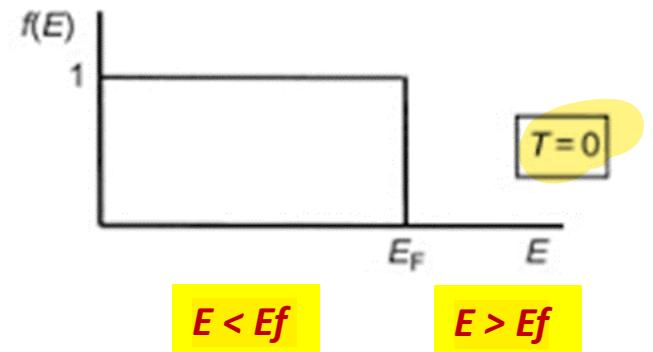
- **Thus that at 0K all electron states below Fermi level are filled**

- **Case #2 $E > E_f$**

$E-E_f$ is positive, then Fermi factor $F_d = \frac{1}{(e^{(\frac{\Delta E}{k_B T})} + 1)}$

At 0K this becomes $F_d = \frac{1}{(e^{(\infty)} + 1)} = 0$

- **Thus that at 0K all electron states above Fermi level are empty**



ENGINEERING PHYSICS

Fermi Factor - Variation with temperature

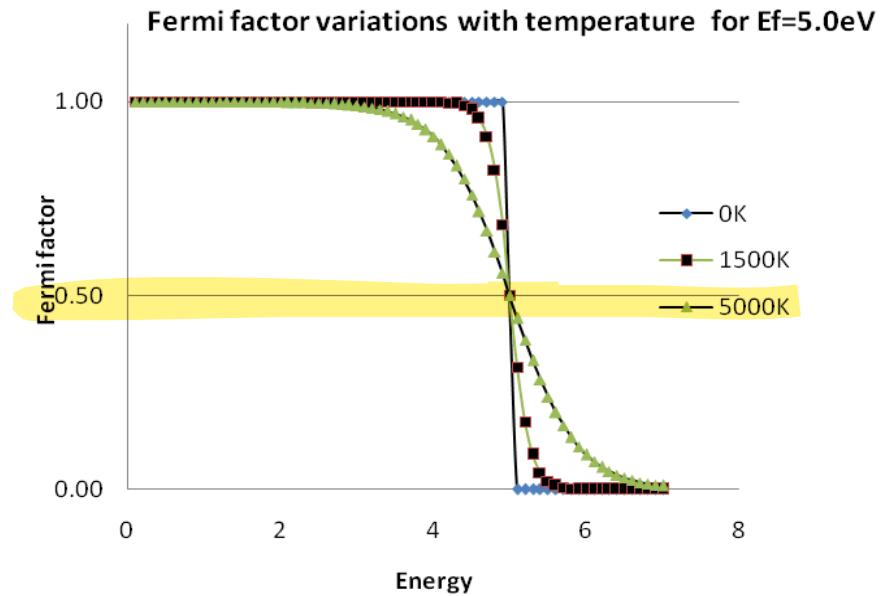
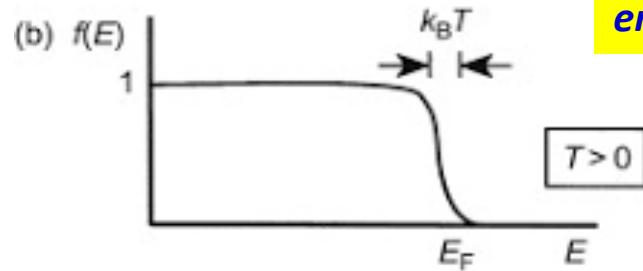
- **For the case when $T > 0 \text{ K}$ and $E = E_f$**

$$\text{Fermi factor } F_d = \frac{1}{e^{\left(\frac{(E-E_f)}{k_B T}\right) + 1}} = \frac{1}{e^{0+1}} = \frac{1}{2} = 0.5$$

- **This gives a probability of occupation of 50% for Fermi energy**



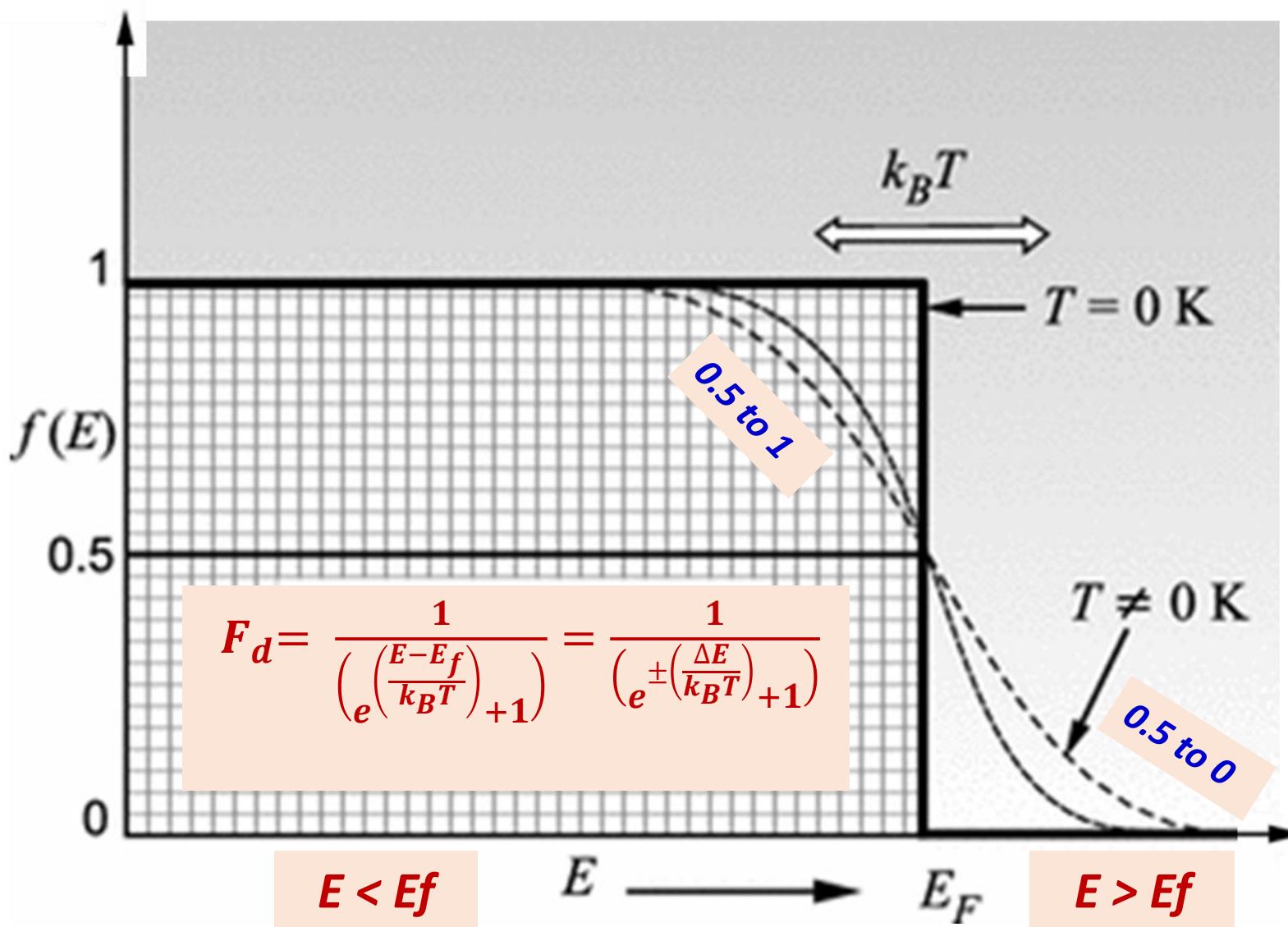
At temperature T , thermal energy available is $k_B T$



Fermi Factor - Variation with temperature

ENGINEERING PHYSICS

Fermi Factor - Variation with energy (E) and Temperature (T)



For $E < E_F$ at $T > 0 \text{ K}$,
 F_d varies from 0.5 to 1

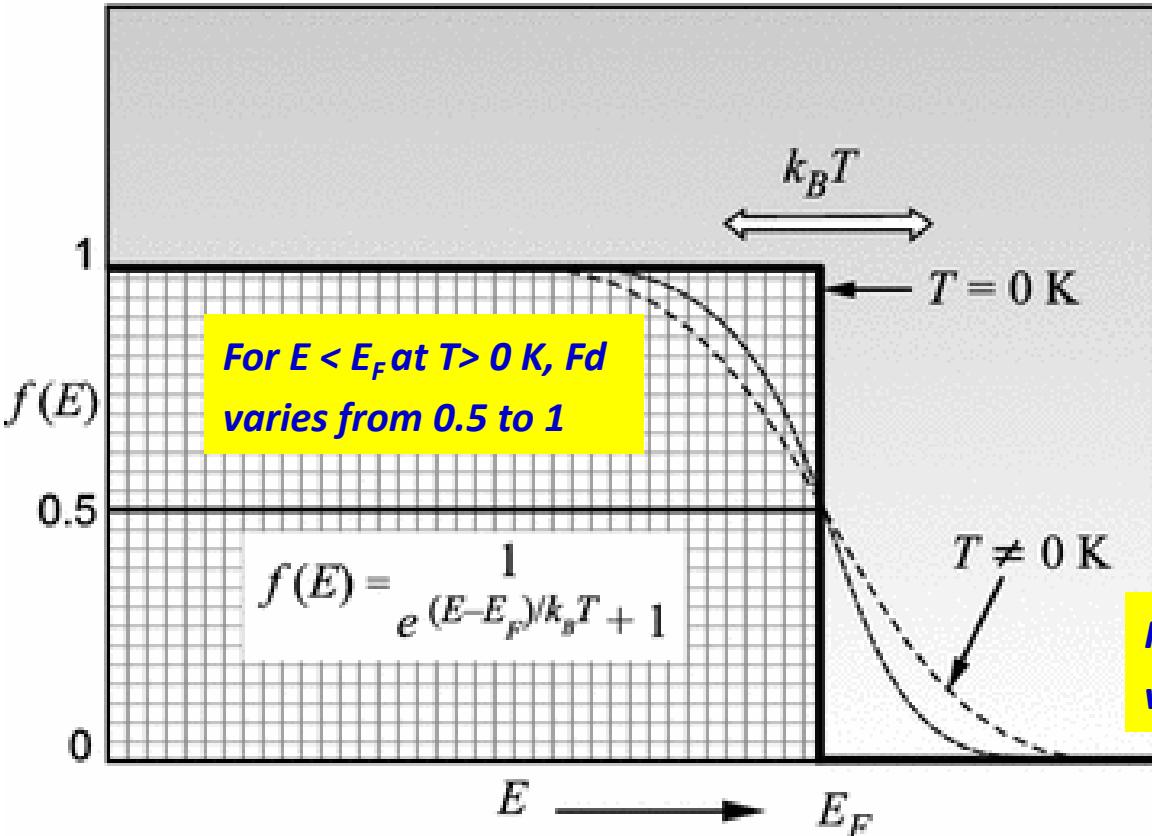
For $E > E_F$ at $T > 0 \text{ K}$,
 F_d varies from 0.5 to 0

Worth noting!
Total probability for a valence electron = 1 (100%)
Eg: Probability 0.01 eV above E_F + Probability 0.01 eV below E_F = 1

ENGINEERING PHYSICS

Fermi Factor - Variation with energy (E) and Temperature (T)

Fermi–Dirac distribution



Let us understand this wrt copper with $EF = 7\text{ eV}$

For 7.01 eV ($E > E_F$ at $T > 0$ K), $\Delta E = 0.01$ eV is +ve, F_d is 40% (0.4)

For 6.99 eV ($E < E_F$ at $T > 0$ K), $\Delta E = 0.01$ eV is -ve, F_d is 60% (0.6)

For 7.02 eV, F_d is 31% (0.31)

For 6.98 eV F_d is 69% (0.69)

For $E > E_F$ at $T > 0$ K, F_d varies from 0.5 to 0

Worth noting!

Total probability for a valence electron = 1 (100%)

Probability 0.01 eV above E_F + Probability 0.01 eV below E_F = 1

- *Valence electrons above the Fermi level contribute to conductivity*
- *No contribution from valence electrons below the Fermi level*
- *Thus, all valence electrons are not conduction electrons*
- *The effective number of electrons above the Fermi level could be*

approximated as $n_{eff} = n \frac{kT}{E_f}$

An example:

- *Effective number of electrons for copper ($E_f = 7\text{eV}$) at 300K will be*

$$n_{eff} = n \frac{kT}{E_f} = n * 0.0036 = n * 0.36\%$$

$$kT = 1.38 \times 10^{-23} \times 300 = 0.025 \text{ eV}$$

- *Thus a small fraction of valence electrons excited above the Fermi level only contribute to conductivity*

- Kinetic energy of the conduction electrons will be equal to Fermi energy

$$E_f = \frac{1}{2}mv_f^2$$

where v_f is called Fermi velocity

$$v_f = \sqrt{\frac{2E_f}{m}}$$

- An example: For copper ($E_f = 7 \text{ eV}$)

$$\text{Fermi velocity, } v_f = 1.06 \times 10^6 \text{ ms}^{-1}$$

- Fermi velocity is greater than the thermal velocity and drift velocity (from CFET) of electrons

Thermal velocity, typical order is 10^5 m/s

Typical order of V_d for an electric field of 1 V/m is 10^{-4} m/s

- As per quantum free electron model, valence electrons near Fermi energy only are excited into conduction band
- At temperature T , thermal energy available is $k_B T$
- Thermal energy required to excite the last electron at the bottom of the energy band at temperature T_f is $k_B T_f$

Then,

$$E_f = k_B T_f$$

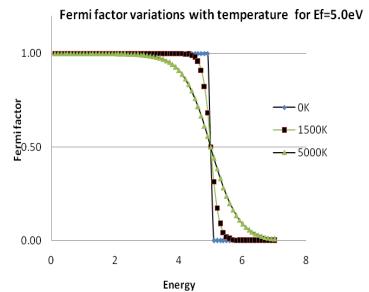
- This temperature is termed **Fermi temperature**
- An example - For Copper ($E_f = 7 \text{ eV}$)
 $\text{Fermi temperature} \approx 81000K$
- Obvious that this is only a representative temperature which highlights all valence electrons cannot be conduction electrons

The concepts which are correct about quantum free electron gas are....

1. Sommerfeld model treats the free electrons as Fermi particles
2. According to QFET all free electrons participate in the conduction process
3. At 0K uppermost filled level will be one unit more than Fermi energy
4. The value of Fermi distribution function at absolute zero is 1 under the condition $E > E_F$

The concepts which are correct about quantized valence electrons are....

1. As the temperature increases, Fermi factor at Fermi level decreases from 0.5 to 0
2. Occupancy probability is zero above Fermi level at 0K
3. Occupancy probability is less than 50% above Fermi level at room temperatures
4. Fermi temperature is hypothetical for monovalent metals only
5. Fermi velocity is smaller than drift velocity but greater than thermal velocity



ENGINEERING PHYSICS

Class 23 . Numericals...

Estimate the probability of occupancy of an energy level 0.1 eV above and below the Fermi level for Copper with $E_f = 7.0\text{eV}$ at 1000K

$$\text{Fermi factor } F_d = \frac{1}{\left(e^{\left(\frac{E-E_f}{k_B T}\right)} + 1\right)}$$

Above means, $E > E_f$

$$E - E_f \text{ is positive, then Fermi factor } F_d = \frac{1}{\left(e^{+\left(\frac{\Delta E}{k_B T}\right)} + 1\right)}$$

Below means, $E < E_f$

$$E - E_f \text{ is negative, then Fermi factor } F_d = \frac{1}{\left(e^{-\left(\frac{\Delta E}{k_B T}\right)} + 1\right)}$$

Logically if probability above is 30%, then corresponding probability below must be 70%!

Logically if probability above is 30%, then corresponding probability of non-occupancy below must also be 30%!

0.1 eV above $E_f, E - E_f = \Delta E = 0.1\text{ eV}$ is +ve

$$\Delta E = 0.1 \times 1.6 \times 10^{-19} \text{ J}, k_B = 1.38 \times 10^{-23}, T = 1000 \text{ K}$$

$$\frac{E - E_f}{k_B T} = + \frac{\Delta E}{k_B T} \text{ and thus, } F_d = 0.238 \text{ or } 23.8 \%$$

Thus, 0.1 eV below must be $100 - 23.8 = 76.2\%$

Find the temperatures at which the occupancy of an energy state 0.3 eV above the Fermi level has an occupancy probability of 0.05

$$\text{Fermi factor } F_d = \frac{1}{\left(e^{\left(\frac{E-E_f}{k_B T}\right)} + 1\right)}$$

$$\text{Thus, } T = \frac{1}{k_B} \cdot \frac{1}{\ln\left(\frac{1}{F_d} - 1\right)} \cdot (E - E_f)$$

Substitution gives, $T = 1181.3 K$

Estimate the energy for which the probability of occupation at 300K is 0.1 for copper with Fermi energy of 7.0eV. Comment on the probability of this level to be 0.5.

$$\text{Fermi factor } F_d = \frac{1}{\left(e^{\left(\frac{E-E_f}{k_B T}\right)} + 1\right)}$$

$$\text{On rearranging, } \frac{E - E_f}{k_B T} = \ln\left(\frac{1}{F_d} - 1\right)$$

$$\text{Thus, } E = E_f + k_B T \cdot \left\{ \ln\left(\frac{1}{F_d} - 1\right) \right\}$$

Substitution gives, $E = 1.129 \times 10^{-18} \text{ J} = 7.056 \text{ eV}$

Comment on the probability of this level to be 0.5 – This probability can never attain for any energy E ($7.056 \text{ eV} > 7 \text{ eV}$) greater than E_f as 0.5 is the probability for $E = E_f$ alone!

Show that the probability of occupancy of an energy level ΔE above the Fermi level is the same as that of the probability of non-occupancy of an energy level ΔE below the Fermi level.

Above means, $E > E_f$

$$E - E_f \text{ is positive, then Fermi factor } F_d = \frac{1}{(e^{+(\frac{\Delta E}{k_B T})} + 1)}$$

Below means, $E < E_f$

$$E - E_f \text{ is negative, then Fermi factor } F_d = \frac{1}{(e^{-(\frac{\Delta E}{k_B T})} + 1)}$$

Probability of non – occupancy = 1 – probability of occupancy

$$E - E_f \text{ is negative, non-occupancy, } 1 - F_d = 1 - \frac{1}{(e^{-(\frac{\Delta E}{k_B T})} + 1)} = \frac{1}{(e^{+(\frac{\Delta E}{k_B T})} + 1)}$$

Show that the sum of the probability of occupancy of an energy level ΔE above the Fermi level and that of ΔE below the Fermi level is unity.

Above means, $E > E_f$

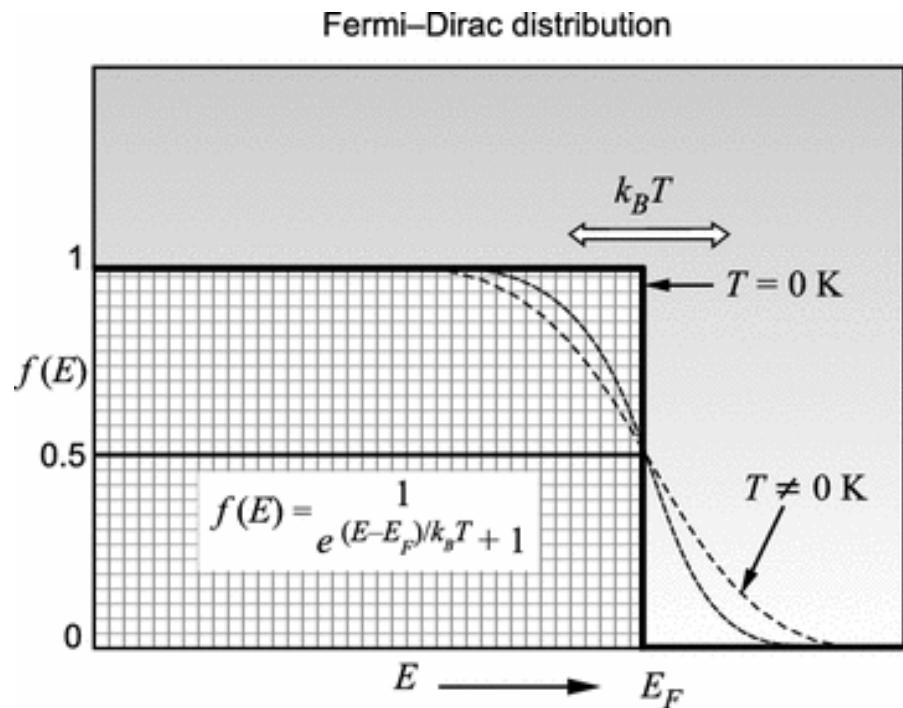
$$E - E_f \text{ is positive, then Fermi factor } F_d = \frac{1}{\left(e^{+\left(\frac{\Delta E}{k_B T}\right)} + 1\right)} \quad \dots \dots 1$$

Below means, $E < E_f$

$$E - E_f \text{ is negative, then Fermi factor } F_d = \frac{1}{\left(e^{-\left(\frac{\Delta E}{k_B T}\right)} + 1\right)} \quad \dots \dots 2$$

Eqn 1 + Eqn 2 = unity

The energy states below E_f in the range kT are emptied at $T > 0\text{K}$, and F_d lies between 1 to 0.5. Justify. If the Fermi energy of Silver is 5 eV, then calculate the effective number of electrons at 400 K. Given that $n = 2 \times 10^{28}/\text{m}^3$



$$n_{eff} = n \frac{kT}{E_f}$$

What are Fermions? Discuss the variation of Fermi factor with energy and temperature. Represent the same graphically.

Discuss how quantum mechanics describes valence electrons in a metal. What are the factors that determine the occupancy of the electron states? Which energy state of electron would have an occupation probability of 50% at any temperature > 0K?

- *Valence electrons occupy discrete energy states following Pauli's exclusion principle. Only electrons close to Fermi level participate in conduction process*
- *Occupation probability described by the Fermi Dirac distribution function applicable to fermions*

- *Fermi factor $F_d = \frac{1}{\left(e^{\left(\frac{E-E_f}{k_B T}\right)} + 1\right)}$ gives the probability of an energy state E to be occupied at a temperature T*

The Fermi level has probability of occupation of 50% for any temperature > 0K

Write an expression for the probability of occupation of an energy level E by valence electrons in a metal. Prove that the probability of occupancy by an electron is zero if $E > E_f$ and unity if $E < E_f$ at $T = 0K$.

What do you mean by Fermi temperature and Fermi velocity of valence electrons in a metal? Estimate the Fermi temperature and Fermi velocity of the electron. Fermi energy of metal is 2 eV.

Discuss the concept of Fermi energy and Fermi factor for valence electrons in a metal. Estimate the Fermi factor of an energy state 0.01 eV below the Fermi level at 500 K.

The Fermi factor $F_d = \frac{1}{e^{\left(\frac{(E-E_f)}{k_B T}\right)} + 1}$ gives the probability of occupancy of an energy state E above or below the Fermi energy at temperature T.

The Fermi factor for an energy state 0.01 eV below the Fermi level at 500 K

$$F_d = \frac{1}{e^{\left(\frac{-0.01 \times 1.6 \times 10^{-19}}{1.38 \times 10^{-23} \times 500}\right)} + 1} = 0.558$$



PES
UNIVERSITY

ENGINEERING PHYSICS

Department of Science and Humanities

ENGINEERING PHYSICS

Unit II : Quantum Mechanics and Simple Quantum Mechanical Systems

➤ *Suggested Reading*

1. *Fundamentals of Physics, Resnik and Halliday, Chapter 41*
2. *Solid state Physics, S.O Pillai, Chapter 6*
3. *Concepts of Modern Physics, Arthur Beiser, Chapter 9*
4. *Learning material prepared by the department-Unit II*

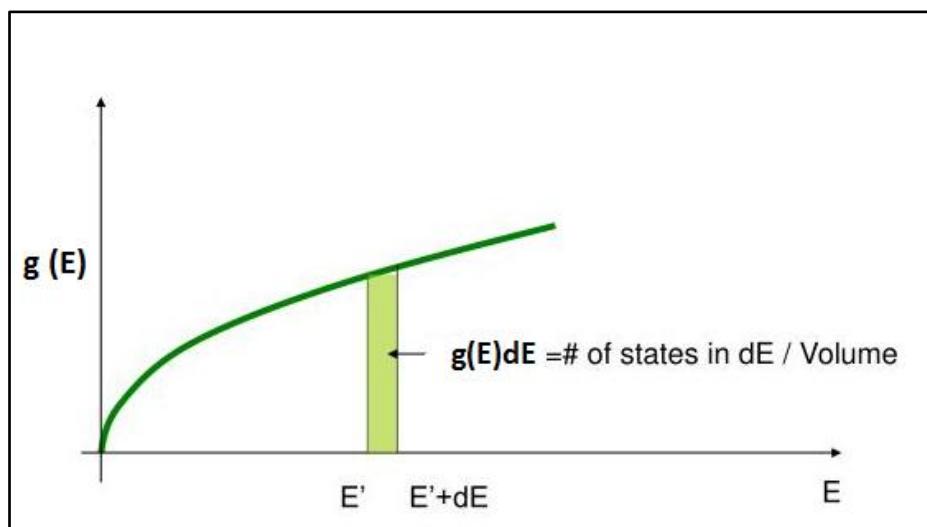
➤ *Reference Videos*

1. [Physics Of Materials-IIT-Madras/lecture-24.html](https://physicsofmaterials.iitm.ac.in/lecture-24.html)

Class #25

- *Density of occupied states*
- *Valence electron concentration in terms of density of occupied states*
- *Fermi energy in terms of electron concentration*
- *Average energy of valence electrons*

- **Density of states, $g(E)dE = \frac{\pi}{2} \left(\frac{8m}{h^2}\right)^{\frac{3}{2}} E^{\frac{1}{2}} dE$**
- **Represents possible number of states of electrons and occupancy is determined by Fermi factor, F_d**
- **The distribution of electrons in energy states vary non-linearly with increasing energy E**



Please review unit II

Density of states filled in the order of increasing energy

- *Product of density of states ($g(E)$) and occupancy probability (F_d)*

$$N(E) = g(E) * F_d$$

- *Probability that an energy state is occupied*

$$F_d = \frac{1}{1 + e^{\left(\frac{E-E_f}{k_B T}\right)}}$$

(Same as multiplying $g(E)$ by a number between 0 and 1 depending the energy relative to the Fermi energy)

- *Density of occupied states ($N(E) = g(E) * F_d$) evaluated for all levels from 0 to E_f provides total count of electrons*

- *Free electron concentration* $n = \int_0^{E_f} N(E) dE$
 $= \int_0^{E_f} g(E) * F_d dE$
 $= \int_0^{E_f} g(E) dE$

(Probability Factor =1 for all energy levels below E_f at 0K)

Substituting for density of states,

$$n = \frac{\pi}{2} \left(\frac{8m}{h^2} \right)^{\frac{3}{2}} \int_0^{E_f} E^{\frac{1}{2}} dE = \frac{\pi}{3} \left(\frac{8m}{h^2} \right)^{\frac{3}{2}} E_f^{\frac{3}{2}}$$

- *Free electron concentration* $n = \int_0^{E_f} N(E) dE$

$$\begin{aligned}&= \frac{\pi}{2} \left(\frac{8m}{h^2} \right)^{\frac{3}{2}} \int_0^{E_f} E^{\frac{1}{2}} dE \\&= \frac{\pi}{3} \left(\frac{8m}{h^2} \right)^{\frac{3}{2}} E_f^{\frac{3}{2}}\end{aligned}$$

- *Fermi energy, if the number of valence electrons per unit volume is known*

$$E_f = \left(\frac{3}{\pi} \right)^{2/3} \left(\frac{h^2}{8m} \right) n^{2/3}$$

ENGINEERING PHYSICS

Variation of Density of Occupied States with Energy

Three distinct results

- *States below $E_f - k_B T$
completely occupied ($F_d = 1$)*
- *States in the range of $k_B T$ below E_f :
Emptied (F_d between 1 and 0.5)*
- *States above E_f in the range $k_B T$
Occupied (F_d between 0.50 and 0.00)*

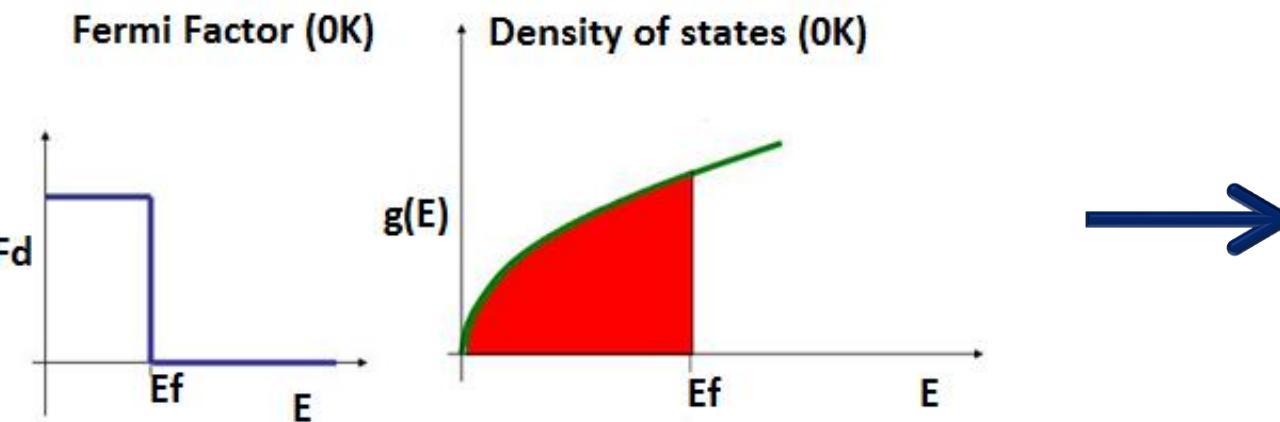
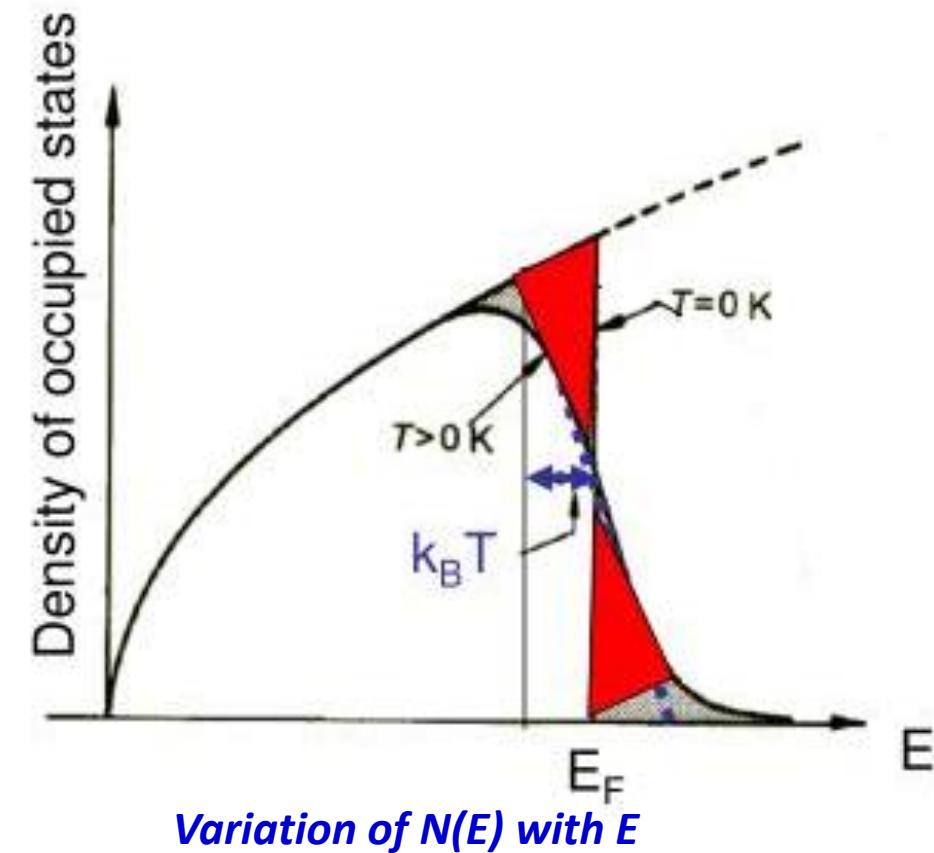
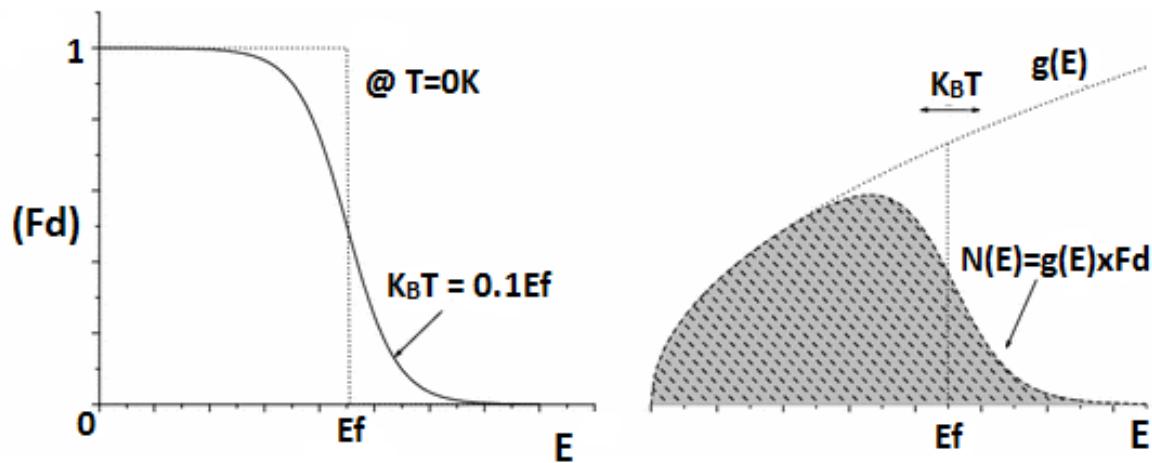


Image courtesy: slideshare



- Distribution of valence electrons show a non linear variation
- Average energy will not be simple average of electron's max and min energy
- Graph of $N(E)$ vs Energy
- The total energy of all electrons in filled states up to E_f is the summation of all $N(E) \cdot E$



Graph of $N(E)$ vs E

- *The average energy of the electron at 0K*

$$= \frac{\text{total energy of all electrons in different energy states}}{\text{total number of electrons}}$$

$$= \frac{\int_0^{E_f} g(E) * E * F_d dE}{\int_0^{E_f} g(E) * F_d dE}$$

$$= \frac{\frac{\pi}{2} \left(\frac{8m}{h^2}\right)^{\frac{3}{2}} \int_0^{E_f} E^{\frac{1}{2}} dE * E}{\frac{\pi}{2} \left(\frac{8m}{h^2}\right)^{\frac{3}{2}} \int_0^{E_f} E^{\frac{1}{2}} dE}$$

- *This gives, average energy $E = \frac{3}{5} E_f = 0.6 * E_f$*

The concepts which are correct about are....

1. The occupancy of the energy states is determined by the factor

$$N(E) = g(E) \times F(E)$$

2. Density of occupied states evaluated for all states between 0 to E_F

is an estimation of valence electron concentration

3. Fermi energy can be estimated in terms of density of occupied states

4. Average energy of valence electron is the simple average of minimum and maximum energy

5. Average energy of valence electrons with highest filled energy as Fermi energy is 40% of Fermi energy

Determine the free electron concentration, the Fermi velocity for electrons in a metal with Fermi energy of 5.10 eV.

Free electron concentration related to Fermi energy as,

$$n = \frac{\pi}{3} \left(\frac{8m}{h^2} \right)^{\frac{3}{2}} E_f^{\frac{3}{2}}$$

with Fermi energy of 5.10 eV, $n = 5.211 \times 10^{28} \text{ m}^{-3}$

$$\text{Fermi velocity } v_f = \sqrt{\frac{2E_f}{m}} = 1.34 \times 10^6 \text{ m/s}$$

Determine the Fermi energy and Fermi temperature for copper with 8.5×10^{28} free electrons per unit volume.

Free electron concentration related to Fermi energy as,

$$n = \frac{\pi}{3} \left(\frac{8m}{h^2} \right)^{\frac{3}{2}} E_f^{\frac{3}{2}}$$

$$E_f = \left(\frac{3}{\pi} \right)^{2/3} \left(\frac{h^2}{8m} \right) n^{2/3}$$

$$E_f = 1.13 \times 10^{-18} J = 7.07 eV$$

$$E_f = k_B T_f$$

Substitution gives, $T_f = 81962 K$

Find the electron density in a metal having Fermi energy of 5.5 eV.

Free electron concentration related to Fermi energy as,

$$n = \frac{\pi}{3} \left(\frac{8m}{h^2} \right)^{\frac{3}{2}} E_f^{\frac{3}{2}}$$

To convert Fermi energy of 5.5 eV into J

Calculate the density of occupied states for copper, with respect to an energy level which is 0.026 eV above the Fermi level at temperature 300 K. Assume Fermi energy of copper as 7 eV.

- *Product of density of states ($g(E)$) and occupancy probability (F_d)*

$$N(E) = g(E) * F_d$$

- *The density of states for electrons per unit volume,*

$$g(E)dE = \frac{\pi}{2} \left(\frac{8m}{h^2}\right)^{\frac{3}{2}} E^{\frac{1}{2}} dE$$

Fermi factor $F_d = \frac{1}{\left(e^{\left(\frac{E-E_f}{k_B T}\right)} + 1\right)}$

The Fermi temperature of two metals A and B are in the ratio 1.103.

If the electron concentration of metal A is $5.86 \times 10^{28} \text{ m}^{-3}$, find the Fermi velocity of electrons in metal B. (Ans: $1.325 \times 10^6 \text{ ms}^{-1}$.)

$$\frac{T_{FA}}{T_{FB}} = 1.103$$

Using n_A we can evaluate E_{FA}

$$E_f = \left(\frac{3}{\pi}\right)^{2/3} \left(\frac{h^2}{8m}\right) n^{2/3}$$

$$E_{fA} = \left(\frac{3}{\pi}\right)^{2/3} \left(\frac{h^2}{8m}\right) n_A^{2/3}$$

$$E_{FA} = 5.52 \text{ eV}$$

$$\frac{T_{FA}}{T_{FB}} = \frac{E_{FA}}{E_{FB}} = \frac{V_{FA}^2}{V_{FB}^2} = 1.103$$

$$V_{FA} = \sqrt{\frac{2E_{FA}}{m}} = 1.393 \times 10^6 \text{ m/s}$$

$$V_{FB}^2 = \frac{V_{FA}^2}{1.103} \text{ gives, } V_{FB} = 1.326 \times 10^6 \text{ m/s}$$

The Fermi energy of silver is 5.5 eV. What is the mean energy of a free electron in silver at 0K? Also, at what temperature a classical free particle will have this kinetic energy?

- *average energy* $E = \frac{3}{5} E_f = 0.6 * E_f$

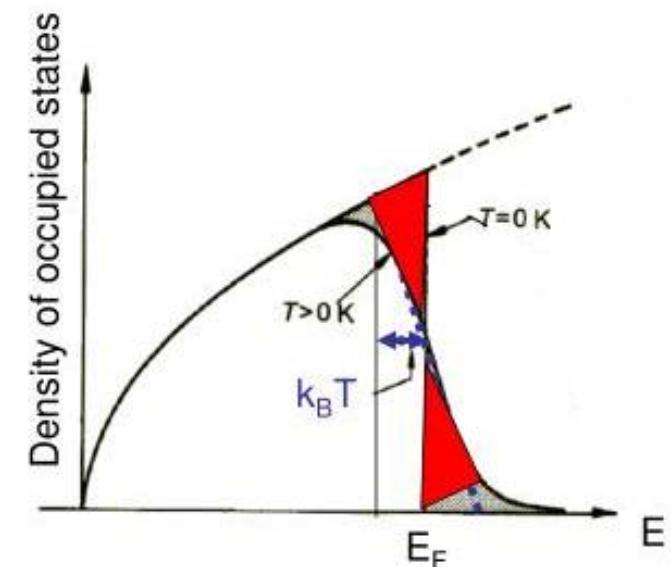
$$\frac{3}{2} k_B T = E_{avg}$$

Discuss the concept of density of states of electrons in metals.

How do we find the distribution of occupied states at a temperature $> 0\text{K}$. Support the answer with suitable graphs.

- Density of states ($g(E) \cdot dE$) gives number of available electron states per unit volume per unit energy range at a certain energy level, E
- The density of states for electrons per unit volume,
$$g(E)dE = \frac{\pi}{2} \left(\frac{8m}{h^2}\right)^{\frac{3}{2}} E^{\frac{1}{2}} dE \quad (\text{for unit volume, } L^3 = 1)$$
- Product of density of states ($g(E)$) and occupancy probability (F_d)

$$N(E) = g(E) * F_d$$



From the expression for the density of states for free electrons in a metal with n electrons per unit volume, obtain an expression for the Fermi energy of electrons at zero kelvin.

- Density of states ($g(E) \cdot dE$) gives number of available electron states per unit volume per unit energy range at a certain energy level, E

- The density of states for electrons per unit volume,

$$g(E)dE = \frac{\pi}{2} \left(\frac{8m}{h^2}\right)^{\frac{3}{2}} E^{\frac{1}{2}} dE \quad (\text{for unit volume, } L^3 = 1)$$

- Product of density of states ($g(E)$) and occupancy probability (F_d)

$$N(E) = g(E) * F_d$$

- Free electron concentration $n = \int_0^{E_f} N(E) dE$
 $= \int_0^{E_f} g(E) * F_d dE$
 $= \int_0^{E_f} g(E) dE$

(Probability Factor =1 for all energy levels below E_f at 0K)

$$n = \frac{\pi}{2} \left(\frac{8m}{h^2}\right)^{\frac{3}{2}} \int_0^{E_f} E^{\frac{1}{2}} dE = \frac{\pi}{3} \left(\frac{8m}{h^2}\right)^{\frac{3}{2}} E_f^{3/2}$$

- Fermi energy, if the number of valence electrons per unit volume is known

$$E_f = \left(\frac{3}{\pi}\right)^{2/3} \left(\frac{h^2}{8m}\right) n^{2/3}$$



PES
UNIVERSITY

THANK YOU

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629



PES
UNIVERSITY

ENGINEERING PHYSICS

Department of Science and Humanities

➤ *Suggested Reading*

1. *Fundamentals of Physics, Resnik and Halliday, Chapter 41*
2. *Solid state Physics, S.O Pillai, Chapter 6*
3. *Concepts of Modern Physics, Arthur Beiser, Chapter 9*
4. *Learning material prepared by the department-Unit III*

➤ *Reference Videos*

1. [Physics Of Materials-IIT-Madras/lecture-26.html](#)

Class #26

- *Specific heat of electrons*
- *Temperature dependence of resistivity*
- *Conductivity dependence on electron concentration*
- *Wiedemann-Franz law*



Merit 1: Heat capacity due to free electrons

- Correct evaluation of electronic specific heat – considering contribution from valence electrons close to the Fermi level
- Heat absorption happens due to this small fraction of electrons
- This effective number in one mole of monovalent metal will be

$$n_{eff} = \frac{k_B T}{E_f} \cdot n = \frac{k_B T}{E_f} \cdot N_a$$

$\frac{k_B T}{E_f}$ is a fraction less than 1% and temperature dependent

- Thus electronic specific heat is a fraction of the value predicted by CFET

$$C_{el} = \frac{dU}{dT} = \frac{\pi^2}{2} \cdot n_{eff} \cdot \frac{k_B^2 T}{E_f}$$

Quantum free electron model gives correct correlation with the experimental results

Merit 2: Temperature dependence of the resistivity

- *As per CFET resistivity arises due to scattering mechanism with stationary ionic centers*
- *For resistance effect, quantum free electron model considers scattering mechanism with thermally vibrating ionic array*
- *Amplitude of vibrations increase with temperature followed by increase in electron scattering*
- *Effective cross sectional area for scattering πr^2 , (r is the amplitude of vibration) is inversely proportional to mean free path*
- *Thus, mean free path reduces as $\lambda \propto 1/T$*

As per QFET,

$$\text{Resistivity } \rho = \frac{m}{ne^2\tau} = \frac{mv_f}{ne^2\lambda}$$

or

$$\text{Conductivity } \sigma = \frac{ne^2\tau}{m} = \frac{ne^2\lambda}{mv_f}$$

Resistivity is inversely proportional to mean free path

Thus, conductivity will be inversely proportional to temperature

or resistivity $\rho \propto T$ as is found experimentally

Merit 3: Conductivity variations with electron concentrations

According to QFET the conductivity expression is given by

$$\sigma = \frac{n_{eff}e^2\tau}{m} = \frac{n_{eff}e^2\lambda}{mv_f}$$

According to the above equation σ not only depends on the number of electrons per unit volume but also depends on the λ/v_F ratio

Merit 4: Relation between electrical conductivity and thermal conductivity

- *As per the quantum model, electrons close to the Fermi energy are responsible for the electrical or thermal conduction*
- *Possible to find a correct relation between the two different physical phenomena (thermal and electrical)*

Thermal conductivity of the metal

$$K = \frac{1}{3} \cdot \frac{C_{el}}{V} \cdot v \cdot L$$

Where the electronic specific heat, $C_{el} = \frac{\pi^2}{2} n_{eff} \cdot \frac{k_B^2 T}{E_f}$,

'V' the volume,

*'v' is the velocity of electrons
and 'L' the mean free path*

ENGINEERING PHYSICS

Relation between electrical and thermal conductivities

- As conduction electrons are located about Fermi energy,

Velocity $v = v_F$, (Fermi velocity)

- Expression for thermal conductivity can be re-written

$$K = \frac{1}{3} \cdot \frac{C_{el}}{V} \cdot v \cdot L$$

$$K = \frac{1}{3} \cdot \frac{1}{V} \cdot \frac{\pi^2}{2} n_{eff} \cdot \frac{k_B^2 T}{E_f} \cdot v_F \cdot v_F \tau = \frac{\pi^2}{6} \cdot n_{eff} \cdot \frac{k_B^2 T}{E_f} \cdot v_F^2 \cdot \tau$$

- n_{eff} is the concentration of free electrons

$$K = \frac{\pi^2}{6} \cdot n_{eff} \cdot \frac{k_B^2 T}{\frac{1}{2} m V_F^2} \cdot \frac{v_F^2}{m} \cdot \tau = \frac{\pi^2}{3} \cdot n_{eff} \cdot \frac{k_B^2 T}{m} \cdot \tau$$

$$Ef = \frac{1}{2} m V_F^2$$

- Expression for electrical conductivity, $\sigma = \frac{n_{eff} e^2 \tau}{m}$

The ratio, $\frac{K}{\sigma} = \frac{\pi^2}{3e^2} k_B^2 T$, is called the Wiedemann-Franz law

- *From the Wiedemann-Franz law,*
- *Lorenz's observation!*

$$\frac{K}{\sigma} = \frac{\pi^2}{3e^2} k_B^2 T, \text{ the Wiedemann-Franz law}$$

Ratio $\frac{K}{\sigma T} = \frac{\pi^2}{3e^2} k_B^2$ is a constant irrespective of the metal

The Lorenz number

- *The Lorenz number has a value = $2.4 \times 10^{-8} W\Omega K^{-2}$*

Short comings of quantum free electron model:

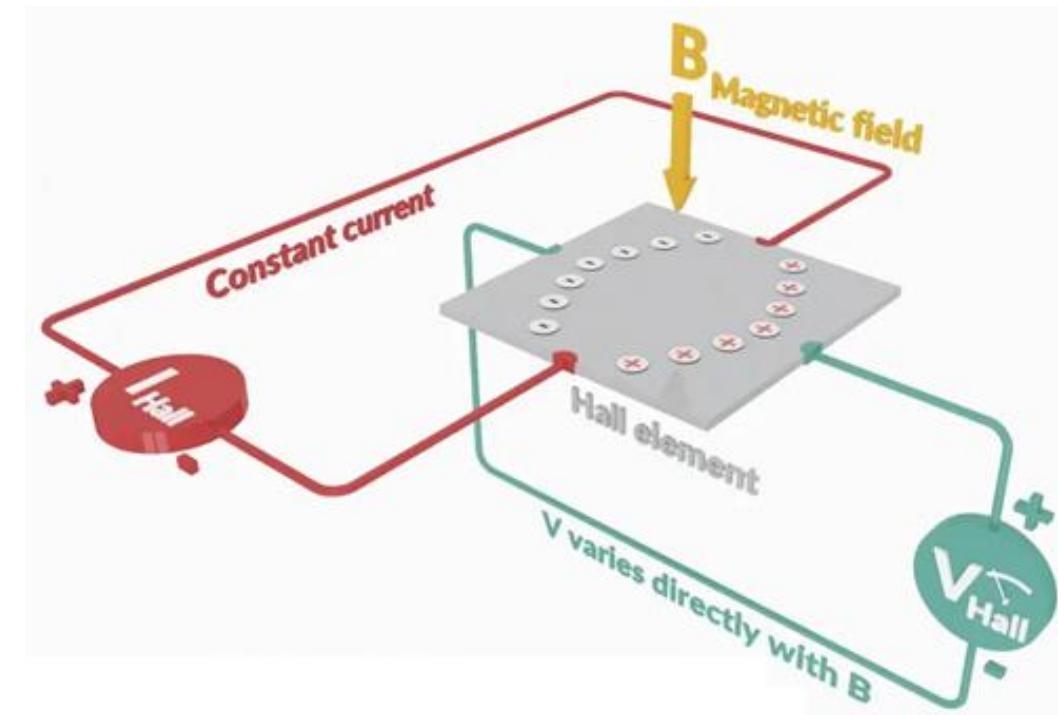
- *Successful in giving correct dependencies of some of the electrical parameters and the specific heat of electrons*
- *Failed to explain*
 - *differences in conduction in metal, semiconductor and insulator*
 - *experimentally observed positive Hall co-efficient observed in some metals like Zinc*
 - *electrical properties of alloys*
- *These demerits reflects that real potentials of ionic centers in metal was ignored in the development of quantum free electron gas model*

A current-carrying conductor is placed in a magnetic field, a force acts on the moving charges due to the Lorentz force: $F = q(v \times B)$

Hall Effect Experiment:

- A current-carrying conductor (like a metal strip)
- A perpendicular magnetic field applied to this conductor
- Measurement of the voltage difference across the conductor, perpendicular to both the current and magnetic field (the Hall voltage).

In the presence of the magnetic field, moving charge carriers experience a sideways force, accumulating on one side of the conductor, creating a voltage difference (the Hall voltage).





The force on a charge carrier is the sum of the electric and magnetic forces:

$$qE_y = qv_d B \quad \text{where,} \quad E_y = \frac{V_H}{d}$$

Substituting v_d

$$q \frac{V_H}{d} = q \left(\frac{I}{nqwd} \right) B$$

Simplifying:

$$\frac{V_H}{d} = \frac{IB}{nqwd^2}$$

The Hall coefficient R_H is defined as:

$$R_H = \frac{V_H}{I} \cdot \frac{d}{Bw}$$

The Hall coefficient R_H can be expressed as:

$$R_H = \frac{1}{nq}$$

where n is the number density of charge carriers and q is the charge of the carrier. For metals with electrons as charge carriers, q is negative, and for materials with holes (like p-type semiconductors), q is positive.

Applications

- Hall Effect can be used to measure carrier concentration and magnetic field intensity.
- It is used to determine type of material i.e. which semiconductor (p type or n- type) or metal.
- It is used to calculate mobility or charge carriers, conductivity of material.
- Hall Effect is used for measurement of direct current, Hall Effect Tong Tester
- In magnetic field sensing equipment
- It is used in phase angle measurement
- In proximity detector
- In Hall effect Sensors and hall probes
- Linear or Angular displacement transducers
- For detecting wheel speed and accordingly assist the ABS – anti-lock braking system.

The concepts which are correct about are....

1. For a given mole of electron gas, the fraction of electron that gain energy kT is

$$n_{eff} = \frac{N_a}{E_f} kT$$

2. Quantum model of free electrons could experimentally correlate the specific heat value
3. As per quantum gas model distance between successive collision is independent of temperature
4. Lorenz number is valid for only monovalent metals

Discuss the molar specific heat of free electrons as per quantum free electron theory. Estimate the molar specific heat of free electron gas at 500 K as per the quantum free electron theory if the Fermi energy of the metal is 3.75 eV.

- Correct evaluation of electronic specific heat – considering contribution from valence electrons close to the Fermi level
- Heat absorption happens due to this small fraction of electrons

- *Using total energy,* $U = \frac{3}{2} \cdot \frac{N_a}{E_f} \cdot k_B^2 T^2$

- *Specific heat*

$$C_{el} = \frac{dU}{dT} = 3 \cdot \frac{N_a}{E_f} \cdot k_B^2 T$$

$$C_{el} = \frac{\pi^2}{2} \cdot n_{eff} \cdot \frac{k_B^2 T}{E_f}$$

Use any one of the equations, both accepted!

Calculate the ratio of the thermal conductivity of a metal to the electrical conductivity of the metal at 500 K.

- *Ratio* $\frac{K}{\sigma T} = \frac{\pi^2}{3e^2} k_B^2$

- *Thus,* $\frac{K}{\sigma} = \frac{\pi^2}{3e^2} k_B^2 T$

$$\frac{K}{\sigma} = 2.4 \times 10^{-8} T$$

How does the quantum free electron explain the temperature dependence of conductivity of metals?

- *For resistance effect, quantum free electron model considers scattering mechanism with thermally vibrating ionic array*
- *Amplitude of vibrations increase with temperature followed by increase in electron scattering*

- *Thus, mean free path reduces as $\lambda \propto 1/T$*

conductivity will be inversely proportional to temperature or resistivity $\rho \propto T$ as is found experimentally



PES
UNIVERSITY

THANK YOU

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629



PES
UNIVERSITY

ENGINEERING PHYSICS

Department of Science and Humanities

ENGINEERING PHYSICS

Unit III : Application of Quantum Mechanics to Electrical Transport in Solids & Magnetism



➤ *Suggested Reading*

1. *Concepts of Modern Physics, Arthur Beiser, Chapters 9 & 10*
2. *Learning material prepared by the department-Unit III*

➤ *Reference Videos*

1. [Physics Of Materials-IIT-Madras/lecture-26.html](#)
2. <https://nptel.ac.in/courses/115/104/115104109/>

Class #27

- *Introduction to band theory*
- *Motion of electron in 1D periodic potential*
- *Bloch function*
- *Kronig-Penney model*

Quantum free electron gas model neglected real potentials of ionic centers in metal

Band theory based on complete quantum mechanical calculations incorporating real potentials in solids

This results in the accurate analysis of the wave function of the electrons



Bloch's theorem, is fundamental approach in quantum mechanics for understanding how electrons behave in periodic potentials, such as in a crystal lattice.

If an electron moves in a periodic potential (like in a crystal), its wavefunction $\psi(x)$ can be written as: $\psi_k(x) = e^{ikx} \cdot V_k(x)$

Where, e^{ikx} a plane wave, describing free motion and $V_k(x)$ is a function with the same periodicity as the lattice, i.e., $V(x + a) = V(x)$ (where a is the lattice spacing). Thus, Bloch function is the product of a plane wave and a periodic function. This will make sure that the **Probability of finding the electron is always dependent on original wave function**

$$|\Psi(x + a)|^2 = |\Psi(x)|^2$$

Importance of Bloch Function in Band Theory

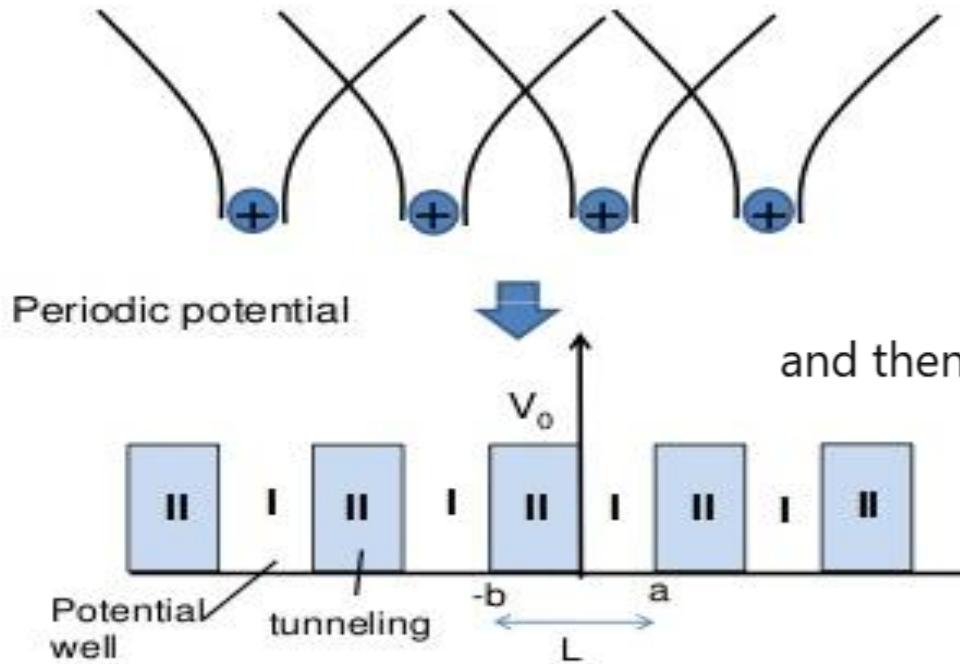
They explain:

- Electron energy bands in solids, origin of band gaps (where electrons are not allowed) and difference between conductors, semiconductors, and insulators.



Bloch Function in Kronig-Penney Model

The **Kronig-Penney model** is a simplified, 1D model that considers the complex atomic potential by a **simplified periodic series of potential wells** (or barriers).



$$V(x) = \begin{cases} 0, & 0 < x < a \\ V_0, & -b < x < 0 \end{cases}$$

Potential distribution

and then repeated with period $d = a + b$, forming an infinite periodic potential.

To solve STIWE

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

Here, wavefunction $\psi(x)$ can be written as: $\psi_k(x) = e^{ikx} \cdot V_k(x)$

Hamiltonian from



Region I: Inside the well ($0 < x < a$), $V(x) = 0$

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0, \quad \text{where } k = \sqrt{\frac{2mE}{\hbar^2}}$$

Solution:

$$\psi_1(x) = Ae^{ikx} + Be^{-ikx}$$

Region II: Inside the barrier ($-b < x < 0$), $V(x) = V_0$

$$\frac{d^2\psi}{dx^2} + \kappa^2\psi = 0, \quad \kappa = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

Solution:

$$\psi_2(x) = Ce^{\kappa x} + De^{-\kappa x}$$

Apply Boundary conditions and Bloch theorem, we get the dispersion relation as

$$\cos(ka) = \frac{ma}{\hbar^2} V_0 \cdot b \cdot \frac{\sin(Ka)}{Ka} + \cos(Ka)$$

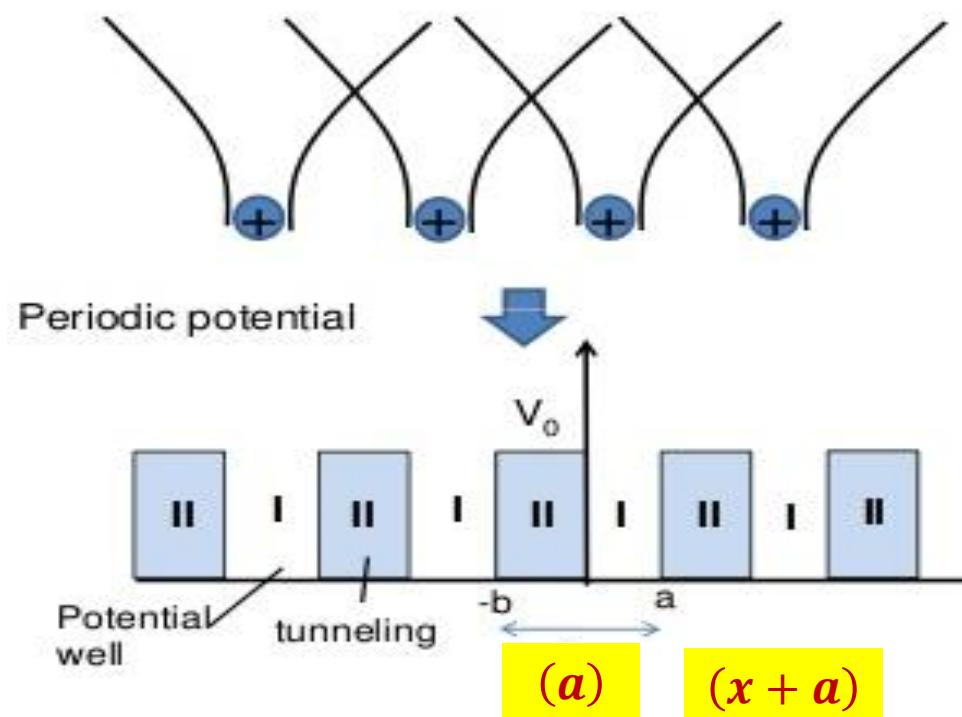
Apply Boundary conditions and Bloch theorem, we get the dispersion relation as

$$\text{Cos}(ka) = \frac{mab}{\hbar^2} V_o \cdot \frac{\text{Sin}(Ka)}{Ka} + \text{cos}(Ka)$$

This equation **relates the energy E** (k and K) to the **wave vector k** (crystal momentum or quais-momentum that connects the Bloch states of an electron in a periodic potential in terms of zones $n \frac{\pi}{a}$).

- *Free electrons in a metal are not free from electrostatic potentials*
- *Move in a periodic potential approximated by rectangular potentials due to the regular arrangement of the ionic centers*

If $V(x)$ is the potential at x then, then $V(x + a) = V(x)$, the periodic potential is invariant under translation through lattice parameter (a)



- *The potential is lower close to positive ions in lattice*
- *The valence electrons of different atoms experience similar potential*

1D lattice of positive ions with the rectangular potential approximation

lattice parameter (a) - periodicity

Bloch Function



Consider wave function associated with valence electrons as,

$$\psi(x) = e^{ikx}, \text{ for periodic lattice, } \psi(x + a) = e^{ik(x+a)}$$

If wave function is modulated by the periodic potential, then

$$\psi(x) = e^{ikx} \cdot V_k(x) \text{ where } k \text{ is the wave number of the electron waves with}$$

$$V_k(x) = V_k(x + a)$$

*This representation of wave function is known as the Bloch function
(wave function as a plane wave modulated by a periodic function -
Bloch theorem)*

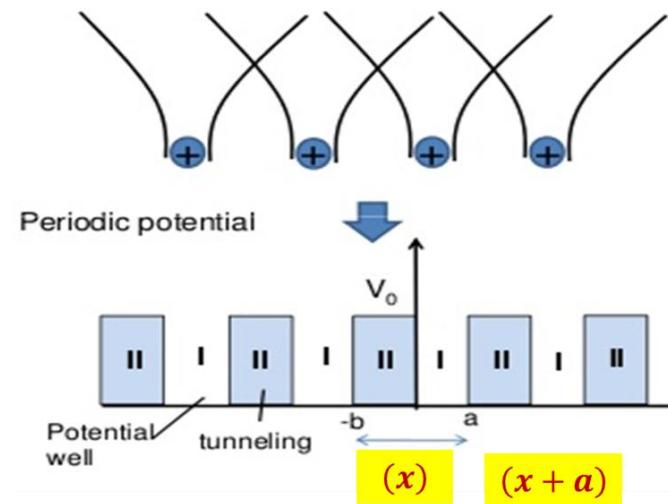
$$\Psi(x) = e^{ikx}$$

$$\Psi(x + a) = e^{ik(x+a)} = e^{ikx} \cdot e^{ika},$$

same function with a modulation (phase term)

Probability of finding the electron is always dependent on original wave function

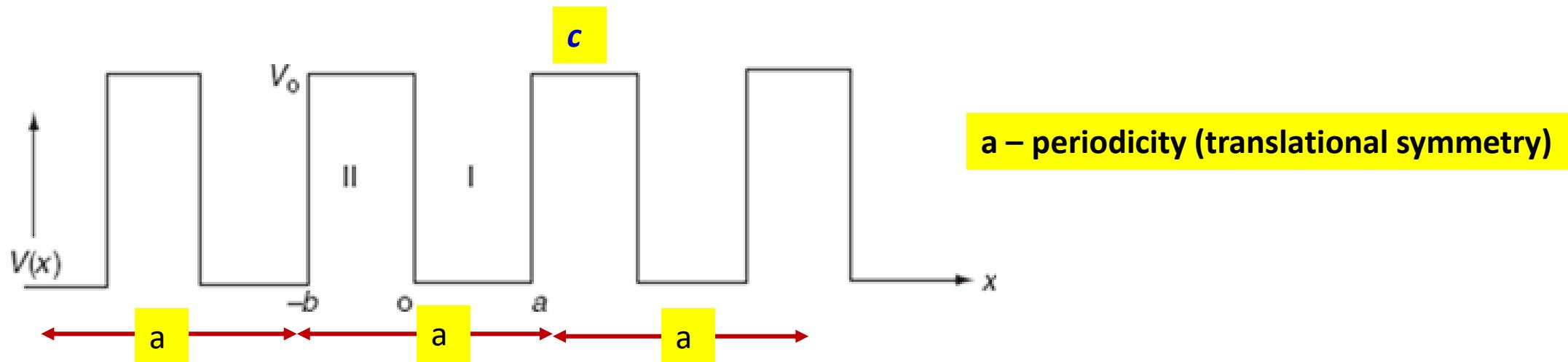
$$|\Psi(x + a)|^2 = |\Psi(x)|^2$$



- Kronig-Penney model approximated the periodic potential as a long chain of coupled finite rectangular wells,*
- Barrier height V_0 , period 'a', and barrier thickness c*

Energies and wave functions of electrons associated with this model can be calculated by solving time-independent 1D Schrödinger's wave equations for the two regions I and II

When an electron is near the positive ion site, potential energy is taken as zero
 In between two positive ions (outside the well), potential energy is assumed to be V_0



Schrödinger's equations are

- For region I with $V=0$ this becomes

$$\frac{\partial^2 \psi_1}{\partial x^2} + \frac{2m}{\hbar^2} E \psi_1 = 0$$

- For region II with $V=V_0$

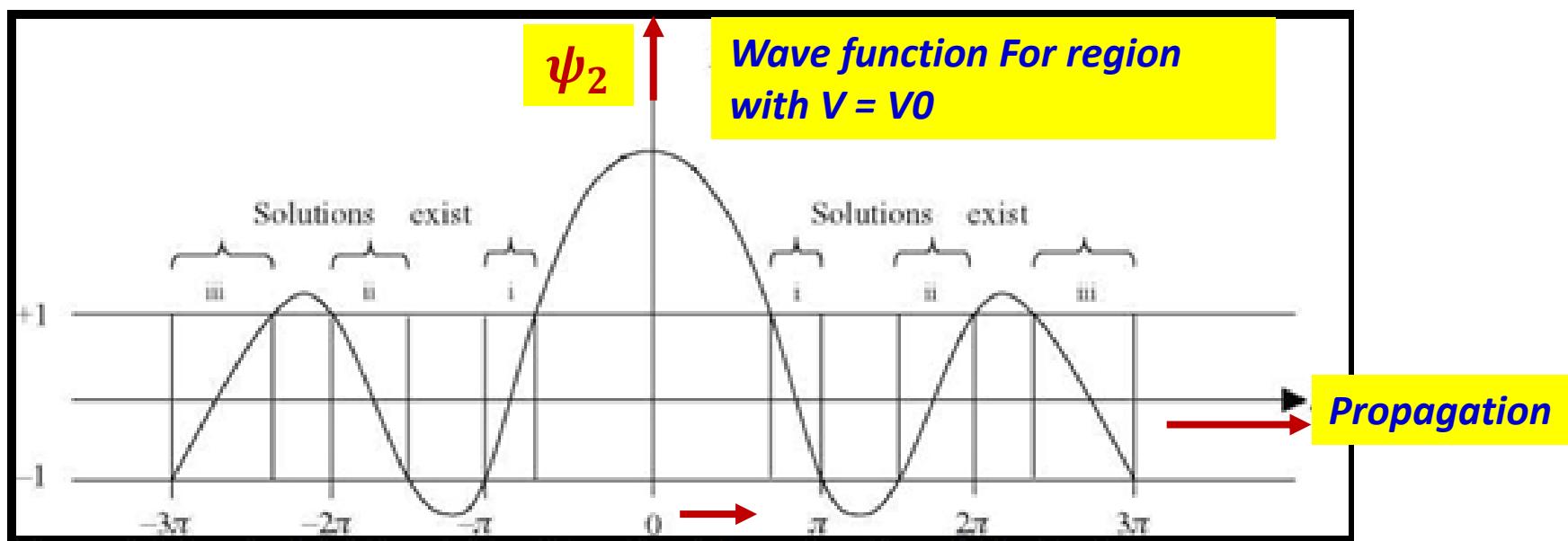
$$\frac{\partial^2 \psi_2}{\partial x^2} - \frac{2m}{\hbar^2} (V_0 - E) \psi_2 = 0 \quad \text{as} \quad \frac{\partial^2 \psi_2}{\partial x^2} - \alpha^2 \psi_2 = 0$$

Using **Bloch theorem** and the boundary conditions for continuity of the wave function, the solution can be obtained.

- A transcendental equation with solutions gives variation of E with propagation k , has discontinuities (forbidden gap)
- Allowed regions, electrons are free to move with energy $E = \frac{\hbar^2 K^2}{2m}$

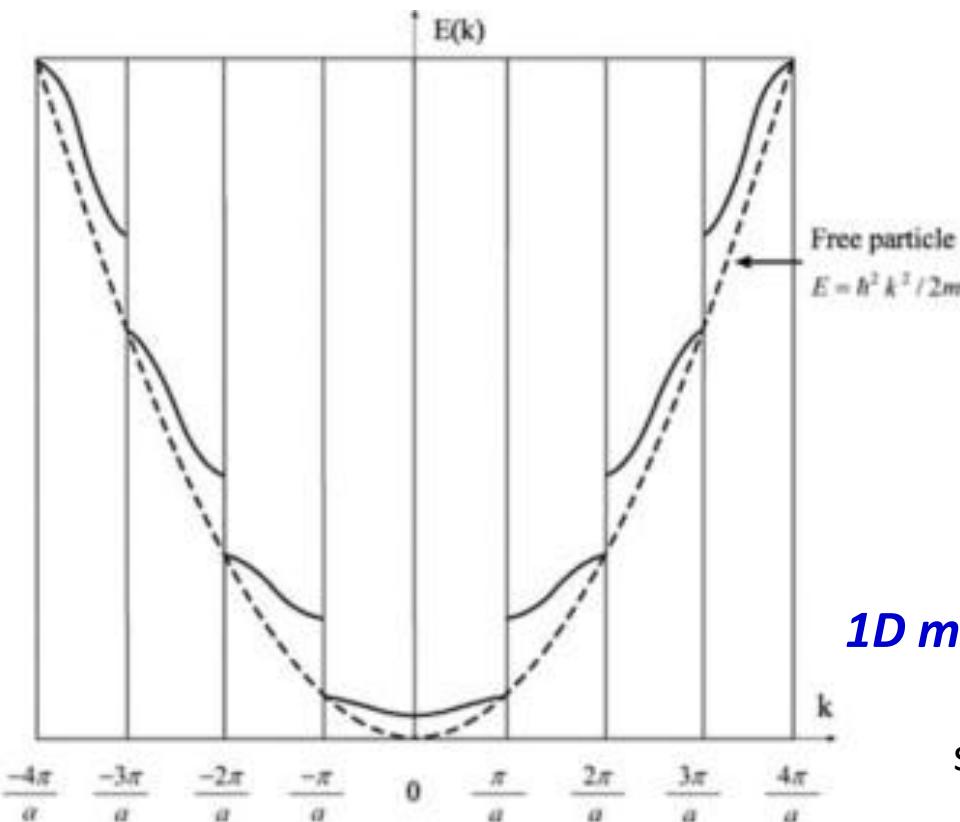
- *Periodic potential inside the solid results in discontinuities in the energy values*
- *Thus, there will be range of allowed energy states and forbidden energy states*
- *Solution and energy exist only for those allowed range of $k = n \frac{\pi}{a}$*
- $n = \pm 1, \pm 2, \dots \dots \dots$

As the original state of electron will be around the positive ion site with $V = 0$



Kronig-Penney Model: E-k diagram

- *E(k)-k diagram for the system show discontinuity in the energy at zone boundary of $k = \pm n \frac{\pi}{a}$*
- *Observed similarity of the $E = E(k)$ curve with the free electron parabola, except at the values of k , where gaps open up*

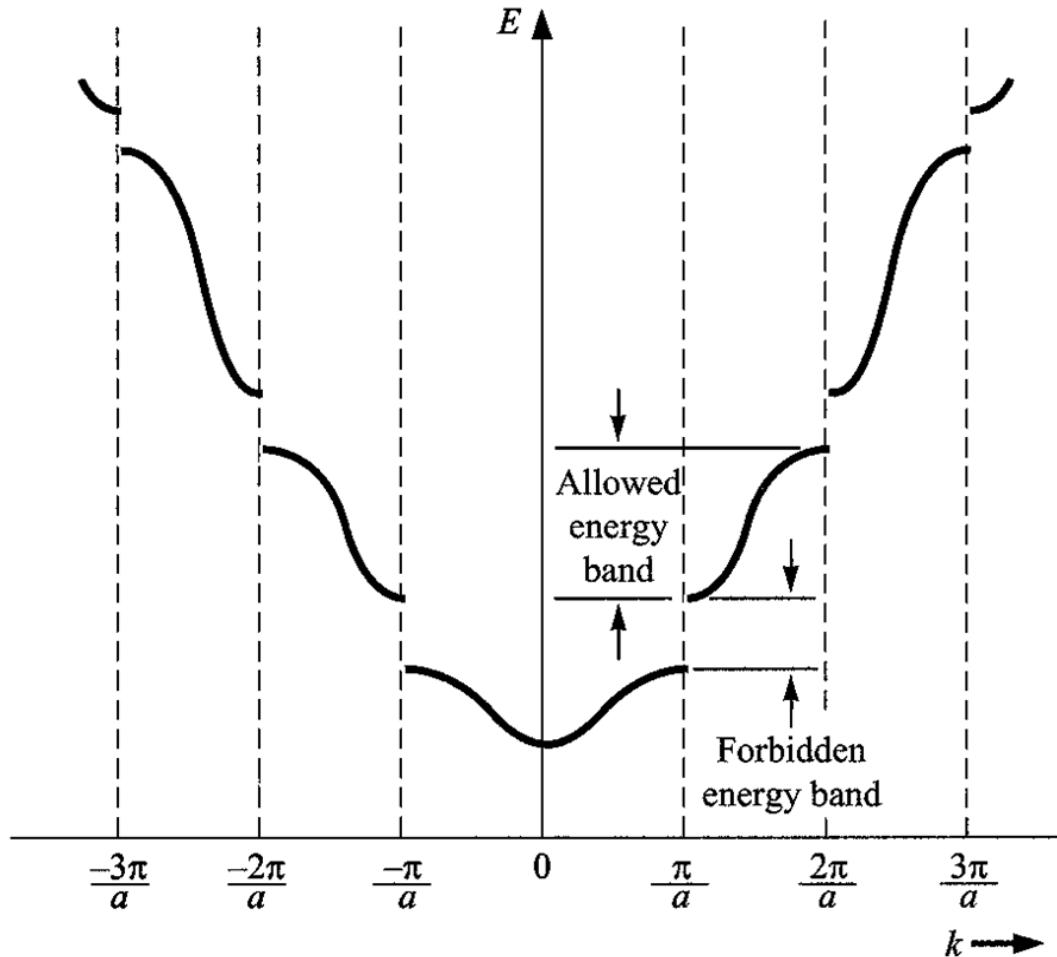


Scattering Power, $P = \frac{mV_0ab}{\hbar^2}$, a=periodicity and b= width of barrier, V_0b is barrier strength
 Very high 'P', (V_0 is very high) – similar to infinite well, if 'P' is zero, (V_0 is zero) – similar to free particle)

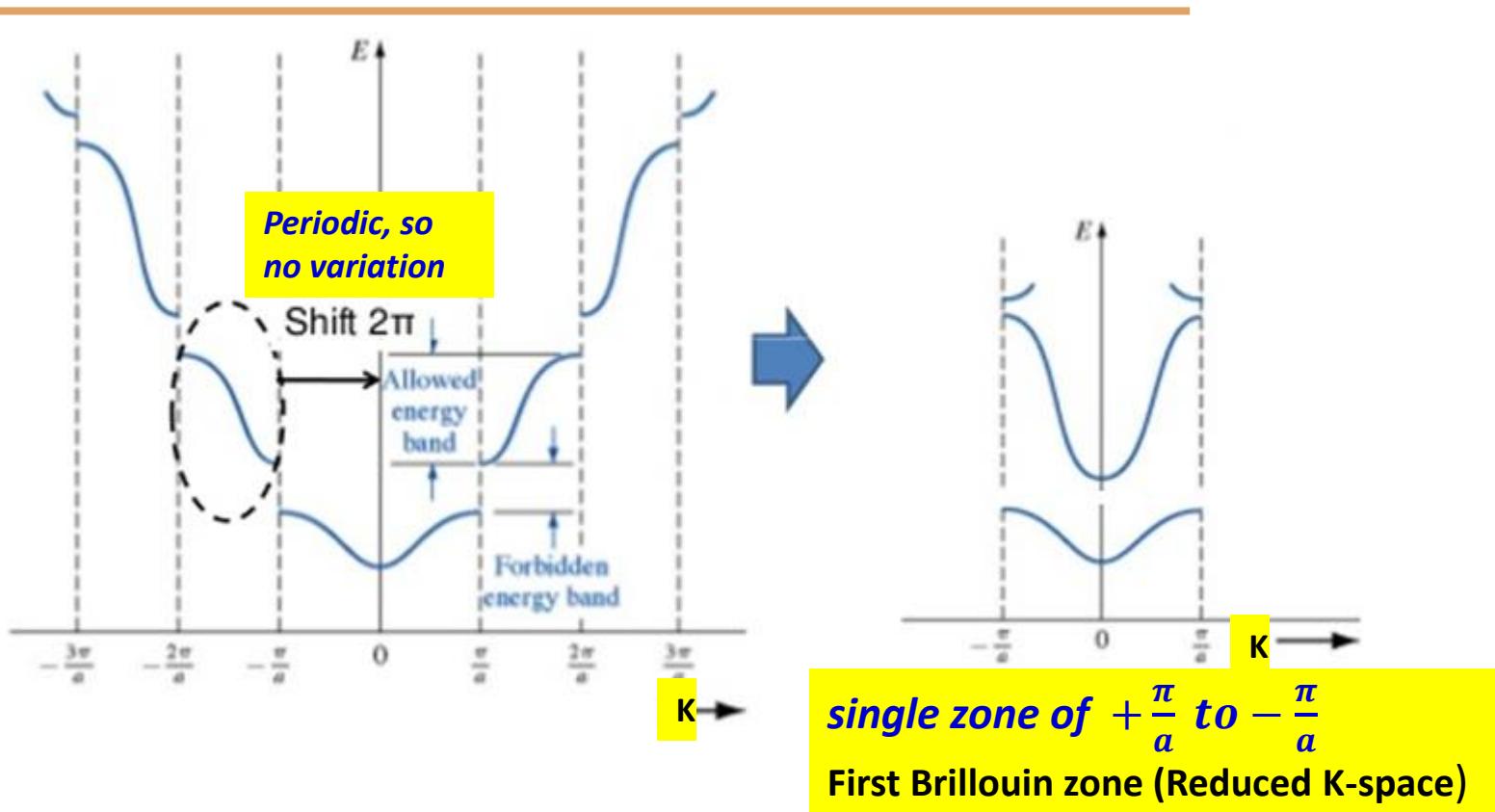
1D model - Energy bands and gaps

Kronig-Penney Model: E-k diagram

KP model: E is discontinuous,
allowed and forbidden bands



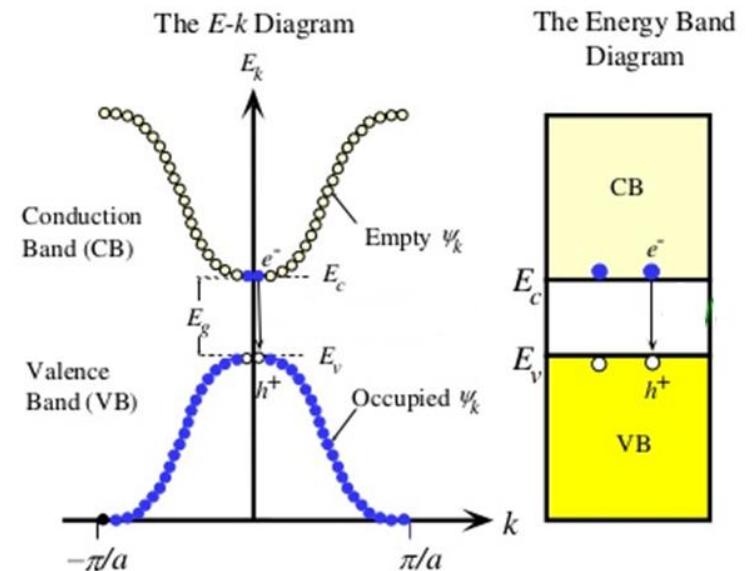
- Since the functions are periodic, it is possible to represent the energy band diagram in a single zone of $+\frac{\pi}{a}$ to $-\frac{\pi}{a}$ (Brillouin zone)



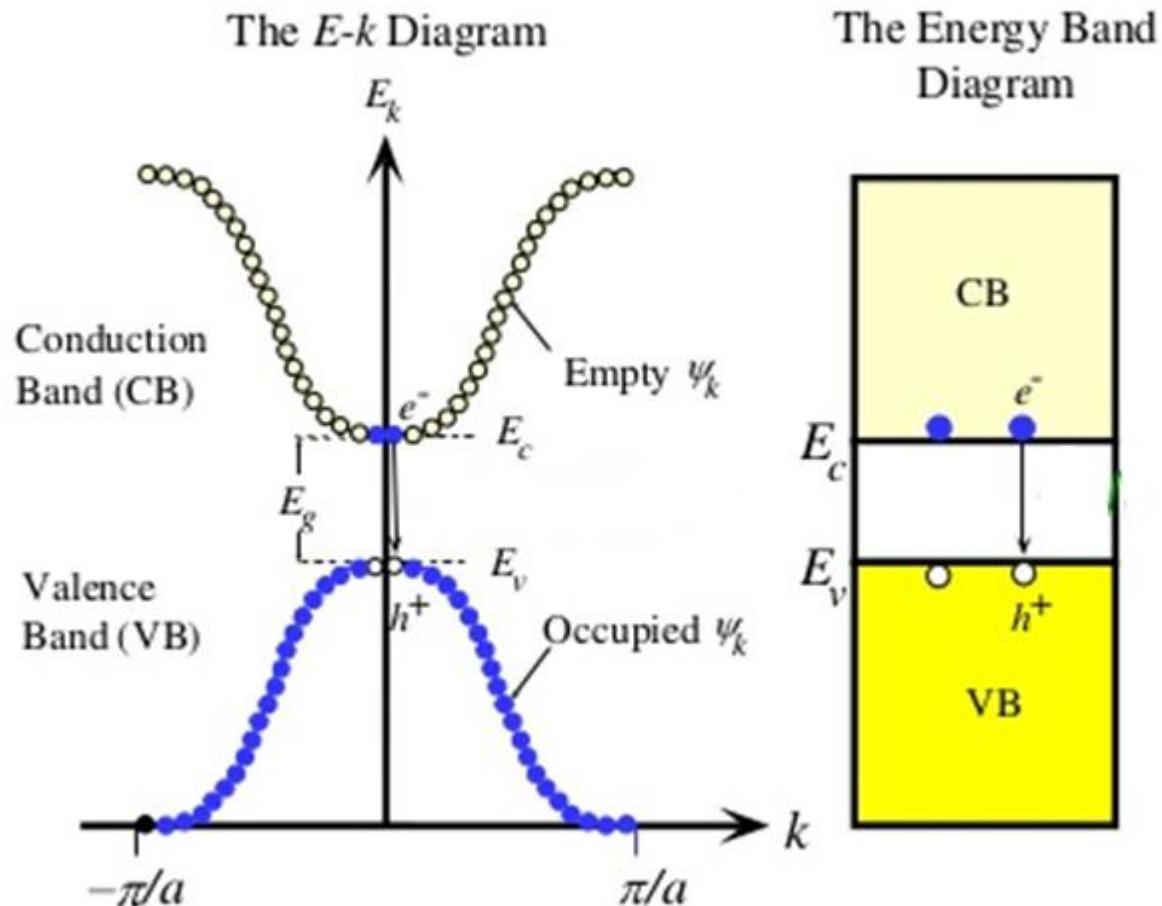
- Completely filled lowest inner band followed by a band of forbidden energy states
- The highest band of allowed states represents valence band
- The upper most occupied states form conduction band

Thus, there are allowed and forbidden energy states for the electrons in solids

Materials are then classified as metals, semiconductors or insulators on the basis of energy band structure



Conduction and valence bands in reduced k space (Brillouin zone)



- ***Case of conductors***

Thus conductors (metals) characterized by a partially filled conduction band (no band gap)

- ***Case of semi-conductors***

Completely filled valence band and completely empty conduction band

Energy gap of 3-5 eV

At normal temperatures, possible for electrons in the valence band to move into the conduction in the case of metals and semiconductors

- ***Case of insulators***

Materials with energy band gap greater than 5eV

Electron conduction is impossible and attempts to excite lead to a dielectric breakdown

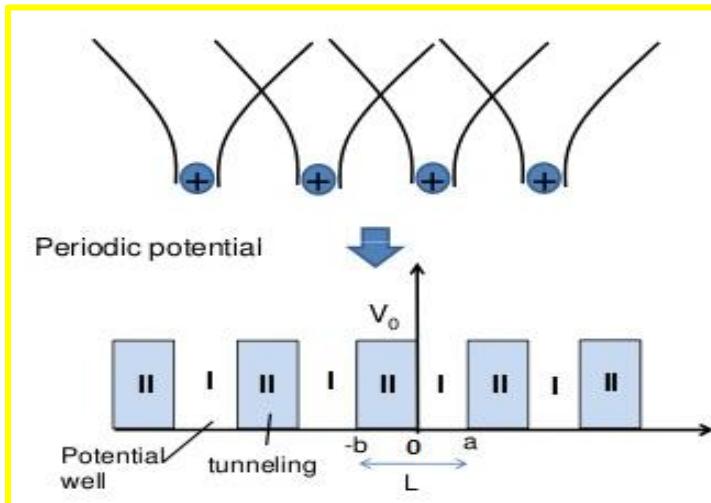


What is Bloch function and how is it different from the free electron wave function?

For the periodically varying potential inside a solid, an acceptable solution of electron wave is of the form $\psi(x) = V_k(x) e^{ikx}$, where $V_k(x + a) = V_k(x)$, called Bloch function. Any plane wave solution is used to represent the free electron wave function.

Outline the Kronig Penny Model to describe the motion of electrons in a metal and discuss how the band structure evolves from this model.

The potential of the solid varies periodically with the periodicity of the space lattice 'a' (inter atomic spacing).

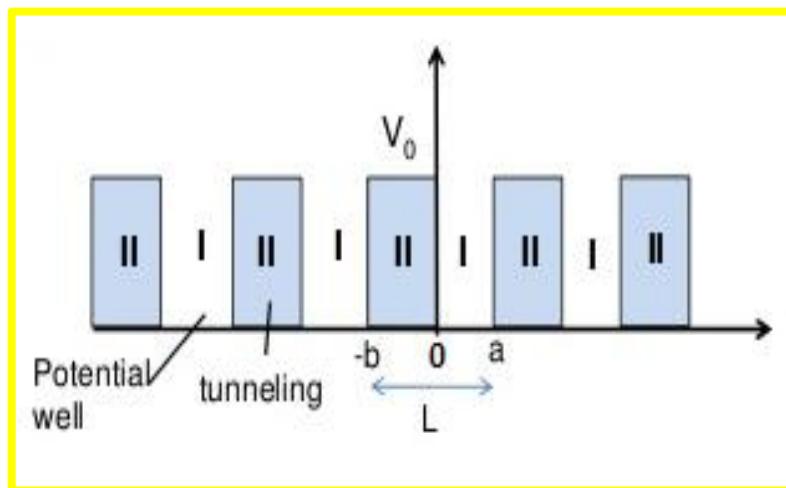


The Kronig-Penney model assumed the periodic potential as a long chain of coupled finite square wells, of barrier height V_0 , with a period 'a', and barrier thickness 'b'.

The solution to Schrodinger's equation is analysed using Bloch theorem, as $\psi(x) = e^{ikx} \cdot V(x)$, where, $V(x)$ is periodic potential, that is $V(x+a) = V(x)$.

Analysis of KP model suggest that solutions are possible only for restricted values of 'E' within certain ranges of the propagation vector 'k' which form the allowed energy bands.

Explain the Schrodinger's equation for an electron moving in a periodic potential field approximated as a long chain of coupled finite square wells, of barrier height V_0 , with a period 'a', and barrier thickness b.



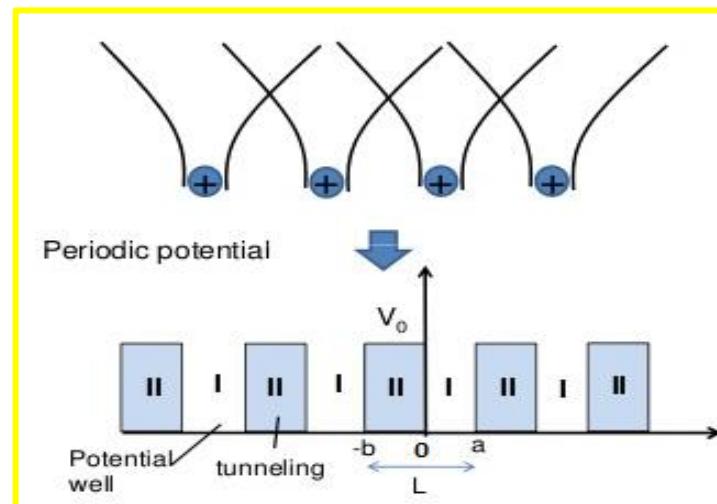
Considering the periodic repetition of the potential well, the time-independent Schrodinger equations for the two regions I and II takes the following forms,

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2m}{h^2} E\psi = 0; \text{ for } 0 < x < a$$

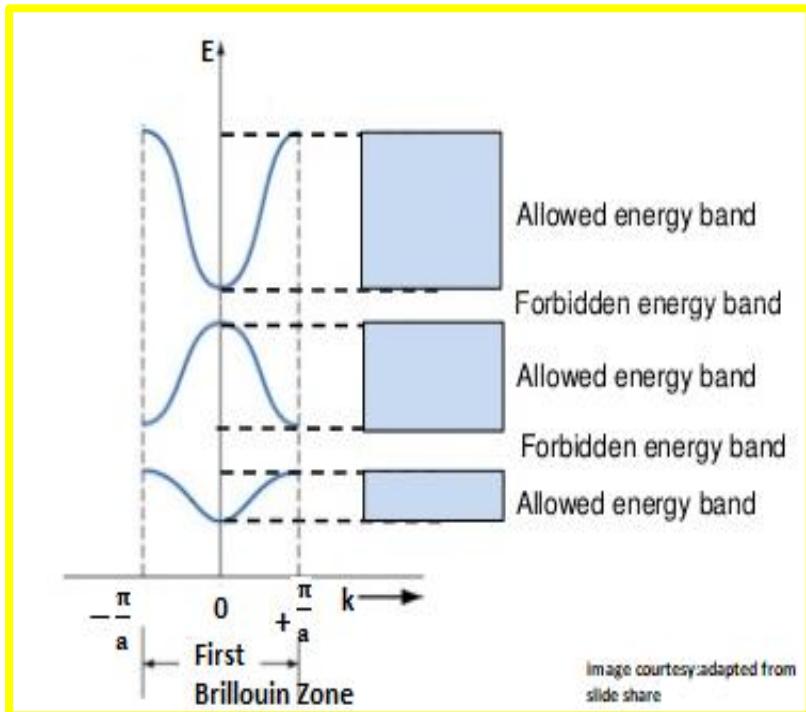
$$\frac{d^2\psi}{dx^2} - \frac{8\pi^2m}{h^2} (E - V_0)\psi = 0; \text{ for } -b < x < 0$$

How does the potential energy of an electron vary in an infinite one-dimensional crystal and how this potential is represented in Kronig-Penny model?

The Kronig-Penney model assumed the periodic potential in a solid as a long chain of coupled finite square wells, of barrier height V_0 , with a period 'a', and barrier thickness 'b'.



Discuss the E-k diagram and give a qualitative picture of the origin of band gaps.



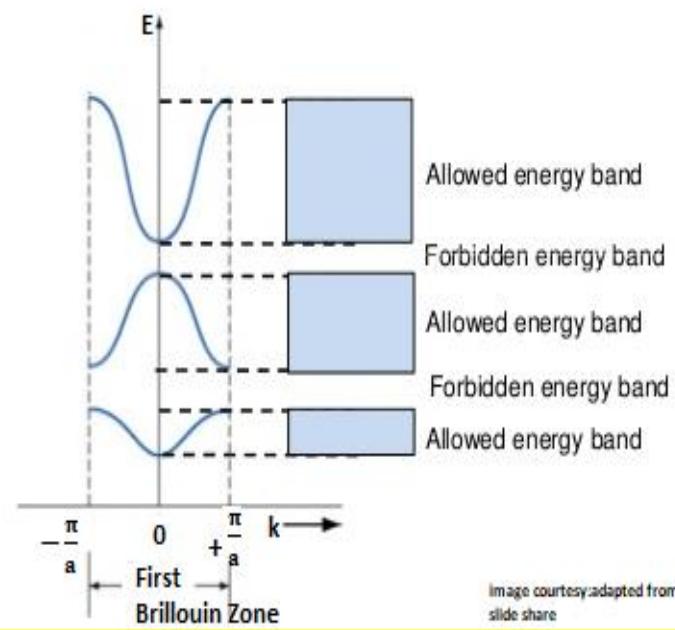
The Kronig-Penney model assumed the periodic potential in a solid as a long chain of coupled finite square wells, of barrier height V_0 , with a period 'a', and barrier thickness 'b'.

The solution to Schrodinger's equation is analysed using Bloch theorem, as $\psi(x) = e^{ikx} \cdot V(x)$, where, $V(x)$ is periodic potential, that is $V(x+a) = V(x)$.

Analysis of KP model suggest that solutions are possible only for restricted values of 'E' within certain ranges of the propagation vector 'k' which form the allowed energy bands.



Distinguish between conductors, insulators and semiconductors on the basis of band theory of solids.



On the basis of band theory in conductors overlapping of valence and conduction bands with large number of conduction electrons even at low temperatures.

In the case of semi-conductors, energy gap between the valence band and conduction band is quite small (3-5 eV). At normal temperatures it is possible for the electrons in the valence band to move into the conduction band.

Insulators possess no effective free electrons, all the bands up to the valence band are completely filled and the conduction band is completely empty with wide forbidden energy region (greater than 5eV) in which the electron conduction is impossible.



PES
UNIVERSITY

THANK YOU

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629



PES
UNIVERSITY

ENGINEERING PHYSICS

Department of Science and Humanities

ENGINEERING PHYSICS

Unit III : Application of Quantum Mechanics to Electrical Transport in Solids & Magnetism



➤ *Suggested Reading*

1. *Concepts of Modern Physics, Arthur Beiser, Chapters 9 & 10*
2. *Learning material prepared by the department-Unit III*

➤ *Reference Videos*

1. [Physics Of Materials-IIT-Madras/lecture-26.html](#)
2. <https://nptel.ac.in/courses/115/104/115104109/>

Week #8 Class #28

- *Concept of effective mass*

Motion of electrons in the crystal is governed by the energy

equation $E = \frac{\hbar^2 k^2}{2m}$ which shows energy is nonlinearly dependent on the propagation constant k

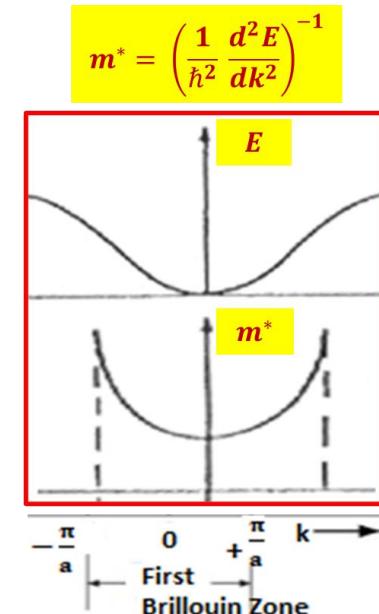
Differentiating the expression twice with respect to k

$$\frac{d^2 E}{dk^2} = \frac{\hbar^2}{m^*}$$

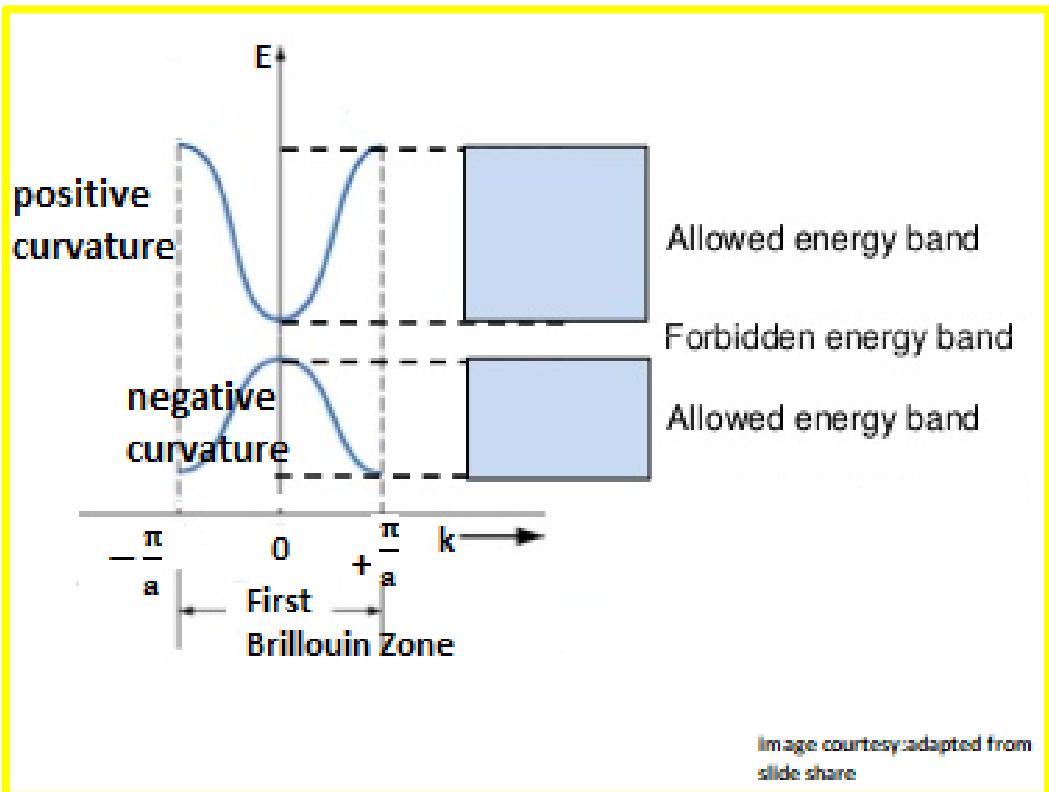
$m^* = \left(\frac{1}{\hbar^2} \frac{d^2 E}{dk^2} \right)^{-1}$ is not a constant and depends on the nonlinearity of E

Thus charge carriers have an effective mass which depends on the curvature of $E-k$

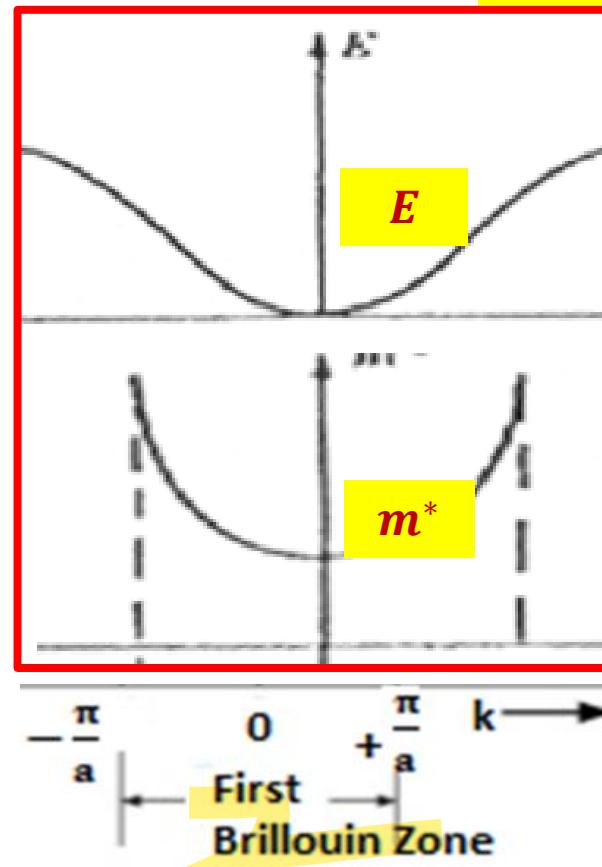
The group velocity (velocity of wave packet or particle) that carries energy through the material can be written as $v_g = 1/\hbar(dE/dk)$



Slope of E-K curve is minimum at the band edges and hence the effective mass of charge carriers are highest at band edges



$$\frac{d^2E}{dk^2} = \frac{\hbar^2}{m^*} \rightarrow m^* = \frac{\hbar^2}{\frac{d^2E}{dk^2}} \quad m^* = \left(\frac{1}{\hbar^2} \frac{d^2E}{dk^2} \right)^{-1}$$



Effective mass of electrons can be higher or lower than the rest mass of the electrons and depends on the position of electron in the particular band

- Curvature of the E-k is positive in the conduction band the effective mass is positive*
- Curvature in the valence band is negative indicating a negative mass, and indicates the concept of hole conduction in the valence band*
- Effective mass of electrons can be higher or lower than the rest mass of the electrons and depends on the position of electron in the particular band*
- Concept of effective mass helps to understand mobility of charge carriers*
- Expression for electrical conductivity, $\sigma = \frac{n_{eff} e^2 \tau}{m^*}$*

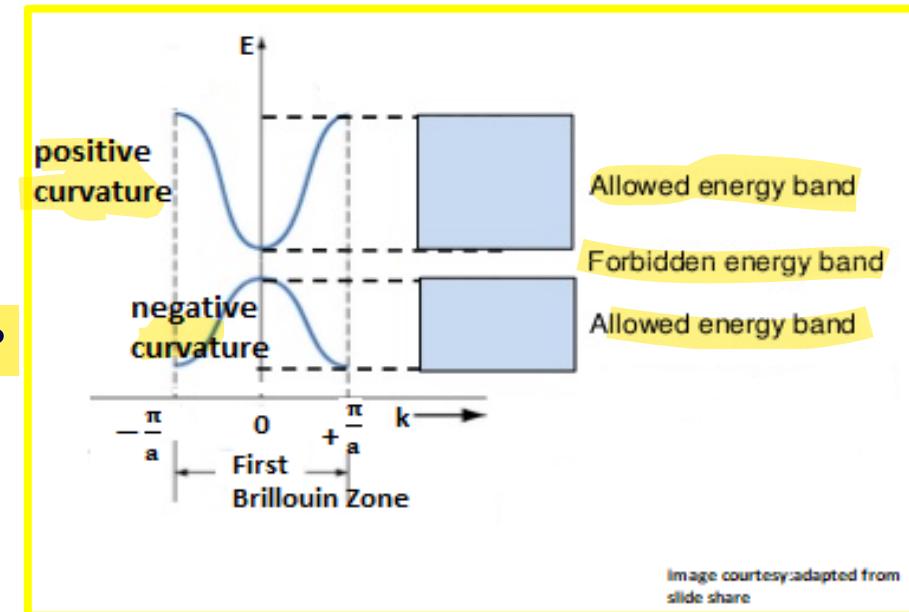


Image courtesy:adapted from slide share

Draw the E-K graph for electrons in metal as per the band theory of solids and discuss the concept of the effective mass of electrons in the conduction band of the metal.

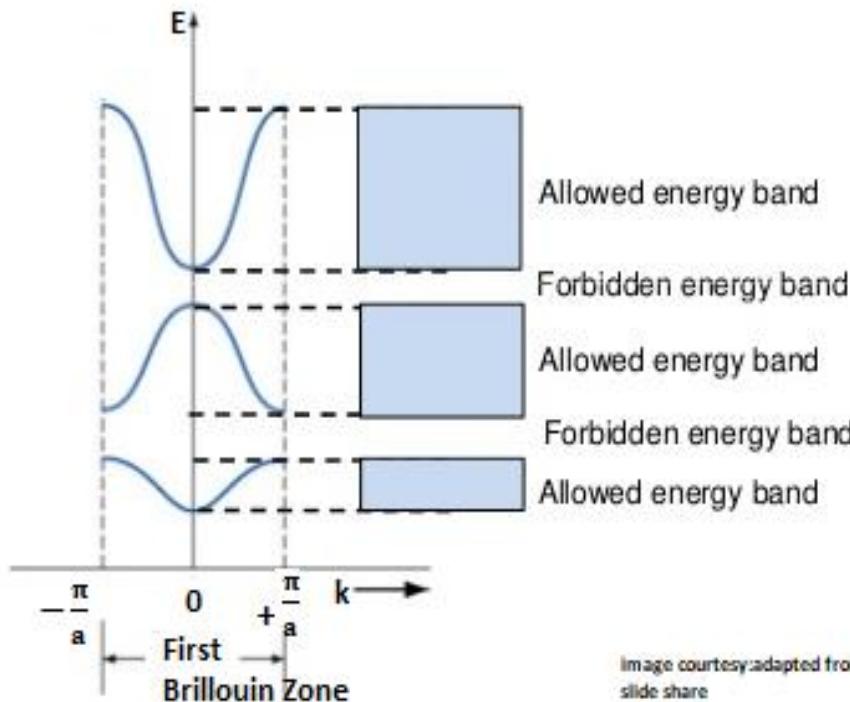


Image courtesy: adapted from slide share

The mass of electron in the periodic potential of a crystal is different from the free electron mass and is referred to as effective mass. In terms of energy and propagation

constant, effective mass is given by $m^* = \left(\frac{1}{\hbar^2} \frac{d^2 E}{dk^2} \right)^{-1}$.

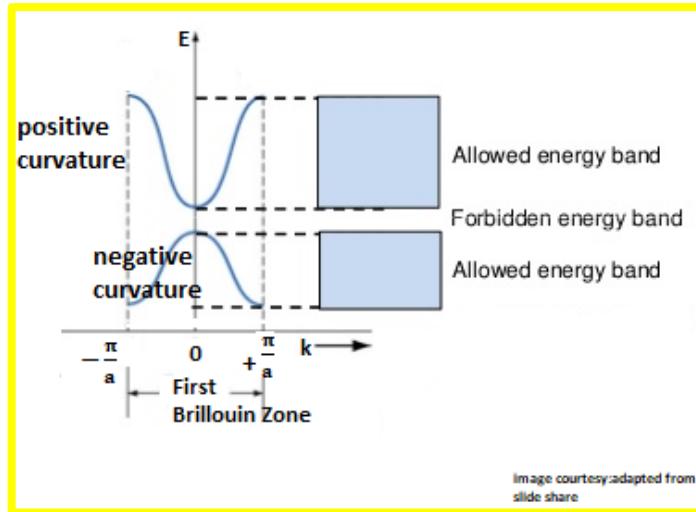
In terms of the curvature of E-k diagram in conduction band and valence band effective mass can be positive or negative.

As the curvature of E-k diagram is positive in the conduction band, the effective mass is positive.

The curvature in the valence band is negative indicating a negative mass and accounts for the concept of hole conduction.



The “effective mass” of electrons depends on the curvature of the E-k plot. Explain this statement.



In terms of energy and propagation constant, effective mass is given by $m^* = \left(\frac{1}{\hbar^2} \frac{d^2 E}{dk^2} \right)^{-1}$.

The curvature of E-k diagram in conduction band and valence band indicates whether the effective mass is positive or negative.

As the curvature of E-k diagram is positive in the conduction band, the effective mass is positive.

The curvature in the valence band is negative indicating a negative mass (concept of hole conduction).

Conceptual Questions

“The mass of an electron in the periodic potential of a solid is different from the free electron mass” Is the statement true or false? Can the effective mass be positive and negative? If yes, what are the specific conditions for the same.

True, the mass of electron in the periodic potential of a crystal is different from the free electron mass and is referred to as effective mass.

In terms of energy and propagation constant, effective mass is given by

$$m^* = \left(\frac{1}{\hbar^2} \frac{d^2 E}{dk^2} \right)^{-1}.$$

In terms of the curvature of E-k diagram in conduction band and valence band effective mass can be positive or negative.

As the curvature of E-k diagram is positive in the conduction band, the effective mass is positive.

The curvature in the valence band is negative indicating a negative mass (concept of hole conduction).



Explain the E-k relationship for a free electron and relate it to the electron mass.

The E-k relationship for free electrons is governed by the energy equation $E = \frac{\hbar^2 k^2}{2m}$ which shows that the energy is nonlinearly dependent on the propagation constant k .

Differentiating the expression twice with respect to k

$$\frac{d^2 E}{dk^2} = \frac{\hbar^2}{m^*}$$

That is, $m^* = \left(\frac{1}{\hbar^2} \frac{d^2 E}{dk^2} \right)^{-1}$ is not a constant and depends on the non-linearity of E and designated as 'effective mass'. This means that the charge carriers have an effective mass which depends on the curvature of energy (E)-propagation constant (k) diagram.



Explain the terms (i) Periodic potential (ii) Bloch function and (iii) Effective mass

(i) Periodic Potential:

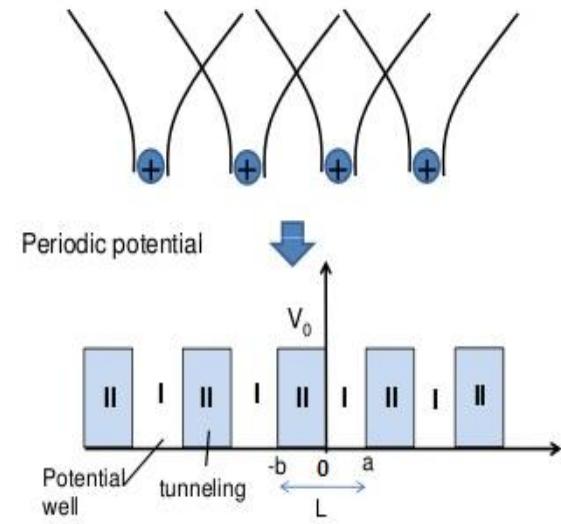
If the potential of a solid varies periodically with the periodicity of the space lattice 'a' (inter atomic spacing).

It is assumed that the potential energy of the electron is zero near the nucleus of the positive ion in the lattice and maximum when it is half way between the adjacent nuclei.

If $V(x)$ is periodic potential, then $V(x+a) = V(x)$

(i) Bloch function:

For the periodically varying potential inside a solid, an acceptable solution of electron wave is of the form $\psi(x) = U_k(x) e^{ikx}$, where $U_k(x + a) = U_k(x)$, called Bloch function.





Explain the terms (i) Periodic potential (ii) Bloch function and (iii)Effective mass

(i) Effective mass

the mass of electron in the periodic potential of a crystal is different from the free electron mass and is referred to as effective mass.

In terms of energy and propagation constant,

effective mass is given by $m^* = \left(\frac{1}{\hbar^2} \frac{d^2 E}{dk^2} \right)^{-1}$.



PES
UNIVERSITY

THANK YOU

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629



PES
UNIVERSITY

ENGINEERING PHYSICS

Department of Science and Humanities

For an Engineer in todays time - A world without magnetic materials!

- *Not possible for efficient generation and use of electricity*
- *No Nonpolluting electric vehicles as they rely on efficient motors utilizing advanced magnetic materials*
- *No telecommunications industry with faster data transmission and miniaturization of devices, both of which require development of improved magnetic materials*

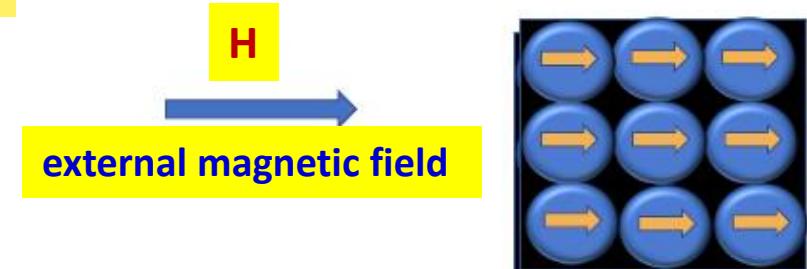
ENGINEERING PHYSICS

Introduction to Magnetic materials: Review of basics



PES
UNIVERSITY

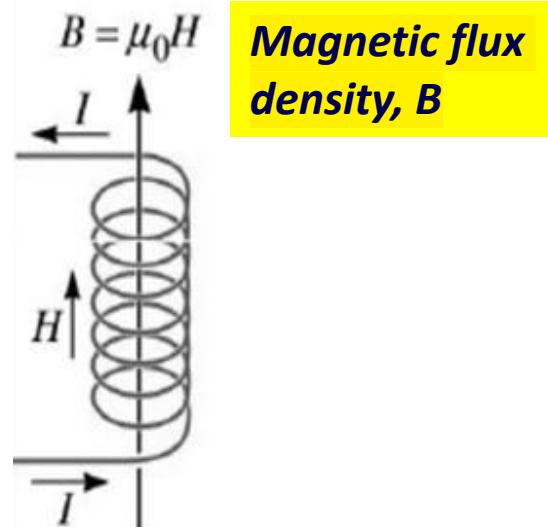
- Materials placed in an external magnetic field H responds differently
- The intensity of magnetization (M) : Dipole strength per unit volume



$$M = \frac{\mu}{V} \quad \text{Magnetic dipole moment, } \mu$$

Also, Magnetization $M \propto H$ or $M = \chi H$

- Magnetic susceptibility : $\chi = \frac{M}{H}$, ability to get magnetized
- Magnetic field strength: $H = \frac{nI}{l}$



- Magnetic flux density : $B_0 = \mu_0 H$

$$\mu_0 = 4\pi \times 10^{-7} \text{ H/m}$$

- Magnetization of the material:

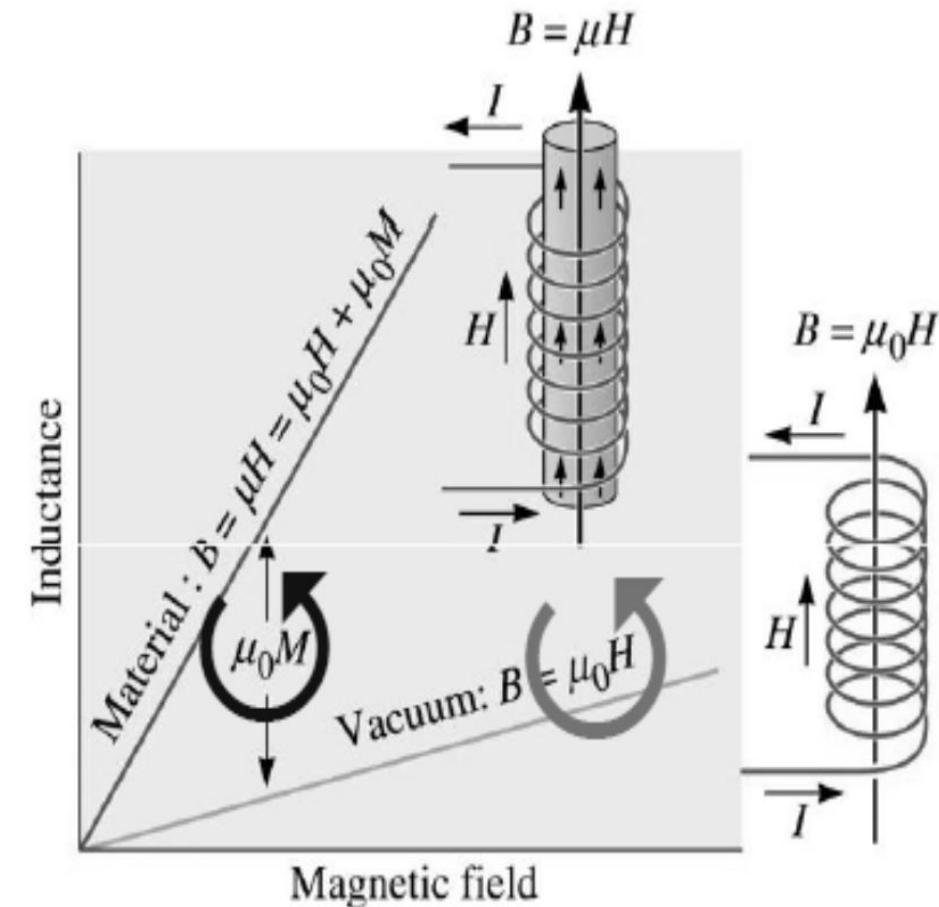
When a material of susceptibility χ_m is introduced inside a solenoid

$$B = \mu_0 H + \mu_0 M = \mu_0 (H + M)$$

$$= \mu_0 (H + \chi_m H) = \mu_0 (1 + \chi_m) H$$

- Relative permeability can be defined as,

$$\mu_r = (1 + \chi_m)$$



ENGINEERING PHYSICS

Origin of Magnetism in Materials – Atomic level analysis

- For orbiting electrons, (orbit of radius r with speed v , the period of rotation T),

current $I = \frac{e}{T} = \frac{e\omega}{2\pi} = \frac{ev}{2\pi r}$

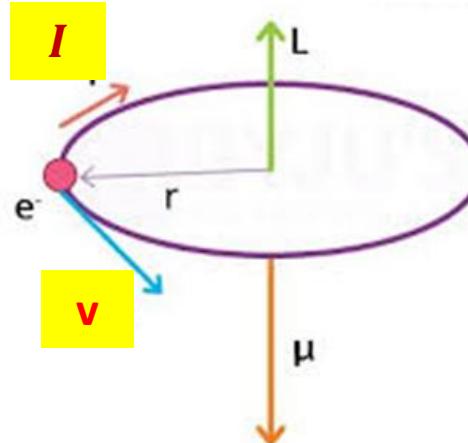
$$\mu_e = IA = I \times \pi r^2 = \frac{ev}{2\pi r} \pi r^2 = \frac{evr}{2} = \frac{e\omega r^2}{2}$$

- Angular momentum of orbiting electron, $\mathbf{L} = m_e v r$

In terms of \mathbf{L} ,

$$\mu_{orb} = \left(\frac{e}{2m_e} \right) L$$

WKT, linear velocity, $v = r\omega$



Due to the negative charge of the electron, the vectors μ and \mathbf{L} are in opposite directions and perpendicular to the plane of the orbit

Gyro-magnetic ratio (or magneto-gyric ratio), γ

the ratio, $= \left(\frac{\mu_{orb}}{L} \right) = \frac{e}{2m_e}$ is called gyromagnetic ratio

ENGINEERING PHYSICS

Origin of Magnetism in materials – Atomic level analysis

- Magnetic effect of the orbital motion of the electron is very small (sometimes ‘zero’) because of cancellation of the magnetic moments of electrons orbiting in opposite directions

- Magnetic moment due to the spin (electrons have property of spin apart from orbital motion) of the electrons is significant and almost twice that of the orbital contribution

$$\mu_{\text{Spin}} = \sqrt{s(s+1)} \frac{e\hbar}{2m} \quad \text{quantized spin}$$

- Total magnetic moment of an atom = Sum of orbital and spins magnetic moments $\mu_e = \mu_{\text{Spin}} + \mu_{\text{orb}} = g_e \frac{e\hbar}{2m}$

Lande ‘g’ factor – Spectroscopic splitting factor

where g_e is the Lande ‘g’ factor

$$g_e = 1 + \frac{j(j+1) + s(s+1) - l(l-1)}{2j(j+1)}$$

- Bohr magneton is $\mu_B = \frac{e\hbar}{2m} = 9.27 \times 10^{-27} \text{ J/T}$

Bohr magneton- smallest unit of magnetic moment

Nuclear magnetic response

Net contribution of orbital, spin and nuclear magnetic responses of all atoms decide the magnetic behavior (susceptibility) of the material

For nucleus, $\mu_{\text{nucleus}} =$

$g_e \cdot \frac{e\hbar}{2m_p}$, will be negligible as mass of proton is 1836 times more than electron!

J-total orbital quantum number



Total magnetic moment of an atom = Sum of orbital and spins

magnetic moments $\mu_e = \mu_{spin} + \mu_{orb} = g_e \frac{e\hbar}{2m}$

where **is the Lande 'g' factor** $g_e = 1 + \frac{j(j+1)+s(s+1)-l(l-1)}{2j(j+1)}$

From this the smallest non zero value of the spin magnetic moment due to electrons (when $s=j$ and $l=0$) is obtained as

$$\mu_s = \frac{e\hbar}{m}, \text{twice the orbital magnetic moment}$$

j - total angular momentum quantum number

To represent the total angular momentum of a given particle, by combining its orbital angular momentum (l) and its intrinsic angular momentum (i.e., spin, s)

ENGINEERING PHYSICS

Larmor precession

- Consider an orbiting electron, magnetic moment
- In the presence of an external magnetic field (B), the magnetic moment experiences a torque $\tau = \mu \times B$
- This torque produces a change in angular momentum ΔL and the magnetic moment precess around the applied field (like a spinning top) called **Larmor precession**

Expression for Larmor frequency (precession angular velocity)- ω_L

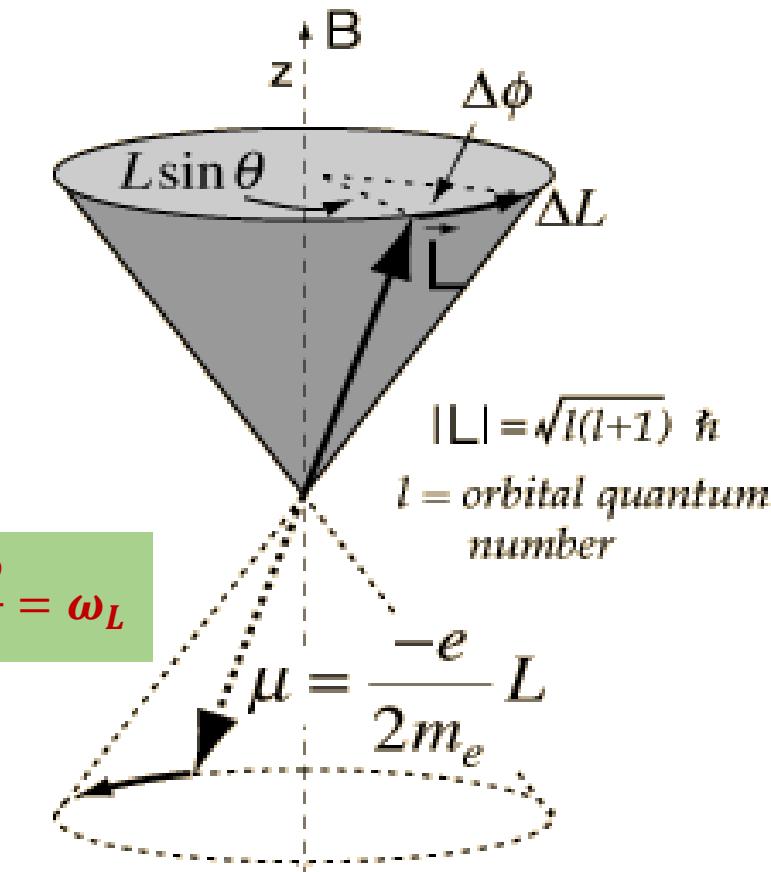
$$\text{Torque } \tau = \frac{\text{change in ang.momentum } (\Delta L)}{\text{time } (\Delta t)}$$

$$\tau = \mu \times B = |\mu B \sin \theta| = \frac{\Delta L}{\Delta t} = \frac{L \sin \theta \times \Delta \phi}{\Delta t} = L \sin \theta \omega_L$$

$$\tau = |\mu B \sin \theta| = L \sin \theta \omega_L$$

- The precession angular velocity (Larmor frequency) is given

by $\frac{d\phi}{dt} = \omega_L = \frac{\mu B}{L} = \frac{e}{2m_e} B$



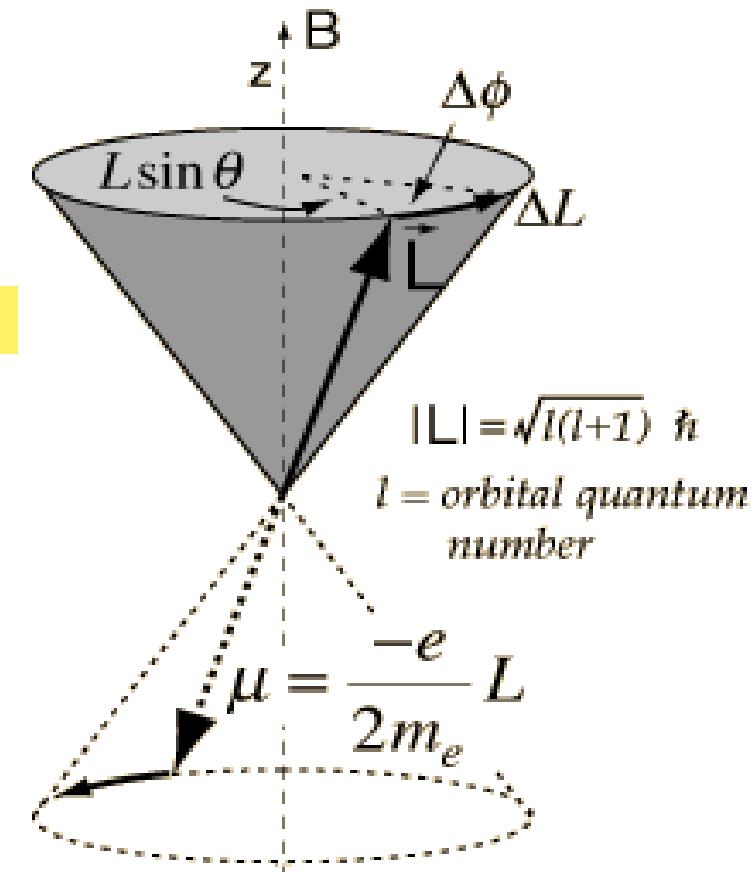
In Figure, ΔL is an arc, $\Delta L = \text{radius} * \text{angle} = L \sin \theta \times \Delta\phi$

Larmor precession frequency: Importance

- Larmor precession forms the basis of Magnetic Resonance Spectroscopy – An important material characterization technique

e.g.: Electron spin resonance (14GHz/T)

Nuclear magnetic resonance (Larmor precession frequency for protons is 7.8 MHz/T)



Magnetic moment due to a precessing charge

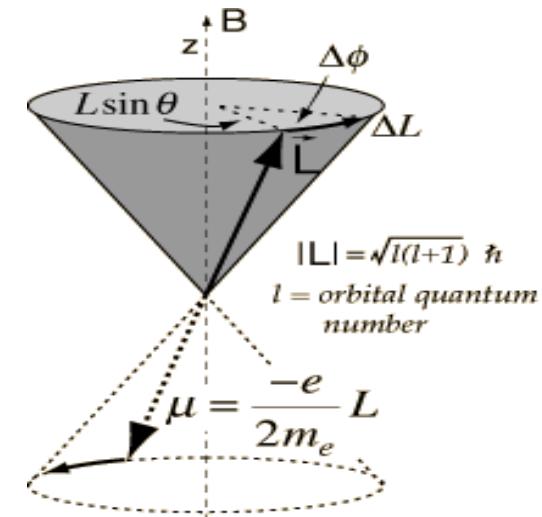
Magnetic moment

$$\mu_e = IA = \frac{e\omega r^2}{2}$$

- Magnetic moment induced due to precession

$$\mu_{ind} = \frac{1}{2} e\omega_L r^2$$

Larmor frequency (precession angular velocity)- $\omega_L = \frac{e}{2m_e} B$



Substituting for Larmor frequency, $\mu_{ind} = \frac{1}{2} e\omega_L r^2 = -\frac{Be^2 r^2}{4me}$

Negative sign because induced moment opposes the field that induced the precession (Lenz's law)

For ***N_a*** number of atoms/unit volume with each atom contains ***Z*** number of electrons (atomic number - Z)

The total induced magnetization $M = N_a Z \mu_{ind} = -\frac{N_a Z e^2 r^2 B}{4m} = \frac{N_a Z e^2 r^2 \mu_0 H}{4m}$

WKT, $B = \mu_0 H$

Thus, induced susceptibility $\chi_m = \frac{M}{H} = -\frac{N_a Z e^2 r^2 \mu_0}{4m}$

All materials have inherent diamagnetic response due to the paired electron up to valence level!

Unpaired valence electrons generate other magnetic responses, para and ferro magnetic!

Magnetic moment induced due to precession, $\mu_{ind} = \frac{1}{2} e\omega_L r^2$

Larmor frequency (precession angular velocity)- $\omega_L = \frac{e}{2m_e} B$

Substituting for Larmor frequency, $\mu_{ind} = \frac{1}{2} e\omega_L r^2 = -\frac{Be^2r^2}{4me}$

Negative sign because induced moment opposes the field that induced the precession (Lenz's law)

For ***N_a*** number of atoms/unit volume with each atom contains ***Z*** number of electrons (atomic number - Z)

The total induced magnetization $M = N_a Z \mu_{ind} = -\frac{N_a Ze^2 r^2 B}{4m} = \frac{N_a Ze^2 r^2 \mu_0 H}{4m}$

WKT, $B = \mu_0 H$

Thus, induced susceptibility $\chi_m = \frac{M}{H} = -\frac{N_a Ze^2 r^2 \mu_0}{4m}$



A magnetic field of 1T is applied to an electron undergoing orbital motion. Calculate the precessional frequency

Solution: Given: $B = 1 \text{ T}$

To find: $\omega_L = ?$

$$\omega_L = (e/2me) B = (1.6 \times 10^{-19} / 2 \times 9.1 \times 10^{-31}) \times 1$$

$$\omega_L = 87.8 \times 10^9 \text{ rad/s}$$

Estimate the magnetic field required to produce a precessional frequency 67.5 MHz in proton.

$$\text{Based on Larmor precession, } B = \frac{2m_{\text{proton}}\omega_L}{e}$$



- The total magnetic moment of an atom is the vector sum of orbital and spins magnetic moments
- The spin magnetic moment of the electron is twice that of the orbital momentum
- The magnetization in magnetic materials is mainly because of the electron motion around the nucleus
- All materials exhibit diamagnetic behavior



PES
UNIVERSITY

THANK YOU

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629



PES
UNIVERSITY

ENGINEERING PHYSICS

Department of Science and Humanities

Class #48

- *Diamagnetic materials*
- *Paramagnetic materials*
- *Ferromagnetic materials*

Diamagnetic materials - Diamagnetism

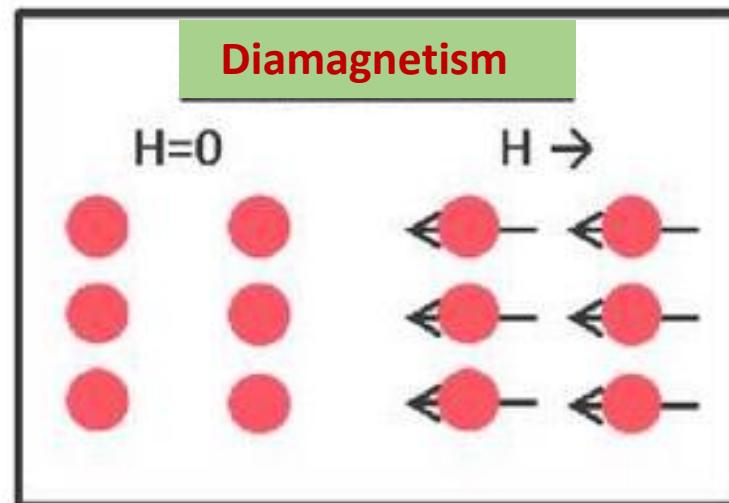
- In diamagnetic materials, the magnetic moments of orbiting electrons '*add up to zero*' in the absence of an external magnetic field
- In the presence of an external field, the magnetic moments of orbiting electrons align opposite to the applied field
- Atoms without unpaired electrons are diamagnetic
- Diamagnetic materials have negative susceptibility (χ_d) and permeability, $\mu_r < 1$
- The classical diamagnetic susceptibility is given by

$$\chi_d \propto \frac{N_a Ze^2 \langle r^2 \rangle \mu_0}{m}$$

Susceptibility is independent of temperature

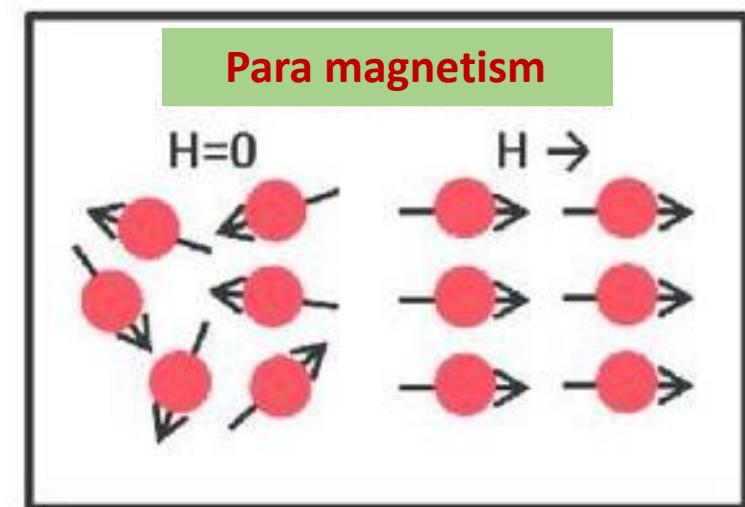
Superconductors show perfect diamagnetism

Examples: water, sodium chloride, some plastics, and many metals including copper



Paramagnetic materials

- Materials where atoms with unpaired electrons and are weakly attracted by magnetic fields
- Presence of randomly oriented magnetic permanent magnetic dipoles even in the absence of external field
- In the presence of an external magnetic field, magnetic dipoles align to the applied direction leading to a net weak magnetization
- If thermal energy $K_B T$ is greater than magnetic energy $\mu \cdot B$ ($K_B T > \mu \cdot B$), increased thermal agitation and zero magnetization
- Paramagnetic materials have positive susceptibility (χ_p)
Susceptibility is temperature dependent



Examples: Aluminium, Oxygen, Sodium

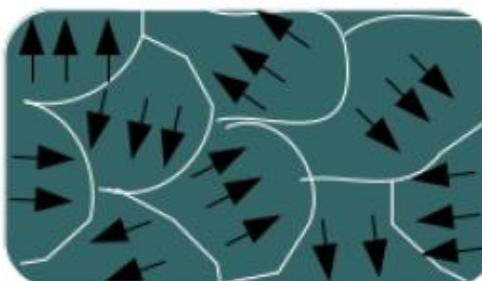
- These materials shows spontaneous magnetization and can be easily magnetized
- Very high magnetic susceptibilities, ranging from 1000 up to 100,000
- High ordering of unpaired electron spins - magnetic domains
- Ferromagnetic materials shows sharp hysteresis
- Phase change (phase transition) from Ferro to Paramagnetic occur above Curie temperature

Examples: Iron, nickel, cobalt

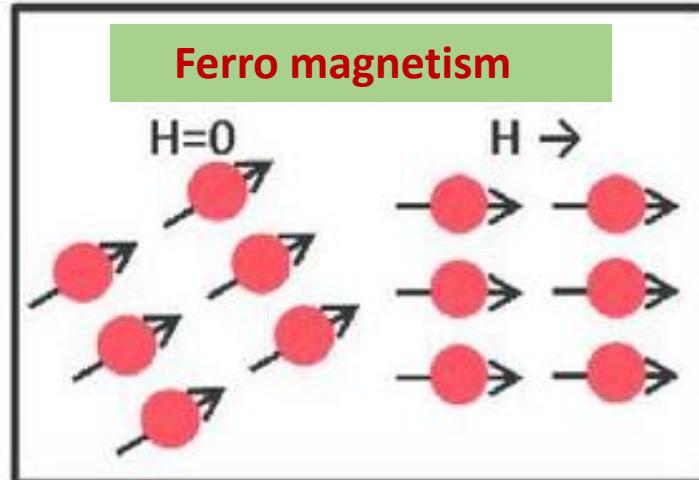
Susceptibility is
temperature dependent

Some applications

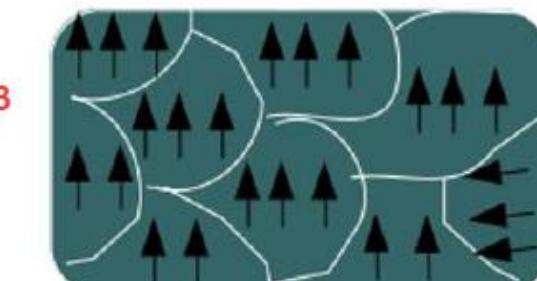
fabrication of magnets, Electromagnets, Transformers, magnetic storage, hard disks etc.



B=0



Domain alignment



B>0

Class #49

- ***Ferromagnetic materials***
- ***Antiferromagnetic materials***
- ***Ferrimagnetic materials***
- ***Susceptibility v/s temperature plots***
- ***B-H curve: Hysteresis and memory effect***
- ***Soft ferromagnetic materials***
- ***Hard ferromagnetic materials***
- ***GMR – Giant magneto resistance effect***

1. Ferromagnetic materials

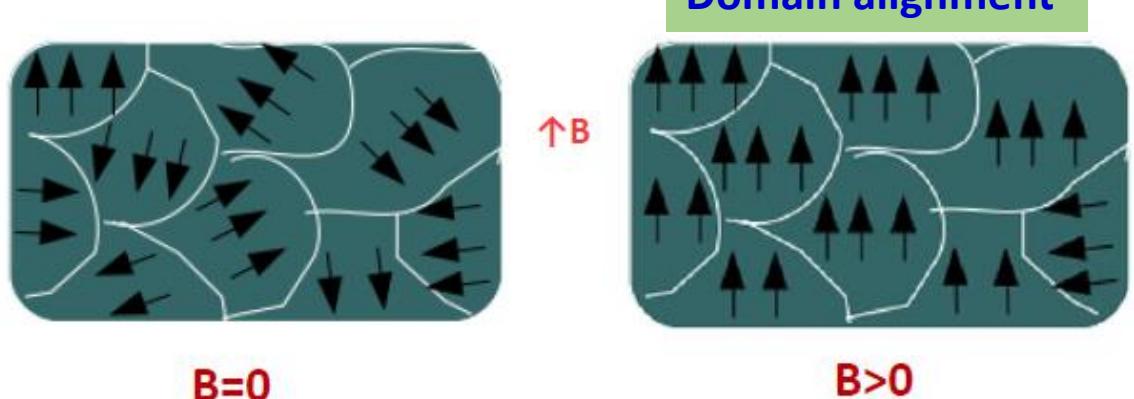
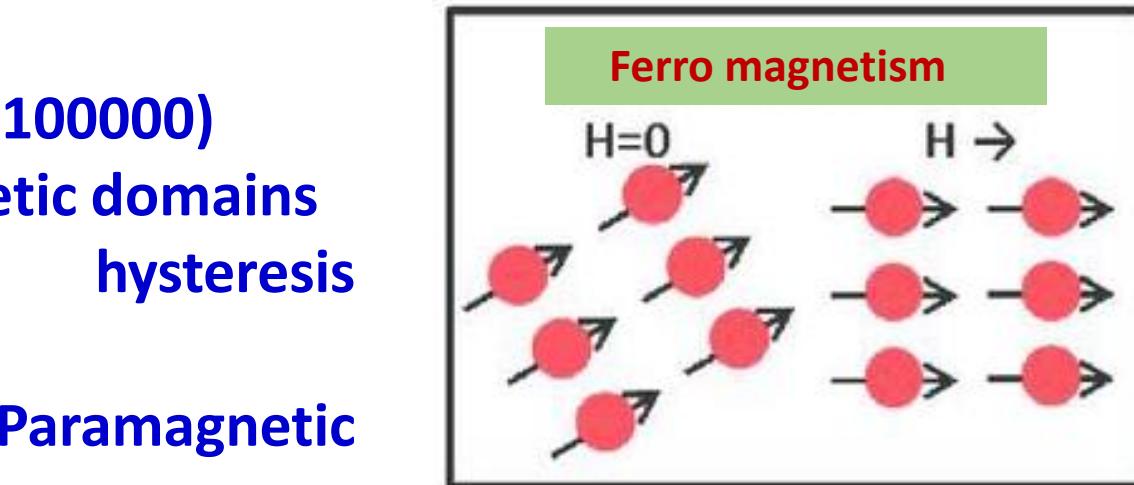
- Shows spontaneous magnetization and can be easily magnetized
- High magnetic susceptibilities, (from 1000 up to 100000)
- High ordering of unpaired electron spins - magnetic domains
- Ferromagnetic materials shows sharp hysteresis characteristics
- Phase change (phase transition) from Ferro to Paramagnetic occur above Curie temperature

Susceptibility is temperature dependent

Examples: Iron, nickel, cobalt

Some applications

fabrication of magnets, Electromagnets,
Transformers, magnetic storage, hard disks etc.



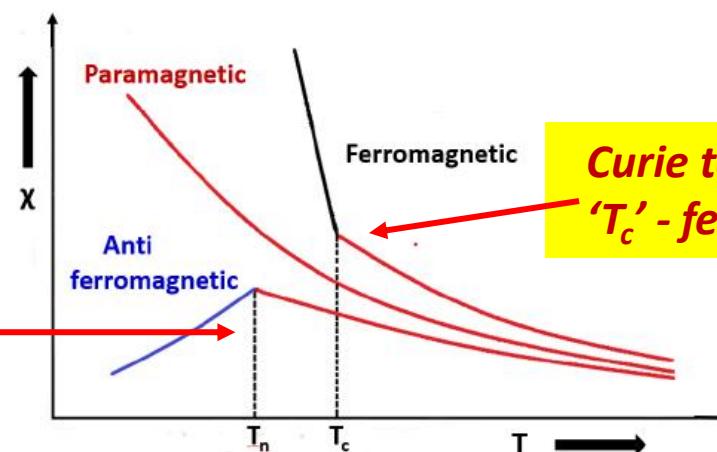
2. Anti-Ferromagnetic materials

- Electron spins (magnetic dipoles) exhibit a degree of ordering within the domain
- Adjacent domains are aligned opposite to each other (equal dipole moments and antiparallel)
- Thus net magnetisation of the material is zero below a certain temperature called as the **Neel temperature ' T_N '**
- Above the Neel temperature the materials behave as paramagnetic

e.g.: **MnO, NiO, CoO, etc.**

**Neel temperature
' T_N ' - antiferro**

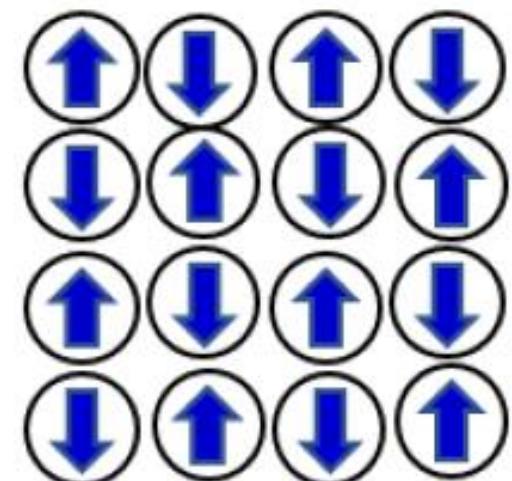
Above Neel temperature anti-ferro materials as paramagnetic



**Curie temperature
' T_c ' - ferro**

Above Curie ferro materials as paramagnetic

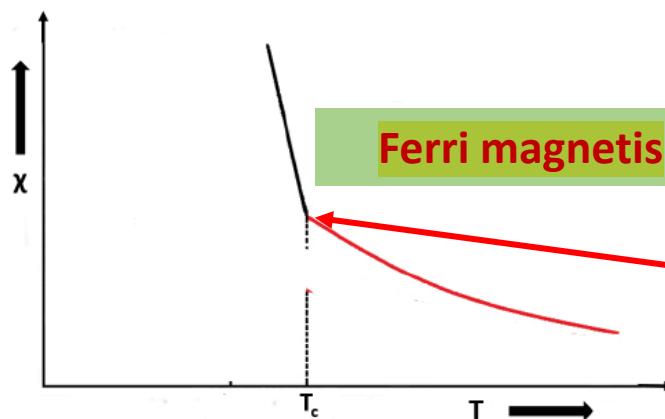
Anti-Ferro magnetism



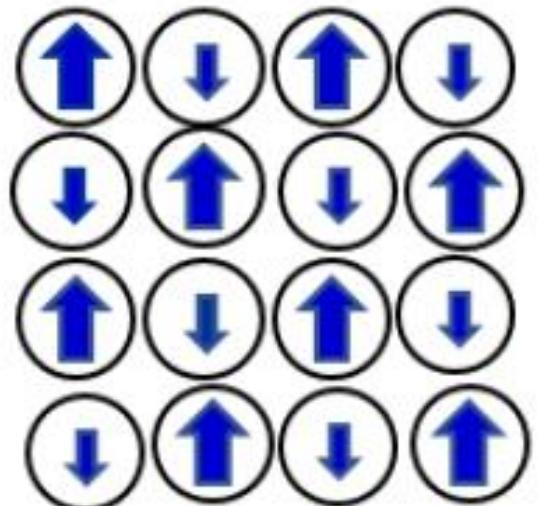
3. Ferrimagnetic materials

- Materials with electron spins are ordered but antiparallel and unequal
- Show a net non-zero magnetization
- Ferri-magnetic materials generally contains two cations with different magnetic moments (e.g.: NiFe_2O_4 , CoFe_3O_4 , and $\text{BaFe}_{12}\text{O}_{19}$ etc.)
- Exhibits spontaneous magnetization (similar to ferromagnetic materials)

Susceptibility is temperature dependent: Above T_c the materials display paramagnetic behavior



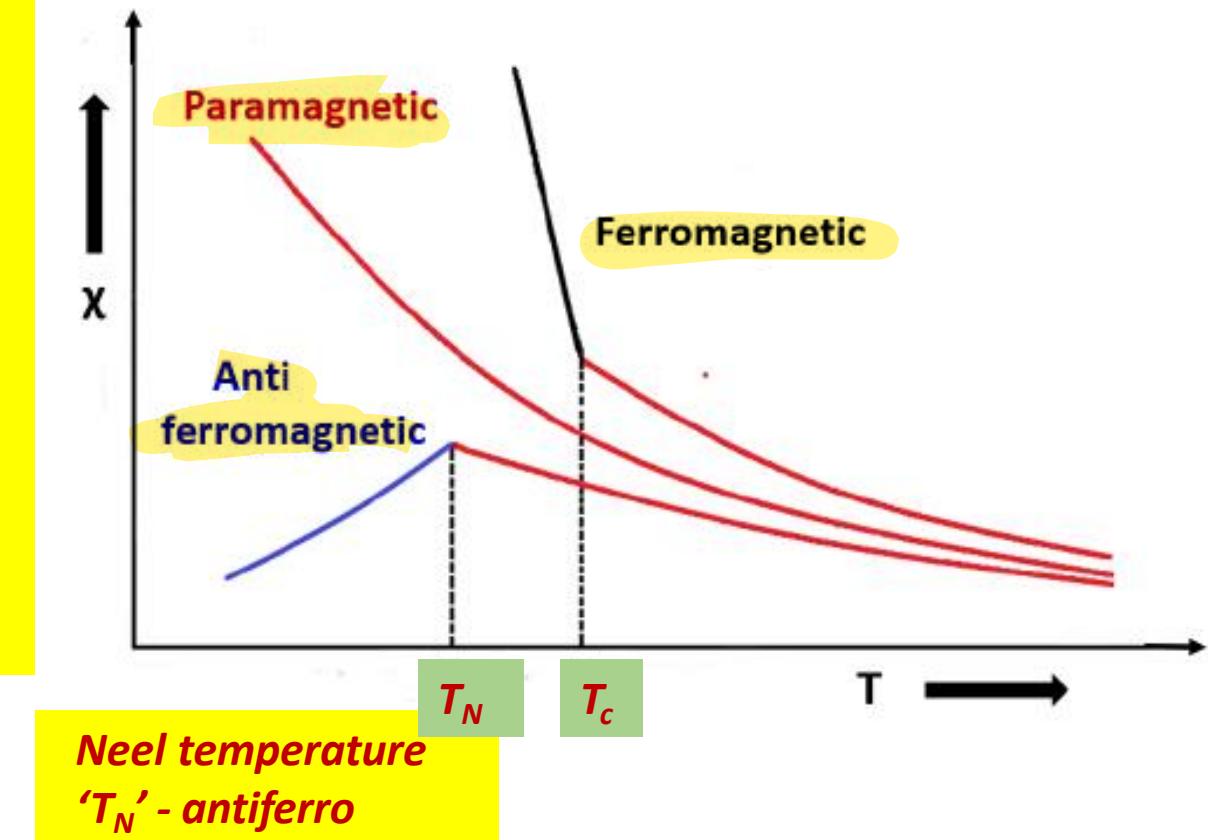
Ferri magnetism



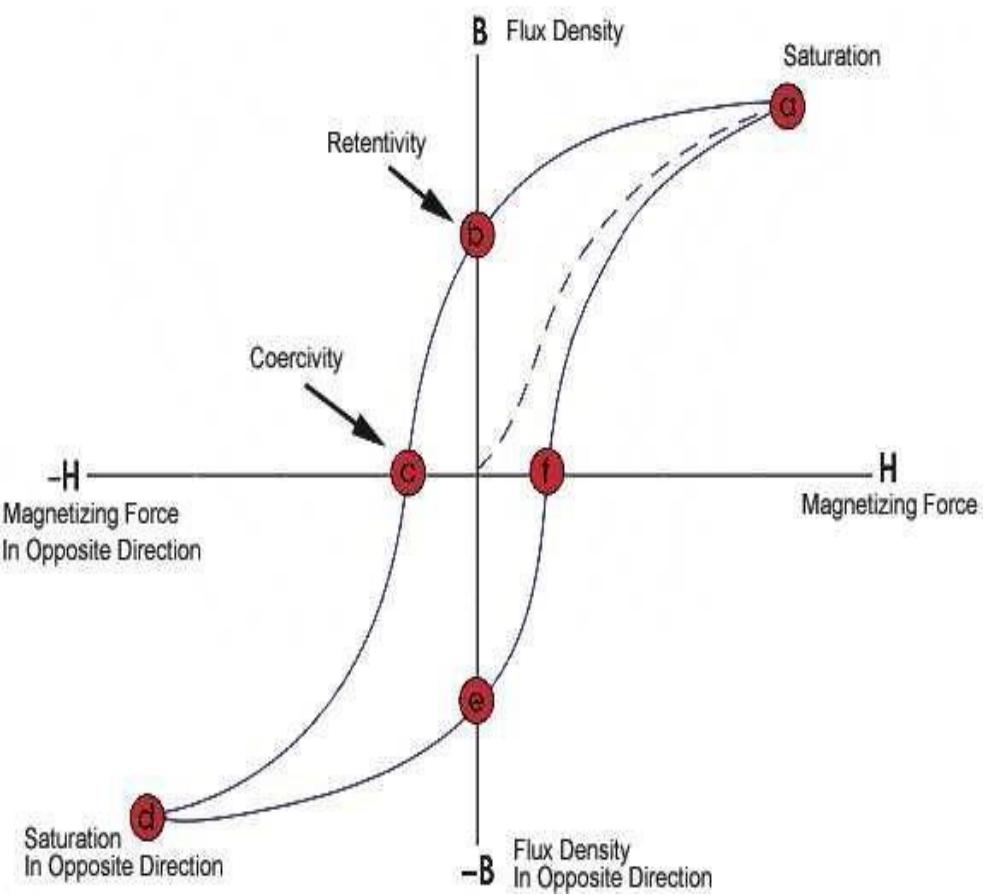
Curie temperature
' T_c ' - ferro

Above Curie ferro materials
as paramagnetic

- **Paramagnetic materials – Curie's law**
- **Ferromagnetic materials – Curie-Weiss' law and exhibit a paramagnetic behavior above the Curie temperature**
- **Antiferromagnetic materials – above Neel temperature material behaves as paramagnetic**



- Magnetization (flux density, B) of a ferromagnetic material in the presence of an external magnetic field (H) forms ***hysteresis loop***
- When all the spin are aligned magnetization shows a ***saturation value***
- When the external field is removed ($H=0$), still maintain net magnetization (remnant magnetization) - ***retentivity*** of the material
- Remnant magnetization can be removed if a coercive field H_c is applied in the reverse direction - ***coercivity***
- Further flipping of magnetization in ***opposite direction***



ENGINEERING PHYSICS

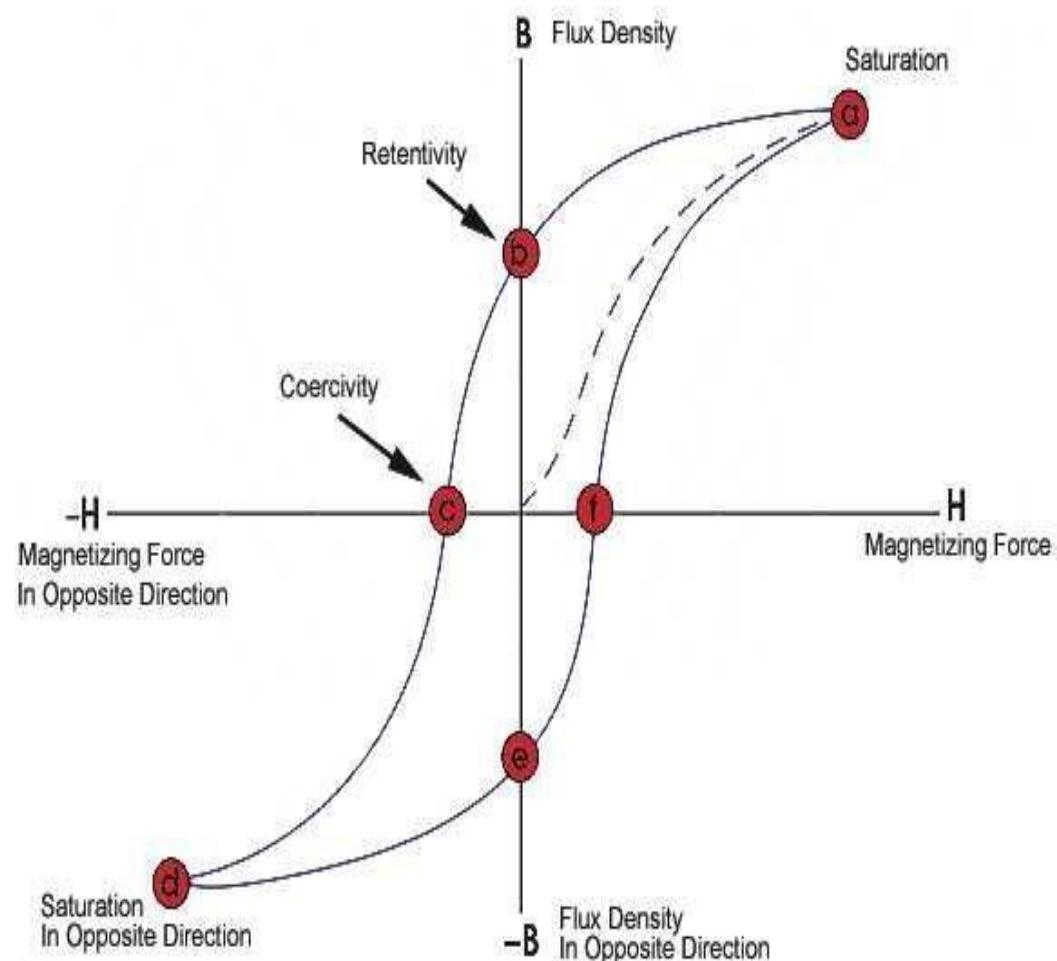
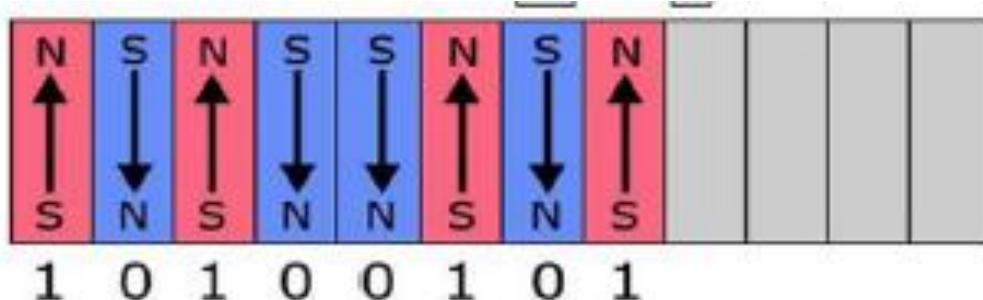
Ferromagnetic materials: Hysteresis as memory effect



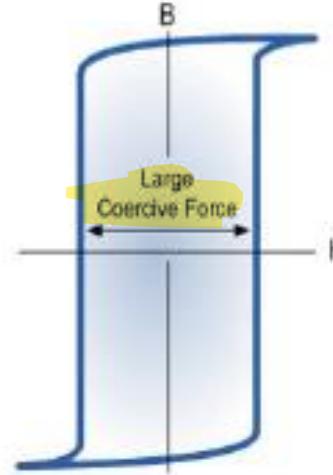
PES
UNIVERSITY

- Hysteresis show memory effect
- Memory effect: previous experience of external fields and can be used as memory materials

Examples: Iron, nickel, cobalt



Classification of ferromagnetic materials based on nature of Hysteresis



Hard ferromagnetic material

Difficult to demagnetise

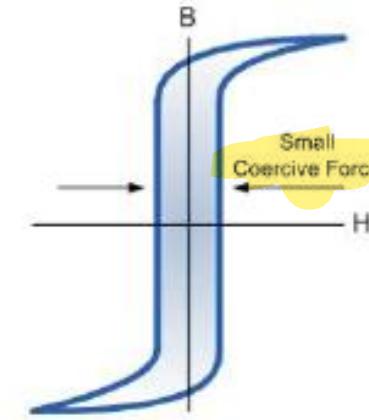
Exhibit very high retentivity and large coercivity

Low permeability

Area under the hysteresis curve is large indicating amount of energy loss

Hard, brittle and difficult to shape

Applications: permanent magnets, Memory devices



Soft ferromagnetic material

Easily magnetisable and de magnetisable

Large saturation magnetisation

Low coercive field (Coercivity is small)

Hysteresis loop is narrow and has low losses

• Examples: Iron and Iron alloys

• Applications: Transformers, motors or inductors.

ENGINEERING PHYSICS

Giant Magneto Resistance effect - GMR



PES
UNIVERSITY

- **Giant magneto-resistance (GMR)- Quantum mechanical magneto resistance effect**
- **Large change in electrical resistance with applied magnetic field**
- **Observed in layered magnetic materials**
e.g: Magnetic metallic multilayers : Fe/Cr and Co/Cu

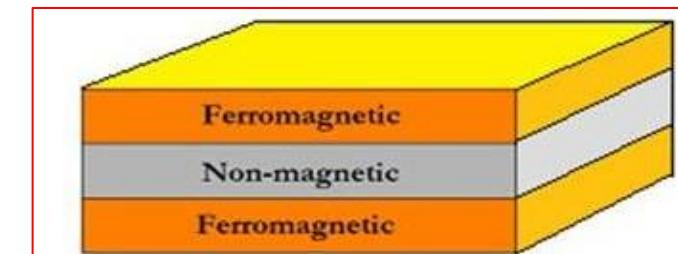
Principle: spin scattering of electrons in the non magnetic layer is less when magnetization is parallel

Resistance increases when magnetization is anti-parallel

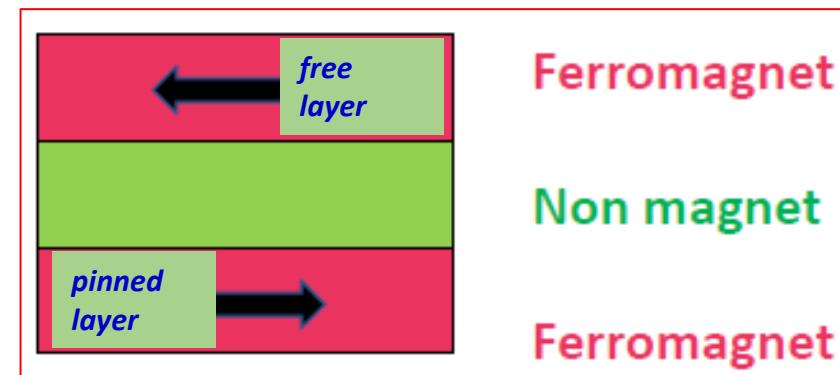
Applications:

In magnetic memories and sensors

Practical GMR devices have one pinned layer (magnetization is fixed) and another free layer (magnetization is varied)



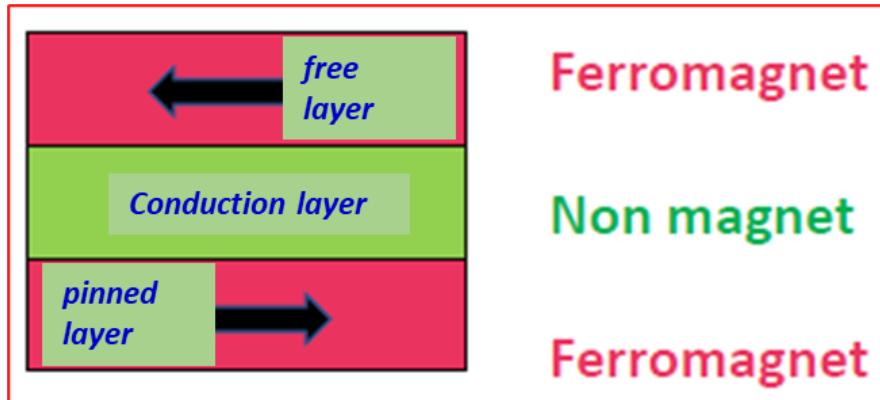
GMR in % is,
$$GMR = \frac{R_{\uparrow\downarrow} - R_{\uparrow\uparrow}}{R_{\uparrow\uparrow}}$$



ENGINEERING PHYSICS

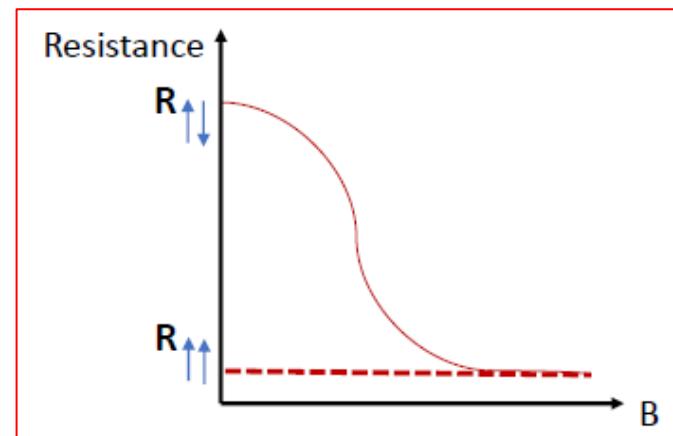
Giant Magneto resistance

- The resistance to current flow depends on the direction of magnetization of the two layers
- Most scattering occurs at the interfaces of the ferromagnetic and the conduction layer

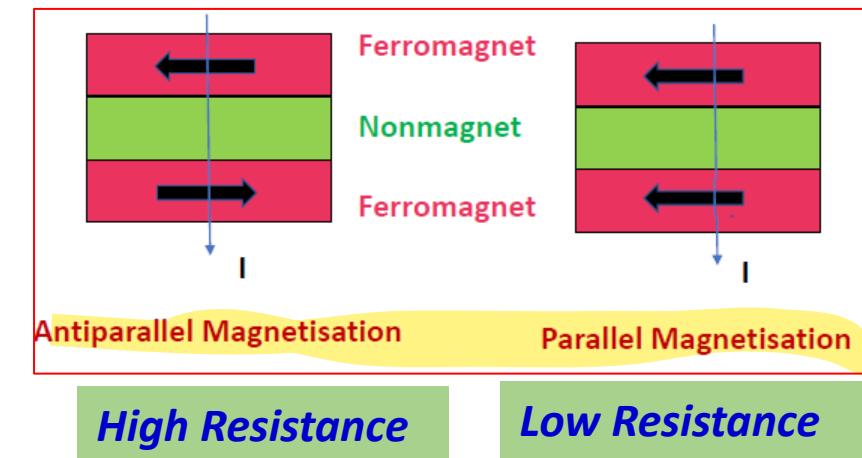


magnetic layers - 3-5nm and
non-magnetic layer - 25nm

$$GMR = \frac{R_{\uparrow\downarrow} - R_{\uparrow\uparrow}}{R_{\uparrow\uparrow}}$$



GMR depends on geometry of the device,
temperature and thickness of
ferromagnetic and non-magnetic layers



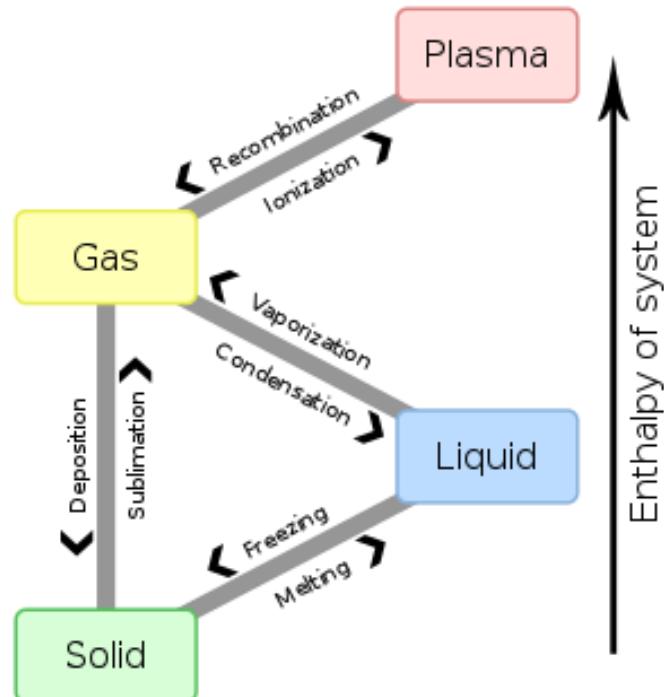
Test your understanding (Answer True/False)

- **The paramagnetic materials exhibits hysteresis property**
- **The net magnetization in Ferri magnetic materials is equal to zero**
- **Diamagnetic materials have permanent dipoles**
- **Ferromagnetic materials have very small susceptibility as compared to paramagnetic materials**

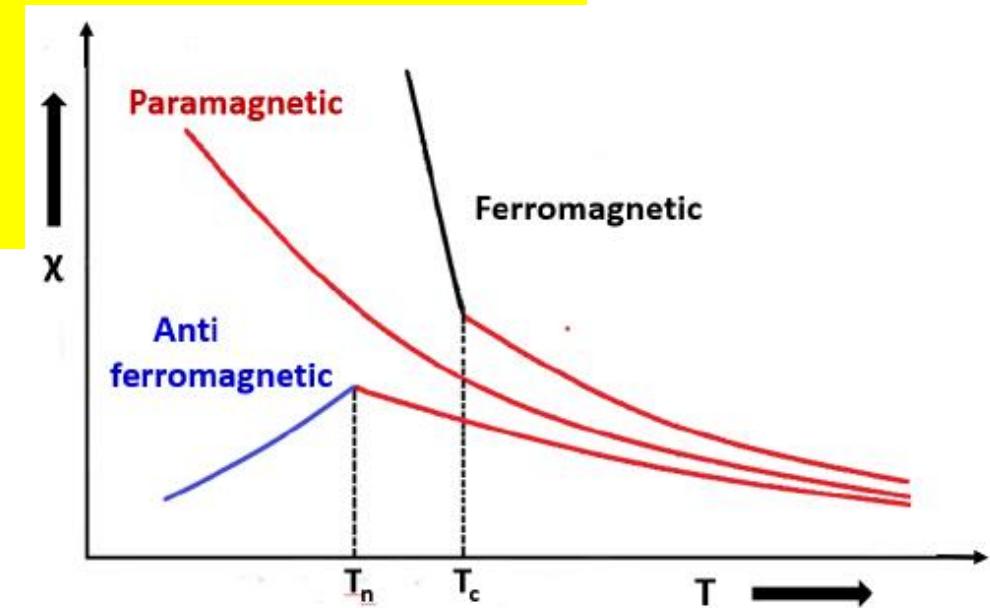
Evaluate the Larmor angular frequency in a magnetic field of 8 tesla.

$$\text{Larmor precession frequency, } \omega_L = \frac{e}{2m_e} B$$

What is a phase transition? Give an example of magnetic phase transition



Phase transition changes the state of the system.
Solid to liquid
Ferro to para



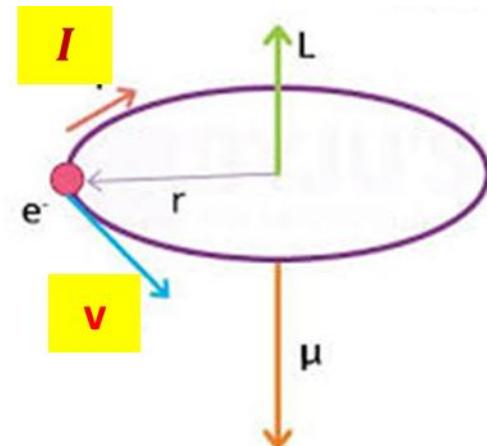
Find the expression for orbital magnetic moment and hence estimate the magnetic moment of an electron that revolves around a nucleus in an orbit of 0.53 Åo radius. The frequency of revolution is 6.6×10^{15} Hz.

- For orbiting electrons, (orbit of radius r with speed v , the period of rotation T),

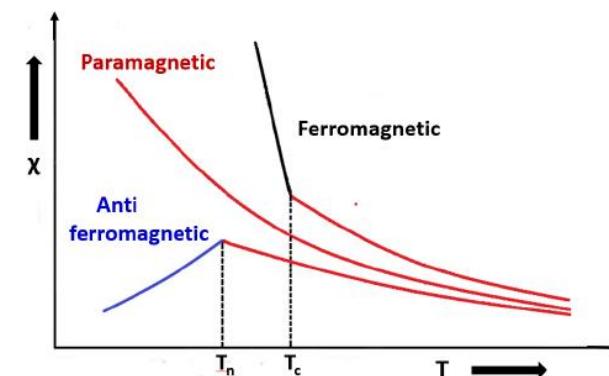
$$I = \frac{e}{T} = \frac{e\omega}{2\pi} = \frac{ev}{2\pi r}$$

$$\mu_e = IA = I \times \pi r^2 = \frac{ev}{2\pi r} \pi r^2 = \frac{evr}{2} = \frac{e\omega r^2}{2}$$

$$\mu_e = ef \times \pi r^2$$



Discuss graphically the variation of magnetic susceptibility of various types of magnetic materials as a function of temperature



Why does a magnetic dipole in an atom precess about the applied magnetic field.

- In the presence of an external magnetic field (B), the magnetic moment experiences a torque $\tau = \mu \times B$
- This torque produces a change in angular momentum ΔL and the magnetic moment precess around the applied field (*like a spinning top*) called *Larmor precession*

$$\text{Larmor precession frequency, } \omega_L = \frac{e}{2m_e} B$$

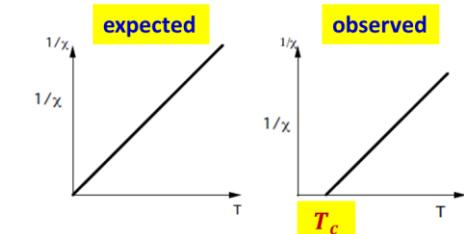
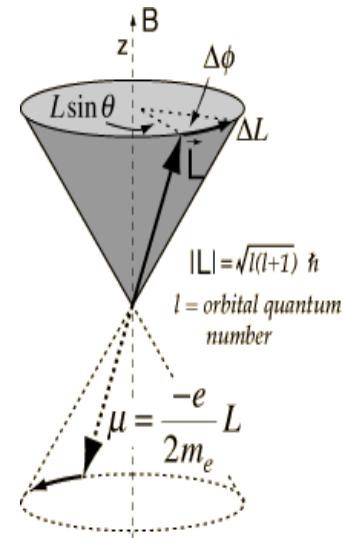
What is Curie-Weiss' law and how is it different from Curie's law? Demonstrate with graphs

Concept of Weiss' Molecular Field

- The variation of $\frac{1}{\chi}$ v/s T is expected to be a straight line passing through the origin, but some materials show a positive intercept T_c on the temperature axis (a deviation from expected temperature dependence)
- Weiss showed that this is due to a molecular field from the neighboring dipoles, as λM

Curie-Weiss law gives the magnetic susceptibility, $\chi = \frac{c}{T-T_c}$

Curie's law, $\chi = \frac{c}{T}$



Write the expression for magnetic moments of an atom from quantum mechanical ideas and compare between the spin magnetic moment and orbital magnetic moment.

- Magnetic moment due to the spin (electrons have property of spin apart from orbital motion) of the electrons is significant and almost twice that of the orbital contribution $\mu_{Spin} = \sqrt{s(s+1)} \frac{e\hbar}{2m}$
- Total magnetic moment of an atom = Sum of orbital and spins magnetic moments $\mu_e = \mu_{Spin} + \mu_{orb} = g_e \frac{e\hbar}{2m}$

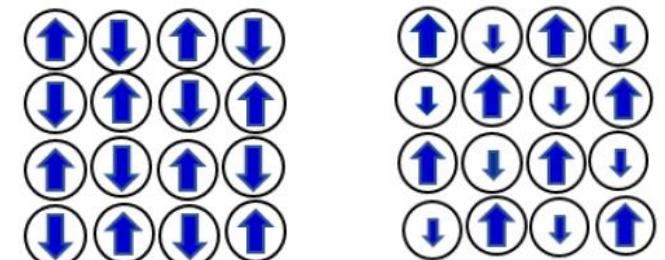
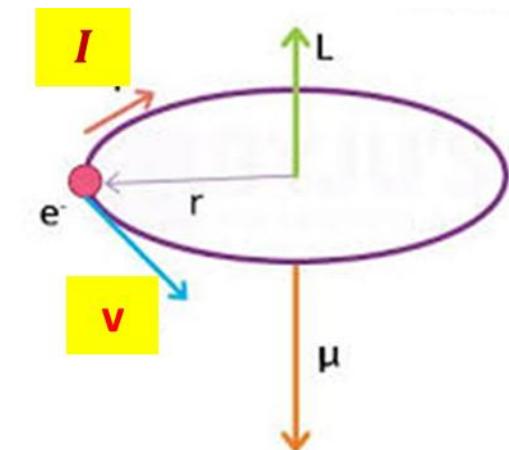
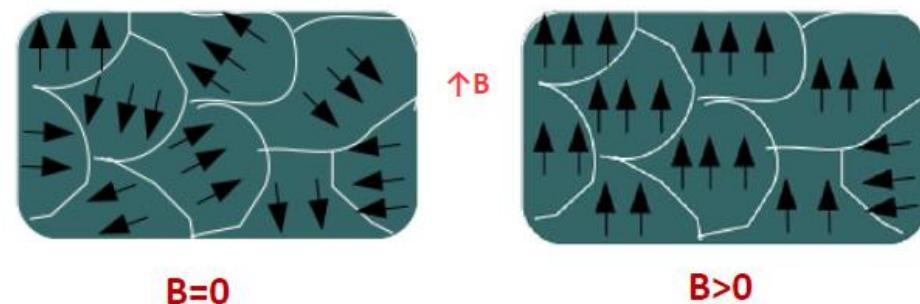
Elaborate on spin ordered magnetic materials and their classification

Spin ordered magnetic materials

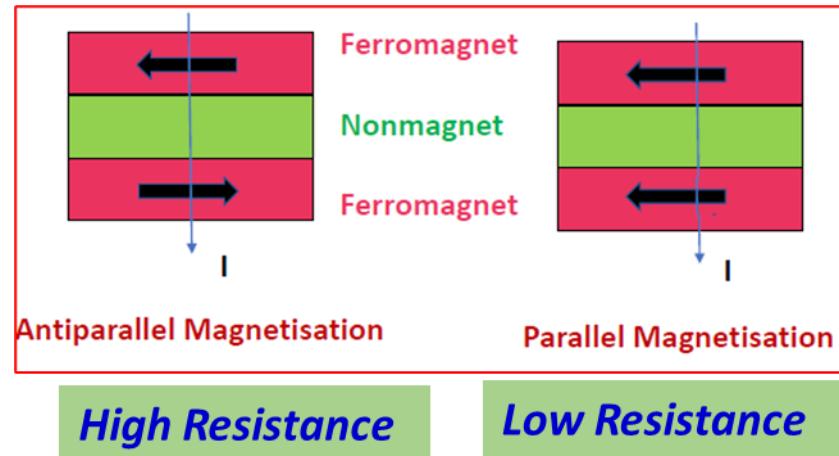
Ferromagnetic materials

Antiferromagnetic materials

Ferrimagnetic materials



Discuss giant magneto resistance and explain its application as a memory device



The resistance to current flow depends on the direction of magnetization of the two layers

In magnetic memories and sensors

Practical GMR devices have one pinned layer (magnetization is fixed) and another free layer (magnetization is varied)

What is Larmor precession? Obtain an expression for Larmor frequency.

Elaborate on Curie's law for paramagnetic materials. What are the arguments proposed by Weiss to modify Curie's law?



PES
UNIVERSITY

THANK YOU

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629



PES
UNIVERSITY

ENGINEERING PHYSICS

Department of Science and Humanities

Class 45

- *Quantum theory of paramagnetism*
- *Average magnetization at low B*
- *Average magnetization at high B & Brillouin function*
- *Langevin's theory of paramagnetism*
- *Weiss' molecular field*

Curie proposed the Curie law – 1895

Langevin proposed the theory of Diamagnetism and paramagnetism – 1905

Wiess proposed the theory of Ferromagnetism – 1906

Physics of magnetism with quantum principles (theory of electron spins and exchange interactions) - 1920

Three principal sources for the magnetic moment of a free atom

Electron's spin

Electron's orbital angular momentum about the nucleus

Change in the orbital moment induced by an applied magnetic field

Classical theory assumed that permanent magnetic moment of an atom/ion rotates freely and can possess any orientations with respect to applied magnetic field. In Quantum theory magnetic moments are quantized (cannot have arbitrary values)

As per quantum theory, for N number of atoms per unit volume of the medium with J as the total angular momentum quantum number of each atom , the possible quantized magnetic moment will be

$$\mu_j = j g_e \mu_B$$

The possible components of the magnetic moment in the direction of the applied field are given by,

$$\mu_z = m_j g_e \mu_B$$

For a given J , the allowed orientations (m_j values) are $-j$ to $+j$ in steps of one. This generates $2j + 1$ different values of m_j .

Where, m_j is magnetic quantum number associated with j (from $-j$ to $+j$) with $2J+1$ orientations relative to applied field.

ENGINEERING PHYSICS

Quantum theory of Paramagnetism – Magnetic energy and Average Magnetization

The quantized magnetic moments of a molecule/atom/ion in a material in the direction of an applied magnetic field can be written as $\mu_z = g_e \mu_B m_j$

where g_e is the Lande g factor,

μ_B is the Bohr magneton

m_j is the total angular momentum quantum number

- Magnetic energy of interaction of the magnetic moments with an external magnetic field B is given by

$$E_j = \mu_j \cdot B$$

$$E_j = g_e \mu_B m_j \mu_0 H$$

- For a paramagnetic material with N atoms per unit volume, the net magnetization is the statistical average of the allowed

orientations, $M = N \left[\frac{\sum_{m_j=-j}^j m_j g \mu_B * e^{m_j g \mu_B \mu_0 H / kT}}{\sum_{m_j=-j}^j e^{m_j g \mu_B \mu_0 H / kT}} \right]$

Magnetic field 'would like' the dipoles aligned but thermal vibrations (kT) 'would like' to randomize and disorder magnetic dipoles! Competition between two mechanisms!

- The average magnetization will depend on the exponent

$$e^{m_j g \mu_B \mu_0 H / kT}$$

Two possible cases, $E_j < kT$ (low magnetization) and $E_j > kT$ (high magnetization)

Case 1: ($m_j g \mu_B \mu_0 H \ll kT$) the thermal energy is much higher than the magnetic interaction energy, magnetization can be simplified

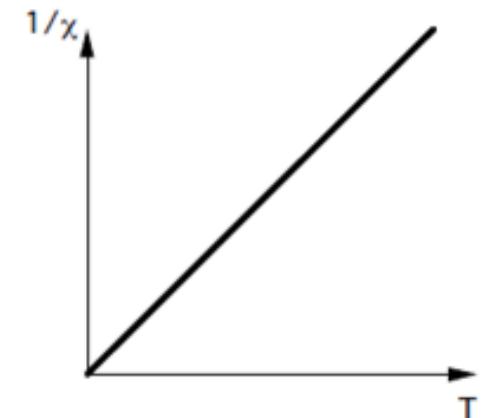
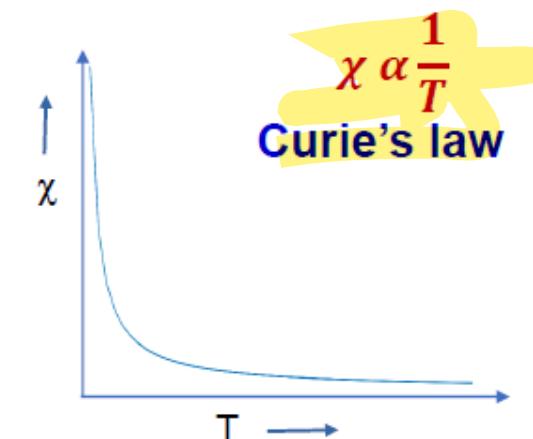
$$M = N \left[\frac{\sum_{-m_j=j}^j m_j g \mu_B * e^{m_j g \mu_B \mu_0 H / kT}}{\sum_{-m_j=j}^j e^{m_j g \mu_B \mu_0 H / kT}} \right]$$

On simplification, $M \propto \frac{Ng\mu_B\mu_0H}{kT}$

Thus, magnetic Susceptibility $\chi = \frac{M}{H} \propto \frac{Ng\mu_B\mu_0H}{kT} \propto \frac{C}{T}$

Which is classical Curie's law for paramagnetic materials

Curie's law is obeyed under conditions of low magnetization ($\mu_0 H \ll kT$),



*Paramagnetic susceptibility in the case $E \ll K_B T$
(Low magnetization)*



Case 2: ($m_j g \mu_B \mu_0 H \gg kT$) the magnetic interaction energy is much higher than the thermal energy , then the magnetization

$$M = N \left[\frac{\sum_{m_i=j}^j m_j g \mu_B * e^{m_j g \mu_B \mu_0 H / kT}}{\sum_{m_j=j}^j e^{m_j g \mu_B \mu_0 H / kT}} \right]$$

can be simplified as,

$$M = Ng\mu_B J \cdot B_j(a), \text{ where 'a' is } g\mu_B \mu_0 H / kT$$

$$\text{Where } B_j(a) = \left[\frac{2j+1}{2j} \coth \left(\frac{2j+1}{2j} a \right) - \frac{1}{2j} \coth \left(\frac{a}{2j} \right) \right]$$

Since, $m_j g \mu_B \mu_0 H \gg kT$, expansion of exponential term is not possible, thus we introduce Brillouin function

At low temperatures, all dipoles align along applied field H and lead to saturation of magnetization M_s

Is the Brillouin function which describes the field induced magnetization when $m_j g \mu_B \mu_0 H \gg kT$



At low temperatures, all dipoles align along applied field H , and lead to saturation of magnetization M_s

Thus, when $\frac{g\mu_B\mu_0H}{kT} \gg 1$ (*saturation magnetization*)

Brillouin function $B_j(a) \approx 1$

$$B_j(a) = \left[\frac{2j+1}{2j} \coth\left(\frac{2j+1}{2j}a\right) - \frac{1}{2j} \coth\left(\frac{a}{2j}\right) \right]$$

The Brillouin function is special_function, where 'a' ($\frac{g\mu_B\mu_0H}{kT}$) is a real variable and j is a positive integer or half-integer used in the calculation of magnetization. It describes the dependency of Magnetization (M) on applied field 'B' and microscopic magnetic moments of the materials (in terms of j)

Therefore, $M = Ng\mu_B J \cdot B_j(a) = Ng\mu_B J = M_s$

Hence, Magnetization can be written as, $M = Ng\mu_B J \cdot B_j(a) = M_s \cdot B_j(a)$



As per quantum theory of paramagnetism, we have the magnetization as

$$M = Ng\mu_B J \cdot B_j(a), \text{ where 'a' is } g\mu_B\mu_0 H / kT$$

$B_j(a)$ is the Brillouin function

We can infer from this equation that, it is similar to Langevin's expression with only difference is that in classical Langevin's theory dipoles can be oriented in all possible directions (classical approach)

The Brillouin and Langevin functions are a pair of special functions. In the Classical limit, magnetic moments can be continuously aligned in the field and j can assume all values. Then Brillouin function reduces to Langevin function.

Thus for large number of allowed orientation of magnetic dipole (classical approach, in the limit of j ($j=\infty$)), Brillouin function reduces to Langevin's function $L(a)$

$$B_j(a) = \left[\frac{2j+1}{2j} \coth \left(\frac{2j+1}{2j} a \right) - \frac{1}{2j} \coth \left(\frac{a}{2j} \right) \right] = \coth(a) - \frac{1}{a} = L, \text{ Langevin function}$$

Thus, Quantum result approaches the classical result!!



As per quantum theory of paramagnetism, we have the magnetization as

$$\mathbf{M} = N g \mu_B \mathbf{J} \cdot \mathbf{B}_j(a), \text{ where 'a' is } \frac{g \mu_B \mu_0 H}{kT}$$

$B_j(a)$ is the Brillouin function

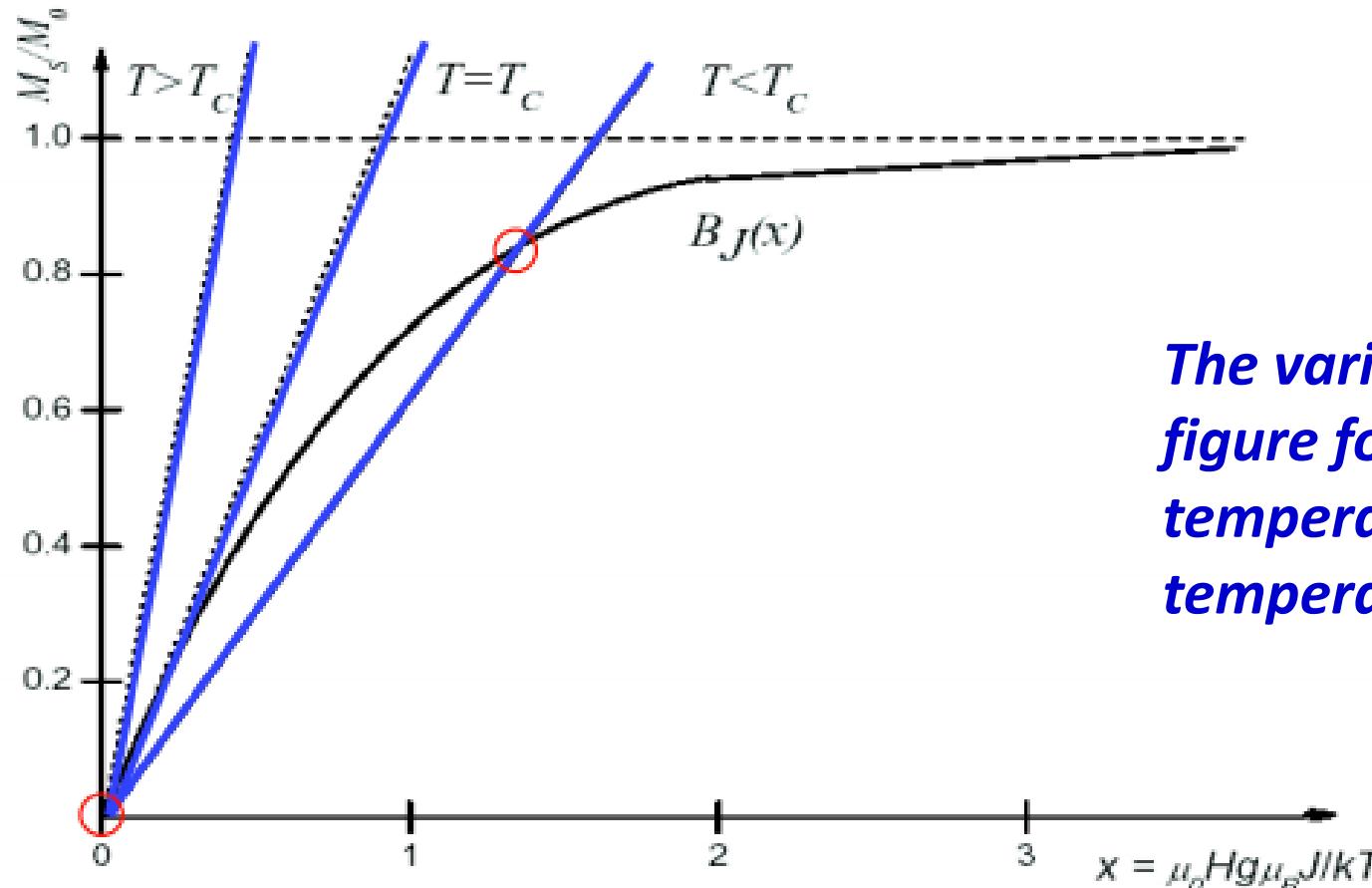
For large number of allowed orientation of magnetic dipole (classical approach, in the limit of j ($j=\text{infinity}$)), Brillouin function reduces to Langevin's function $L(a)$

$$B_j(a) = \left[\frac{2j+1}{2j} \coth\left(\frac{2j+1}{2j}a\right) - \frac{1}{2j} \coth\left(\frac{a}{2j}\right) \right]$$

When $j = \infty$, the first term reduces to $\coth(a)$ and second term to $1/a$

Thus, $B_\infty(a) = \coth(a) - \frac{1}{a}$ which is Langevin function

Thus, Quantum result approaches the classical result!!



The variation of M/M_s is represented in the figure for three different cases of the temperature (as compared to T_c the curie temperature of the material)

Importance of this study?! This theory leads naturally into the theory of Ferromagnetism

Brillouin function like classical Langevin function varies between zero to one, and with other values depend on the 'j' involved.

ENGINEERING PHYSICS

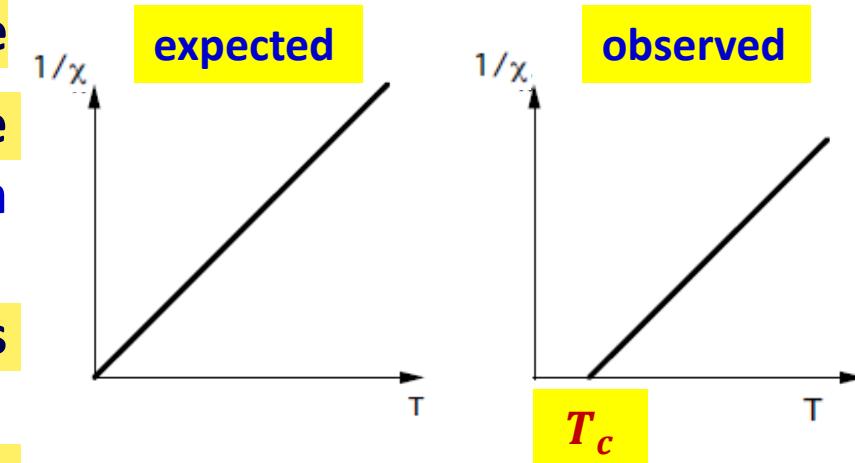
Weiss' molecular field: *Concept of Weiss Molecular Field*



PES
UNIVERSITY

Curie's law, $\chi = \frac{C}{T}$, based on individual magnetic moment don't interact with one another, only acted on by applied field and thermal agitation.

- The variation of $\frac{1}{\chi}$ v/s T is expected to be a straight line passing through the origin, but some materials show a positive intercept T_c on the temperature axis (a deviation from expected temperature dependence)
- Weiss showed that this is due to a 'molecular field' (a fictitious internal field) from the neighboring dipoles, as λM
- This field represents the interaction of the dipoles which leads to spontaneous magnetization



*Variation of inverse
of magnetic
susceptibility with
temperature*

Therefore, Curie's law is modified as, $\chi = \frac{M}{H(\text{total})} = \frac{M}{H + \lambda M} = \frac{C}{T} \rightarrow M(T - \lambda C) = CH$

Curie-Weiss law gives the magnetic susceptibility, $\chi = \frac{C}{T - T_c}$

$$\chi = \frac{M}{H} = \frac{C}{T - \lambda C}$$

Curie-Weiss law correctly describes the susceptibility variation

$\lambda C = T_c$, measure of strength of interaction

ENGINEERING PHYSICS

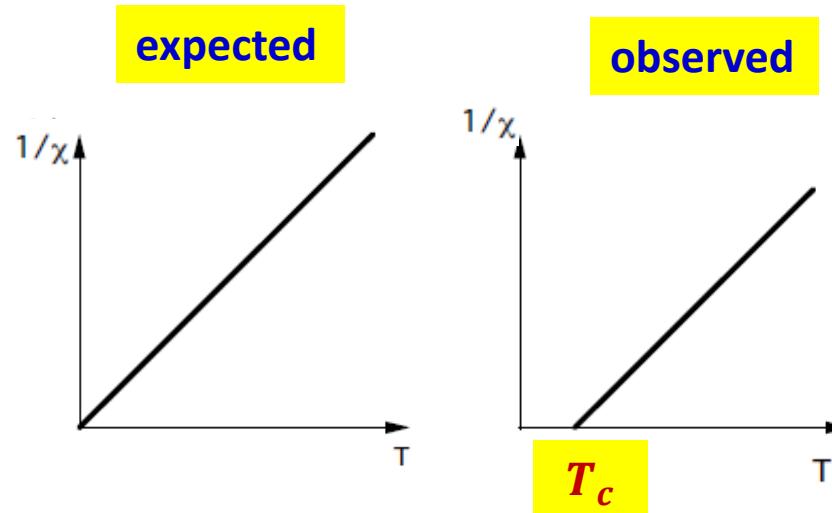
Weiss' molecular field: *Concept of Weiss Molecular Field*



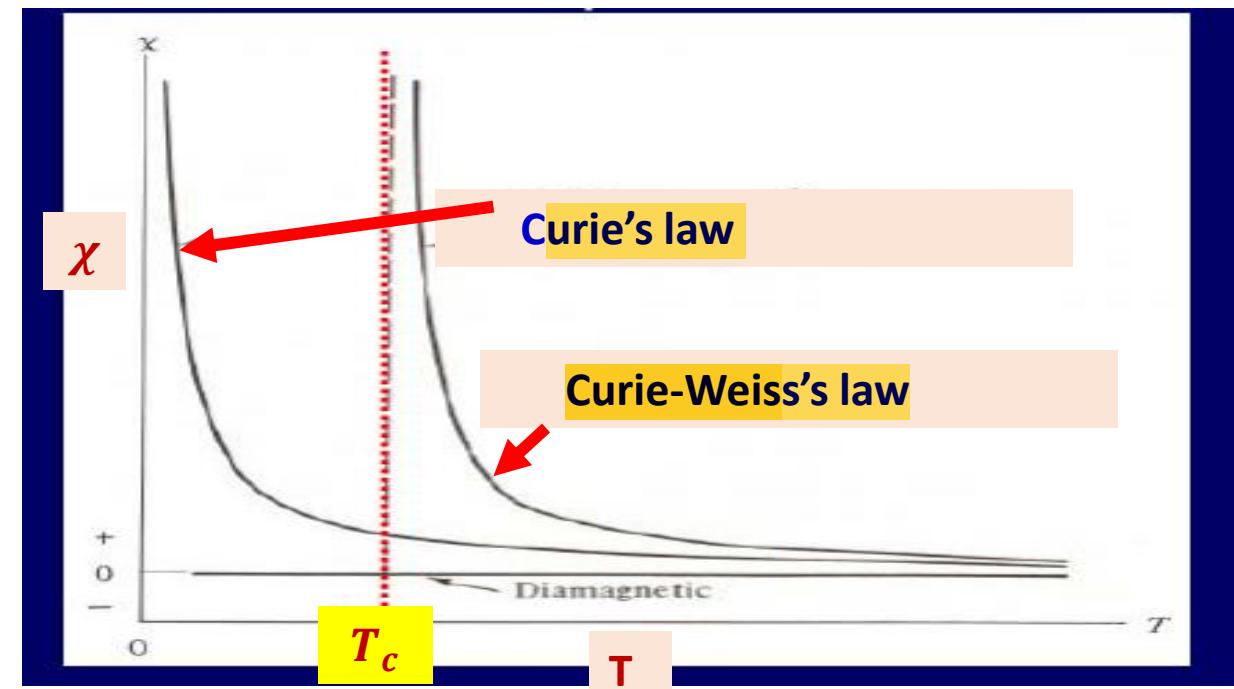
PES
UNIVERSITY

Curie's law, $\chi = \frac{C}{T}$, based on individual magnetic moment don't interact with one another, only acted on by applied field and thermal agitation.

- Weiss showed that this is due to a 'molecular field' (a fictitious internal field) from the neighboring dipoles, as λM
- This field represents the interaction of the dipoles which leads to spontaneous magnetization



Variation of inverse of magnetic susceptibility with temperature



Obtain an expression for magnetic interaction energy of a magnetic dipole in an external field.

Arrive at an expression for magnetization of a paramagnetic materials when placed in an external magnetic field such that the thermal energy dominates magnetic interaction energy.



PES
UNIVERSITY

THANK YOU

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629



PES
UNIVERSITY

ENGINEERING PHYSICS

Department of Science & Humanities

ENGINEERING PHYSICS

Unit III : Application of Quantum Mechanics to Electrical Transport in Solids



➤ *Suggested Reading*

1. *Concepts of Modern Physics, Arthur Beiser, Chapter 10*
2. *Learning material prepared by the department-Unit III*

➤ *Reference Videos*

1. <https://nptel.ac.in/courses/115/104/115104109/>
2. <https://physlab.org/class-demo/meissner-effect/>

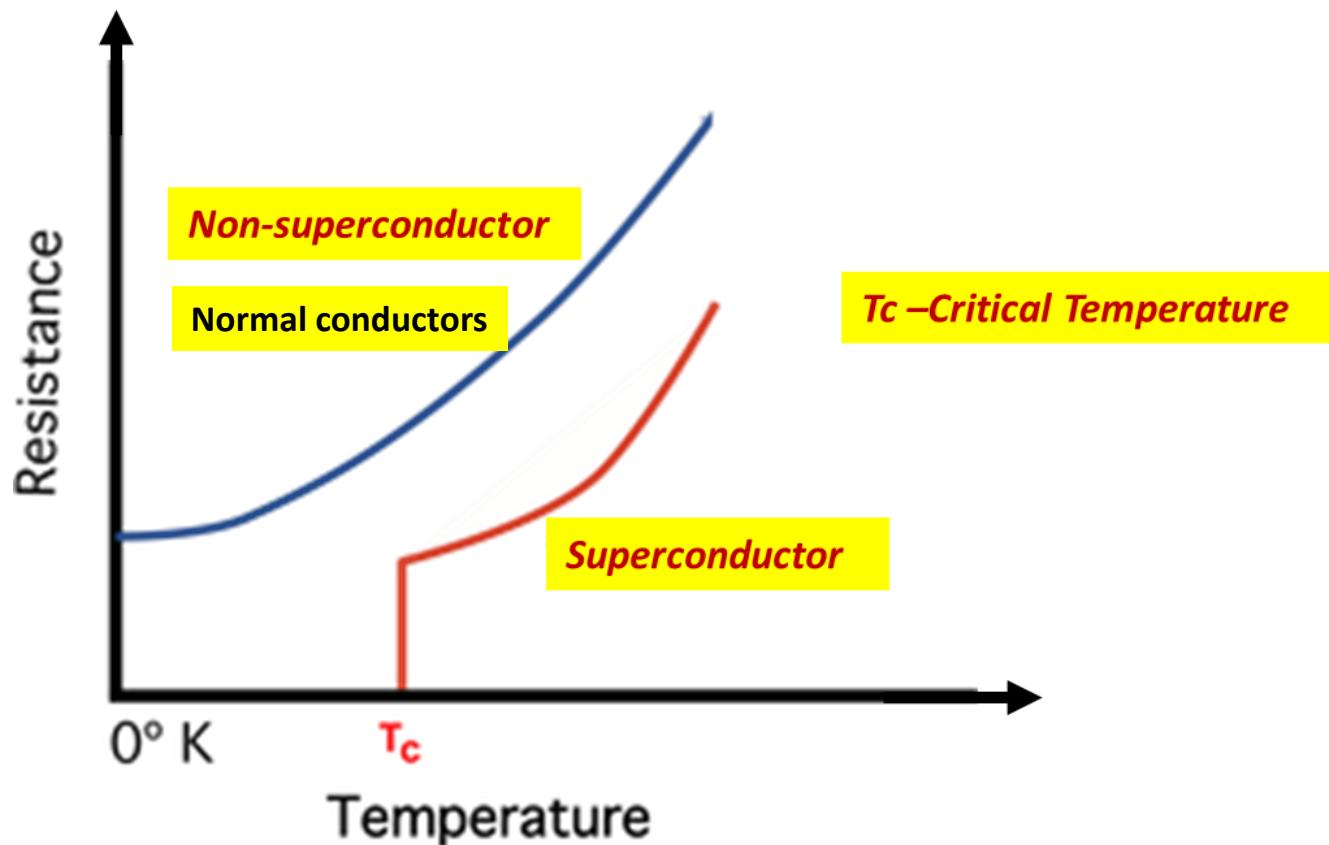
Class #29

Superconductivity as a phenomenon

- *Meissner effect & Critical Field*
- *Type I and type II superconductors*
- *BCS Theory of Superconductors*

Superconductivity as an unusual electrical phenomenon

Superconductivity was discovered by H. Kammerlingh Onnes in 1911.



Superconductivity:

An unusual property of certain metals, alloys, and ceramics in which electrical resistance drops to zero when the temperature is reduced below a critical value (T_c - known as the transition temperature)

Material	T_c [K]
Pb	7.2
Nb	9.2
Nb-Ti alloys	~ 9.6
Nb_3Sn	18.1
Nb_3Ge	23.2
$Y_1Ba_2Cu_3O_{7-x}$ (YBCO)	90
$Bi_2Sr_2Ca_1Cu_2O$ (Bi2212)	80
$Bi_2Sr_2Ca_2Cu_3O$ (Bi2223)	125

ENGINEERING PHYSICS

General properties of superconductors: Effect of magnetic field

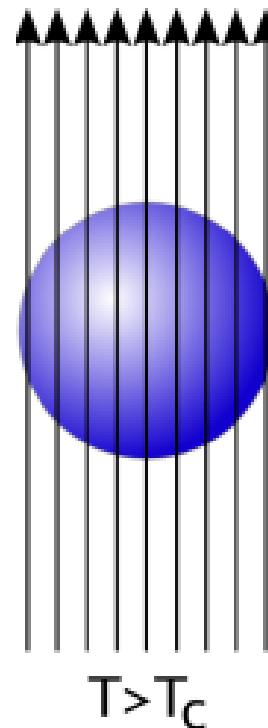
Diamagnetic property: Meissner effect

Superconductors exhibit unique features other than their ability to perfectly conduct current

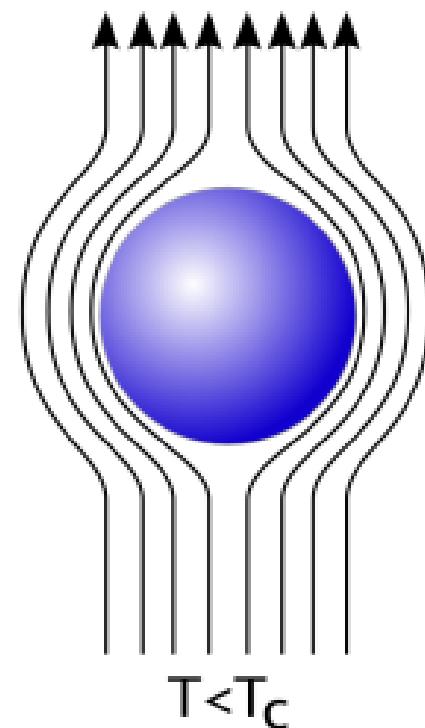
Superconductors expel magnetic fields during the transition to the superconducting state- like a perfect diamagnetic material

This property is called Meissner effect

Normal state, $B \neq 0$



Superconducting state, $B = 0$



ENGINEERING PHYSICS

General properties of superconductors

Critical field

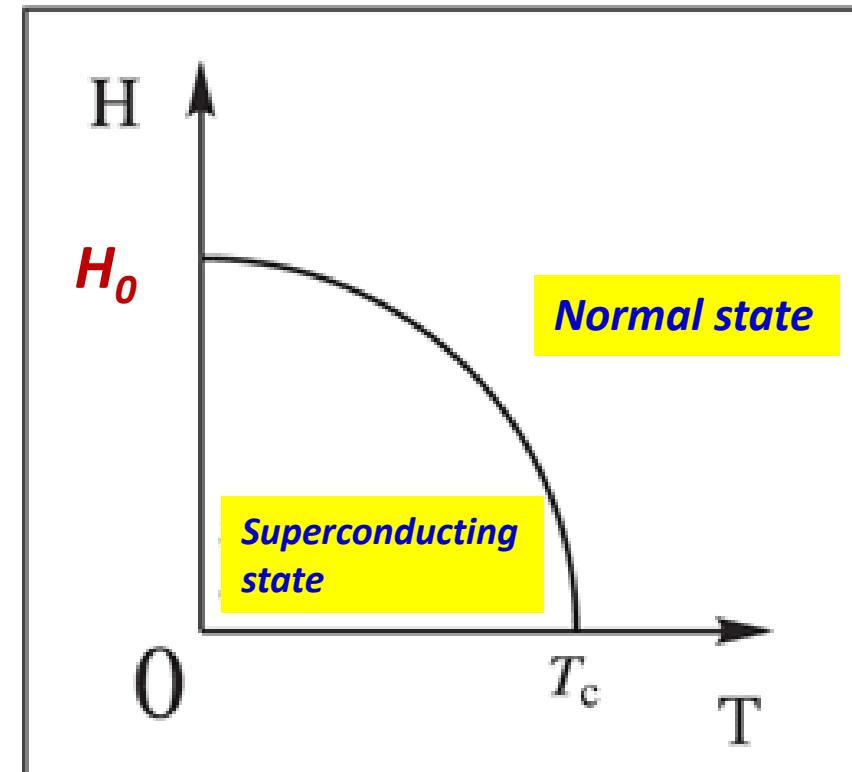
Presence of strong external fields – drives superconducting material to normal conducting state (destruction of superconducting property)

Magnetic field at which the material loses its superconducting state - Critical Field (H_c)

The critical field strength is temperature dependent

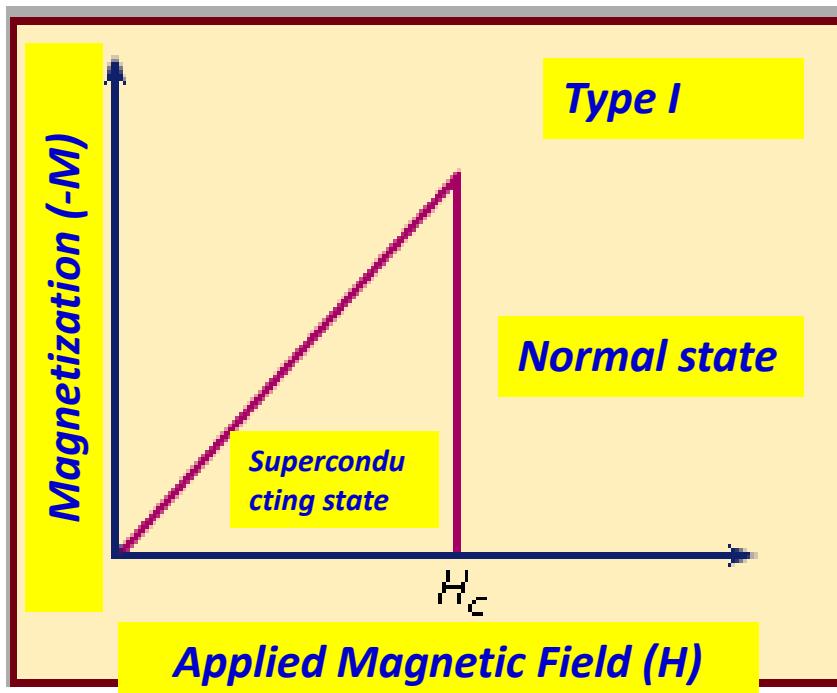
and is given by
$$H_c = H_0 \left[1 - \left(\frac{T}{T_c} \right)^2 \right]$$

H_0 is the magnetic field required to destroy the superconducting property at 0 K



Critical Field (H_c) increases if temp decreases

Type I superconductors (Soft superconductors):



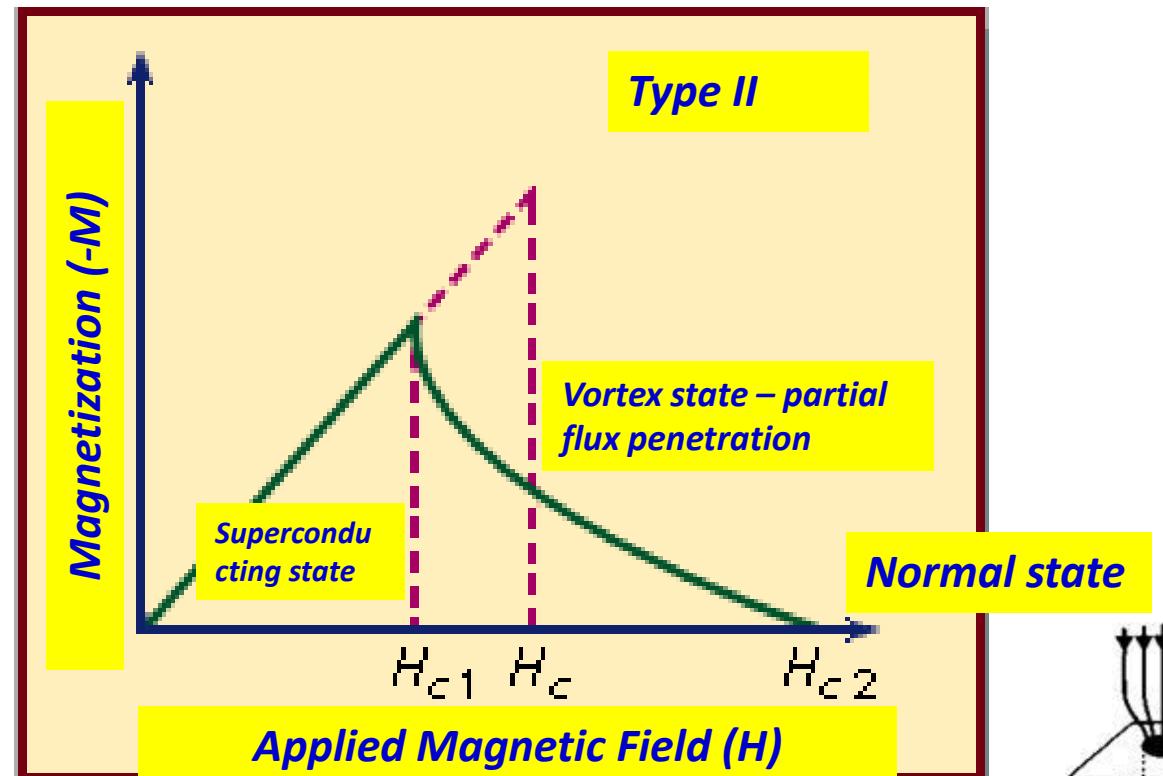
Type I superconductors exhibit complete Meissner effect

In the presence of external magnetic field $H < H_c$, the material in superconducting state

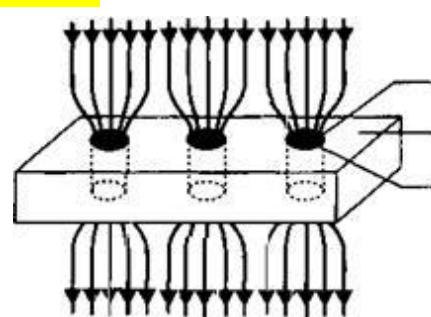
*As soon as H exceeds H_c , the material become normal
Type I material has very low values of H_c*

Examples for Type I superconductors - Aluminum, Lead and Indium etc.

Type II superconductors:



*Type II superconductors have two critical fields H_{c1} and H_{c2} and practically important
Behave as perfect superconductor up to H_{c1}
Above H_{c1} magnetic flux starts to penetrate
(mixed state –Vortex state) up to H_{c2}
Above H_{c2} material behave as normal
 H_{c1} and H_{c2} – lower critical field and upper
critical filed*

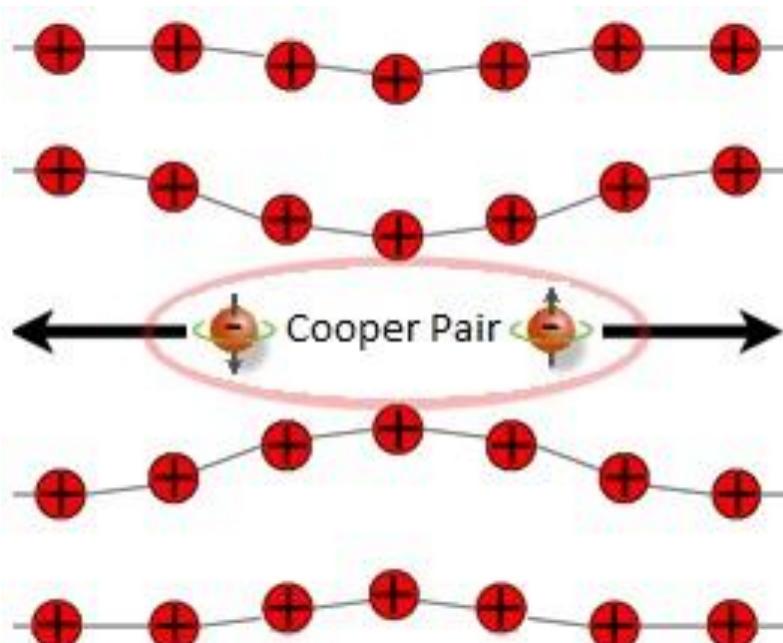


*Examples for type II superconductors:
Transition metals and alloys containing
niobium, silicon and vanadium.*

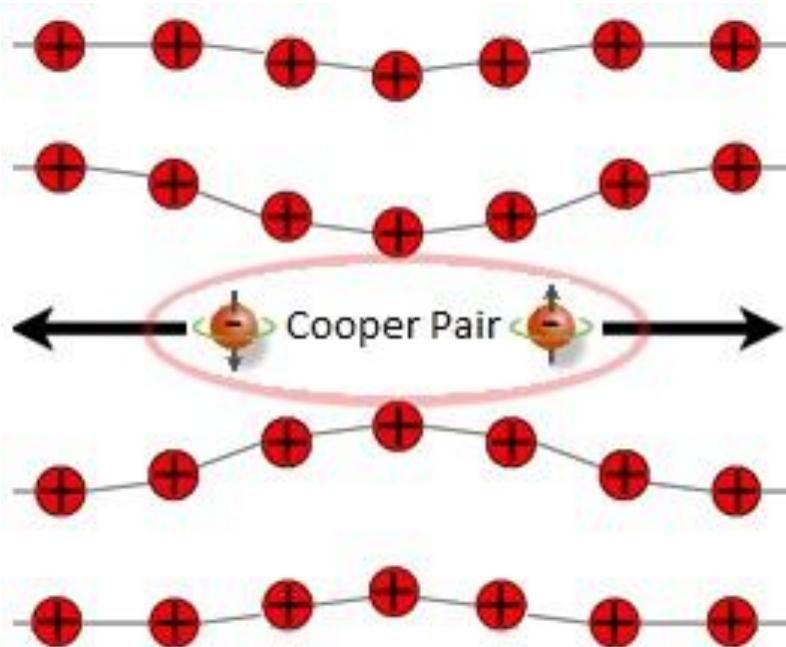
Vortex state – partial flux penetration through filaments

- *Current in the superconductor persists for a long time.*
- *Not observed in Mono valent metals.*
- *Exhibited by metals for which the valence electrons number are between 2 & 8.*
- *Observed in metals having a higher resistivity at normal temperatures .*
- *Destroyed by applying high magnetic fields or excessive currents.*
- *Ferro and anti ferromagnetic materials are not superconductors.*

Theory of superconductivity was given by J. Bardeen, L.N. Cooper and J.R. Schrieffer in the year 1957



- **Based on the formation of Cooper pairs**
- **During electron flow, because of opposite polarity between electron and ion core, results in lattice distortion (phonons)**
- **Lattice distortion results in the interaction of another electron – as interaction between two electrons via lattice**
- **If the electrons have equal and opposite spins and opposite momentum, electron-lattice (phonon field)-electron interaction exceed Coulomb repulsive force forming Cooper pairs (quantum pairs – bosons, electrons – fermions, Higgs particles and photons - bosons)**



- *The energy required to separate the pairs is far too large compared to the thermal energy available*
- *Cooper pairs collectively move through the lattice with small velocity*
- *Low speed reduces collisions and decreases resistivity, which explains superconductivity*
- *The attraction between the electrons in the Cooper pair can be separated by a small increase in temperature, which results in a transition back to the normal state*

- **MAGLEV VEHICLES – Magnetic levitation based on Meissner effect**
- **MRI – Magnetic response imaging**

The concepts which are correct are....

1. *Superconductivity cannot be destroyed by a high magnetic field or excessive currents.*
2. *Materials in the superconducting state, expels the magnetic lines of force.*
3. *Type I superconductors exhibits mixed state Meissner effect.*
4. *The electrons in the Cooper pair have either equal spins or opposite momentum.*

ENGINEERING PHYSICS

Class 33 . Numericals...

Superconducting tin has a critical temperature of 3.7 K with critical field of 0.0306 T. Find the critical field at 2 K.

$$H_c = H_0 \left[1 - \left(\frac{T}{T_c} \right)^2 \right]$$

Given, $T_c = 3.7 \text{ K}$, $H_0 = 0.0306 \text{ T}$

$$H_c = 0.0306 \left[1 - \frac{(2)^2}{(3.7)^2} = 0.0217 \text{ T} \right]$$

ENGINEERING PHYSICS

Class 33 . Numericals...

Calculate the critical field for a Superconducting wire at 4.2 K.

Critical temperature for lead is 7.18 K and $H_c(0)$ is 6.5×10^4 T.

$$H_c = H_o \left[1 - \left(\frac{T}{T_c} \right)^2 \right]$$

Given, $T_c = 7.18$ K, $H_0 = 6.5 \times 10^4$ T

$$H_c = 6.5 \times 10^4 \left[1 - \frac{(4.2)^2}{(7.18)^2} \right] = 42.76 \times 10^3 \text{ T}$$

ENGINEERING PHYSICS

Class 33 . Conceptual questions...

Explain BCS theory.

Explain Meissner effect.

ENGINEERING PHYSICS

Class 33 . Conceptual questions...

Justify the negative magnetic moment observed in superconductors.

**Explain the validity of Meissner effect in type I and type II superconductors.
Which interaction is responsible for superconductivity?**

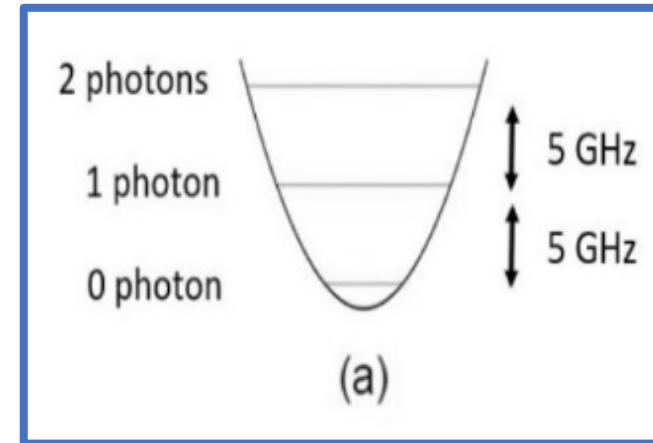
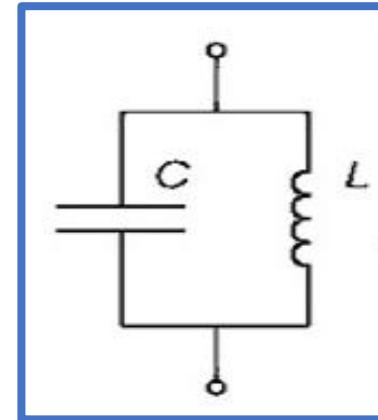
Superconducting Qubits – Transmon Oscillator

As we know as **LC circuit is known as tank circuit producing harmonic oscillations**

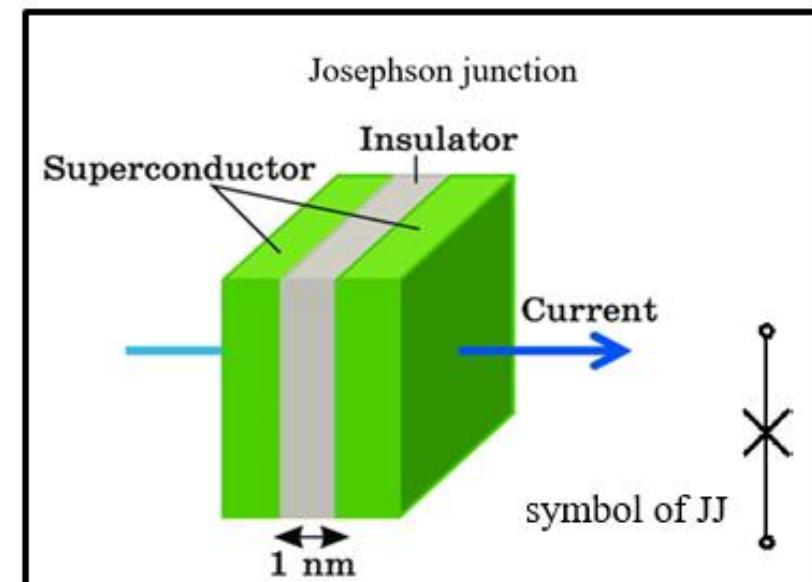
In the case of the LC circuit the total energy in the circuit is $\frac{1}{2}Li^2 + \frac{1}{2}CV^2$ which can be written in terms of the magnetic flux and the charges as is $H = \frac{1}{2L}\varphi^2 + \frac{1}{2C}q^2$.

In operator notation, (Hamiltonian operator) $\hat{H} = \frac{1}{2L}\hat{\varphi}^2 + \frac{1}{2C}\hat{Q}^2$

By modifying this harmonic LC circuit (**linear**) can be used for realizing Quantum computing circuit elements. An example is Transmon oscillator where anharmonicity (**nonlinear element**) is introduced by replacing the inductor element with **Josephson Junction**. This results in energy levels with controllable excitation energies and this can be the equivalent of an **artificial atom**.



Quantum LC Oscillator – Harmonic with equally spaced energy states



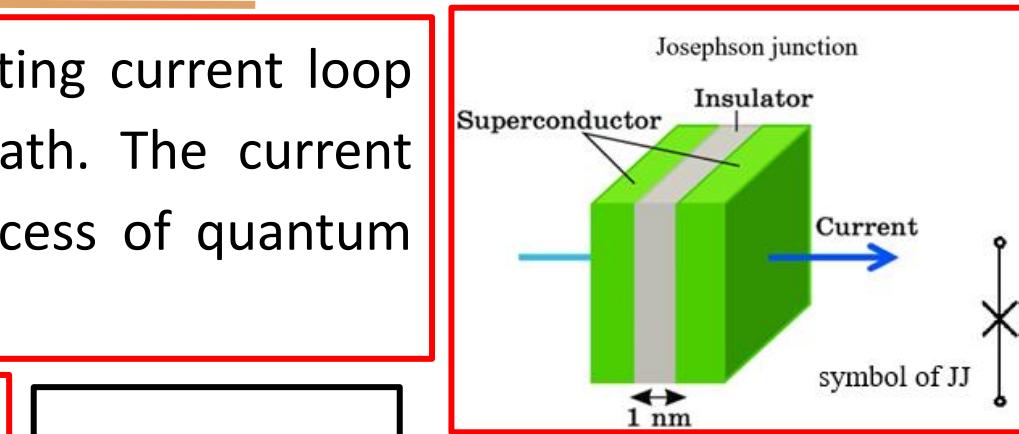
Superconducting Qubits – Transmon Qubits

Superconducting Josephson junction (JJ) - a superconducting current loop with a thin layer of insulating material in the current path. The current continues to flow crossing the insulating layer by the process of quantum tunnelling of the Cooper pairs.

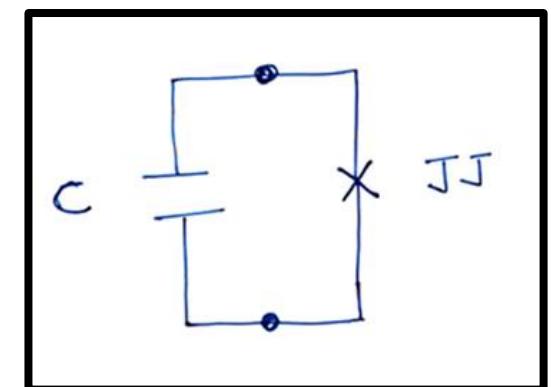
The current through the JJ can be written as

$I = I_c \sin \phi$ where ϕ is the phase difference introduced by the JJ junction and the energy in the circuit is given by $E = E_j \cos \phi$

Thus, the total energy of the system is cosine function which is nonlinear.



$$I = I_c \sin(\phi)$$

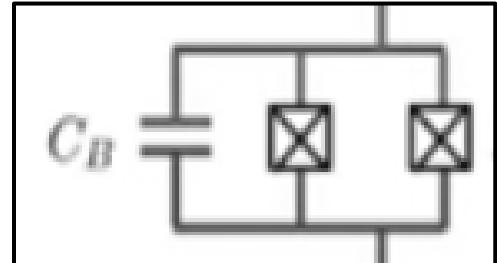


Transmon Oscillator

Thus Qubit states can be optimized using this modified Transmon oscillator (like, ground state and the first excited states in the Transmon qubit correspond to the $|0\rangle$ and $|1\rangle$ states). The qubit excitation is achieved using microwave pulses of the precise frequency influencing the anharmonicity. Thus, the qubit in the $|0\rangle$ state can be excited to the $|1\rangle$ using electromagnetic energy pulses .

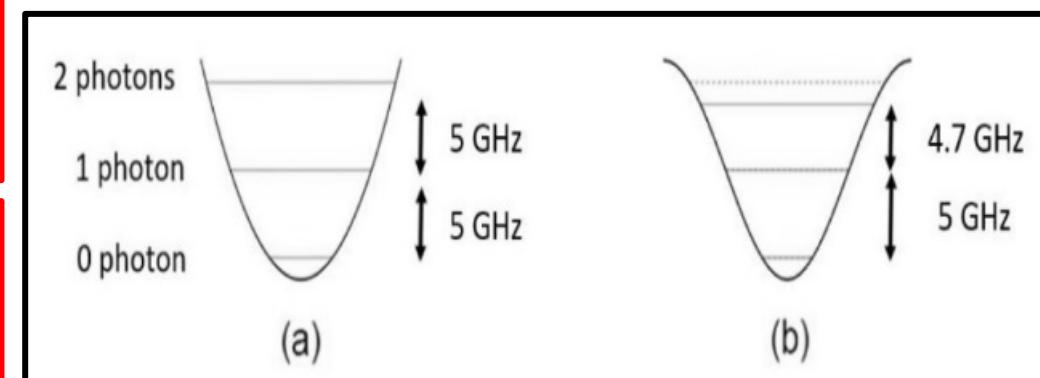
Superconducting Qubits – Transmon Qubits and Cooper Pair Box

A pair of Josephson Junction in parallel with the capacitor element effectively creates what is referred to as a Cooper Pair Box (CPB), which has a pair of distinct energy states between which the switching can take place.



The graphical representation shows the differences in the excitation energy states of the LC oscillator with harmonicity and cooper pair box with anharmonicity.

Cooper Pair Box



Transmon qubits are preferred over other qubit possibilities like atomic, nuclear, molecular, spin or polarization states because of the following reasons:

- easier to fabricate and scale up to circuit level electronics
- noise resistant by providing sufficient isolation from the environment
- controlled accurately with microwave pulses
- easy integration of the technology with standard IC fabrication methods

Structure of a Transmon Qubit

A transmon is essentially a modified LC circuit where:

- Inductor (L) is replaced with a Josephson junction (a nonlinear, superconducting element).
- Capacitor (C) remains.

Why Use a Josephson Junction?

- A Josephson junction behaves like a nonlinear inductor.
- This nonlinearity causes the energy levels to be unequally spaced—allowing you to define a qubit with the lowest two states ($|0\rangle$ and $|1\rangle$).
- The third level ($|2\rangle$) is sufficiently far to avoid accidental excitation during operations.

The Josephson junction introduces nonlinearity

The large capacitor (shunting capacitor) improves stability

The result is a quantum two-level system optimized for computation



PES
UNIVERSITY

THANK YOU

Muhammad Faisal, Ph.D.

Associate Professor, Department of Science and Humanities

muhammadfaisal@pes.edu

+91 80 50829629