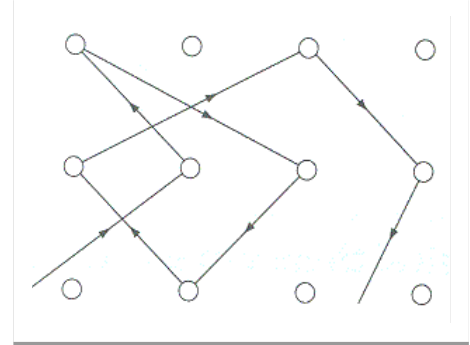


1 Basics of CFET, expressions for electrical parameters

Drude and Lorentz proposed the classical free electron theory of electrical conductivity of metals (as early as 1904). The model of conductivity of free electrons is based on the following assumptions:

- (1) The valence electrons of the atoms of the metal contribute to the conduction process either electrical or thermal. The electrons move in an array of ion cores (which are nuclei surrounded by inner electrons excluding the valance electrons). All the valance electrons are free electrons and are treated as conduction electrons which are in a state of random motion (like the molecules in an ideal gas).
- (2) The effect of positive ion cores on the electrons is considered to be constant and hence neglected.
- (3) The electrostatic repulsion between the electrons is neglected.
- (4) The electrons in the metal are considered equivalent to molecules in a gas and the gas laws are made applicable to the electrons in a metal. Accordingly, the distribution of energy and velocity is assumed to follow Maxwell-Boltzmann statistics.



The average velocity of electrons in the metal is dependent on the temperature of the metal and is termed as the thermal velocity of electrons $v_{th} = \sqrt{\frac{3kT}{m}}$. At 300K the thermal velocity of the electrons is $v_{th} \approx 10^5 \text{ m s}^{-1}$.

However this random motion of the electrons do not contribute to a net drift of electrons across the metal and hence no current flows through the material

The conduction electrons in the lattice are scattered by collisions with the ionic cores and other electrons. The mean time between collisions is the relaxation time of the electrons in the metal and the distance between successive collisions is the mean free path. Taking the mean lattice parameter of 10nm as the mean free path λ , the relaxation time can be estimated

$$\tau = \frac{\lambda}{v_{th}} \approx 10^{-15} \text{ s}.$$

Drift Velocity : In the presence of an Electric field E the electrons show a net drift across the metal in a direction opposite to that of the electric field. The velocity of the electrons across the metal in the presence is known as the drift velocity v_d .

The force equation for the electron's motion can be described by $m \frac{dv}{dt} = eE - kmv$ where the last term accounts for the loss of energy due to the scattering which is proportional to the momentum of the electrons and k is the coefficient of scattering loss.

In the equilibrium condition this leads to an average velocity for the electrons which is the drift velocity $v_d = \frac{eE}{km}$

Dimensionally k should be $(\text{time})^{-1}$.

The decay of the drift velocity to zero in the absence of the electric field yields that $k = \frac{1}{\tau}$ where τ is the relaxation time – the time between successive collisions or the time for the drift velocity to fall to $1/e$ times its steady value in the presence of an electric field.

The drift velocity $v_d = \frac{e\tau E}{m} = \mu E$ where $\mu = \frac{e\tau}{m}$ is the **electron mobility or the charge carrier mobility**. The mobility $\mu = \frac{e\tau}{m} = \frac{v_d}{E}$ is the drift velocity per unit electric field.

The drift velocity of electrons is extremely low compared to the thermal velocity. To illustrate, the drift velocity of electrons experiencing an electric field of 1V/m is of the order of 10^{-4} ms^{-1} .

Expression for Electrical conductivity:

The current through a conductor with an electron concentration n of cross section A and length L at an applied electric field E can be evaluated as

$$I = ne v_d A \text{ where } v_d \text{ is the drift velocity given by } v_d = \frac{e\tau E}{m}$$

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

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

$$\text{metal } \sigma = \frac{ne^2\tau}{m} = ne\mu$$

$$\text{The resistivity of the metal is } \rho = \frac{1}{\sigma} = \frac{m}{ne^2\tau} = \frac{1}{ne\mu}.$$

The resistivity is inversely proportional to the concentration of free electrons and the relaxation time of electrons in the metal.

2 Experimental temperature dependence of the resistivity

Experiments show that resistivity of metals in general vary linearly with temperature in the normal operating temperatures. At these temperatures the resistivity ρ_{sc} results from the scattering of the electrons moving with high thermal velocities in random directions.

However at very low temperatures the resistivity ρ_{res} is found to saturate to a non zero finite value, which is dependent on the impurity concentration in the metal.

Hence two independent types of resistivities determine the total resistivity of the metal. Since the phenomena are independent of each other the net resistivity would be the sum of the two resistivity components which is known as the Mattheissen's rule .

$$\rho = \rho_{res} + \rho_{sc}$$

Hence $\frac{m}{ne^2\tau} = \frac{m}{ne^2\tau_{res}} + \frac{m}{ne^2\tau_{sc}}$. This gives us the effective relaxation time as $\frac{1}{\tau} = \frac{1}{\tau_{res}} + \frac{1}{\tau_{sc}}$

3 Draw backs of CFET and quantum corrections.

The classical free electron theory failed to correlate the experimental results of many a phenomena such as the temperature dependence of resistivity, specific heat of electrons etc.

- a. According to the classical free electron theory the resistivity of a metal is given by $\rho = \frac{m}{ne^2\tau}$

. For a given material the temperature dependence of resistivity arises from the

temperature dependence of the relaxation time $\tau = \frac{\lambda}{v_{th}}$. Since the mean free path of the electrons is assumed to be a constant for a wide range of metals, the temperature dependence of the thermal velocity should affect the relaxation time. For a given

temperature $v_{th} = \sqrt{\frac{3k_B T}{m}}$ and hence $v_{th} \propto \sqrt{T}$ $\therefore \tau \propto T^{-\frac{1}{2}}$. Since the resistivity $\rho \propto \tau^{-1}$, the temperature dependence should be given by $\rho \propto \sqrt{T}$. But the experimental observations show that $\rho \propto T$ and hence the classical free electron theory fails to explain the correct temperature dependence of resistivity of metals.

- b. The contribution of electrons to the specific heat of the metal can be estimated using the principle that the specific heat $C_{el} = \frac{dU}{dT}$.

Considering one mole of a mono valent material the energy of the electrons $U =$

$$\frac{3}{2} k_B T \cdot N_{avg}$$

Hence the specific heat of the electrons should be equal to $C_{el} = \frac{dU}{dT} = \frac{3}{2} k_B \cdot N_{avg} = \frac{3}{2} R$

which is a constant.

However the experimental estimation of the specific heat of electrons is only approximately 1% of the theoretical value and is also found to be temperature dependent. Thus the theory fails to explain the actual specific heat dependence of electrons in metals.

- c. The electrical conductivity of metals, given by $\sigma = \frac{ne^2\tau}{m}$, should be dependent on the free electron concentration for a given temperature, assuming that the relaxation time is more or less constant. However, it found that mono valent Copper with lesser electronic concentration has a higher electrical conductivity as compared to trivalent Aluminum. Similarly Zinc with higher electronic concentration has lesser conductivity than Aluminum. Experimental results show that there is no linear dependence of the electronic concentration on the conductivity of metals.

Thus the classical free electron theory fails to explain the experimental observations. It is obvious that some of the assumptions of the CFET are over / underestimations of the physical parameters and hence need to be corrected.

4 Quantum model of valence electrons in a metal - Fermi energy

Metals have a very high concentration of valence electrons $\cong 10^{28} m^{-3}$. According to the quantum mechanical principles these valence electrons in a metal have to be in discrete energy states following Pauli's exclusion principle. This requires the energy states of the atomic levels to split into discrete closely spaced energy states to accommodate all the valence electrons. At 0K such an arrangement leads to a sea of energy levels which have a separation as small as $\cong 10^{-20} eV$. The upper most occupied energy state at 0K is then termed as the Fermi energy of the metal. Thus at 0K all the states below the Fermi energy are filled and all the states about the Fermi energy are empty.

By convention electrons above the Fermi level should contribute to the conduction process and the valence electrons are below the Fermi level. (The electrons in states below the Fermi level do not contribute to the conduction process). Thus according to this model not all the valence electrons in a metal are not conduction electrons.

The effective number of electrons above the Fermi level could be approximated as $n_{eff} = n \frac{kT}{E_f}$.

The effective number of electrons above the Fermi level for copper ($E_f=7eV$) at 300K can be calculated to be $n_{eff} = n \frac{kT}{E_f} = n * 0.0036 = n * 0.36\%$. Thus a small fraction of the available valence electrons are excited into states above the Fermi level.

This quantum model of the free electrons gives rise to the following modifications to the free electron theory:

- The valence electrons in the metal are arranged in discrete energy states following Pauli's exclusion principle. Only electrons close to the Fermi level participate in the conduction process
- The conduction electrons in a metal move in array of positive ions, colliding with the ionic centers and other electrons resulting in the resistance of the material.
- The electrostatic interactions namely, the electron – electron interaction and the electron – ion interactions are negligible.
- The electrons undergo random scattering due to the vibrating ionic centers giving rise to resistance to flow of electrons.

5 Fermi Dirac statistics, Fermi factor

The occupation probabilities of electrons in the different energy state at different temperatures are estimated using the Fermi Dirac statistics for Fermions. (All particles with spin $\pm \frac{1}{2}$ are classified as Fermions. Fermions follow the Fermi Dirac statistics for particles which are indistinguishable.)

The 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

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

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

At 0K this becomes $F_d = \frac{1}{\left(e^{-[\infty]} + 1 \right)} = 1$. This implies that at 0K all electron states below the Fermi level are filled states.

- If $E > E_f$ then for $E - E_f$ is positive, then

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

At 0K this becomes $F_d = \frac{1}{\left(e^{[\infty]} + 1 \right)} = 0$.

This implies that at 0K all electron states above the Fermi level are empty states.

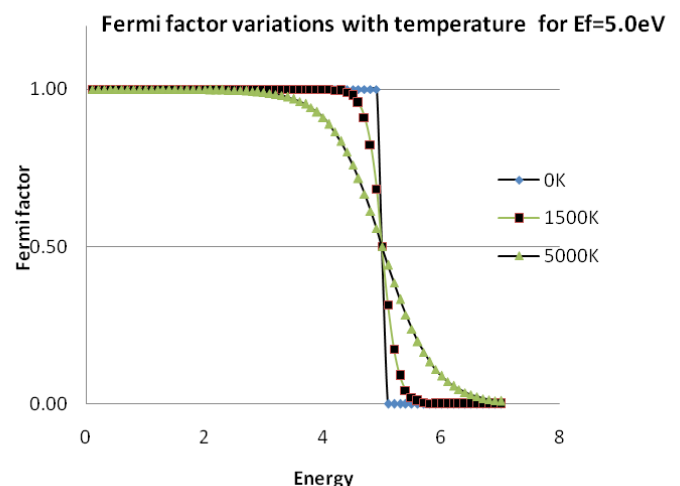
- For $T > 0$ and $E = E_f$ the Fermi factor

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

. This

gives a probability of occupation of 50% for the Fermi energy.

The Fermi energy has a weak temperature dependence and is given by



$$E_f = E_{f0} \left[1 - \frac{\pi^2}{12} \left(\frac{k_B T}{E_{f0}} \right)^2 \right]$$

where E_{f0} is the Fermi energy at zero Kelvin. At normal temperature ranges the ratio of $\frac{k_B T}{E_{f0}}$ is very low and hence can be approximated to be a constant equal to the value at zero Kelvin.

6 Fermi temperature

The arrangement of electrons in discrete energy states leads to the concept that only electrons near the Fermi energy are excited into the conduction band and it may be really difficult to excite all the valence electrons into the conduction band. If the temperature of the metal is T then $k_B T$ is the thermal energy available to the electrons in the metal. The thermal energy required to excite the last electron at the bottom of the energy band if termed as $k_B T_f$, then at temperature T_f the electron would have an energy $E_f = k_B T_f$. This temperature is termed as the Fermi temperature of electrons in the metal.

Evaluating the temperature for Copper with Fermi energy as 7 eV gives the value of the Fermi temperature as approximately 81000K. It is obvious that at such high temperatures the metal cannot be in the solid state and hence this is only a representative temperature which highlights the point that all valence electrons cannot be conduction electrons.

7 Fermi velocity

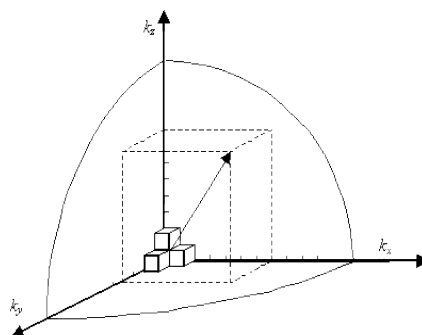
From the above analysis it is clear that only a small fraction of electrons close to the conduction band can be taking part in the conduction processes. The electrons excited into the conduction band have energies very close to the Fermi energy. These conduction electrons then possess a kinetic energy which may be equal to the Fermi energy.

The kinetic energy of the electrons near the Fermi energy is $E_f = \frac{1}{2} m v_f^2$ where v_f the Fermi velocity of conduction electrons is. Fermi velocity for conduction electrons in Copper gives $v_f = 1.06 \times 10^6 \text{ m s}^{-1}$.

This velocity is greater than the thermal velocity of electrons (as per the CFET). The electrons in the conduction band are in a state of random motion and the scattering of the electrons by the lattice is the origin of the electrical resistance of the metal.

8 Density of states derivation

The electrons in a metal can be approximated to the particle in a box in three dimensions, since under normal conditions the electrons cannot escape the boundaries of the metal. Consider a mono valent metal in the form of a cube of side L . Inside the metal the electrons can be assumed to be moving in a zero potential field.



The three dimensional Schrödinger's wave equation can be written as three one dimensional Schrödinger's wave equation and their corresponding solutions analysed.

$$\frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} + E \psi(x) = 0 \quad \text{which gives the Eigen energy value for the x component as}$$

$$E_{n_x} = \frac{h^2 n_x^2}{8mL^2}$$

Similarly the energy in the other two dimensions can be evaluated as $E_{n_y} = \frac{h^2 n_y^2}{8mL^2}$ and $E_{n_z} = \frac{h^2 n_z^2}{8mL^2}$

The total energy of the electron is given by

$$E_n = \frac{h^2}{8mL^2} (n_x^2 + n_y^2 + n_z^2) = \frac{h^2}{8mL^2} R^2 \quad \text{----- (1) where } R^2 = n_x^2 + n_y^2 + n_z^2$$

The number of states with energy E can be evaluated by studying the variation of the combinations of n_x , n_y and n_z . It can be deduced that every combination of n_x , n_y and n_z result in an energy state as per equation (1). When n_x , n_y and n_z are equal the energy state is unique and is non degenerate. It is also noted that the energy states can be degenerate with degeneracy of 3 when two of the three n_x , n_y and n_z are equal and degeneracy of 6 when all the three are not equal. This can be evaluated analyzing the n space formed by n_x , n_y and n_z . It is also realized that every combination of n_x , n_y and n_z gives additional unit volume in **n space** from which we conclude that evaluating the number of states is equivalent to evaluating the volume of the **n space**. It is also noticed that the degenerate energy states with the same energy values lie on the surface of an octant of a sphere with the center at the origin. Hence it is sufficient to find the volume of the octant of a sphere of radius R to evaluate the number of energy states up to R i.e., the combination of n_x , n_y and n_z .

The sensitivity of the increase in the states with increasing n_x , n_y and n_z can be found from the change in the volume of the octant if the radius changes from R to R+dR realizing that $R \gg dR$.

The volume of the shell of thickness dR is then given by $\frac{\pi R^2 dR}{2}$

$$E_n \leq E_o \quad \text{gives us } R^2 = \frac{E_n}{E_o} \quad \text{and} \quad dR = \frac{dE}{2 \left(\frac{E_n E_o}{2} \right)^{\frac{1}{2}}}$$

The number of energy states between E and E+dE is given by

$$\frac{\pi R^2 dR}{2} = \frac{\pi}{4} \frac{E_n}{E_o} \frac{dE}{\left(\frac{E_n E_o}{2} \right)^{\frac{1}{2}}} = \frac{\pi}{4} \cdot \frac{E_n^{\frac{1}{2}}}{E_o^{\frac{3}{2}}} dE$$

Substituting for $E_o = \frac{h^2}{8mL^2}$ we get the number of energy states between E and E+dE as

$$\frac{\pi}{4} \cdot \left(\frac{8mL^2}{h^2} \right)^{\frac{3}{2}} E^{\frac{1}{2}} \cdot dE$$

Taking into consideration the Pauli's exclusion principle, two electrons can be accommodated in one energy state, the number of electrons states per unit volume can be estimated and is called as the density of states.

The density of states for electrons in a metal gives the number of electron states per unit volume with energy E

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

This shows that the distribution of electrons in energy states vary non- linearly with increasing energy E.

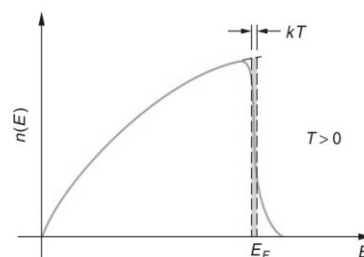
The probability that an energy state is occupied is given by the fermi factor

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

And hence the occupancy of the states described by N(E) is determined by the factor

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

The states below $E_f - k_B T$ are completely occupied as F_d is 1. The states in the range of $k_B T$ below the Fermi level are emptied and the probability of occupancy F_d is between 1 and 0.5. The states above E_f in a range $k_B T$ are now occupied and the probability of occupancy lies between 0.50 and 0.00.



9 Expression for Fermi energy, average electron energy

The Fermi energy of metals can be evaluated from the fact that all available electrons occupy energy levels below the Fermi level E_f . This means that the density of occupied states

$N(E) = g(E) * F_d$ when evaluated for all levels from 0 to E_f , should result in the total count of electrons in the metal, ie.,

$$\text{The total free electronic concentration } n = \int_0^{E_f} N(E) dE = \int_0^{E_f} g(E) * F_d dE.$$

We know that F_d has to be 1 for all energy levels below E_f at 0K and hence

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

This relation helps to relate the Fermi energy and the concentration of free electrons. Thus if the concentration of free electrons is known, the Fermi energy of the system at 0K can be evaluated as

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

10 Average energy of electrons in a metal at 0K

Since the distribution of electrons in the different energy states shows a non linear variation, the average energy of the electron is not the simple average of the electron's max and min energy. From the graph of $N(E)$ vs E we observe that $N(E)$ states have energy E which implies that the total energy of all electrons in filled states upto E_f should be the summation of all $N(E)*E$

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

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

This on integration gives the average energy $E = \frac{3}{5} E_f = 0.6 * E_f$

11 Merits of Quantum free electron theory:

a) Heat capacity due to free electrons

The electronic specific heat (contribution to the specific heat from the conduction electrons) can be evaluated in the light of the fact that only electrons close to the Fermi level participate in the conduction. Hence the heat absorption happens due to that fraction of electrons. This number can be estimated as the effective number of electrons (in one mole of the metal for a

mono valent metal) in the conduction process as $n_{eff} = \frac{N_a}{E_f} * k_B T$.

Hence if the average thermal energy of the electrons is taken to be $\frac{3}{2} k_B T$ then the total energy of electrons in one mole of the material

$$U = n_{eff} * \frac{3}{2} k_B T = \frac{3}{2} k_B T \frac{N_a}{E_f} * k_B T = \frac{3}{2} * \frac{N_a}{E_f} * k_B^2 T^2$$

$$\text{Hence the specific heat } C_{el} = \frac{dU}{dT} = 3 * \frac{N_a}{E_f} * k_B^2 T = 3 R * \frac{kT}{E_f}.$$

Thus the electronic specific heat is temperature n_x , n_y and n_z dependent and is a fraction of the value predicted by the CFET. This analysis gives the correct correlation with the experimental results.

A more accurate evaluation of the electronic specific heat of mono valent metals results in the

$$\text{relation } C_{el} = \frac{\pi^2}{2} \frac{N k_B^2 T}{E_f}$$

b) Temperature dependence of the resistivity

According to the classical free electron theory resistivity of the electrons originates from the scattering mechanism in which the ionic centers are stationary.

The quantum free electron theory takes into account the thermal vibrations of the ionic array which accounts for the scattering of electrons. The amplitude of the random vibrations of the lattice ions increase with increasing temperature and hence increase the probability of electron scattering. This reduces the mean free path of the electrons.

When the ions vibrate the lattice presents an effective cross sectional area for scattering of r^2 where r is the amplitude of vibration. The electron mean free path λ is inversely proportional to the scattering cross section and hence $\lambda \propto 1/T$

The expression for conductivity $\sigma = \frac{n e^2 \tau}{m} = \frac{n e^2 \lambda}{m v_f}$ shows that the conductivity is proportional to the mean free path. Hence the conductivity will be inversely proportional to temperature or resistivity $\rho \propto T$ as is found experimentally.

c) Relation between electrical conductivity and thermal conductivity (Wiedemann-Franz law and Lorenz number)

From the discussions of the electronic arrangement it is obvious that the electrons close to the Fermi energy are responsible for the electrical or thermal conduction and hence it should be possible to find a relation between the two.

It is known that the thermal conductivity of the metal $K = \frac{1}{3} \cdot \frac{C}{V} \cdot v \cdot L$

Where C is the electronic specific heat given by $C_{el} = \frac{\pi^2}{2} N \cdot \frac{k_B^2 T}{E_f}$,

V the volume, v is the velocity of electrons and L the mean free path. The mean free path of electrons is given by $L = v \cdot \tau$. Taking velocity to be the Fermi velocity v_F (since most of the conduction electrons are located about the Fermi energy) the expression for the thermal conductivity can be written as

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

where $n = \frac{N}{V}$ is the concentration of free electrons.

$$K = \frac{\pi^2}{3} \cdot n \cdot \frac{k_B^2 T}{E_f} \cdot \frac{m v_F^2}{2m} \cdot \tau = \frac{\pi^2}{3} \cdot n \cdot \frac{k_B^2 T}{E_f} \cdot \tau$$

The electrical conductivity of the metal is then given by $\sigma = \frac{ne^2\tau}{m}$

The ratio of the thermal conductivity to electrical conductivity can be calculated as

$$\frac{K}{\sigma} = \frac{\pi^2}{3e^2} k_B^2 T.$$

This is the Wiedemann-Franz law. It was noticed by Lorenz that the ratio $\frac{K}{\sigma T} = \frac{\pi^2}{3e^2} k_B^2$ is a constant irrespective of the metal and is called the Lorenz number.

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

12 Demerits of quantum free electron theory

The quantum free electron theory though successful in giving correct dependencies of some of the electrical parameters and the specific heat of electrons, was not able to explain

- Differences in conduction in metal, semiconductor and insulator. The origin of the band gap in semiconductors and insulators are not explained.
- Experimentally observed positive Hall co-efficient observed in some metals like Zinc.

These demerits could be reflective of the real potentials of the ionic centers in the metal which was ignored in the development of the model. The presence of the potentials can significantly affect the wave function of the electrons.

13 Motion of electron in periodic potential (one dimensional treatment)

The free electrons in a metal are not free from electrostatic potentials and move in a periodic potential due to the regular arrangement of the ionic centers.

The potential is lower close to the positive ions in the lattice (and in some cases basis) positions. The electrons experience a potential with the same periodicity as the lattice. The coulombic potential in the real crystal can be approximated by rectangular potentials.

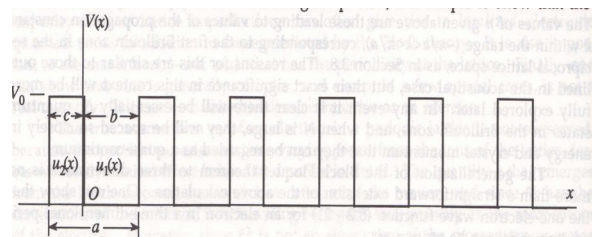
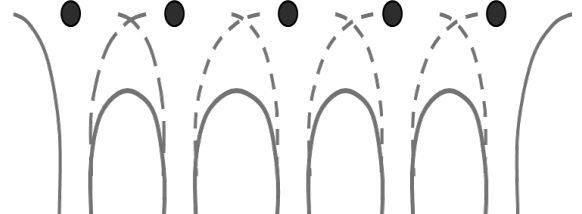
If $V(x)$ is the potential at x then, it can be seen from the figure that

$V(x+a) = V(x)$ which means that the potential is periodic and invariant under the translation through the lattice parameter.

However the wave function of the electrons

$\psi(x) = e^{ikx}$ is affected by the periodic potential and can be written as

$\psi(x) = e^{ikx} \cdot V_k(x)$ where k is the wave number of the electron waves. This is known as the Bloch function.



14 Kronig Penny model, allowed energy zones/energy bands

In the Kronig-Penney model the periodic potential is approximated as a long chain of coupled finite square wells, of barrier height V_0 , with a period 'a', and barrier thickness c .

The wave function of the electron is a modulated wave of the form $\psi(x) = e^{ikx} \cdot V_k(x)$.

A solution to the Schrödinger's equation exists if the dispersive wave number of the electron k is related to the energy through the equation

$$\cos(ka) = \frac{ma}{\hbar^2} V_0 \cdot c \cdot \frac{S \in(Ka)}{Ka} + \cos(Ka)$$

where $K = \sqrt{\frac{2m(E)}{\hbar^2}}$. We notice that the above is a transcendental equation and has approximate solutions.

The left hand side of the equation is bound with upper and lower limits of +1 to -1. The right side of the equation has oscillations of decreasing amplitude with increasing Ka . However, the solutions exist only for

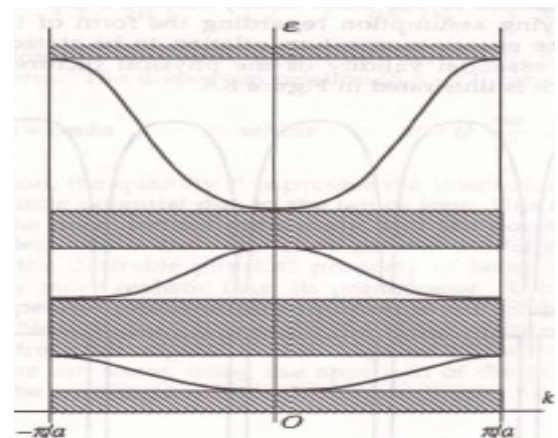
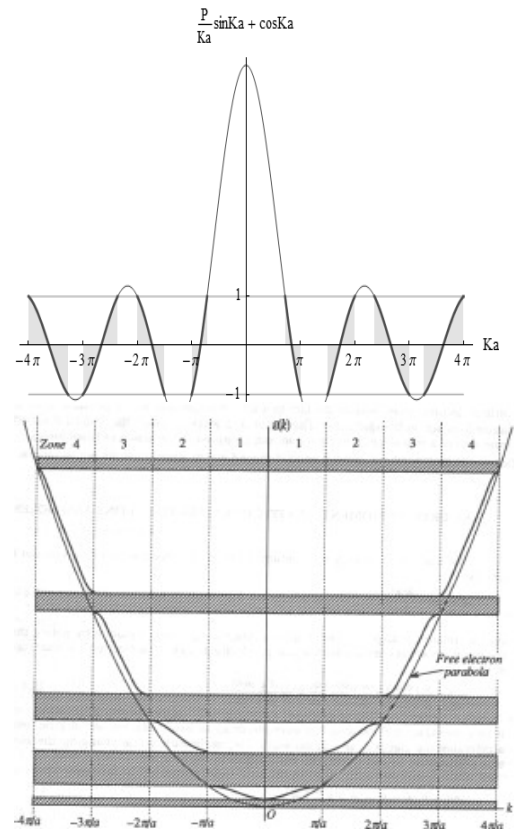
those allowed range of $K = n \frac{\pi}{a}$. Thus there exists a range of allowed energy states and forbidden energy states.

In the limit $\frac{ma}{\hbar^2} V_0 \cdot c$ tends to infinity $s \in(Ka) = 0$ which implies $K = \frac{n\pi}{a}$ and hence the energy $E_n = \frac{\hbar^2 \pi^2}{2ma^2}$

In the limit $\frac{ma}{\hbar^2} V_0 \cdot c$ tends to zero $\cos(Ka) = 1$ which implies $k = K$ and hence the energy $E = \frac{\hbar^2 K^2}{2m}$ which is the solution for a free particle.

The $E(k) - k$ diagram for the system show discontinuity in the energy at the zone boundary of $k = \pm n \frac{\pi}{a}$. (The parabolic variation of E for the free electrons is shown for comparison).

Since the functions are symmetric (and periodic with period of $2 \frac{\pi}{a}$), it is possible to represent the energy band diagram in a single zone of $\frac{+\pi}{a} \text{ to } -\frac{\pi}{a}$. The lowest band (shaded) is the completely



filled inner band followed by a band of forbidden energy states. The next band of allowed states represents the valence band. The conduction band is above energy band gap.

Materials are then classified as metals, semiconductors or insulators on the basis of the Fermi energy of the material.

In the case of conductors the Fermi level is in the uppermost band the conduction band. All states below the Fermi level are filled and all levels above the Fermi energy are empty. Thus metal are characterized by a partially filled conduction band.

In the case of materials with a completely filled valence band and completely empty conduction band, the Fermi energy is theoretically the midpoint of the energy band gaps. Materials with energy gap of 3-5 eV are classified as semiconductors. Materials with energy band gap greater than 5eV At normal temperatures it is possible for the electrons in the valence band to move into the conduction in the case of metals and semiconductors.

Concept of Effective mass

The moment of the electrons in the crystal 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

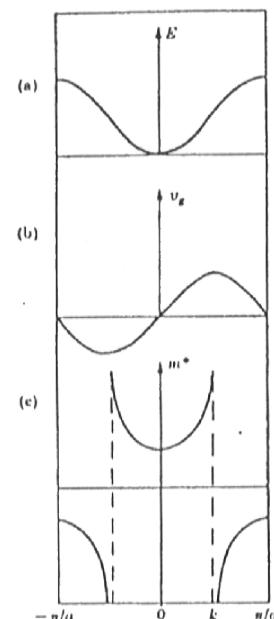
$$\frac{d^2 E}{dk^2} = \frac{\hbar^2}{m^*}$$

it is observed that $m^* = \left(\frac{1}{\hbar^2} \frac{d^2 E}{dk^2} \right)^{-1}$ is not a constant and depends on the non linearity of E . This means that the charge carriers have an effective mass which depends on the curvature of $E-k$. Higher curvature (larger $\frac{d^2 E}{dk^2}$) means smaller effective mass and smaller curvature results in higher effective mass.

It can be seen that the slope of the $E-K$ curve is minimum at the band edges and hence the effective mass of the charge carriers are highest at the band edges.

Since curvature of the $E-k$ is positive in the conduction band the effective mass is +ve and the curvature in the valence band is negative indicating a negative mass. However, this can be construed to be the motion of a charge carrier with a charge of the opposite type as that of electrons. This leads to the concept of hole conduction in the valence band. The effective mass of can be higher or lower than the rest mass of the electrons and depends on the position of the electron in the particular band.

The concept of the effective mass helps understand the mobility of charge carriers in a system particularly in semiconductors. In most compound semiconductors the effective mass of electrons and holes are much smaller than the rest mass of electrons. These materials exhibit a higher mobility of charge carriers.



Problem set

1. 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 $6.22 \times 10^7 (\Omega\text{m})^{-1}$. (Ans :
2. 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 $2.7 \times 10^3 \text{ kg m}^{-3}$.
3. Find the relaxation time and mobility of conduction electrons in a metal having 6.5×10^{28} electrons m^{-3} if the resistivity of the metal is $1.43 \times 10^{-8} \text{ ohm m}$
4. There are 10^{20} electrons per m^{-3} in a material having a resistivity of 0.1 ohm -m . Find the charge mobility and the electric field needed to produce a drift velocity of 1ms^{-1} .
5. A copper wire of radius 1mm and length 10 meter carries a direct current of 5 ampere. Calculate the drift velocity of electrons in copper if $n = 5 \times 10^{28}/\text{m}^3$.
6. 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.
7. Calculate the relaxation time of conduction electrons in a metal of resistivity of $1.55 \times 10^{-8} \Omega - \text{m}$ and an electronic concentration of 6×10^{28} per m^3 .
8. 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.
9. Estimate the probability of occupancy of an energy level 0.1 eV above the Fermi level for Copper with $E_F = 7.0\text{eV}$ for i) 100K ii) 300K iii) 1000K
10. Find the temperatures at which the occupancy of an energy state 0.3 eV above the Fermi level has an occupancy probability of i) 0.01 and ii) 0.05
11. Calculate the Fermi energy of electrons in a mono valent metal with atomic weight $132.9 \times 10^{-3} \text{ kg / mol}$ and density of $1.9 \times 10^3 \text{ kg/m}^3$ at 0K.
12. 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.
13. 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: $1.325 \times 10^6 \text{ ms}^{-1}$.)
14. Calculate the density of states with energy between 4eV and 4.005eV in copper with fermi energy of 7.02eV.($E = 4\text{eV} = 4 \times 1.6 \times 10^{-19} \text{ J}$ and $dE = .005 \times 1.6 \times 10^{-19} \text{ J}$ mass of electron = $9.1 \times 10^{-31} \text{ kgs}$)

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