

Module 6 : PHYSICS OF SEMICONDUCTOR DEVICES

Lecture 30 : Energy Band Diagram

Objectives

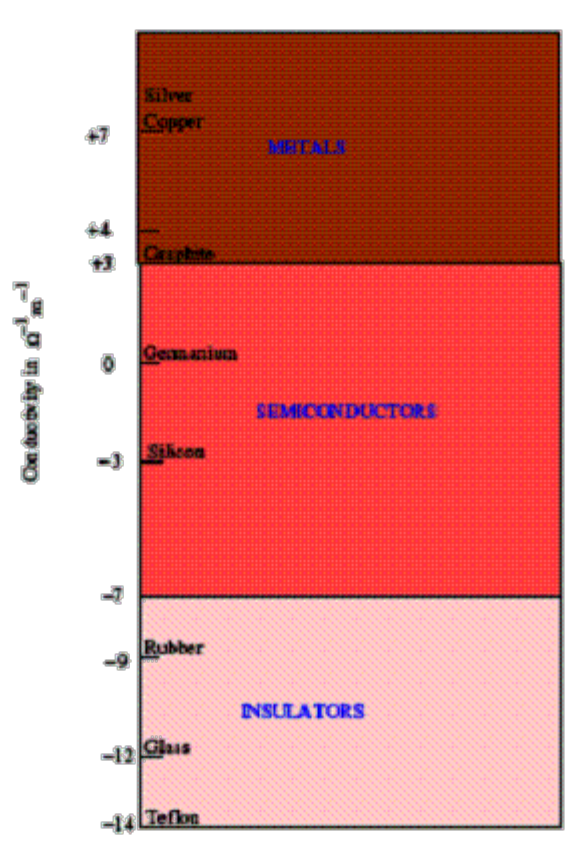
In this course you will learn the following

- Difference between electrical properties of metals, semiconductor and insulators.
- Band theory of metals and semiconductors.
- Free electron theory of metals and concept of Fermi energy.
- Calculation of density of state for free electrons.

Modern electronics, which has revolutionized our way of life, is based on interesting properties of a class of material known as **semiconductors**.

Semiconductors have resistivity values intermediate between those of metals and insulators. While typical metallic resistivity is between 10^{-8} to 10^{-6} ohm-m, that of silicon, which is a representative semiconductor is 3×10^3

ohm-m. Materials with resistivities higher than 10^8 ohm-m are considered to be insulators. Glass, rubber and many plastics are typical insulators.



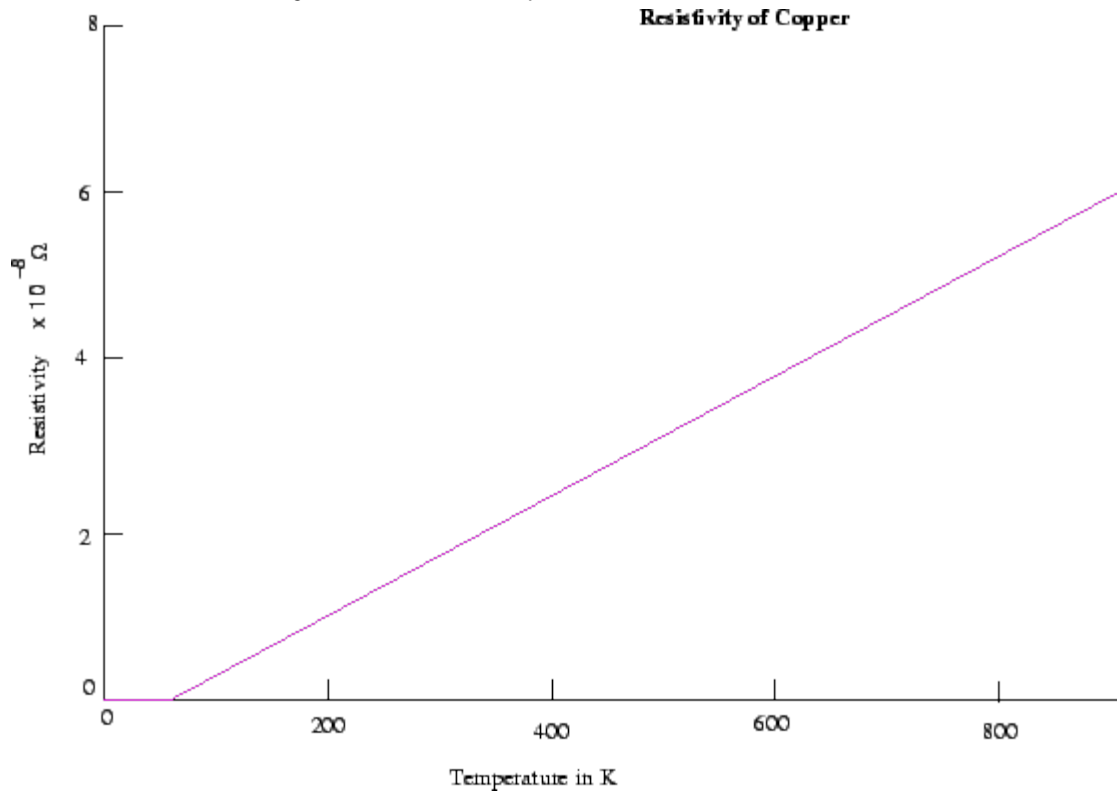
Temperature coefficient of resistivity :

The resistivity of metals increase with the increase of temperature. This is because with increase in temperature, ions in a solid vibrate more causing electrons to scatter more frequently from them. The semiconductors, on the other hand, have a negative temperature coefficient of resistivity, i.e., their resistivity decreases with increase in temperature.

An empirical formula for resistivity of metal is

$$\rho(T) = \rho_{ref}[1 + \alpha(T - T_{ref})]$$

where ρ_{ref} is the resistivity at a reference temperature T_{ref} , usually taken to be 0 °C or 20 °C. The constant α is known as the coefficient of resistivity, which is a small positive number (For Cu $\alpha \simeq 0.004/^\circ\text{C}$).

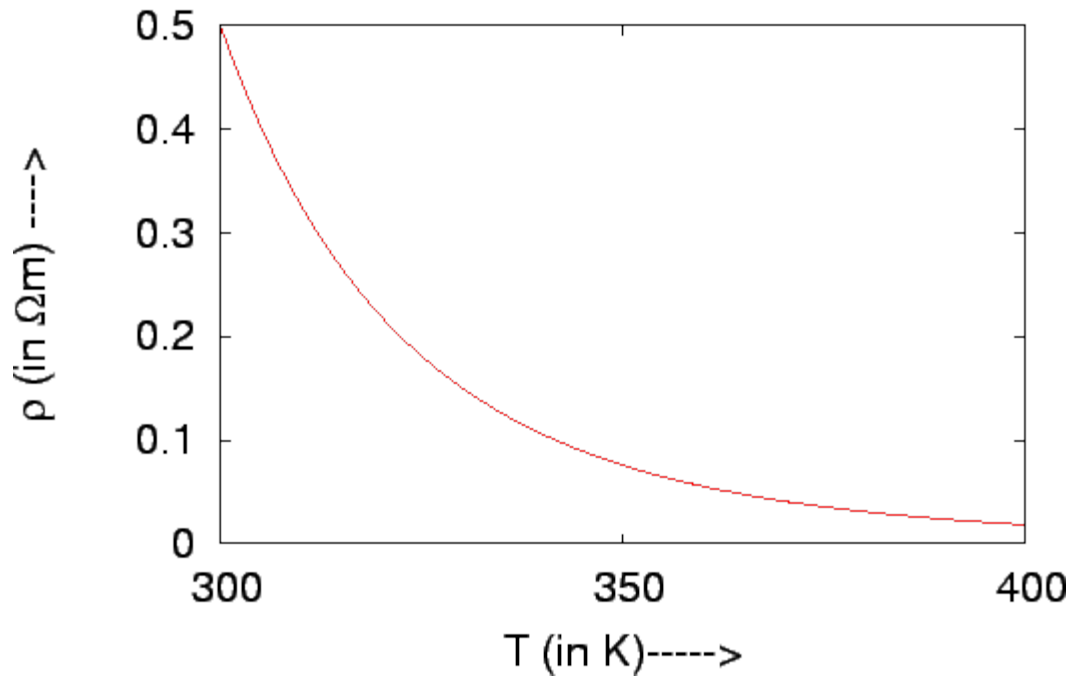


An corresponding formula for resistivity of semiconductors (or of insulators) is

$$\rho(T) = \rho_0 \exp\left[\left(\frac{1}{T} - \frac{1}{T_0}\right) \frac{\Delta E}{2k}\right]$$

where ρ_0 is the resistivity at 0 °C (i.e. at 273 K) and T is the absolute temperature at which the resistivity is measured. Here k is Boltzmann constant and ΔE is the bandgap energy, which, for semiconductors is of the order of 1 eV and much larger for insulators.

Resistivity (ρ) of Ge with Temperature (T)



Charge carriers

Conductivity arises due to motion of charge carriers in a material when placed in an electric field. The primary charge carriers in a metal are electrons. In gases and solutions, the carriers could be charged ions. The density of carriers in a metal is very high, being of the order of 10^{29} per m^3 .

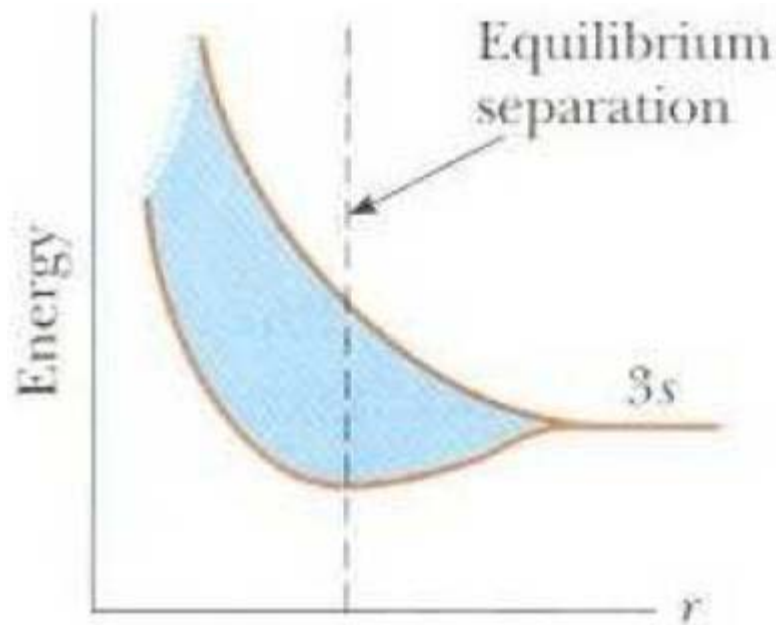
Charge carriers in semiconductors are electrons and vacancies, the latter being known as **holes**. Typical carrier density in a semiconductor is about 10^{16} which is substantially lower than that of metals. Insulators have negligible carrier densities.

Energy Band Diagram

Electrical properties of materials are best understood in terms of their electronic structure. We know that the energy levels of isolated atoms are discrete. When atoms are brought together to form a solid, these energy levels spread out into **bands** of allowed energies. The effect is qualitatively understood as follows by considering what happens when a collection of N atoms, which are initially far apart are brought closer.

When the spacing r between adjacent atoms is large, each atom has sharply defined energy levels which are denoted by $1s, 2s, 2p, 3s$ etc. As the atoms are far apart their orbitals do not overlap. In particular if each atom is in its

ground state, the electrons in each atom occupy identical quantum states. As the distance starts decreasing, the orbitals overlap. The electrons of different atoms cannot remain in the same state because of **Pauli Exclusion Principle**. Pauli principle states that a particular state can at most accommodate two electrons of opposite spins. Thus when N atoms are brought together, the levels must split to accommodate electrons in different states. Though they appear continuous, a band is actually a very large number of closely spaced discrete levels.

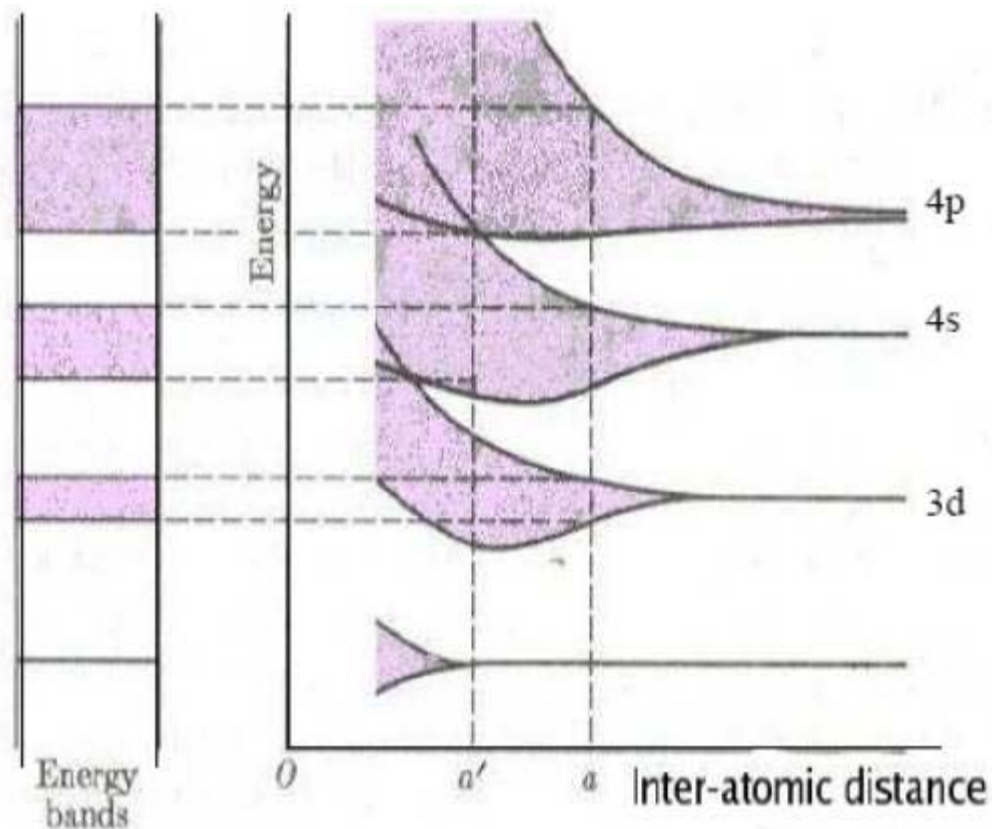


[See the animation](#)

Conductors, Insulators and Semiconductors :

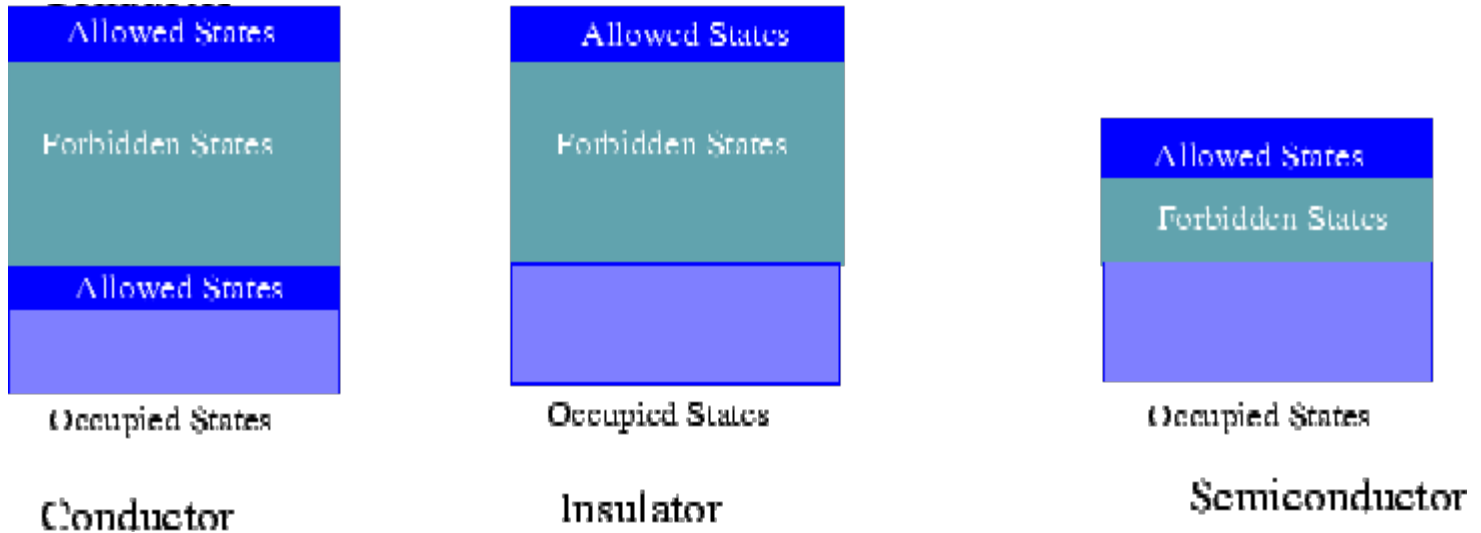
When an electric field is applied to any substance, the electrons can absorb energy from the field and can move to higher energy levels. However, this is possible only when empty states with higher energies exist close to the initial states in which the electrons happen to be in. If there is a substantial energy difference between the occupied electron state and the higher unoccupied state, the electron cannot absorb energy from the electric field and conduction cannot take place. Thus **conduction takes place only in partially occupied bands**.

In case of a metal, the bands which arise from different atomic orbitals overlap and the electrons can absorb energy from an electric field (or absorb thermal or light energy). The electrons in such partially filled bands are called **free electrons**.



For an insulator there is a wide gap (eV) between the lower occupied band, known as the **valence band**,

and the higher unoccupied band, called the **conduction band**. No electron can exist in this **forbidden gap**. To promote electrons from lower levels to higher levels would require a great amount of energy. It is incorrect to say that electrons in an insulator are not free to move around. In fact, they do. However, as there are as many electrons as there are states, the electrons only trade places resulting in no net movement of charges.



Semiconductors, like insulator have band gaps. However, the gap between the top of the valence band and the bottom of the conduction band is much narrower than in an insulator. For comparison, the gap in case of Silicon is 1.1 eV while that for diamond, which is an insulator is about 6 eV.

Quantum Mechanical Concepts

Formation of bands can only be understood on the basis of quantum mechanics. Earlier, we had seen that an object behaves both as particle and as wave. According to de Broglie theory, an electron having a momentum p has an associated wave with a wavelength h/p . Schrödinger proposed an equation for the wave associated with a particle of

mass m having a total energy E which is moving in a potential V . The Schrödinger equation, which is as fundamental to quantum mechanics as Newton's laws are to classical mechanics, is given by

$$-\frac{\hbar^2}{2m}\nabla^2\psi = (E - V)\psi$$

According to quantum mechanical hypothesis, the **wavefunction** $\psi(\vec{r})$ is interpreted as the probability amplitude of a particle of energy E being at a point \vec{r} . The square of the wavefunction $|\psi(\vec{r})|^2$ gives the probability density at the point, so that the probability of finding the particle anywhere in space given by $\int_{\text{all space}} |\psi(\vec{r})|^2 d^3r$ is unity.

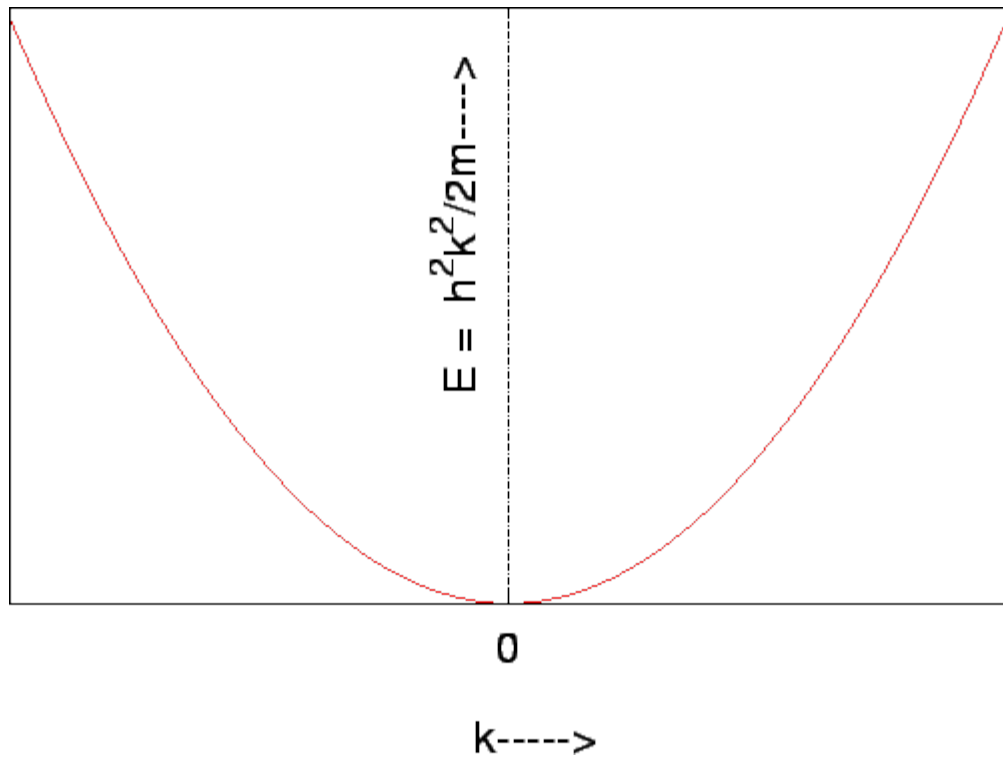
This is called the normalization of the wavefunction. It is also postulated that the wavefunction and its first derivative are continuous and single valued.

Wavefunction of a Free Electron

The energy- momentum relationship for a free electron is given by

$$E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m}(k_x^2 + k_y^2 + k_z^2)$$

The $E - k$ relationship (known as the *dispersion relation*) is a parabola.



Free Electron Model of a Metal

The valence electrons in a metal are detached from the individual atoms and move in the metal like a gas of free particles. This leaves the atomic cores positively charged. In the free electron model of a metal, it is assumed that this positive charge of the cores is uniformly distributed throughout the metal. Such an assumption essentially removes any details of the crystal structure of the metal. Nevertheless, it is a good starting point in understanding behaviour of electrons in a metal.

As the interaction between the electrons themselves are also ignored, one can simply consider the motion of a single electron which is moving in a constant potential, which can be conveniently taken to be zero. The electron can be taken to be confined within a box of dimension $L \times L \times L$ within which the potential is constant (taken to be zero)

and outside which it is infinite. The Schrödinger equation for the electron within the box is

$$-\frac{\hbar^2}{2m} \left[\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} \right] = E\psi$$

Defining $k^2 = 2mE/\hbar^2$, the equation reads

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} + k^2 \psi = 0 \quad (A)$$

The equation may be solved by separation of variables by substituting

$$\psi(x, y, z) = \psi_x(x)\psi_y(y)\psi_z(z)$$

in eqn. (A) and dividing the resulting equation by $\psi_x\psi_y\psi_z$. We get

$$\frac{1}{\psi_x} \frac{\partial^2 \psi_x}{\partial x^2} + \frac{1}{\psi_y} \frac{\partial^2 \psi_y}{\partial y^2} + \frac{1}{\psi_z} \frac{\partial^2 \psi_z}{\partial z^2} + k^2 = 0$$

Since k^2 is constant and the first three terms depend upon x, y, z separately, the above equation can be satisfied

for all values of x, y, z only if each of the three terms is constant, i.e.

x, y, z

$$\frac{1}{\psi_x} \frac{\partial^2 \psi_x}{\partial x^2} + k_x^2 = 0$$

$$\frac{1}{\psi_y} \frac{\partial^2 \psi_y}{\partial y^2} + k_y^2 = 0$$

$$\frac{1}{\psi_z} \frac{\partial^2 \psi_z}{\partial z^2} + k_z^2 = 0$$

with $k_x^2 + k_y^2 + k_z^2 = 0$.

The solutions of the above with boundary condition (i.e. vanishing of wavefunction at the walls) gives

$$\psi_x(x) = A \sin(k_x x)$$

where $k_x = n_x \pi / L$, n_x being any non-zero positive integer. Thus the complete solution (with normalization constant) is

$$\psi(x, y, z) = \frac{2^{3/2}}{\sqrt{V}} \sin k_x x \sin k_y y \sin k_z z$$

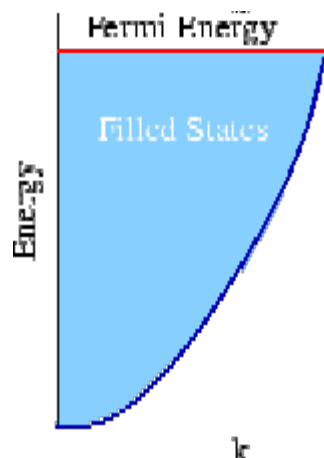
and the energy

$$E = \frac{\hbar^2 \pi^2}{2m} \left(\frac{n_x^2}{L^2} + \frac{n_y^2}{L^2} + \frac{n_z^2}{L^2} \right) (B)$$

where $V = L^3$ is the volume of the crystal.

At absolute zero temperature, electrons fill up available states from minimum energy upwards satisfying Pauli exclusion principle. Each distinct energy level, specified by a combination of n_x, n_y and n_z is occupied by two electrons of

opposite spins. The maximum value of energy is known as **Fermi energy** and is denoted by E_F .



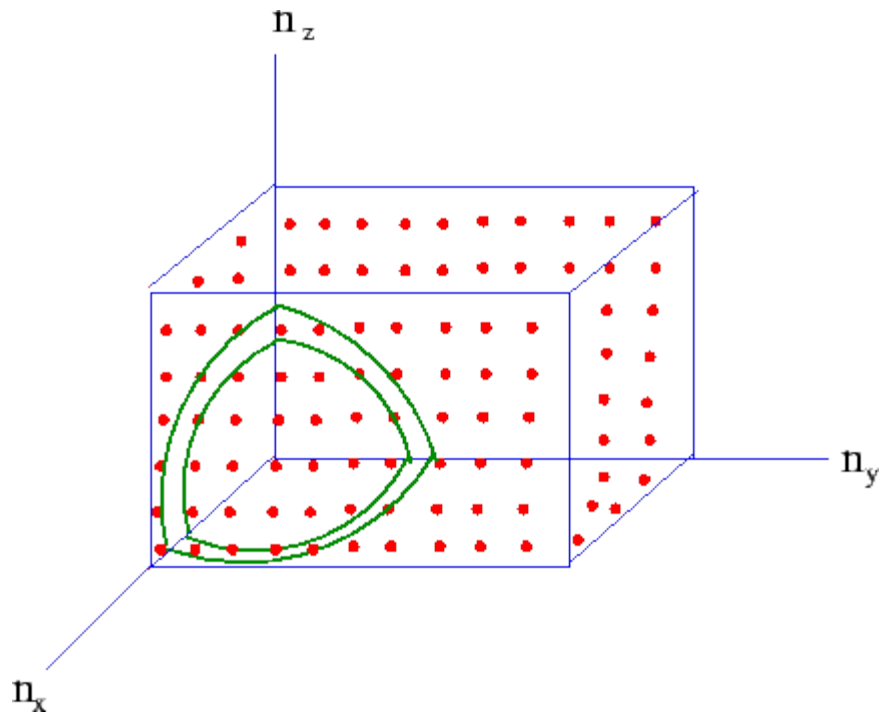
Density of States

Density of states at an energy E is the number of states per unit volume available per unit energy interval with

energy between E and $E + dE$. This would require counting of states, i.e., enumeration of different values of n_x, n_y, n_z corresponding to the energy of states within this interval. This is obviously a difficult task. However, given the large dimension of a crystal, the states are very closely packed and one can essentially treat the k — values as continuous.

Equation of constant energy given by eqn. (B) is a sphere in $n_x - n_y - n_z$ space with a radius $\sqrt{2mEL}/\pi\hbar$.

As the points in this space are separated from the adjacent ones by one unit in each direction, each point effectively occupies a volume $(2\pi)^3/V$ in the k — space. Thus a unit volume in k — space contains $V/(2\pi)^3$ number of states. As each k — state can accommodate two electrons (corresponding to two distinct spin states), the number of electrons per unit volume of k — space is $V/4\pi^3$.



Since the constant energy surface in k — space is a sphere, we can define **Fermi wave vector** k_F as the radius of a sphere corresponding to the Fermi energy E_F by

$$E_F = \frac{\hbar^2 k_F^2}{2m}$$

The volume of Fermi sphere being $4\pi k_F^3/3$, the number of electrons N that lie within such a sphere is

$$N = \frac{4\pi}{3} k_F^3 \times \frac{V}{4\pi^3} \equiv \frac{V}{3\pi^2} \left(\frac{2mE_F}{\hbar^2} \right)^{3/2} \quad (C)$$

which gives the density n as equal to

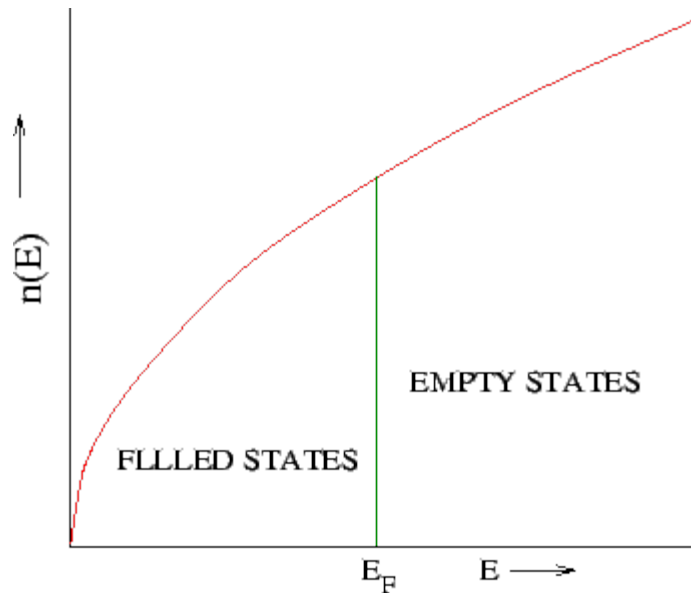
$$n = \frac{N}{V} = \frac{k_F^3}{3\pi^2}$$

Using eqn. (C), we can obtain an expression for the density of states $n(E)$. Since, by definition, $n(E)dE$ is the number of states lying within energy interval E and $E + dE$, we may simply subtract the number of states below energy E from the number below $E + dE$. We have

$$\begin{aligned} n(E)dE &= \frac{1}{3\pi^2} \left[\frac{2m}{\hbar^2} \right]^{3/2} [(E + dE)^{3/2} - E^{3/2}] \\ &\simeq \frac{1}{3\pi^2} \left[\frac{2m}{\hbar^2} \right]^{3/2} [E^{3/2}(1 + \frac{3dE}{2E}) - E^{3/2}] \\ &= \frac{1}{2\pi^2} \left[\frac{2m}{\hbar^2} \right]^{3/2} E^{1/2} dE \end{aligned}$$

The unit of density of states $n(E)$ is $(\text{eV})^{-1} \text{m}^{-3}$.

Density of States and Fermi Energy



[See the animation](#)

Free electron theory can be used to explain, reasonably satisfactorily, several qualitative properties of metals, such as, thermal and electrical conductivity, magnetic properties, heat capacity etc. However, as the theory totally ignores the crystalline structure of metals, it fails to provide a distinction between metals, semiconductors and insulators. The atoms in a crystal are arranged in a periodic arrangement. Consequently, the electrons in the crystal are subject to a periodic potential rather than a uniform potential assumed in the free electron model. If this potential is assumed to be weak, the electrons do not become completely free but nearly so. The model is known as **nearly free electron model**.

Recap

In this course you have learnt the following

- Metals have free charge carriers. With increase in temperature, the resistivity of a metal increases.
- Pure (intrinsic) semiconductors are very similar to insulators. For a semiconductor, the resistivity decreases with increase in temperature.
- Metals have partially occupied band which allow charge carriers to move even when a small amount of energy is supplied. Semiconductors have occupied valence band and unoccupied conduction band. Carriers can be thermally excited from valence band to conduction band.
- Insulators are similar to semiconductor in their band structure. However, the band gap is much larger than in a semiconductor.
- Behaviour of simple metals can be described by a free electron theory in which an electron is taken to move in a constant potential. At zero temperature the electron states are occupied from the lowest energy state to a state of maximum energy, known as Fermi energy.
- Density of state is the number of states per unit volume of a substance per unit energy interval. For free electrons the density of state is proportional to the square root of energy.