3 Electrons in a Crystal

3.1 Fermi Energy and Fermi Surface

In the preceding chapters, we considered essentially only one electron, which was confined to the field of atoms of a solid.

However, in a solid of one cubic centimeter at least 10^{22} valence electrons can be found.

Now we will consider how these electrons are distributed among the available energy levels.

The Fermi Energy : "Highest energy that the electrons assume at T=0K"

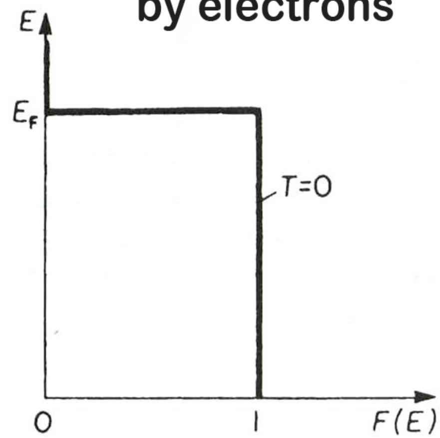
This definition can occasionally be misleading , particularly when dealing with semiconductors.

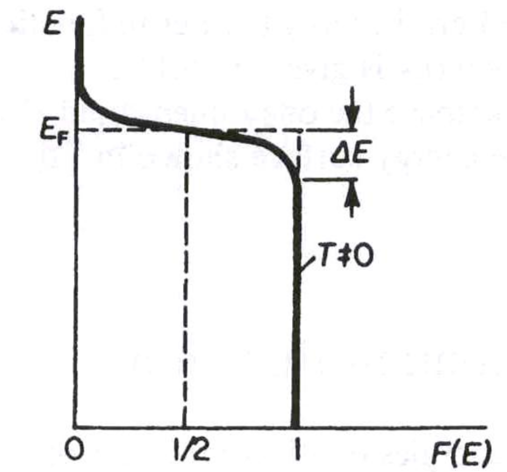
More accurate definition of the Fermi energy is that the value of the Fermi distribution function F(E), equal 1/2

3.2 Fermi Distribution Function

The kinetic energy of an electron gas is governed by Fermi-Dirac statistics which states that the probability that a certain energy level is occupied by electrons is given by the Fermi Function, F(E)

Fermi function, F(*E*) : The probability that a certain energy level is occupied by electrons



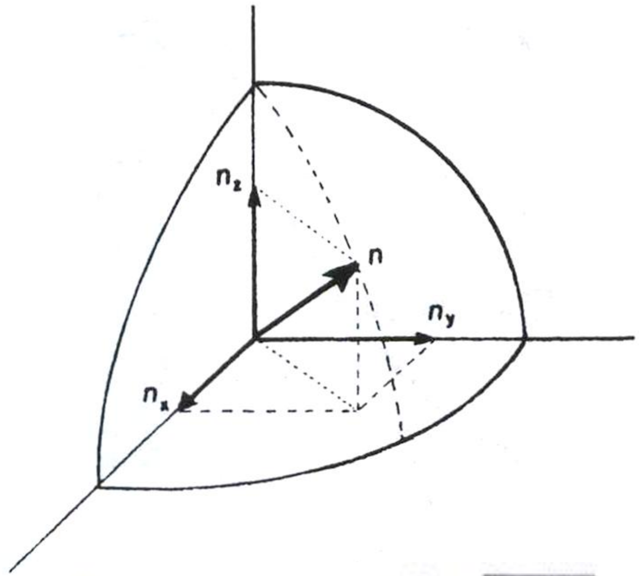


$$F(E) = \frac{1}{\exp\left(\frac{E - E_F}{k_B T}\right) + 1}.$$

At high energy (E >> E_F) : approximated by classical Boltzmann distribution

$$F(E) \approx \exp\left[-\left(\frac{E - E_F}{k_B T}\right)\right].$$

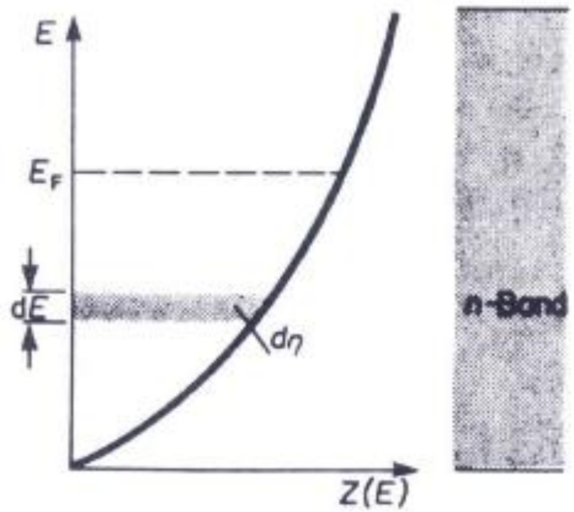
3.3 Density of States (free electron model)



$$E_n = \frac{\pi^2\hbar^2}{2ma^2}(n_x^2 + n_y^2 + n_z^2),$$

$$n^2 = n_x^2 + n_y^2 + n_z^2.$$

$$\eta = \frac{1}{8}\cdot\frac{4}{3}\pi n^3 = \frac{\pi}{6}\left(\frac{2ma^2}{\pi^2\hbar^2}\right)^{3/2} E^{3/2}.$$



$$\frac{d\eta}{dE} = Z(E) = \frac{\pi}{4}\left(\frac{2ma^2}{\pi^2\hbar^2}\right)^{3/2} E^{1/2}$$

$$= \frac{V}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} E^{1/2}$$

Number of energy states per unit energy in the energy interval ΔE, **density of states**

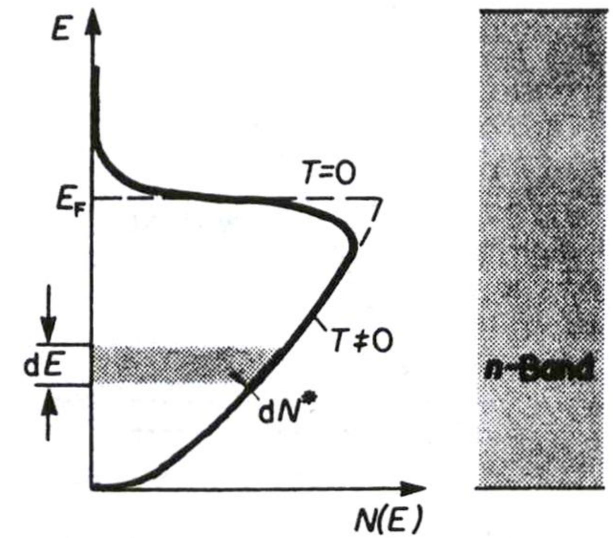
$$d\eta = Z(E)\cdot dE,$$

3.4 Population Density

$$N(E) = 2 \cdot Z(E) \cdot F(E)$$

$$N(E) = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} E^{1/2} \frac{1}{\exp\left(\frac{E - E_F}{k_B T}\right) + 1}.$$

$$dN^* = N(E)\,dE.$$



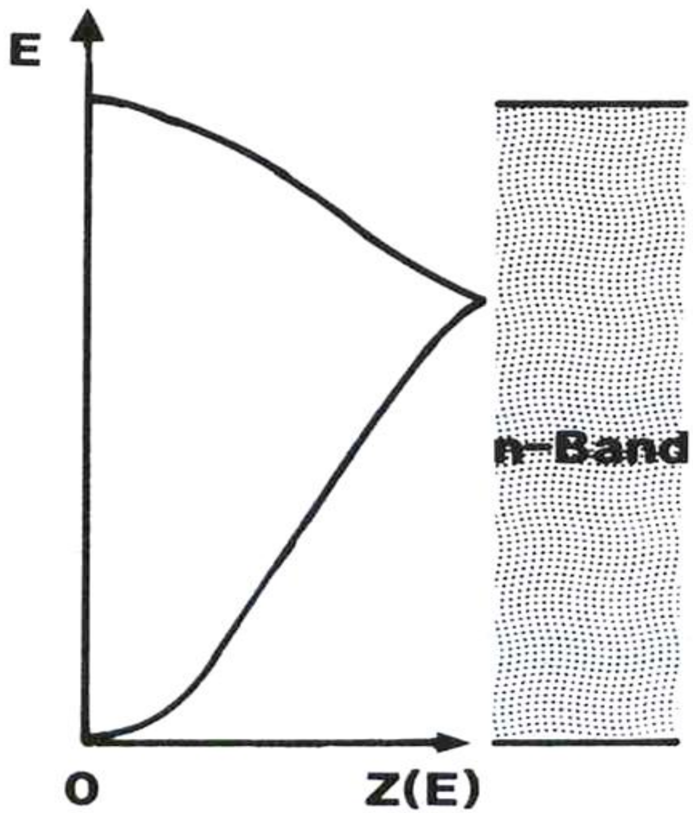
N* represents the number of electrons that have an energy equal to of smaller than the energy E_n.

$$N^* = \int_0^{E_F} N(E)\,dE = \int_0^{E_F} \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} E^{1/2} dE = \frac{V}{3\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} E_F^{3/2}.$$

$$E_F = \left(3\pi^2 \frac{N^*}{V}\right)^{2/3} \frac{\hbar^2}{2m}. \quad E_F = \left(3\pi^2 N'\right)^{2/3} \frac{\hbar^2}{2m}.$$

Where, N′ represents the number of electrons per unit volume

3.5 Complete Density of States Function Within a Band

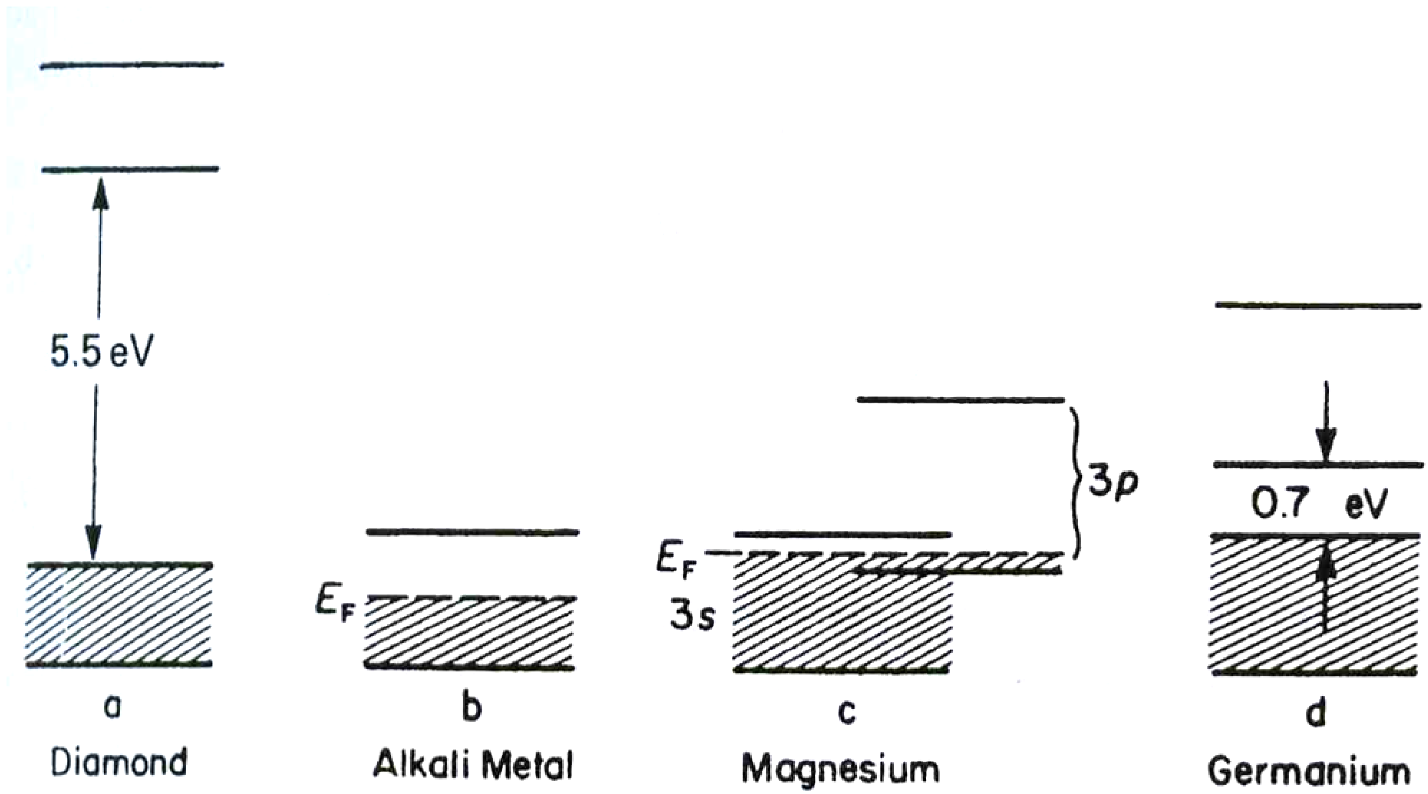


- Low energy : free electronlike

- Higher energy : fewer energy state available

Z(*E*) decrease with increasing E

3.6 Consequences of the Band Model



3.7 Effective Mass

$$\upsilon_g = \frac{d\omega}{dk} = \frac{d(2\pi v)}{dk} = \frac{d(2\pi E/h)}{dk} = \frac{1}{\hbar}\frac{dE}{dk}.$$

$$a = \frac{d\upsilon_g}{dt} = \frac{1}{\hbar}\frac{d^2E}{dk^2}\frac{dk}{dt}. \qquad \frac{dp}{dt} = \hbar\frac{dk}{dt}.$$

$$a = \frac{1}{\hbar^2}\frac{d^2E}{dk^2}\frac{dp}{dt} = \frac{1}{\hbar^2}\cdot\frac{d^2E}{dk^2}\cdot\frac{d(m\upsilon)}{dt} = \frac{1}{\hbar^2}\frac{d^2E}{dk^2}F,$$

$$a = \frac{F}{m}.$$

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