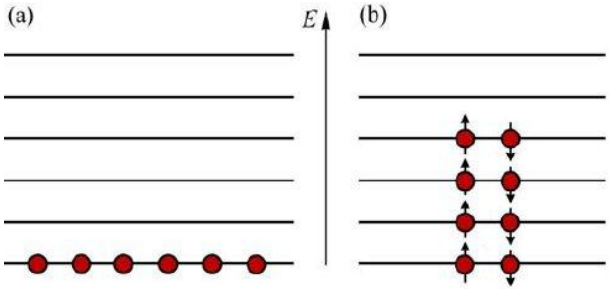
Semiconductors

Carrier statistics and Density of States

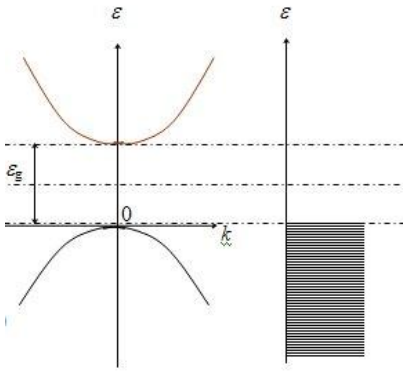
In the previous chapter we derived a microscopic expressions for the conductivity and the mobility in an electric field for free carriers based on the band structure of a periodic systems. We introduced a concept of the *effective mass* as we progressed from classical to semi-classical microscopic description to account for the QM nature of an electron. Here we shall further investigate QM effects in materials with non-zero value of the energy gap – ε_g.

We saw that the conductivity σ was a function of the temperature and identified possible source of that as *n(T)* where *n* is carrier concentration. Hence, further investigation of this dependence require a closer investigation the source of the temperature dependence of carrier concentration. Once again, the QM properties of an electron have to be taken into account, specifically: (i) wave character of electrons; (ii) Pauli exclusion principle. The former results in only a finite number of solutions of Schrödinger equation within the energy range ε and $\varepsilon+d\varepsilon$. The latter results in that an eigenstate can only be occupied by two electrons of opposite spin.



Energy level occupancy in a classical case (a) vs Pauli Exclusion Principle (b).

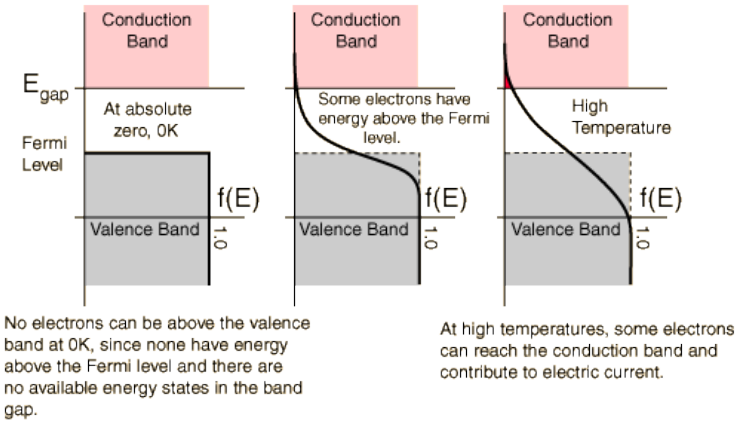
Now, we shall reduce the full *ε(k)* dependence to a simple energy diagram:



The Fermi-Dirac distribution gives the probability of an energy state to be occupied at a given temperature:

$$f(\varepsilon) = \frac{1}{e^{(\varepsilon-\varepsilon_F)/k_BT}+1}$$

Resulting in the following picture:



No electrons can be above the valence band at 0K, since none have energy above the Fermi level and there are no available energy states in the band gap.

At high temperatures, some electrons can reach the conduction band and contribute to electric current.

Ref: http://hyperphysics.phy-astr.gsu.edu

An important point to observe here is a finite (albeit small) electron concentration in the conduction band at non-zero temperature.

Intrinsic semiconductors.

Now we are ready to look into the microscopic parameter of interest – the electron concentration. This, as in the case of the free-electron model involves counting the number of electrons, except this time these will be electrons in the conduction band. We remember that density of electrons in the energy interval ε, $\varepsilon + \Delta\varepsilon$ = density of states times probability for occupancy times energy interval:

$dN = D(\varepsilon) \cdot f(\varepsilon,T) \cdot d\varepsilon$

$$N = \int_0^\infty D(\varepsilon) f(\varepsilon,T) d\varepsilon$$

Where for a free-electron model:

$$D(\varepsilon) = \frac{dN}{d\varepsilon} = \frac{1}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}} \varepsilon^{\frac{1}{2}}$$

This in case of semiconductors translates to:

$$D_c(\varepsilon) = Cm^*_c{}^{\frac{3}{2}} (\varepsilon - \varepsilon_c)^{\frac{1}{2}}$$

$$D_v(\varepsilon) = Cm^*_v{}^{\frac{3}{2}} (\varepsilon_v - \varepsilon)^{\frac{1}{2}}$$

where, m_c*=conduction band effective mass, m_v*=valence band effective mass, and C= constant.

And considering that im most cases

Assume CB occupancy <<1, $$f(\varepsilon) \approx \frac{1}{e^{(\varepsilon-\varepsilon_F)/k_BT}} = e^{-\left(\frac{\varepsilon-\varepsilon_F}{k_BT}\right)}$$

Probability of hole in VB, 1- $f(\varepsilon) \approx 1 - \frac{1}{e^{(\varepsilon-\varepsilon_F)/k_BT}} = e^{-\left(\frac{\varepsilon_F-\varepsilon}{k_BT}\right)}$

Number of electrons in CB:

$$n = \int_{\varepsilon_c}^{\infty} f \times D_c d\varepsilon \approx C m^*_c{}^{\frac{3}{2}} \int_{\varepsilon_c}^{\infty} (\varepsilon - \varepsilon_c)^{\frac{1}{2}} \times e^{-\frac{(\varepsilon-\varepsilon_F)}{k_B T}} d\varepsilon$$

substitute y=(ε-ε_c)/$k_B T$

$$n \approx C(m^*_c\, k_B T)^{\frac{3}{2}} \times e^{-\frac{(\varepsilon_c-\varepsilon_F)}{k_B T}} \int_0^{\infty} y^{\frac{1}{2}} \times e^{-y} dy$$

Which results is:

$$n = 2\frac{(2\pi m^*_c\, k_B T)^{\frac{3}{2}}}{h^3} \times e^{-\frac{(\varepsilon_c-\varepsilon_F)}{k_B T}} = N_c \times e^{-\frac{(\varepsilon_c-\varepsilon_F)}{k_B T}}$$

where N_c is the effective number density of *accessible* states at ε_c

Similarly the hole density, *p* is given by

$$p = 2\frac{(2\pi m^*_v\, k_B T)^{\frac{3}{2}}}{h^3} \times e^{-\frac{(\varepsilon_F-\varepsilon_v)}{k_B T}} = N_v \times e^{-\frac{(\varepsilon_F-\varepsilon_v)}{k_B T}}$$

In an **intrinsic** semiconductor the only source of electrons in the CB is thermal excitation from the VB

$\Rightarrow$ $$\boxed{n_i = n = p = W^{\frac{1}{2}} T^{\frac{3}{2}} \times e^{-\frac{\varepsilon_g}{2k_B T}}}$$

n_i=**intrinsic carrier density**

NB $\varepsilon_g/2$ rather than ε_g appears in the above equation because creation of an electron in the CB *automatically* generates a hole in the VB.

How does the **Fermi energy** change with *T*?

From calculation of n_i and $D(\varepsilon)$, $\frac{N_c}{N_v} = \left(\frac{m^*_c}{m^*_v}\right)^{\frac{3}{2}} = e^{\left(\frac{2\varepsilon_F - \varepsilon_c - \varepsilon_v}{k_B T}\right)}$

$$\Rightarrow \qquad \varepsilon_F = \frac{1}{2}(\varepsilon_c - \varepsilon_v) + \frac{3}{4}k_B T \ln\left(\frac{m^*_c}{m^*_v}\right)$$

⇒ When *T*=0 K or $m_c^* = m_v^*$, ε_F lies in the middle of the band gap

Law of mass action

$$np \approx N_c \times N_v \times e^{-\frac{\varepsilon_g}{k_B T}} = W \times T^3 \times e^{-\frac{\varepsilon_g}{k_B T}}$$

This is an important relationship because it shows that the product of carrier densities in a nondegenerate semiconductor at a given temperature is dependent only on the densities of states, ie on the effective masses, and on the energy gap. It holds for intrinsic as well as extrinsic material. It is referred to as the *law of mass action.*

MODILITY AND CONDUCTIVITY

It both electrons and holes are present, both contribute to the electrical conductivity

$$\sigma = ne\mu_e + pe\mu_h$$

where μ is the **mobility**.

Remember that the free electron model is a good approximation for electrons in the CB or holes in the VB of a semiconductor, therefore the expression for electrical conductivity is used

$$\sigma = \frac{ne^2\tau}{m^*}$$

or resistivity, $1/\sigma$

$$\rho = \frac{m^*}{ne^2\tau}$$

Mobilty, the drift velocity per unit electric field, $\mu = |v_D|/E$, for electrons is defined as

$$\mu_e = \frac{e\tau_e}{m_e^*}$$

and for holes

$$\mu_h = \frac{e\tau_h}{m_h^*}$$

ENERGY GAP OF SELECTED SEMICONDUCTORS

MATERIAL	E_g ($T = 300$ K)	E_g ($T = 0$ K)	E_0 (LINEAR EXTRAPOLATION TO $T = 0$)	LINEAR DOWN TO
Si	1.12 eV	1.17	1.2	200 K
Ge	0.67	0.75	0.78	150
PbS	0.37	0.29	0.25	
PbSe	0.26	0.17	0.14	20
PbTe	0.29	0.19	0.17	
InSb	0.16	0.23	0.25	100
GaSb	0.69	0.79	0.80	75
AlSb	1.5	1.6	1.7	80
InAs	0.35	0.43	0.44	80
InP	1.3		1.4	80
GaAs	1.4		1.5	
GaP	2.2		2.4	
Grey Sn	0.1			
Grey Se	1.8			
Te	0.35			
B	1.5			
C (diamond)	5.5