

ELEC4705 – Fall 2009

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LECTURE 1

Filling the states and determining n and p

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9.1. Introduction – Density of Carriers

In the previous lectures we have determined that the energy levels present for an electron in a crystal are described by a band structure consisting of allowed energy bands and band gaps. We wish now to determine the number of carriers (current carrying particles) present in a material per unit volume. To do this we need to determine how many states are present at a particular energy (previously we only determined the total number of states in a band) and the probability of a state being occupied at a particular temperature.

To calculate the carrier concentrations in energy bands we therefore need to know in mathematical form the following quantities:

- (a) The distribution of energy states or levels as a function of energy within the energy band ($g(E)$), i.e. $g(E)$ is the density of states in energy at E .
- (b) The probability of each of these states being occupied by an electron ($f(E)$).

Once these are determined we can then find the density of electrons in the system as by integration over the band structure:

$$n = \int_0^{+\infty} g(E) f(E, E_F, T) dE \quad (9.1)$$

and for holes we will have (as the probability of a state being empty is $1 - f(E)$):

$$p = \int_0^{+\infty} g(E) (1 - f(E, E_F, T)) dE \quad (9.2)$$

9.2. Density of States in Conduction Band

To determine the number of states in an energy band as a function of volume we first determine the distribution and density of states in k space and then use the approximately quadratic relationship between energy and momentum for nearly free electrons at the top or bottom of a band.

Consider a semiconductor for which the bottom of the conduction band has spherical constant energy surfaces for free electrons with a mass m^* . (Spherical is 3D version of parabolic $E(k)$.) A 3-D k -space is shown in figure 1.

As we saw in the last lecture a piece of material of size $L_x \times L_y \times L_z$ will act like a large potential well for the electrons. This will produce a regular lattice of allowed energy states in k space separated by “momentum distances” of $2\pi/L_x$, $2\pi/L_y$ and $2\pi/L_z$. Due the finite size of

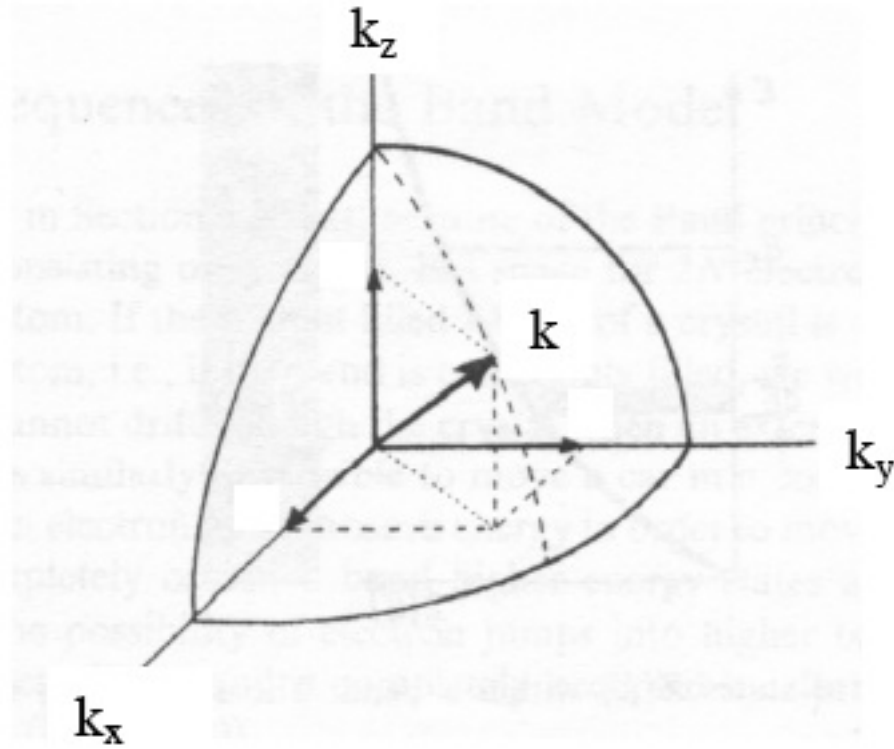


Figure 1. A 3D k-space

the crystal each unit cell in k space containing a single allowable energy level has an volume of,

$$\frac{2\pi}{L_x} \times \frac{2\pi}{L_y} \times \frac{2\pi}{L_z} = (2\pi)^3 / (L_x \times L_y \times L_z) = (2\pi)^3 / V \quad (9.3)$$

So considering the spin factor 2, the *density of states* in k-space will be

$$N_{3D}(k) = 2V / (2\pi)^3 \quad (9.4)$$

And dividing by the crystal volume we obtain the *density of states per unit volume* in k-space will be

$$n_{3D}(k) = 2 / (2\pi)^3 \quad (9.5)$$

Now we wish to find the *density of states in energy per unit volume* $g(E)$.

In k space we take two sphere's with radius's K and $K + \delta K$ centered on the origin. As we have a simple one-to-one relationship between momentum and energy the number of states between these two spheres

must be equal in K space and the energy domain (E). We can define a density of states in energy $g(E)$ and write:

$$g(E) \delta E = g(E) (dE/dK) \partial k \quad (9.6)$$

Assuming the $E = \hbar^2(k_x^2 + k_y^2 + k_z^2)/2m$ – quadratic like dispersion – and the number of states in k space is the volume $4/3\pi K^3$ times the density of states n_{3D} we can obtain dE/dK and derive the density of states function,

$$\begin{aligned} g(E) \frac{\hbar^2 K}{m} \delta K &= \left(\frac{4\pi}{3} 3K^2 \delta K \right) \times (2/(2\pi)^3) \\ g(E) &= \frac{m}{\pi^2 \hbar^3} \sqrt{2mE} \end{aligned} \quad (9.7)$$

9.3. Occupancy of Available Energy Levels

We have determined $E(k)$ and a density of states. We also need a way of determining if a state is filled or not at a given temperature. According to the Pauli exclusion principle, no more than one electron can occupy a given state. In equilibrium the average number of particles that occupy a state depends on its energy. The average occupation is governed by Fermi-Dirac distribution function which is given by equation 9.8 and shown in figure 2. $E_F(T)$ is called the fermi level in semiconductors which is dependent on temperature, The higher the T the more *smearing* is present in the function. E_F represents the highest energy that the electrons assume at $T = 0K$. At any temperature above absolute zero the probability of occupation of the energy level at $E = E_F$ is $1/2$. (Note there may not be an actual state at the Fermi energy!)

$$f(E, E_F, T) = \frac{1}{\exp\left(\frac{E - E_F(T)}{k_B T}\right) + 1} \quad (9.8)$$

The important features of the Fermi-Dirac distribution are:

- Its value is between zero and one.
- It passes 0.5 when $E = E_F$.
- $f(E)$ can be considered as the probability of states being occupied.
- $f(E)$ is a decreasing function of energy.
- At low temperature, the transition from one to zero becomes very sharp.

If $T=0$ we have $f(E, E_F, T) = \Theta(E_F^0 - E)$ where $\Theta(x)$ is the Heaviside unit step function. So all the states below E_F^0 are fully filled and the above ones are empty. For $T \neq 0$ as we can see the transition

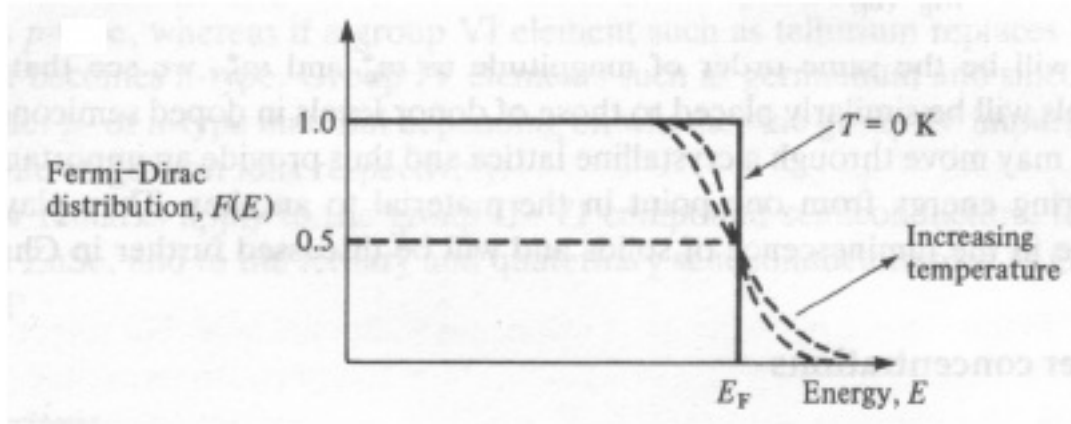


Figure 2. Fermi Dirac Distribution

from 1 to 0 broadens as the temperature rises, with a width roughly $8 k_B T$.

Note 1:

We have fermi temperature as $T_F = E_F^0 / k_B$

Note 2:

For $E \gg E_F$ we have Boltzmann distribution given by:

$$f(E, E_F, T) \simeq \exp\left(-\frac{E - E_F}{k_B T}\right) \quad (9.9)$$

Note 3:

The distribution of holes are given by:

$$\bar{f}(E, E_F, T) = 1 - f(E, E_F, T) = \frac{1}{\exp\left(\frac{E_F(T) - E}{k_B T}\right) + 1} \quad (9.10)$$

9.4. Carrier Concentrations

Returning to the calculation of carriers concentrations, we have that the density of electrons in conduction band as in equation 9.1, i.e.

$$n = \int_{E=0}^{+\infty} g(E) f(E, E_F, T) dE \quad (9.11)$$

where we define $E = 0$ as the bottom of the conduction band.

As the conduction band is well away from E_f ($E_f \approx E_g/2$) we have $E \gg E_F$ and we use the Boltzmann approximation for $f(E)$ as in 9.12

which as mentioned above is valid for the tail of the distribution when E is well away from E_F .

$$\begin{aligned} f(E, E_F, T) &= \frac{1}{\exp\left(\frac{E - E_F(T)}{k_B T}\right) + 1} \approx \exp\left(-\frac{E - E_F(T)}{k_B T}\right) \\ &= \exp\left(-\frac{E - E_c}{k_B T}\right) \exp\left(-\frac{E_c - E_F}{k_B T}\right) \end{aligned} \quad (9.12)$$

Then from equation 9.11 we will have

$$n = \exp\left(-\frac{E_c - E_F}{k_B T}\right) \int_{E=0}^{+\infty} g(E) \exp\left(-\frac{E - E_c}{k_B T}\right) dE \quad (9.13)$$

We define the effective density of states in conduction band as

$$N_c = \int_{E=0}^{+\infty} g(E) e^{-(E - E_c)/k_B T} dE \quad (9.14)$$

$$= \frac{1}{4} \left(\frac{2m^* k_B T}{\pi \hbar^2}\right)^{3/2}. \quad (9.15)$$

Doing the same for holes we will have,

$$N_v = \frac{1}{4} \left(\frac{2m^* k_B T}{\pi \hbar^2}\right)^{3/2}. \quad (9.16)$$

And so the density of electrons and holes will be given by:

$$n = N_c \exp\left(-\frac{E_c - E_F}{k_B T}\right) \quad (9.17)$$

$$p = N_v \exp\left(-\frac{E_F - E_v}{k_B T}\right) \quad (9.18)$$

These quantities are the per unit volume density of carriers present in a material. They can be functions of positions ($n(x, y, z)$ and $p(x, y, z)$).

9.4.1. Intrinsic Semiconductors

A perfect semiconductor crystal containing no impurities or lattice defects is called an intrinsic semiconductor. As the carriers are generated in pairs, the concentration n of electrons in the conduction band equals the concentration p of holes in the valence band and we can define,

$$n = p = n_i$$

where n_i is the intrinsic carrier concentration.

Therefore we can obtain a value for E_f

$$N_c \exp\left(-\frac{E_c - E_F}{k_B T}\right) = pN_v \exp\left(-\frac{E_F - E_v}{k_B T}\right) \quad (9.19)$$

$$k_B T \ln\left(\frac{N_c}{N_v}\right) = E_c - E_F - E_F + E_v \quad (9.20)$$

$$E_F = \frac{E_c + E_v}{2} - \frac{k_B T}{2} \ln\left(\frac{N_c}{N_v}\right) \quad (9.21)$$

$$E_{Fi} \approx \frac{1}{2}E_g \quad (9.22)$$

Which we had actually assumed before and is now confirmed. This is shown in figure 3

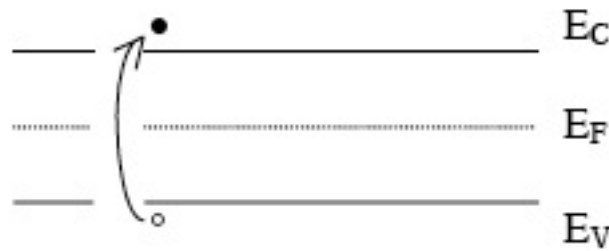


Figure 3. Band Structure

we also have the mass action law as below:

$$np = n_i^2 \quad (9.23)$$

where:

$$n_i = \sqrt{N_c N_v} e^{-(E_c - E_v)/k_B T} \quad (9.24)$$

$$n_i = \sqrt{N_c N_v} e^{-E_g/2k_B T} \quad (9.25)$$

It is important in devices to control n and p concentrations and suppress the influence of intrinsic concentration. These equations are important in establishing upper limits in semiconductor operating temperature. We generally require $n_i \ll$ (minimum doping density in device) and practically, this means we need doping concentrations above 10^{14} cm^{-3} .