ELEC4705 – Fall 2009

Tom Smy

LECTURE 1
Filling the states and determining n and p

Contents

ELEC4705 – Fall 2009 1

Lecture 1. Filling the states and determining n and p 1

9.1. Introduction – Density of Carriers 4

9.2. Density of States in Conduction Band 4

9.3. Occupancy of Available Energy Levels 6

9.4. Carrier Concentrations 8

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 quantaties:

(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:

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

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

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

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

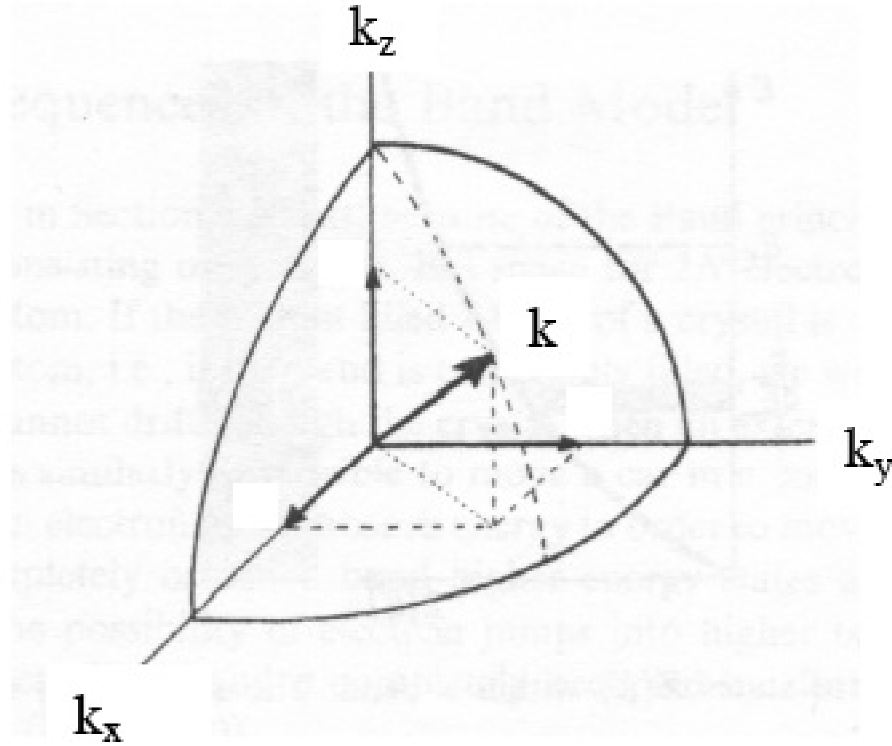

Figure 1. A 3D k-space

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

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

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

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

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

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

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

In k space we take two spheres with radius's $K = \sqrt{k_x^2 + k_y^2 + k_z^2}$ 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:

$$g(E)\,\delta E \;=\; g(E)\,(dE/dK)\,\partial k \tag{9.6}$$

Assuming quadratic like dispersion:

$$E \;=\; \hbar^2(k_x^2 + k_y^2 + k_z^2)/2m = \hbar^2 K^2/2m \tag{9.7}$$

$$\frac{dE}{dK} \;=\; \hbar^2 K/m \tag{9.8}$$

and the number of states in k space is the volume $V_{sh} = 4/3\pi K^3$ times the density of states n_{3D} we can obtain dE/dK and derive the density of states function,

$$g(E)\,\frac{dE}{dK}\delta K \;=\; \frac{V_{sh}}{dK}\,\delta K\, n_{3D}(k) \tag{9.9}$$

$$g(E)\,\frac{\hbar^2\,K}{m}\delta K \;=\; (\frac{4\pi}{3}\,3K^2\,\delta K) \times (2/(2\pi)^3)$$

$$g(E) \;=\; \frac{m}{\pi^2\hbar^3}\sqrt{2mE} \tag{9.10}$$

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 9.11 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!)

$$f(E,\,E_F,\,T) \;=\; \frac{1}{\exp\,(\frac{E\,-\,E_F(T)}{k_B\,T})\,+\,1} \tag{9.11}$$

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.

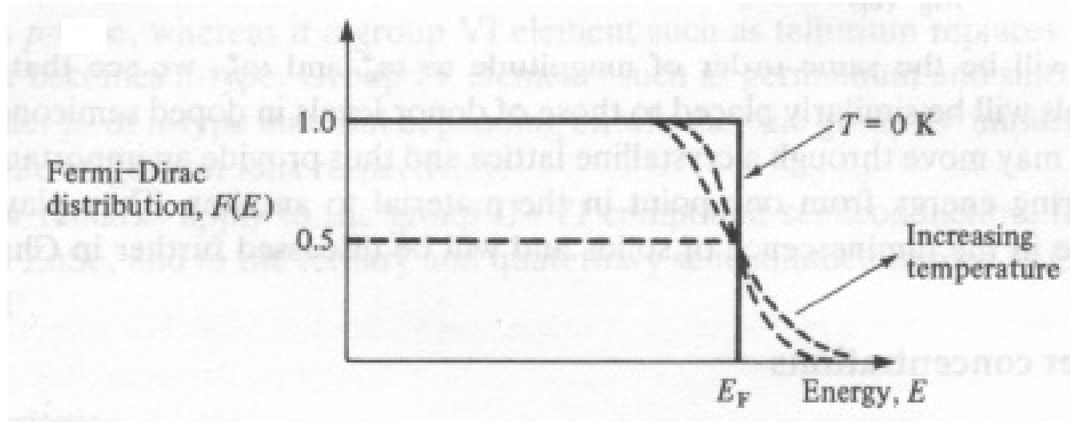

Figure 2. Fermi Dirac Distribution

- 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 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:

$$f(E,\, E_F,\, T) \;\simeq\; \exp\,(-\frac{E \,-\, E_F}{k_B\, T}) \tag{9.12}$$

Note 3:
The distribution of holes are given by:

$$\overline{f}(E,\, E_F,\, T) \;=\; 1 \,-\, f(E,\, E_F,\, T) \;=\; \frac{1}{\exp\,(\frac{E_F(T)\,-\,E}{k_B\, T}) \,+\, 1} \tag{9.13}$$

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.

$$n = \int_{E=0}^{+\infty} g(E)\, f(E,\, E_F,\, T)\, dE \tag{9.14}$$

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

As the conduction band is well away from E_f ($E_f \approx Eg/2$) we have $E \gg E_F$ and we use the Boltzmann approximation for $f(E)$ as in 9.15 which as mentioned above is valid for the tail of the distribution when E is well away from E_F.

$$\begin{aligned} f(E,\, E_F,\, T) &= \frac{1}{\exp\left(\frac{E - E_F(T)}{k_B T}\right) + 1} \approx \exp\left(-\frac{E - E_F(T)}{k_B T}\right) \\ &= \exp\left(-\frac{E - E_c}{k_B T}\right) \exp\left(-\frac{E_c - E_F}{k_B T}\right) \end{aligned} \tag{9.15}$$

Then from equation 9.14 we will have

$$n = \exp\left(-\frac{E_c - E_F}{k_B T}\right) \int_{E=0}^{+\infty} g(E)\, \exp\left(-\frac{E - E_c}{k_B T}\right) dE \tag{9.16}$$

We define the effective density of states in conduction band as

$$N_c = \int_{E=0}^{+\infty} g(E)\, e^{(-(E - E_c)/k_B T}\, dE \tag{9.17}$$

$$= \frac{1}{4}\left(\frac{2m^* k_B T}{\pi \hbar^2}\right)^{3/2}. \tag{9.18}$$

Doing the same for holes we will have,

$$N_v = \frac{1}{4}\left(\frac{2m^* k_B T}{\pi \hbar^2}\right)^{3/2}. \tag{9.19}$$

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

$$n = N_c \exp\left(-\frac{E_c - E_F}{k_B T}\right) \tag{9.20}$$

$$p = N_v \exp\left(-\frac{E_F - E_v}{k_B T}\right) \tag{9.21}$$

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

$$N_c \exp(-\frac{E_c - E_F}{k_B T}) = pN_v \exp(-\frac{E_F - E_v}{k_B T}) \quad (9.22)$$

$$k_B T \ln(\frac{N_c}{N_v}) = E_c - E_F - E_F + E_v \quad (9.23)$$

$$E_F = \frac{E_c + E_v}{2} - \frac{k_B T}{2} \ln(\frac{N_c}{N_v}) \quad (9.24)$$

$$E_{Fi} \approx \frac{1}{2} E_g \quad (9.25)$$

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

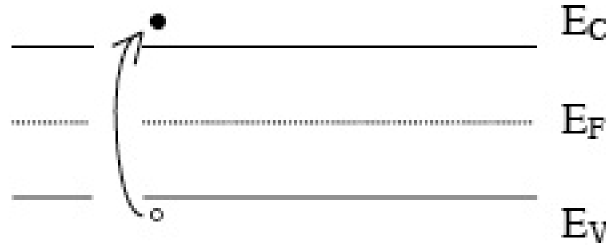

Figure 3. Band Structure

we also have the mass action law as below:

$$np = n_i^2 \quad (9.26)$$

where:

$$n_i = \sqrt{N_c N_v} e^{-(E_c - E_v)/k_B T} \quad (9.27)$$

$$n_i = \sqrt{N_c N_v} e^{-E_g/2k_B T} \quad (9.28)$$

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 $10^{14}\ cm^{-3}$.