Notes for Lecture 9

DOS, n, and p

In the previous lecture, we considered doping, and the "Fermi level," which we will understand is the chemical potential only for the purpose of this course.

9.1 Density of States

The concept of DOS is of basic importance in much of physics – it is the number of states available between energy E and $E + dE$. Thus it can be written as

$$\frac{dN}{dE}$$

where N is the number of (quantum) states and E is the energy. In addition, sometimes the DOS per volume is defined simply as the DOS: in this case, the DOS would be

$$\frac{1}{V} \cdot \frac{dN}{dE}$$

where V is the system volume.

For any dispersion relation in 1D, DOS is inversely proportional to the slope of the dispersion, i.e. the group velocity v_g. This is because for any small segment of the dispersion, which can be approximated as a line segment, the number of quantum states is proportional to dk. This is due to the fact that k values are discrete ("quantized") and they are equally spaced. I.e., $dN \propto |dk|$, and thus, DOS $\propto |dk/dE| = 1/(\hbar|v_g|)$, proving that the DOS is inversely proportional to $|v_g|$. In higher dimensions (3D, e.g.), the general idea holds up. I.e., where v_g is small, some interesting things happen, but these are not necessary the maxima of the DOS, but the singularities of the DOS.

Eqs. (T2.6a, T2.6b)[1] of the textbook give the density of states (DOS) for the electron and the hole in a semiconductor. The derivation will be worked out in a homework problem. The symbol $g(E)$ is used for the DOS. It is defined as "per-volume" DOS. So, the SI unit of $g(E)$ is 1/(J m^3). In this course, 1/(eV cm^3) or 1/(eV Å^3) will be more useful.

9.2 Fermi Function and Hole Occupation

Let us re-visit the Fermi function (Eq. (7.9)):

$$f(E) = \frac{1}{\exp(\beta(E - E_F)) + 1} \tag{9.1}$$

Here, I merely changed some notations. $\beta = (k_B T)^{-1}$ is a common notation in physics. The convention of using E_F (Fermi energy/level) for μ (chemical potential), as discussed in LN 8 at length.

Let us note that, since $f(E)$ is the average occupation of a unique (cf. LN 7) quantum state at energy E, $1 - f(E)$ gives the average "un-occupation" (or vacancy) of that state. That is, if $f(E)$ is defined for an electron energy level (as usual), then $1 - f(E)$ is the **hole occupation** associated with that energy level. The following should be derivable by you from the above equation.

$$1 - f(E) = \frac{1}{1 + \exp(\beta(E_F - E))} \tag{9.2}$$

Exercise T2.2 is interesting. Exercise T2.3 is discussed at length on the course wiki page.

9.3 Equilibrium Carrier Distribution

With the DOS and the Fermi function in hand, we can count the number of carriers! The number of electrons between energy E and $E + dE$ per volume would be given by $g(E)f(E)$. The number of holes between energy E and $E + dE$ per volume would be given by $g(E)(1 - f(E))$.

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[1] When this note refers to equation/figure/table numbers of the textbook, I will use this format T<number>.

Study Fig. T2.16 carefully and completely with this in mind. Also, Figs. T2.17 and T2.18.

All of these pertain only to the equilibrium. Q: What in our formula (gf or $g(1-f)$) is/are valid only for the equilibrium state?Most of these short questions and their answers have been discussed in class.

9.3.1 n, p and n_i, p_i

The number of carriers per volume has the standard notation: n for the electron and p for the hole. Steps of Eqs. T2.8a,b leading to Eqs. T2.13a,b and T2.14a,b should be followed by you. Q: What is the physical dimension of N_c and N_v defined in Eqs. T2.13a,b? Q': What is the physical dimension of $F_{1/2}$ defined in Eq. T2.12? Answering these two questions correctly, you should be able to ascertain that Eqs. 2.14a,b make sense dimensionally.

Notice that Eqs. T2.14a,b are general for any value of E_F.

Depending on the position of E_F, we distinguish **degenerate semiconductor** or **non-degnerate semiconductor**. The word "degenerate" here is slightly different from the same word used in QM. Here, it refers to the concept of quantum degeneracy of identical particles, rather than having two wave functions at the same energy state. If the temperature is such that the quantum statistics (i.e. the Fermi function or the Bose function) is important, then the system is said to be **degenerate**, since the identical nature of particles is important. If the temperature is such that the quantum statistics is not important, then the system is said to be **non-degenerate**. So, any system will become degenerate at low temperature! Since an electronic energy scale is very high compared to RT (room temperature), any metallic materials that you see around you are in quantum degenerate state! However, for many semiconductors, E_F is far away from the VBM and the CBM, making them **non-degenerate** semiconductors. For them, $f(E)$ for $E \geq E_c$ can be written as

$$f(E) \approx \frac{1}{\exp(\beta(E-E_F))} = \exp(-\beta(E-E_F)) \qquad \text{for } E \geq E_c \tag{9.3}$$

There, $f(E) \ll 1$ for any electron in the CB. Likewise, $1 - f(E)$ for $E \leq E_v$ can be written as (using Eq. 9.2):

$$1 - f(E) \approx \exp(-\beta(E_F - E)) \qquad \text{for } E \leq E_v \tag{9.4}$$

So, for non-degenerate semiconductors, the occupancy of an electron carrier (Eq. 9.3) and the occupancy of a hole carrier (Eq. 9.4) are both very small compared to 1. Notice also that both these occupancies are approximated by the Boltzman function

$\exp(-\beta \times$ energy rel. to chem. pot.), keeping in mind that the hole energy is given by $-(E-E_F)$, i.e. the negative of the electron energy. Namely, "non-degenerate" means classical statistics (where the Boltzman statistics is valid), while "degenerate" means quantum statistics (where the Fermi statistics or the Bose statistics must be used without any further approximation).

As you can see, the mathematics of the degenerate semiconductors can be a bit challenging, due to the somewhat complicated nature of $F_{1/2}$. However, for a non-degenerate semiconductor, $F_{1/2}$ gets simplified – it becomes a constant times the Boltzman factor for the CBM or the VBM.

In the following mathematical treatment, we will deal exclusively with non-degenerate semiconductors.

So, for non-degenerate semiconductors, we get (cf. Eqs. T2.16a,b)

$$n = N_c \exp(-\beta(E_c - E_F)) \tag{9.5}$$

$$p = N_v \exp(-\beta(E_F - E_v)) \tag{9.6}$$

For an intrinsic semiconductor, let us use the subscript i for n and p. Then, $n_i = p_i$, by the charge conservation. We might *assume* that intrinsic semiconductors are non-degenerate. Then, using the above results, we get

$$n_i = p_i = N_c \exp(-\beta(E_c - E_i)) = N_v \exp(-\beta(E_i - E_v)) \tag{9.7}$$

where E_i is defined as E_F for an intrinsic semiconductor.

What is the value E_i? From Eq. 9.7, and the fact that $N_v/N_c = (m_p^*/m_n^*)^{3/2}$ (from Eqs. T2.13a,b), we get

$$E_i = \frac{E_c + E_v}{2} + \frac{3}{4} k_B T \ln\left(\frac{m_p^*}{m_n^*}\right) \tag{9.8}$$

This result means that as $T \to 0$, the Fermi level of an intrinsic semiconductor approaches the middle of the gap, justifying our "forced assignment" of E_F as such for a semiconductor in LN 8, and also justifying our assumption made above that intrinsic semiconductors are non-degenerate. Q: The above reasoning is perfect in any physical sense. But, mathematically, we have *not* actually proved that $E_F = \frac{E_c+E_v}{2}$ *at* $T = 0$. Why is this?

From Eq. 9.7,

$$N_c = n_i \exp(\beta(E_c - E_i)) \tag{9.9}$$

$$N_v = n_i \exp(\beta(E_i - E_v)) \tag{9.10}$$

Plugging these into Eqs. 9.5,9.6, we get the following important result

$$n = n_i \exp(\beta(E_F - E_i)) \tag{9.11}$$

$$p = p_i \exp(\beta(E_i - E_F)) \tag{9.12}$$

For given effective masses, temperature, and energy gap ($E_G = E_c - E_v$), n_i and p_i can be readily calculated (Eqs. T2.21 and T2.13a,b). If E_F is known, then n and p can be calculated also.

Notice that

$$np = n_i p_i \tag{9.13}$$

This is due to the "law of mass action." $dn/dt = A - Bnp$, if A is the "generation rate for an electron-hole pair" and B is the "recombination rate for an electron-hole pair." For small doping, these rates A and B are independent of doping, namely they are the intrinsic properties of the host crystal. In an equilibrium state, $dn/dt = 0$, and thus, $np = A/B$, independent of the Fermi level. Thus, this applies both to intrinsic and extrinsic semiconductors, giving $n_i p_i = np$.

Exercise 2.4 should be studied by you.