Chapter one: The Semiconductor in Equilibrium

This chapter deals with the semiconductor in equilibrium:

Equilibrium (Thermal equilibrium)

- No external forces such as voltages, electric fields, magnetic fields, or temperature gradients are acting on the semiconductor

- All properties of the semiconductor will be independent of time at equilibrium

- Equilibrium is our starting point for developing the physics of the semiconductor. We will then be able to determine the characteristics that result when deviations from equilibrium occur

1.1 CHARGE CARRIERS IN SEMICONDUCTORS

Current is the rate at which charge flow

- ➤ two types of carriers can contribute the current flow (Electrons in conduction band and Holes in valence band)
- ➤ The density of electrons and holes is related to the density of state function and Fermi-Dirac distribution function

This statement is written in equation form as

$$n(E)dE = g_c(E)f_F(E)dE \qquad (1)$$

n (E)dE density of electrons in CB at energy levels between E and $E+dE$

$$p(E)dE = g_v(E)\big(1 - f_F(E)\big)dE \qquad (2)$$

P(E)dE = density of holes in VB at energy levels between E and $E+dE$

[The **density of states** (**DOS**) of a system describes the number of states that are available to be occupied by the system at each level of energy.

Distribution functions are the probability density functions used to describe the probability with which a particular particle can occupy a particular energy level. When we speak of *Fermi-Dirac distribution function*, we are particularly interested in knowing the chance by which we can find a fermion in a particular energy state of an atom. Here, by fermions, we mean the electrons of an atom which are the particles with ½ spin, bound to Pauli Exclusion Principle.]

To find the thermal-equilibrium electron and hole concentrations, we need to determine the position of the Fermi energy E_F with respect to the bottom of the conduction-band energy E_c and the top of the valence-band energy E_v. To address this question, we will initially consider an intrinsic semiconductor.

Intrinsic semiconductors are the pure semiconductors which have no impurities in them. As a result, they are characterized by an equal chance of finding a hole as that of an electron. This in turn implies that they have the Fermi-level exactly in between the conduction and the valence bands.

DENSITY OF STATES FUNCTION

Since current is due to the flow of charge, an important step in the process is to determine the number of electrons and holes in the semiconductor that will be available for conduction. The number of carriers that can contribute to the conduction process is a function of the number of available energy or quantum states since, by the Pauli Exclusion Principle, only one electron can occupy a given quantum state. When we discussed the splitting of energy levels into bands of allowed and forbidden energies, we indicated that the band of allowed energies was actually made up of discrete energy levels. We must determine the density of these

allowed energy states as a function of energy in order to calculate the electron and hole concentrations.

To find the DOS, we need to know the energy of the particle in 3D box, which can be get it from the solution of the Schrodinger's equation, i.e.

$$E = \frac{\hbar^2 k^2}{2m} \qquad (3)$$

where $n = 1, 2, 3, \ldots$ and $k = n\pi/a$, with a the length of the box.

At this point, associated with each value of n is an energy.

The volume V_k of a single quantum state is

$$V_k = \left(\frac{\pi}{a}\right)^3 \qquad (4)$$

We can now determine the density of quantum states in k space. A differential volume in k space is shown in Figure 3.26b and is given by $4k2dk$, so the differential density of quantum states in k space can be written as

$$g(k)dk = 2\left(\frac{1}{8}\right)\frac{4\pi k^2 dk}{\left(\frac{\pi}{a}\right)^2} \qquad (5)$$

The first factor, 2, takes into account the two spin states allowed for each quantum state; the next factor, 1/8, takes into account that we are considering only the quantum states for positive values of k_x, k_y, and k_z. The factor $4k2dk$ is again the differential volume and the factor $(\pi/a)^3$ is the volume of one quantum state. Equation (5) may be simplified to

$$g(k)dk = \frac{\pi k^2 dk}{\pi^3} a^3 \qquad (6)$$

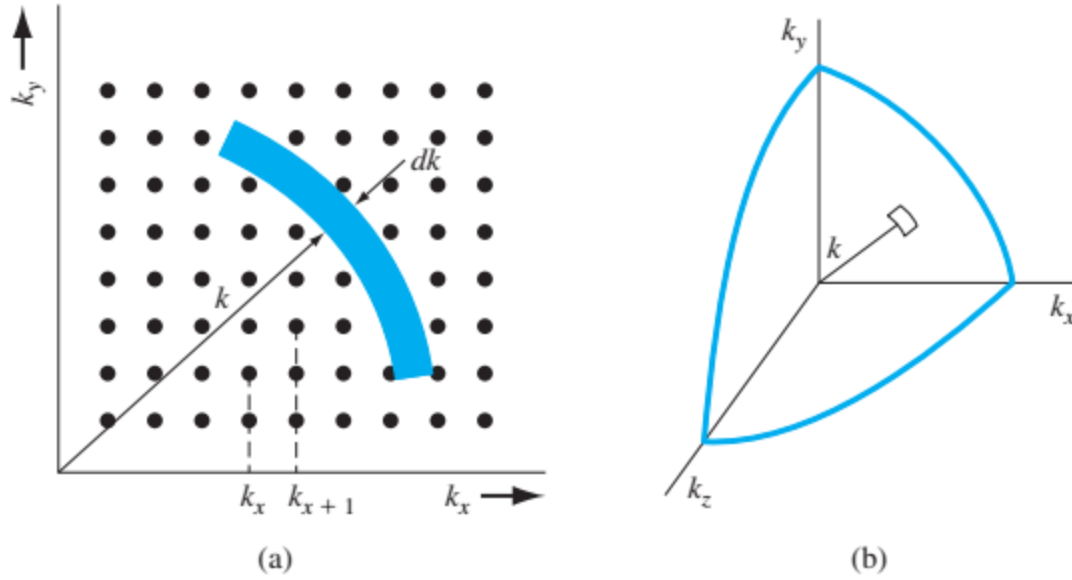Equation (6) gives the density of quantum states as a function of momentum, through the parameter k.

Figure1 (a) A two-dimensional array of allowed quantum states in *k* space. (b) The positive one-eighth of the spherical *k* space.

We can now determine the density of quantum states as a function of energy *E*. For a free electron, the parameters *E* and *k* are related by using (3),

$$k = \frac{1}{\hbar}\sqrt{2mE} \qquad (7)$$

And

$$dk = \frac{1}{\hbar}\sqrt{\frac{m}{2E}}\,dE \qquad (8)$$

Then,; substituting the expressions for k^2 and *dk* into Equation (6), the number of energy states between *E* and *E dE* is given by

$$g(k)dE = \frac{\pi a^3}{\pi^3}\left(\frac{2mE}{\hbar^2}\right)\cdot\frac{1}{\hbar}\sqrt{\frac{m}{2E}}\,dE \qquad (9)$$

Or

$$g(E)dE = \frac{4\pi^3}{h^3}\cdot(2m)^{3/2}\sqrt{E}\,\mathrm{d}E \qquad (10)$$

4

Equation (10) gives the total number of quantum states between the energy E and E dE in the crystal space volume of a^3. If we divide by the volume a^3, then we will obtain the density of quantum states per unit volume of the crystal. Equation (10) then becomes

$$g(E) = \frac{4\pi(2m)^{3/2}}{h^3}\sqrt{E} \tag{11}$$

Example: Calculate the density of states per unit volume over a particular energy range.

Hint, consider the density of states for a free electron given by Equation (11). Calculate the density of states per unit volume with energies between 0 and 1 eV.

Ans. The volume density of quantum states, from Equation (10), is

$$N = \int_0^1 g(E)\, dE = \frac{4\pi(2m)^{3/2}}{h^3}\int_0^1 \sqrt{E}\, dE$$

Then $N = \frac{4\pi(2m)^{3/2}}{h^3}\frac{2}{3}E^{3/2}$,   The density of states is now

$N = \frac{4\pi(9.11x10^{-31})^{3/2}}{(6.625x10^{-34})^3}\cdot\frac{2}{3}(1.6x10^{-19})^{3/2} = 4.5x10^{27}m^{-3}$.

Or   N=4.5x10^{21} states/cm^3

Comment

The density of quantum states is typically a large number. An effective density of states in a semiconductor, as we will see in the following sections and in the next .

H.W: For a free electron, calculate the density of quantum states (#/cm3) over the energy range of (a) $0 \leq E \leq 2.0$ eV and (b) $1 \leq E \leq 2$ eV.