University of Anbar
College of Science – Dept. of Physics

Lectures of Semiconductors #1

for 3th level of physics students
Lecture 7 : Introduction to the Quantum Theory of Solids/3

by
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The E versus k diagram for GaAs.

The valence band maximum and the conduction band minimum both occur at k = 0.

The electrons in the conduction band tend to settle at the minimum conduction band energy which is at k = 0.

Similarly, holes in the valence band tend to congregate at the uppermost valence band energy.

In GaAs, the minimum conduction band energy and maximum valence band energy occur at the same k value.

A semiconductor with this property is said to be a **direct bandgap semiconductor**; transitions between the two allowed bands can take place with no change in crystal momentum $\hbar k$.
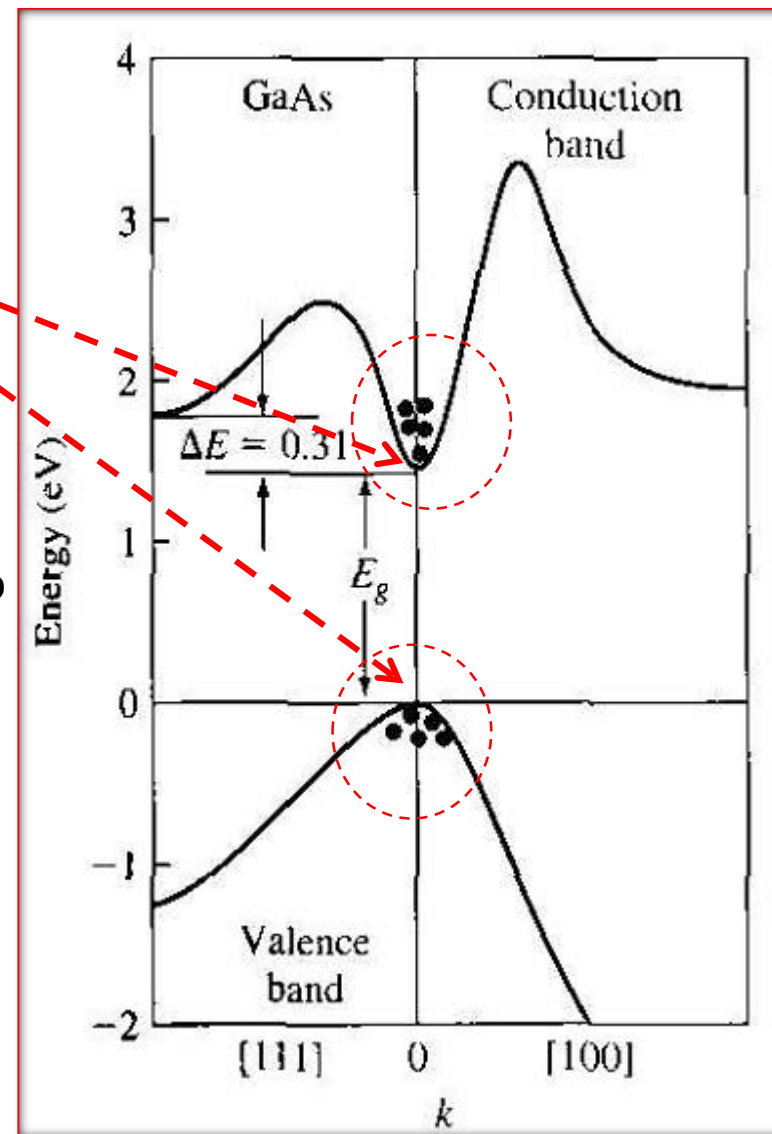
This direct nature has significant effect on the optical properties of the material. GaAs and other direct bandgap materials are ideally suited for use in semiconductor lasers and other optical devices.

The maximum in the valence band energy occurs at k = 0

The minimum in the conduction hand energy occurs not at k = 0, but along the [100] direction.

The difference between the minimum conduction band energy and the maximum valence band energy is still defined as the bandgap energy E_g. A semiconductor whose maximum valence band energy and minimum conduction band energy do not occur at the same k value is called an indirect bandgap semiconductor.

When electrons make a transition between the conduction and valence bands, we must invoke the law of conservation of momentum. A transition in an indirect bandgap material must necessarily include an interaction with the crystal so that crystal momentum is conserved.

Some compound semiconductor, such as Gap and AIAs, have indirect bandgaps
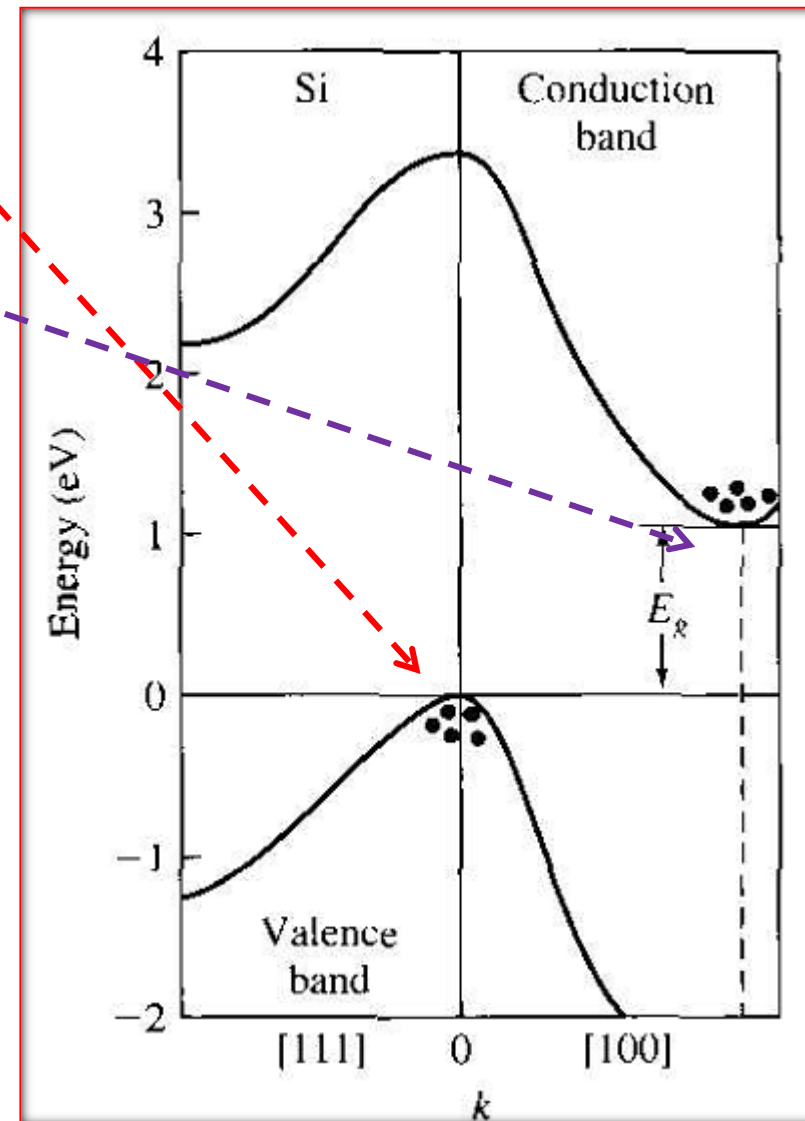
3.3.2 Additional Effective Mass Concepts

❖ The curvature of the E versus k diagrams near the minimum of the conduction band energy is related to the effective mass of the electron. We may note from the beside figure , that the curvature of the conduction band at its minimum value for GaAs is larger than that of silicon, so the effective mass of an electron in the conduction hand of GaAs will be smaller than that in silicon.

❖ For the one-dimensional E versus k diagram, the effective mass was defined by

Equation ,$\frac{1}{\hbar^2}\frac{d^2E}{dk^2} = \frac{1}{m^*}$. A complication occurs in the effective mass concept in a real crystal. A three-dimensional crystal can be described by three k vectors. The curvature of the E versus k diagram at the conduction band minimum may not be the same in the three k directions.
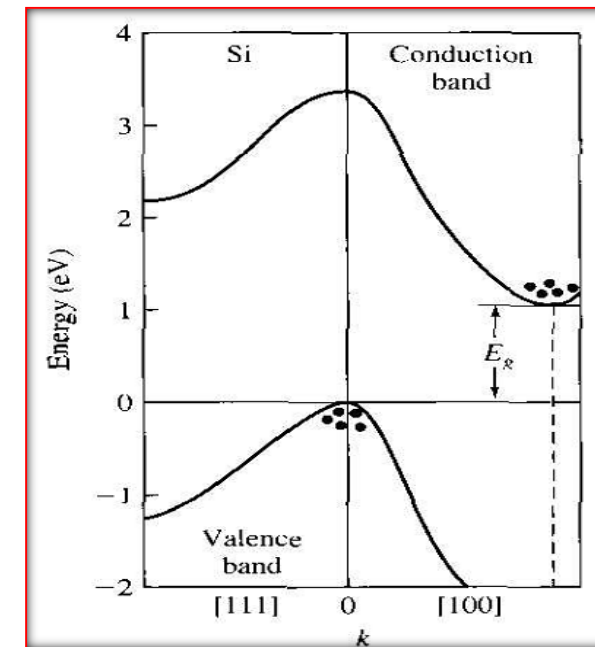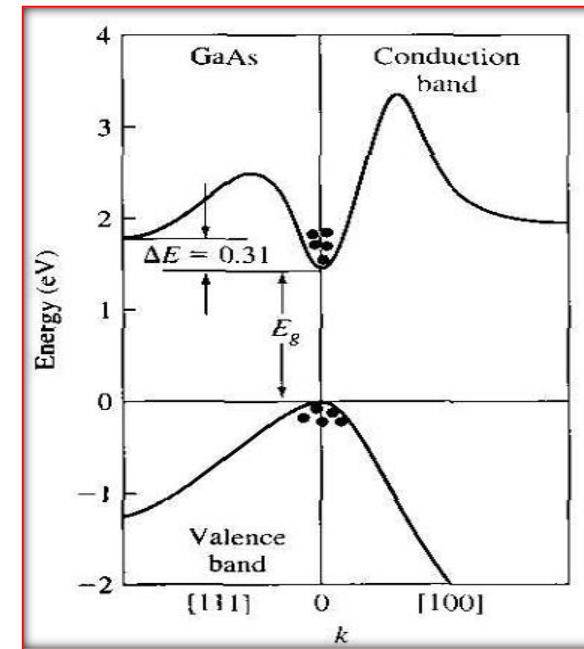
3.4 : DENSITY OF STATES FUNCTION

We can determine the density of quantum states in k space. A differential volume in k space is given by($4\pi\,k^2$ dk) , so the differential density of quantum states in k space can be written as
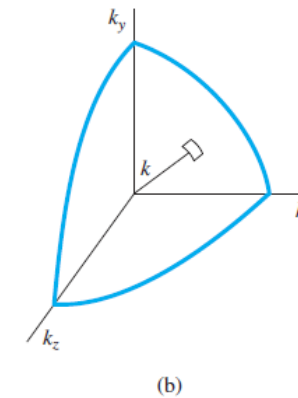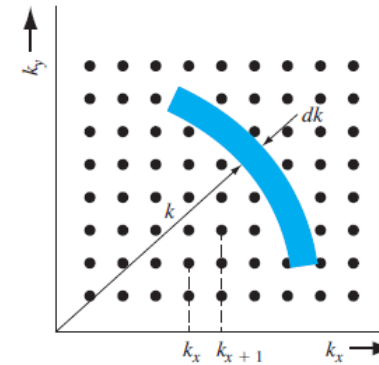
$$g_T(k)dk = 2\left(\frac{1}{8}\right)\frac{4\pi k^2 dk}{\left(\frac{\pi}{a}\right)^3} = \frac{k^2 dk}{\pi^2}a^3 \qquad \ldots\ldots\ldots.(28)$$

$$\hbar = h/2\pi \ , \quad dk = \frac{1}{\hbar}\sqrt{\frac{m}{2E}}dE \ , \quad k^2 = \frac{2mE}{\hbar^2} \qquad V_k = \left(\frac{\pi}{a}\right)^3$$

$$g_T(E)\,dE = \frac{4\pi a^3}{h^3}\cdot(2m)^{3/2}\cdot\sqrt{E}\,dE \qquad \ldots\ldots\ldots\ldots\ldots\ldots.(29)$$

$$g(E) = \frac{4\pi(2m)^{3/2}}{h^3}\sqrt{E} \qquad \ldots\ldots\ldots\ldots\ldots.(30)$$

The density of quantum states is a function of energy E. As the energy of this free electron becomes small, the number of available quantum states decreases. This density function is really a double density, in that the units are given in terms of states per unit energy per unit volume.

The volume density of quantum states is

$$N = \int_{E_1}^{E_2} g(E)\,dE \qquad \dots\dots\dots\dots\dots\dots\dots(31)$$

$$= \frac{4\pi(2m)^{3/2}}{h^3} \int_{E_1}^{E_2} \sqrt{E}\,dE \qquad \dots\dots\dots\dots\dots\dots(32)$$

$$= \frac{2}{3}\,\frac{4\pi(2m)^{3/2}}{h^3}\left(E_2{}^{3/2} - E_1{}^{3/2}\right) \qquad \dots\dots\dots\dots\dots\dots(33)$$

3.4.2 Extension to Semiconductors

The relationship between energy and momentum of a free electron was given by :

$$E = \frac{p^2}{2m} = \frac{k^2\hbar^2}{2m} \quad ………………………………(34)$$

The E versus k curve near $k = 0$ at the bottom of the conduction band can be approximated as a parabola, so we may write

$$E = E_c + \frac{\hbar^2 k^2}{2m_n^*} \quad ……………………(35)$$

where E_c is the bottom edge of the conduction band and m^* is the electron effective mass.

$$E - E_c = \frac{\hbar^2 k^2}{2m_n^*} \quad ………………………(36)$$

The general form of the E versus k relation for an electron in the bottom of a conduction band is the same as the free electron, except the mass is replaced by the effective mass. We can then think of the electron in the bottom of the conduction band as being a "free " electron with its own particular mass.
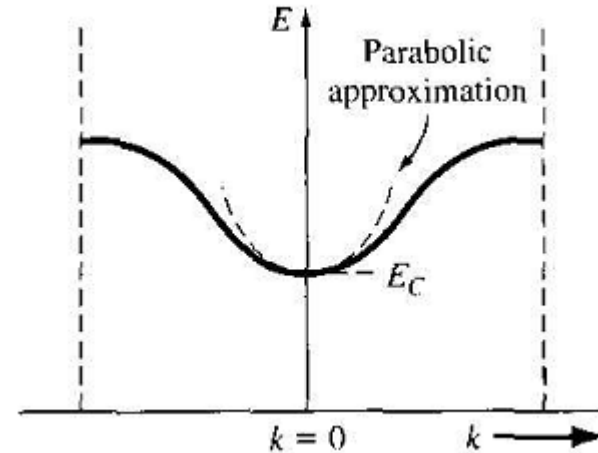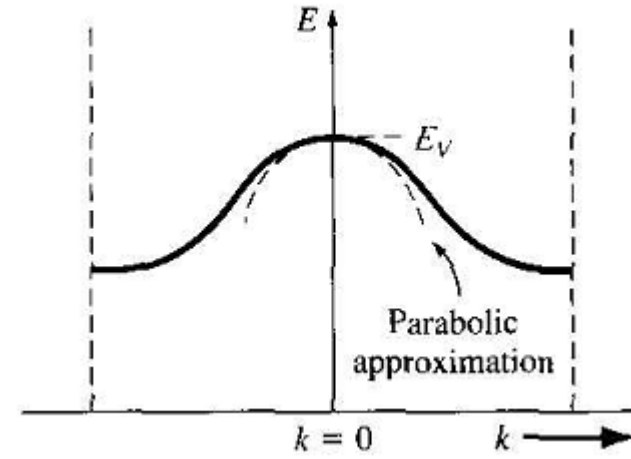
To describe the density of allowed electronic energy states in the conduction band us we can rewrite eq. (46) as :

$$g_c(E) = \frac{4\pi(2m_n{}^*)^{3/2}}{h^3} \sqrt{E - EC} \quad \dots \dots \dots \dots \dots \dots \dots \dots \dots \dots . . (36)$$

Eq. (33) is valid for $E \geq E_c$. As the energy of the electron in the conduction band decreases, the number of available quantum states also decreases.

The density of quantum states in the valence hand can be obtained by using the same infinite potential well model, since the hole is also confined in the semiconductor crystal and can be treated as a "free" particle. The effective mass of the hole is m_p^*. Figure showed the valence energy band in the reduced k space. We may also approximate the E versus k curve near $k = 0$ by a parabola for a "free" hole, so that
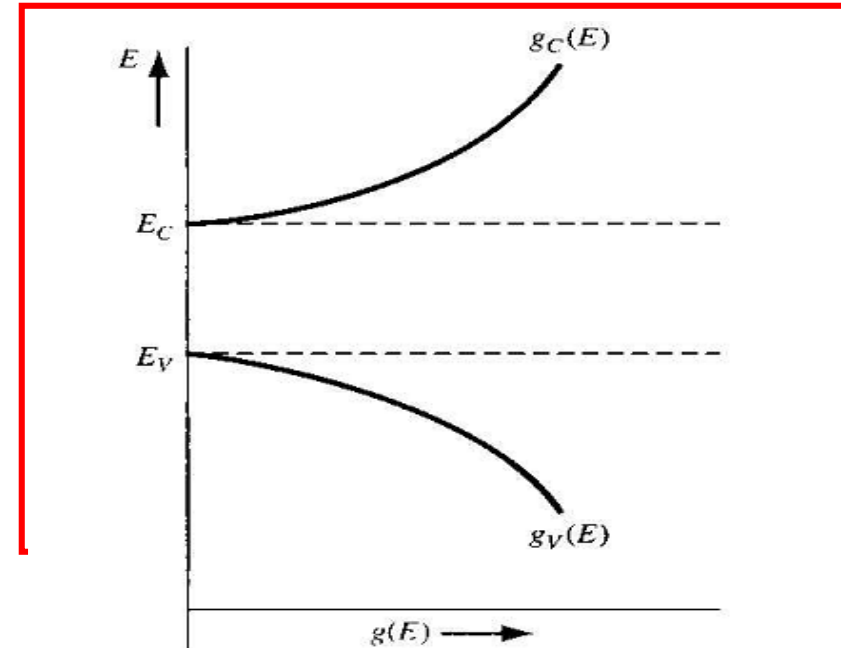

Parabolic approximation

$$E = Ev - \frac{\hbar^2 k^2}{2m_p^*} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (37)$$

$$Ev - E = \frac{\hbar^2 k^2}{2m_p^*} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (38)$$

$$g(E) = \frac{4\pi(2m_p^*)^{3/2}}{h^3} \sqrt{Ev - E} \quad \ldots\ldots\ldots\ldots (39)$$

Equation (56) is valid for $E \leq EC$.

* $g(E) = 0 \; for \; Ev < E \; < EC$

If the electron and hole effective masses were equal, then the functions $g(E)_C$ and $g(E)_v$ would be symmetrical about the energy midway between E_C and E_v or the midgap energy.
E_{midga}

Example:

Determine the total number of energy states in silicon between E_C and $E_v + kT$ at
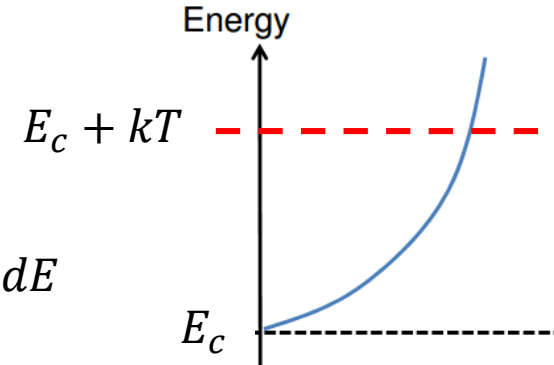
T = 300 K. Where $\dfrac{m_e^{\,*}}{m_{eo}} = 1.08$.

Solution :

Energy

$$E_c + kT \quad \text{-----}$$

$$N = \int_{E_c}^{E_c+kT} g_c(E)\,dE = gc(E) = \int_{E_c}^{E_c+kT} \frac{4\pi(2m_n^{\,*})^{3/2}}{h^3}\sqrt{E - E_C}\,dE$$

$$E_c \quad \text{-----}$$

$$= \int_{E_c}^{E_c+kT} \frac{4\pi(2m_n^{\,*})^{3/2}}{h^3} E^{1/2}\,dE$$

$$= \int_{0}^{kT} \frac{4\pi(2m_n)^{3/2}(m_n^{\,*}/m_n)^{3/2}}{h^3} E^{1/2}\,dE$$

$$= \frac{4\pi(2m_n^{\,*})^{3/2}(m_n^{\,*}/m_n)^{3/2}}{h^3} \cdot \frac{2}{3} E^{3/2} \Big]_{0}^{kT}$$

$$= \frac{4\pi(2\times1.08\times9.11\times10^{-31})^{3/2}}{(6.625\times10^{-34})^3}\left(\frac{2}{3}\right)(0.0259\times1.6\times10^{-19})^{3/2}$$

$$= 2.12\times10^{19}\,cm^{-3}$$

3.5 : STATISTICAL MECHANICS

3.5.1 Statistical Laws

In determining the statistical behavior of particles, we must consider the laws that the particles obey. There are three distribution laws determining the distribution of particles among available energy states.

1. the Maxwell-Boltzmann probability function. In this case, the particles are considered to be distinguishable by being numbered, for example, from 1 to N. with no limit to the number of particles allowed in each energy state. The behavior of gas molecules in a container at Fairly low pressure is an example of this distribution.

2. the Bose-Einstein function. The particles in this case are indistinguishable and, again, there is no limit to the number of particles permitted in each quantum state. The behavior of photons, or black body radiation, is an example of this law. And the particles have integer n of spin (n = 0,1,2 …..)

3. the Fermi-Dirac probability function. In this case, the particles are again indistinguishable, but now only one particle is permitted in each quantum state. Electrons in a crystal obey this law. And the particles have spin (S= 0,1,2 …..) .

In each case, the particles are assumed to be noninteracting

The particles with half-integer spins, such as 1/2, 3/2, 5/2, are known as **fermions**, while the particles with integer spins, such as 0, 1, 2, are known as **bosons**

3.5.2 The Fermi-Dirac Probability Function

The most probable distribution function as

$$\frac{N(E)}{g(E)} = f(E) = \frac{1}{1 + \exp(\frac{E - EF}{kT})}$$

E_F = Fermi energy or Fermi level

k = Boltzmann constant

= 1.38 $\times 10^{-23}$ J/K = 8.6 $\times 10^{-5}$ eV/K

T = absolute temperature in K

Density of states tells us how many states exist at a given energy E. The Fermi function *f(E)* specifies how many of the existing states at the energy E will be filled with electrons. The function f(E) specifies, under equilibrium conditions, the probability that an available state at an energy E will be occupied by an electron. It is a probability distribution function.

$$f(E) = \frac{1}{1 + e^{(E - E_f)/kT}}$$

Fermi-Dirac distribution: Consider $T \to 0$ K

For $E < E_F$:

$$f(E < E_F) = \frac{1}{1+\exp(-\infty)} = 1$$

For $E > E_F$:

$$f(E > E_F) = \frac{1}{1+\exp(+\infty)} = 0 \quad : \exp(+\infty) = \infty$$
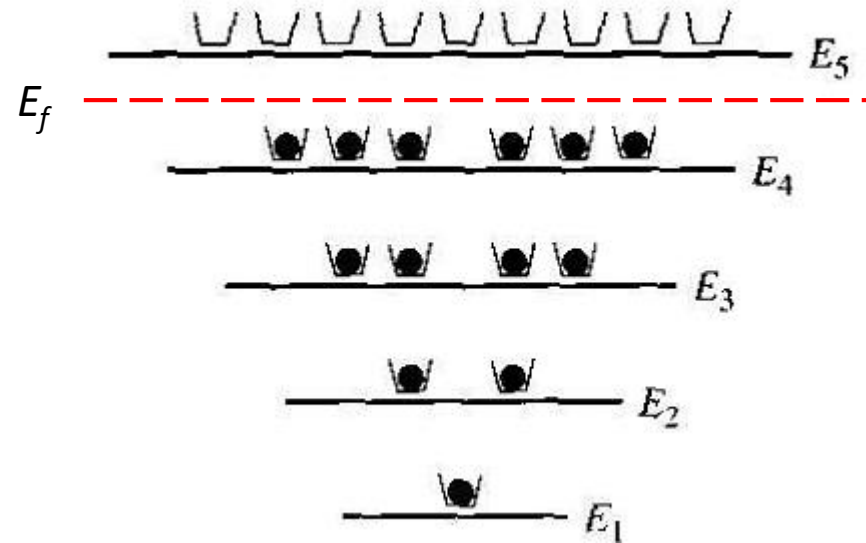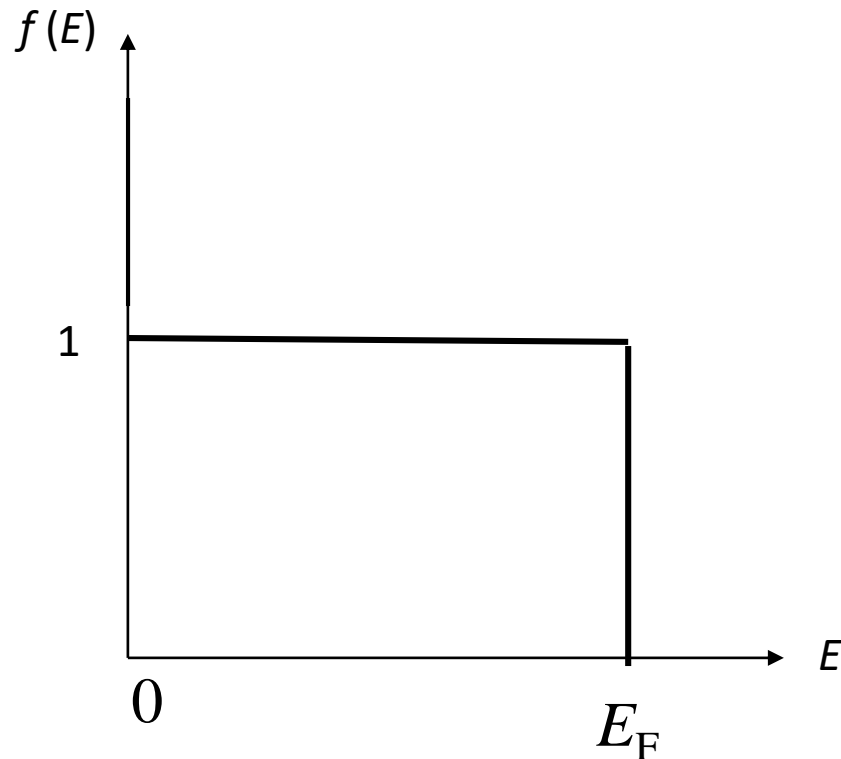
Fermi-Dirac distribution: Consider $T > 0$ K

- If $E = E_F$ then $f(EF) = \frac{1}{2}$

- If $E \geq E_F + 3kT$ then $\exp\left(\dfrac{E - E_F}{kT}\right) \gg 1$

Thus the following approximation is valid: $f(E) = \exp\left(\dfrac{-(E - E_F)}{kT}\right)$

i.e., most states at energies $3kT$ above E_F are empty.

- If $E \leq E_F - 3kT$ then $\exp\left(\dfrac{E - E_F}{kT}\right) \ll 1$

Thus the following approximation is valid: $f(E) = 1 - \exp\left(\dfrac{E - E_F}{kT}\right)$

So, $1 - f(E)$ = Probability that a state is empty, decays to zero.

So, most states will be filled.

kT (at 300 K) = 0.025eV, E_g(Si) = 1.1eV, so $3kT$ is very small in comparison.

- consider a case in which the density of quantum states g(E) is a continuous function of energy

If N_o electrons in this system, then the distribution of these electrons among the quantum states at $T = 0\ K$ is shown by the dashed line. The electrons are in the lowest possible energy state so that all states below E_F are filled and all states above E_F are empty. If g(E) and N_o are known for this particular system, then the Fermi energy E_F can be determined.

$$g(E)$$

$$n(E)$$

$$N_o = \int_0^{E_F} g(E)\, dE$$
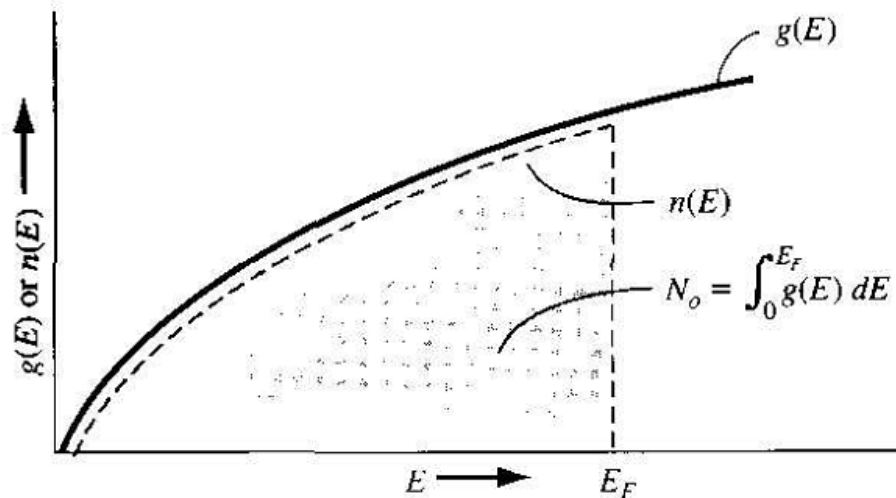
Consider the situation when the temperature increases above T = O K. Electrons gain a certain amount of thermal energy so that some electrons can jump to higher energy levels, which means that the distribution of electrons among the available energy states will change.
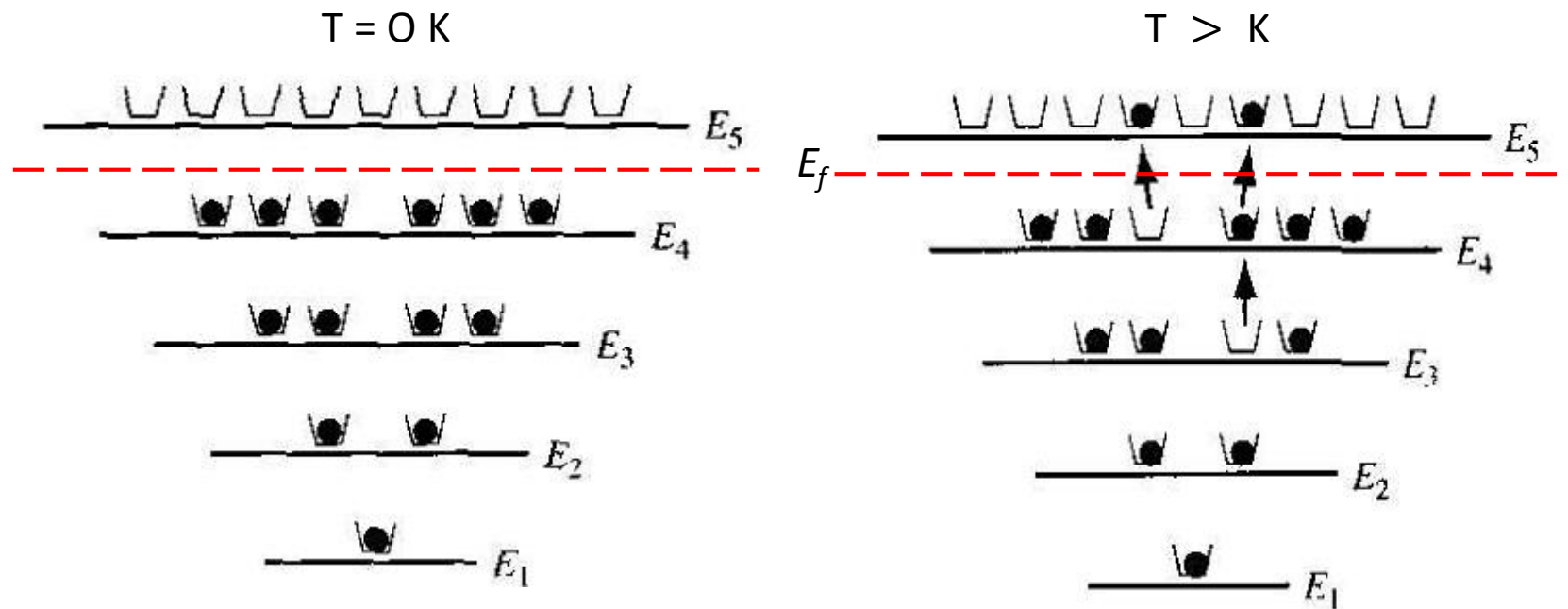
The change in the electron distribution among energy levels for T > O K can be seen by plotting the Fermi-Dirac distribution function. If we *let E = E$_F$* and T > OK

$$E = E_F \text{ then } f(E_F) = \tfrac{1}{2}$$

The probability of a state being occupied at $E = E_F$ is (1/2)
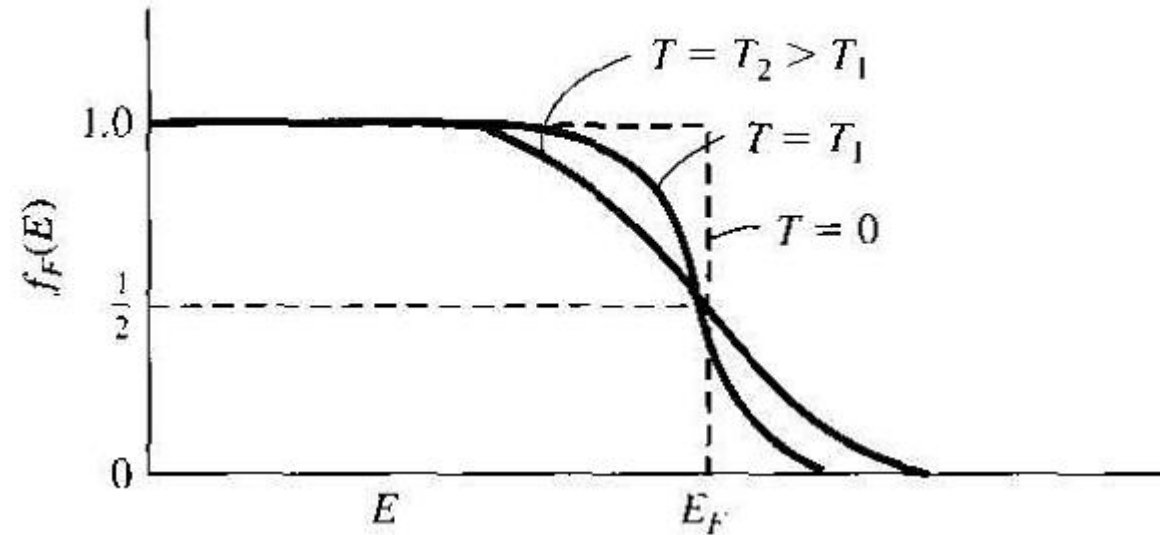
EXAMPLE:

Determine the probability that an energy level 3kT above the Fermi energy is occupied by an electron.

Solution :

$$f(E) = \frac{1}{1 + e^{(E - E_f)/kT}} = \frac{1}{1 + e^{3kT/kT}} = 0.0474$$

H.W : E3.4 , E3.5 , E3.6 and E3.7 P. s 93 and 94

the probability of a state a distance dE above E_F occupied is the same as the probability of a state a distance dE below E_F empty. The function f_F (E) is symmetrical with the function $(1 - f_F(E))$ about t Fermi energy, E_F
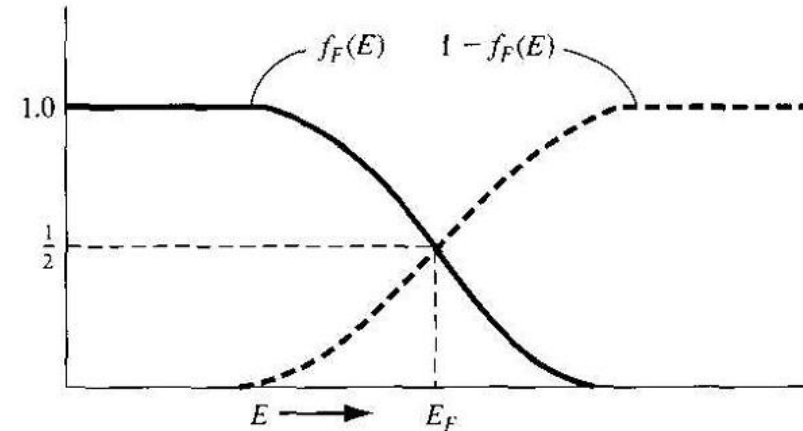
Consider the case when E - E_F >> kT . where the exponential term in the denominator of Equation $f(E) = \dfrac{1}{1+ e^{(E-E_f)/kT}}$ is much greater than unity. We may neglect the 1 in the denominator, so the Femi-Dirac distribution function becomes

$$f(E) \approx e^{-(E-E_f)/kT}$$

This equation is known as the **Maxwell - Boltzmann** approximation, or simply the Boltzmann approximation to the Fermi-Dirac distribution function.
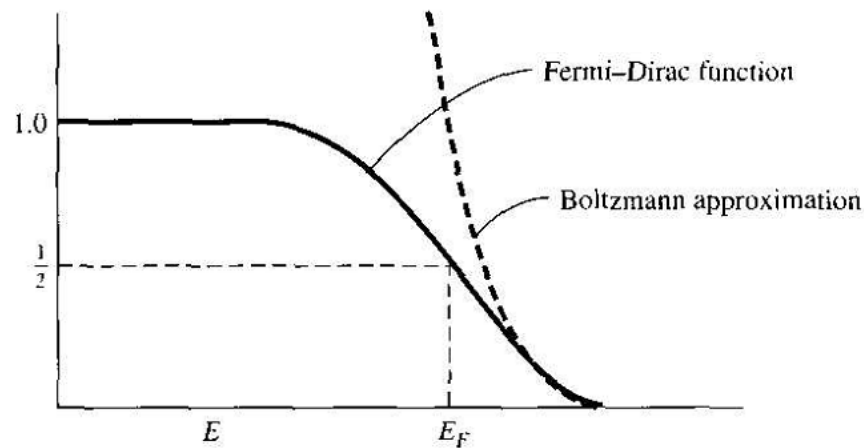
This figure gives an indication of the range of energies over which the approximation is valid.

To determine the energy at which the Boltzmann approximation may be considered valid. Calculate the energy, in terms of kT and E_F . at which the difference between the Boltzmann approximation and the Fermi-Dirac function is 5 percent of the Fermi function.

Solution :

$$\frac{\exp -(E- E_f)/kT - \dfrac{1}{1+\exp~(E- E_f)/kT}}{\dfrac{1}{1+\exp~(E- E_f)/kT}} = 0.05$$

If we multiply both numerator and denominator by the $1 + \exp~(E - E_f)/kT$ function, we have

$$\exp -(E - E_f)/kT . \left(1 + \exp \frac{E- E_f}{kT} \right) - 1 = 0.05$$

$$\exp -(E - E_f)/kT = 0.05$$

$$(E - E_f) = kT ln \left(\frac{1}{0.05} \right) \approx 3kT$$

H.W : Solve the odd problems of ch.3