James Maxwell (1831–1879)
Established velocity
distribution of gases

Ludwig Boltzmann (1844–1906)
Established classical statistics

Enrico Fermi (1901–1954)
Established quantum statistics

13

Classical and quantum statistics

Classical Maxwell–Boltzmann statistics and quantum mechanical Fermi–Dirac statistics are introduced to calculate the occupancy of states. Special attention is given to analytic approximations of the Fermi–Dirac integral and to its approximate solutions in the non-degenerate and the highly degenerate regime. In addition, some numerical approximations to the Fermi–Dirac integral are summarized.

Semiconductor statistics includes both classical statistics and quantum statistics. Classical or Maxwell–Boltzmann statistics is derived on the basis of purely classical physics arguments. In contrast, quantum statistics takes into account two results of quantum mechanics, namely (*i*) the Pauli exclusion principle which limits the number of electrons occupying a state of energy E and (*ii*) the finiteness of the number of states in an energy interval E and $E + \mathrm{d}E$. The finiteness of states is a result of the Schrödinger equation. In this section, the basic concepts of classical statistics and quantum statistics are derived. The fundamentals of ideal gases and statistical distributions are summarized as well since they are the basis of semiconductor statistics.

13.1 Probability and distribution functions

Consider a large number N of free classical particles such as atoms, molecules or electrons which are kept at a constant temperature T, and which interact only weakly with one another. The energy of a single particle consists of *kinetic energy* due to translatory motion and an internal energy for example due to rotations, vibrations, or orbital motions of the particle. In the following we consider particles with only kinetic energy due to translatory motion. The particles of the system can assume an energy E, where E can be either a discrete or a continuous variable. If N_i particles out of N particles have an energy between E_i and $E_i + \mathrm{d}E$, the probability of any particle having any energy within the interval E_i and $E_i + \mathrm{d}E$ is given by

$$f(E_i)\,dE \;\; = \;\; \frac{N_i}{N} \tag{13.1}$$

where $f(E)$ is the **energy distribution function** of a particle system. In statistics, $f(E)$ is frequently called the *probability density function*. The total number of particles is given by

$$\sum_i N_i \;\; = \;\; N \tag{13.2}$$

where the sum is over all possible energy intervals. Thus, the integral over the energy distribution function is

$$\int_0^\infty f(E)\,dE \;\; = \;\; \sum_i \frac{N_i}{N} \;\; = \;\; 1 \; . \tag{13.3}$$

In other words, the probability of any particle having an energy between zero and infinity is unity. Distribution functions which obey

$$\int_0^\infty f(E)\,dE \;\; = \;\; 1 \tag{13.4}$$

are called **normalized** distribution functions.

The **average energy** or **mean energy** $\overline{E}$ of a single particle is obtained by calculating the total energy and dividing by the number of particles, that is

$$\overline{E} \;\; = \;\; \frac{1}{N} \sum_i N_i\, E \;\; = \;\; \int_0^\infty E\, f(E)\,dE \; . \tag{13.5}$$

In addition to energy distribution functions, velocity distribution functions are valuable. Since only the kinetic translatory motion (no rotational motion) is considered, the velocity and energy are related by

$$E \;\; = \;\; \tfrac{1}{2}\, m\, v^2 \; . \tag{13.6}$$

The average velocity and the average energy are related by

$$\overline{E} \;\; = \;\; \tfrac{1}{2}\, m\, \overline{v^2} \tag{13.7}$$

$$v_{\text{rms}} \;\; = \;\; \sqrt{\overline{v^2}} \tag{13.8}$$

and is the velocity corresponding to the average energy

$$\overline{E} \;\; = \;\; \tfrac{1}{2}\, m\, v_{\text{rms}}^2 \; . \tag{13.9}$$

In analogy to the energy distribution we assume that N_i particles have a velocity within the interval v_i and $v_i + dv$. Thus,

$$f(v)\, dv \;=\; \frac{N_i}{N} \tag{13.10}$$

where $f(v)$ is the normalized velocity distribution. Knowing $f(v)$, the following relations allow one to calculate the mean velocity, the mean square velocity, and the root-mean-square velocity

$$\bar{v} \;=\; \int_0^\infty v\, f(v)\, dv \;, \tag{13.11}$$

$$\overline{v^2} \;=\; \int_0^\infty v^2\, f(v)\, dv \;, \tag{13.12}$$

$$v_{\text{rms}} \;=\; \sqrt{\overline{v^2}} \;=\; \left[\int_0^\infty v^2\, f(v)\, dv \right]^{1/2} . \tag{13.13}$$

Up to now we have considered the velocity as a scalar. A more specific description of the velocity distribution is obtained by considering each component of the velocity $v = (v_x, v_y, v_z)$. If N_i particles out of N particles have a velocity in the 'volume' element $v_x + dv_x$, $v_y + dv_y$, and $v_z + dv_z$, the distribution function is given by

$$f(v_x, v_y, v_z)\, dv_x\, dv_y\, dv_z \;=\; \frac{N_i}{N} \;. \tag{13.14}$$

Since $\Sigma_i\, N_i = N$, the velocity distribution function is normalized, *i. e.*

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(v_x, v_y, v_z)\, dv_x\, dv_y\, dv_z \;=\; 1 \;. \tag{13.15}$$

The average of a specific propagation direction, for example v_x is evaluated in analogy to Eqs. (13.11 – 13). One obtains

$$\overline{v_x} \;=\; \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} v_x\, f(v_x, v_y, v_z)\, dv_x\, dv_y\, dv_z \;, \tag{13.16}$$

$$\overline{v_x^2} \;=\; \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} v_x^2\, f(v_x, v_y, v_z)\, dv_x\, dv_y\, dv_z \;, \tag{13.17}$$

$$v_{x,\text{rms}} \;=\; \sqrt{\overline{v_x^2}} \;=\; \left[\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} v_x^2\, f(v_x, v_y, v_z)\, dv_x\, dv_y\, dv_z \right]^{1/2} . \tag{13.18}$$

In a closed system the mean velocities are zero, that is $\bar{v}_x = \bar{v}_y = \bar{v}_z = 0$. However, the mean square velocities are, just as the energy, not equal to zero.

13.2 Ideal gases of atoms and electrons

The basis of classical semiconductor statistics is ideal gas theory. It is therefore necessary to make a small excursion into this theory. The individual particles in such ideal gases are assumed to interact weakly, that is collisions between atoms or molecules are a relatively seldom event. It is further assumed that there is no interaction between the particles of the gas (such as electrostatic interaction), unless the particles collide. The collisions are assumed to be (*i*) *elastic* (*i. e.* total energy and momentum of the two particles involved in a collision are preserved) and (*ii*) of very short duration.

Ideal gases follow the universal gas equation (see *e. g.* Kittel and Kroemer, 1980)

$$P V = R T \tag{13.19}$$

where P is the pressure, V the volume of the gas, T its temperature, and R is the universal gas constant. This constant is independent of the species of the gas particles and has a value of $R = 8.314 \, \text{J K}^{-1} \, \text{mol}^{-1}$.
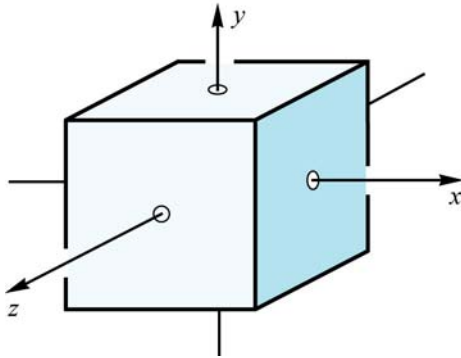

Fig. 13.1. Cubic volume confining one mole ($N_{\text{Avo}} = 6.023 \times 10^{23}$ atoms/mole) of an ideal gas. The pressure of the ideal gas exerted on one side of the cube (shaded area) is calculated in the text.

Next, the pressure P and the kinetic energy of an individual particle of the gas will be calculated. For the calculation it is assumed that the gas is confined to a cube of volume V, as shown in **Fig**. 13.1. The quantity of the gas is assumed to be 1 mole, that is the number of atoms or molecules is given by Avogadro's number, $N_{\text{Avo}} = 6.023 \times 10^{23}$ particles per mole. Each side of the cube is assumed to have an area $A = V^{2/3}$. If a particle of mass m and momentum $m \, v_x$ (along the x-direction) is elastically reflected from the wall, it provides a momentum $2 \, m \, v_x$ to reverse the particle momentum. If the duration of the collision with the wall is dt, then the force acting on the wall during the time dt is given by

$$F = \frac{dp}{dt} \tag{13.20}$$

where the momentum change is $dp = 2 \, m \, v_x$. The pressure P on the wall during the collision with one particle is given by

$$dP = \frac{F}{A} = \frac{1}{A} \frac{dp}{dt} \tag{13.21}$$

where A is the area of the cube's walls. Next we calculate the total pressure P experienced by the wall if a number of N_{Avo} particles are within the volume V. For this purpose we first determine the number of collisions with the wall during the time dt. If the particles have a velocity v_x, then the number of particles hitting the wall during dt is $(N_{\text{Avo}}/V) A \, v_x \, dt$. The fraction of particles

having a velocity v_x is obtained from the velocity distribution function and is given by $f(v_x, v_y, v_z)\, dv_x\, dv_y\, dv_z$. Consequently, the total pressure is obtained by integration over all positive velocities in the x-direction

$$P = \int\limits_{-\infty}^{\infty} \int\limits_{-\infty}^{\infty} \int\limits_{0}^{\infty} \frac{N_{\text{Avo}}}{V} A\, v_x\, dt\, f(v_x, v_y, v_z)\, dv_x\, dv_y\, dv_z\, \frac{2\, m\, v_x}{A\, dt}\ . \tag{13.22}$$

Since the velocity distribution is symmetric with respect to positive and negative x-direction, the integration can be expanded from $-\infty$ to $+\infty$.

$$P = \frac{N_{\text{Avo}}}{V} m \int\limits_{-\infty}^{\infty} \int\limits_{-\infty}^{\infty} \int\limits_{-\infty}^{\infty} v_x^2\, f(v_x, v_y, v_z)\, dv_x\, dv_y\, dv_z = \frac{N_{\text{Avo}}}{V} m\, \overline{v_x^2}\ . \tag{13.23}$$

Since the velocity distribution is isotropic, the mean square velocity is given by

$$\overline{v^2} = \overline{v_x^2} + \overline{v_y^2} + \overline{v_z^2} \quad \text{or} \quad \overline{v_x^2} = \frac{1}{3}\overline{v^2}\ . \tag{13.24}$$

The pressure on the wall is then given by

$$P = \frac{1}{3}\overline{v^2}\, \frac{N_{\text{Avo}}}{V} m\ . \tag{13.25}$$

Using the universal gas equation, Eq. (13.19), one obtains

$$RT = \frac{2}{3} N_{\text{Avo}} \frac{1}{2} m\, \overline{v^2}\ . \tag{13.26}$$

The average kinetic energy of one mole of the ideal gas can then be written as

$$\overline{E} = \overline{E_{kin}} = \frac{3}{2} RT\ . \tag{13.27}$$

The average kinetic energy of one single particle is obtained by division by the number of particles, *i. e.*

$$\boxed{\overline{E} = \overline{E_{\text{kin}}} = \frac{3}{2} kT} \tag{13.28}$$

where $k = R / N_{\text{Avo}}$ is the Boltzmann constant. The preceding calculation has been carried out for a three-dimensional space. In a one-dimensional space (one degree of freedom), the average velocity is $\overline{v^2} = \overline{v_x^2}$ and the resulting kinetic energy is given by

$$\overline{E_{\text{kin}}} = \frac{1}{2} kT \qquad \text{(per degree of freedom)}\ . \tag{13.29}$$

Thus the kinetic energy of an atom or molecule is given by $(1/2) kT$. Equation (13.29) is called the ***equipartition law***, which states that each 'degree of freedom' contributes $(1/2) kT$ to the total kinetic energy.

Next we will focus on the energetic distribution of electrons. The properties which have been derived in this section for atomic or molecular gases will be applied to free electrons of effective mass m^* in a crystal. To do so, the interaction between the electrons and the lattice must be negligible and electron – electron collisions must be a relatively seldom event. Under these circumstances we can treat the electron system as a classical ideal gas.

13.3 Maxwell velocity distribution

The Maxwell velocity distribution describes the distribution of velocities of the particles of an ideal gas. It will be shown that the Maxwell velocity distribution is of the form

$$f_{\mathrm{M}}(v) = A \exp\left(-\frac{(1/2)\, m\, v^2}{kT}\right) \tag{13.30}$$

where $(1/2)\, m\, v^2$ is the kinetic energy of the particles. If the energy of the particles is purely kinetic, the Maxwell distribution can be written as

$$f_{\mathrm{M}}(E) = A \exp\left(-\frac{E}{kT}\right). \tag{13.31}$$

The proof of the Maxwell distribution of Eq. (13.30) is conveniently done in two steps. In the first step, the exponential factor is demonstrated, *i. e.* $f_{\mathrm{M}}(E) = A \exp(-\alpha E)$. In the second step it is shown that $\alpha = 1 / (kT)$.

In the theory of ideal gases it is assumed that collisions between particles are elastic. The total energy of two electrons before and after a collision remains the same, that is

$$E_1 + E_2 = E_1' + E_2' \tag{13.32}$$

where E_1 and E_2 are the electron energies before the collision and E_1' and E_2' are the energies after the collision. The probability of a collision of an electron with energy E_1 and of an electron with energy E_2 is proportional to the probability that there is an electron of energy E_1 and a second electron with energy E_2. If the probability of such a collision is p, then

$$p = B\, f_{\mathrm{M}}(E_1)\, f_{\mathrm{M}}(E_2) \tag{13.33}$$

where B is a constant. The same consideration is valid for particles with energies E_1' and E_2'. Thus, the probability that two electrons with energies E_1' and E_2' collide is given by

$$p' = B\, f_{\mathrm{M}}(E_1')\, f_{\mathrm{M}}(E_2') . \tag{13.34}$$

If the change in energy before and after the collision is ΔE, then $\Delta E = E_1' - E_1$ and $\Delta E = E_2 - E_2'$. Furthermore, if the electron gas is in equilibrium, then $p = p'$ and one obtains

$$f_{\mathrm{M}}(E_1)\, f_{\mathrm{M}}(E_2) = f_{\mathrm{M}}(E_1 + \Delta E)\, f_{\mathrm{M}}(E_2 - \Delta E) . \tag{13.35}$$

Only the exponential function satisfies this condition, that is

$$f_M(E) \;=\; A \exp(-\alpha E) \tag{13.36}$$

where α is a positive yet undetermined constant. The exponent is chosen negative to assure that the occupation probability decreases with higher energies. It will become obvious that α is a universal constant and applies to all carrier systems such as electron-, heavy- or light-hole systems.

Next, the constant α will be determined. It will be shown that $\alpha = 1/kT$ using the results of the ideal gas theory. The energy of an electron in an ideal gas is given by

$$E \;=\; \tfrac{1}{2} m v^2 \;=\; \tfrac{1}{2} m (v_x^2 + v_y^2 v + v_z^2) \; . \tag{13.37}$$

The exponential energy distribution of Eq. (13.36) and the normalization condition of Eq. (13.15) yield the normalized velocity distribution

$$f(v_x, v_y, v_z) \;=\; \left(\frac{m\,\alpha}{2\,\pi} \right)^{3/2} \exp\left[-\frac{1}{2} m\,\alpha\, (v_x^2 + v_y^2 + v_z^2) \right] . \tag{13.38}$$

The average energy of an electron is obtained by (first) calculating the mean square velocities, $\overline{v_x^2}, \overline{v_y^2}, \overline{v_z^2}$ from the distribution and (second) using Eq. (13.37) to calculate E from the mean square velocities. One obtains

$$E \;=\; (3/2)\,\alpha^{-1} \; . \tag{13.39}$$

We now use the result from classic gas theory which states according to Eq. (13.28) that the kinetic energy equals $E = (3/2)\,kT$. Comparison with Eq. (13.39) yields

$$\alpha \;=\; (kT)^{-1} \tag{13.40}$$

which concludes the proof of the Maxwell distribution of Eqs. (13.30) and (13.31).

Having determined the value of α, the explicit form of the normalized *maxwellian velocity distribution* in cartesian coordinates is

$$f_M(v_x, v_y, v_z) \;=\; \left(\frac{m}{2\,\pi\,kT} \right)^{3/2} \exp\left[-\frac{\frac{1}{2} m (v_x^2 + v_y^2 + v_z^2)}{kT} \right] \tag{13.41}$$

Due to the spherical symmetry of the maxwellian velocity distribution, it is useful to express the distribution in spherical coordinates. For the coordinate transformation we note that $f_M(v_x, v_y, v_z)\, dv_x\, dv_y\, dv_z = f_M(v)\, dv$, and that a volume element $dv_x\, dv_y\, dv_z$ is given by $4\,\pi\,v^2\, dv$ in spherical coordinates. The maxwellian velocity distribution in spherical coordinates is then given by

$$f_M(v) \;=\; \left(\frac{m}{2\,\pi\,kT} \right)^{3/2} (4\,\pi\,v^2) \exp\left(-\frac{\frac{1}{2} m v^2}{kT} \right) . \tag{13.42}$$

The maxwellian velocity distribution is shown in *Fig*. 13.2. The peak of the distribution, that is the most likely velocity, is $v_p = (2kT/m)^{1/2}$. The mean velocity is given by $\bar{v} = (8kT)/(\pi m)^{1/2}$. The root-mean-square velocity can only be obtained by numerical integration.
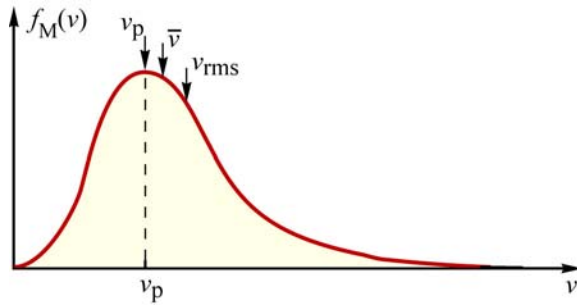

Fig. 13.2. Schematic maxwellian velocity distribution $f_M(v)$ of an ideal elecron gas. The velocity with the highest probability, v_p, is lower than the mean velocity, $\bar{v}$, and the root-mean-square velocity, v_{rms}.

13.4 The Boltzmann factor

The maxwellian velocity distribution can be changed to an energy distribution by using the substitution $E = (1/2)\,m\,v^2$. Noting that the energy interval and the velocity interval are related by $dE = m\,v\,dv$ and that the number of electrons in the velocity interval, $f_M(v)\,dv$, is the same as the number of electrons in the energy interval, $f_{MB}(E)\,dE$, then the energy distribution is given by

$$f_{MB}(E) \;=\; \frac{2}{\sqrt{\pi}} \frac{\sqrt{E}}{(kT)^{3/2}} e^{-E/kT} \tag{13.43}$$

which is the *Maxwell–Boltzmann distribution*.

For large energies, the exponential term in the Maxwell–Boltzmann distribution essentially determines the energy dependence. Therefore, the high-energy approximation of the Maxwell–Boltzmann distribution is

$$f_B(E) \;=\; A\,e^{-E/kT} \tag{13.44}$$

which is the *Boltzmann distribution*. The exponential factor of the distribution, $\exp(-E/kT)$, is called the *Boltzmann factor* or *Boltzmann tail*. The Boltzmann distribution does not take into account the quantum mechanical properties of an electron gas. The applicability of the distribution is therefore limited to the classical regime, *i. e.* for $E \gg kT$.

13.5 The Fermi–Dirac distribution

In contrast to classical Boltzmann statistics, the quantum mechanical characteristics of an electron gas are taken into account in Fermi–Dirac statistics. The quantum properties which are explicitly taken into account are

- The *wave character* of electrons. Due to the wave character of electrons the Schrödinger equation has only a *finite number of solutions* in the energy interval E and $E + dE$.

- The *Pauli principle* which states that an eigenstate can be occupied by only two electrons of opposite spin.

Since the Pauli principle strongly restricts the number of carriers per energy level, higher states are populated even at zero temperature. This situation is illustrated in *Fig*. 13.3, where two

electron distributions are illustrated at zero temperature. The distribution in *Fig*. 13.3(a) does not take into account the Pauli principle while that in *Fig*. 13.3(b) does.
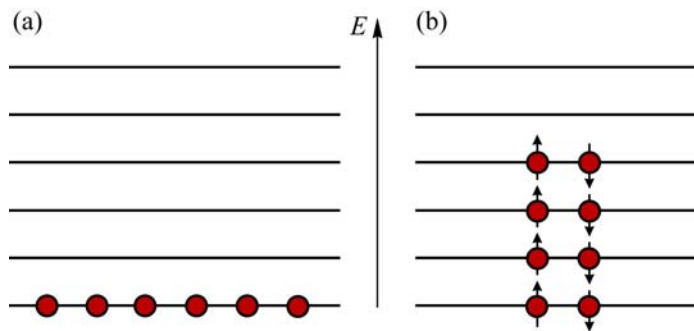

Fig. 13.3. Distribution of electrons at zero temperature among discrete energy levels (a) without Pauli principle and (b) with Pauli principle and spin taken into account. Spin 'up' and 'down' is illustrated by arrows.

The first restriction imposed by quantum mechanics is the *finiteness of states* within an energy interval E and $E + dE$. Recall that the finiteness of states played a role in the derivation of the density of states. The density of states in an isotropic semiconductor was shown to be

$$\rho_{DOS}(E) \; = \; \frac{1}{2\,\pi^2}\left(\frac{2\,m^*}{\hbar^2}\right)^{3/2}\sqrt{E} \tag{13.45}$$

where E is the kinetic energy. Note that for the derivation of the density of states the Pauli principle has been taken into account. Therefore, the states given by Eq. (13.45) can be occupied only by *one* electron. Since the number of states per velocity-interval will be of interest, Eq. (13.45) is modified using $E = (1/2)\,mv^2$ and $dE = mv\,dv$. Note that the number of states per energy interval dE is the same as the number of states per velocity interval dv, *i. e.* $\rho_{DOS}(E)\,dE = \rho_{DOS}(v)\,dv$. The number of states per velocity interval (and per unit volume) is then given by

$$\rho_{DOS}(v) \; = \; \frac{m^{*3}}{\pi^2\,\hbar^3}\,v^2 \tag{13.46}$$

for an isotropic semiconductor.

The *Fermi–Dirac distribution*, also called the Fermi distribution, gives the probability that a state of energy E is occupied. Since the Pauli principle has been taken into account in the density of states given by Eq. (13.45), each state can be occupied by at most one electron. The Fermi distribution is given by

$$f_F(E) \; = \; \left[1 \,+\, \exp\left(\frac{E - E_F}{kT}\right)\right]^{-1} \tag{13.47}$$

where E_F is called the Fermi energy. At $E = E_F$ the Fermi distribution has a value of 1/2. For small energies the Fermi distribution approaches 1; thus low-energy states are very likely to be populated by electrons. For high energies the Fermi distribution decreases exponentially; states of high energy are less likely to the populated. Particles which follow a Fermi distribution are called *fermions*. Electrons and holes in semiconductors are such fermions. A system of particles which obey *Fermi* statistics are called a *Fermi gas*. Electrons and holes constitute such Fermi gases.

An approximate formula for the Fermi distribution can be obtained for high energies. One obtains for $E \gg E_F$

$$f_F(E) \approx \exp\left(-\frac{E - E_F}{kT}\right) = f_B(E) .$$

(13.48)

This distribution coincides with the Boltzmann distribution. Thus the (quantum-mechanical) Fermi distribution and the (classical) Boltzmann distribution coincide for high energies, *i. e.* in the classical regime.

Next we prove the Fermi distribution of Eq. (13.47) by considering a collision between two electrons. For simplification we assume that one of the electrons has such a high energy that it belongs to the classical regime of semiconductor statistics. Quantum statistics applies to the other low-energy electron. During the collision of the two electrons, the energy is conserved

$$E_1 + E_2 = E_1' + E_2'$$

(13.49)

where, as before (Eq. 13.32), E_1 and E_2 are electron energies before the collision and E_1' and E_2' are the energies after the collision.

The probability for the transition $(E_1, E_2) \rightarrow (E_1', E_2')$ is given by

$$p = f_F(E_1) \, f_B(E_2) \left[1 - f_F(E_1')\right] \left[1 - f_B(E_2')\right]$$

(13.50)

where it is assumed that E_2 and E_2' are relatively large energies and the corresponding electron can be properly described by the Boltzmann distribution. The terms $[1 - f_F(E_1')]$ and $[1 - f_B(E_2')]$ describe the probability that the states of energies E_1' and E_2' are empty, and are available for the electron after the collision. Further simplification is obtained by considering that E_2' is large and therefore $[1 - f_B(E_2')] \approx 1$. Equation (13.50) then simplifies to

$$p = f_F(E_1) f_B(E_2) \left[1 - f_F(E_1')\right] .$$

(13.51)

The same considerations are valid for the transition $(E_1', E_2') \rightarrow (E_1, E_2)$. The probability of this transition is given by

$$p' = f_F(E_1') \, f_B(E_2') \left[1 - f_F(E_1)\right] .$$

(13.52)

Under equilibrium conditions both transition probabilities are the same, *i. e.* $p = p'$. Equating Eqs. (13.51) and (13.52), inserting the Boltzmann distribution for $f_B(E)$, and dividing by $f_F(E_1)$ $f_F(E_1') f_B(E_2)$ yields

$$\frac{1}{f_F(E_1')} - 1 = \left[\frac{1}{f_F(E_1)} - 1\right] \exp\left[\frac{E_2 - E_2'}{kT}\right]$$

(13.53)

which must hold for all E_1 and E_1'. This condition requires that

$$\frac{1}{f_F(E)} - 1 = A \exp\frac{E}{kT}$$

(13.54)

where A is a constant. If the value of the constant is taken to be $A = \exp(-E_F/kT)$ one obtains the **Fermi–Dirac distribution**

$$f_F(E) = \left[1 + \exp\left(\frac{E - E_F}{kT}\right)\right]^{-1} \tag{13.54}$$
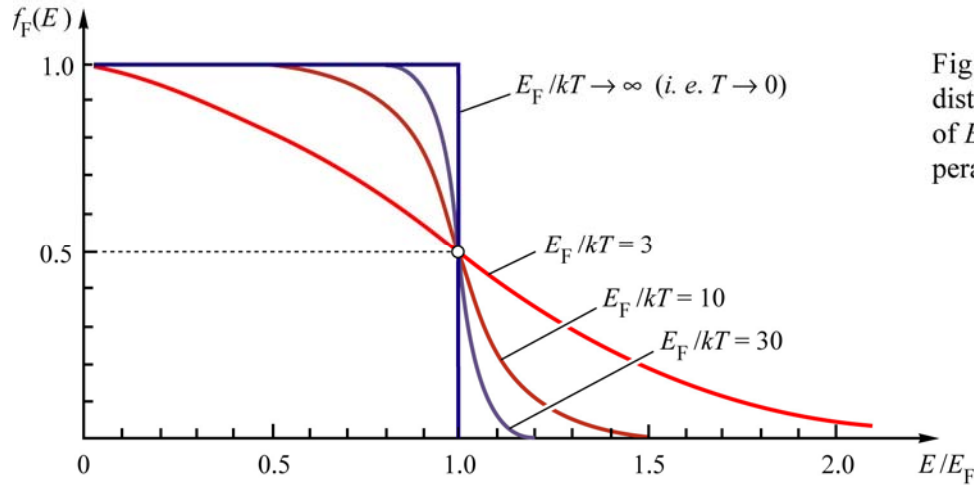
which proves Eq. (13.47).

Fig. 13.4. Fermi–Dirac distribution as a function of E/E_F for different temperatures.

The Fermi–Dirac distribution is shown for different temperatures in **Fig**. 13.4. At the energy $E = E_F$ the probability of a state being populated has always a value of ½ independent of temperature. At higher temperatures, states of higher energies become populated. Note that the Fermi–Dirac distribution is symmetric with respect to E_F, that is

$$f_F(E_F + \Delta E) = 1 - f_F(E_F - \Delta E) \tag{13.55}$$

where ΔE is any energy measured with respect to the Fermi energy.

The Fermi–Dirac velocity distribution of the particles in a Fermi gas is obtained by multiplication of Eq. (13.46) with Eq. (13.47)

$$g(v) = \rho_{DOS}(v)\, f_F(v) = \frac{m^3 v^3}{\pi^2 \hbar^3}\left[1 + \exp\left(\frac{\frac{1}{2}mv^2 - E_F}{kT}\right)\right]^{-1} \tag{13.56}$$

where we have used the fact that the energy of the Fermi gas is purely kinetic, *i. e.* $E = (1/2)\,mv^2$. Note that $g(v)$ is the number of carriers per velocity interval v and $v + dv$ and per unit volume. If the velocity v is expressed in terms of its components, then the spherical volume element, $4\pi v^2\, dv$, is modified to a volume element in rectangular coordinates, $dv_x\, dv_y\, dv_z$. Thus, using $g(v)\, dv = g(v_x, v_y, v_z)\, dv_x\, dv_y\, dv_z$, one obtains

$$g(v_x, v_y, v_z) = \frac{m^3}{\pi^2 \hbar^3}\frac{1}{4\pi}\, v\left\{1 + \exp\left[\frac{\frac{1}{2}\left(v_x^2 + v_y^2 + v_z^2\right) - E_F}{kT}\right]\right\}^{-1} \tag{13.57}$$

which is the Fermi velocity distribution (per unit volume) in cartesian coordinates.

The Fermi distribution of energies of an ideal gas is obtained by multiplication of Eq. (13.45) with Eq. (13.47) and is given by

$$g(E) = \frac{1}{2\pi^2}\left(2\frac{m}{\hbar^2}\right)^{3/2}\sqrt{E}\left[1 + \exp\left(\frac{E - E_F}{kT}\right)\right]^{-1} \tag{13.59}$$

when $g(E)$ is the number of particles in the energy interval E and $E + dE$ and per unit volume.

13.6 The Fermi–Dirac integral of order $j = + 1/2$ (3D semiconductors)

The Fermi–Dirac integral of order $j = + 1/2$ allows one to calculate the free carrier concentration in a three-dimensional (3D) semiconductor. The free carrier concentration in one band, e. g. the conduction band, of a semiconductor is obtained from the product of density of states and the state occupation probability, i. e.

$$n = \int_{E_C}^{E_{top}} \rho_{DOS}(E)\, f_F(E)\, dE \ . \tag{13.60}$$

Integration over all conduction band states is required to obtain the total concentration. The upper limit of integration is the top of the conduction band and can be extended to infinity. This extension of $E_C^{top} \to \infty$ can be done without losing accuracy, since $f_F(E)$ converges strongly at high energies. The two functions, $\rho_{DOS}(E)$, $f_F(E)$, and their product are schematically shown in *Fig*. 13.5 for a semiconductor with three, two, and one, spatial degrees of freedom. The concentration per unit energy $n(E)$ is the product of state density and distribution function.
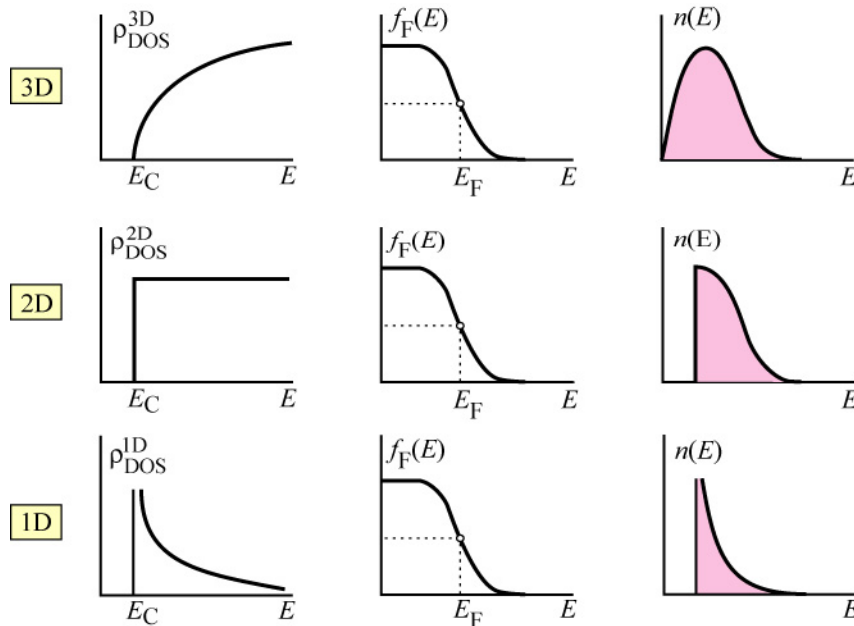

Fig. 13.5. Density of states (ρ_{DOS}), Fermi-Dirac distribution function (f_F) and carrier concentration (n) as a function of energy for a 3D, 2D, and 1D system. The shaded areas represent the total carrier concentration in the conduction band.

Equation (13.60) is evaluated by inserting the explicit expressions for the state density and the Fermi–Dirac distribution (Eq. 13.47). One obtains

$$n = \frac{1}{2\pi^2} \left(\frac{2 m^* kT}{\hbar^2} \right)^{3/2} \int_0^\infty \frac{\eta^{1/2}}{1 + \exp(\eta - \eta_F)} \, d\eta \qquad (13.61)$$

where $\eta = E/kT$ and $\eta_F = -(E_C - E_F)/kT$ is the reduced Fermi energy. η_F is positive when E_F is inside the conduction band. The equation can be written in a more convenient way by using the Fermi–Dirac integral of order j, which is defined by (Sommerfeld, 1928; Sommerfeld and Frank, 1931)

$$F_j(\eta_F) = \frac{1}{\Gamma(j+1)} \int_0^\infty \frac{\eta^j}{1 + \exp(\eta - \eta_F)} \, d\eta \qquad (13.62)$$

where $\Gamma(j+1)$ is the Gamma-function.

Sommerfeld's original definition of the Fermi–Dirac integral omitted the term of the Gamma–function, i. e. $F_j^s(\eta_F) = \int_0^\infty \eta^j / [1 + \exp(\eta - \eta_F)] \, d\eta$. The modern definition of the Fermi–Dirac integral of Eq. (13.62) has the following advantages: (i) Unlike F_j^s, the functions F_j exist for negative orders of j, e. g. $j = -(1/2)$, -1, $-3/2$ etc. (ii) In the non-degenerate limit in which $\eta_F \ll 0$, all members of the $F_j(\eta_F)$ family reduce to $F_j(\eta_F) \to \exp \eta_F$ for all j. (iii) The *derivative* of the Fermi–Dirac integral of integer order j can be expressed as a Fermi–Dirac integral of order $(j-1)$, i. e. $(\partial/\partial \eta_F) F_j(\eta_F) = F_{j-1}(\eta_F)$.

With $j = (1/2)$ and $\Gamma(3/2) = \pi^{1/2}/2$ one obtains

$$n = N_c F_{1/2}(\eta_F) \qquad (13.63)$$

where N_c is the effective state density at the bottom of the conduction band. The Fermi–Dirac integral $F_{1/2}$ is shown in *Fig*. 13.6 along with several approximations which will be discussed later.

For $j = (1/2)$ the Fermi–Dirac integral is

$$F_{1/2}(\eta_F) = \frac{1}{\Gamma(3/2)} \int_0^\infty \frac{\eta^{1/2}}{1 + \exp(\eta - \eta_F)} \, d\eta . \qquad (13.64)$$

The evaluation of the integral cannot be done analytically. Even though the numerical calculation of the Fermi–Dirac integral is straightforward, it proves frequently convenient to use *approximate* analytic solutions of $F_{1/2}(\eta_F)$.

For analytic approximations of the Fermi–Dirac integral $n/N_c = F_{1/2}(\eta_F)$, the inverse function is frequently used, that is the reduced Fermi energy η_F is expressed as a function of n/N_c. A number of analytic approximations developed prior to 1982 have been reviewed by Blakemore (Blakemore, 1982). To classify various approximations, we differentiate between non-degeneracy and degeneracy. In the *non-degenerate* regime, the Fermi energy is below the bottom of the conduction band, $E_F \ll E_C$. In the *degenerate* regime the Fermi energy is at or above the bottom of the conduction band.
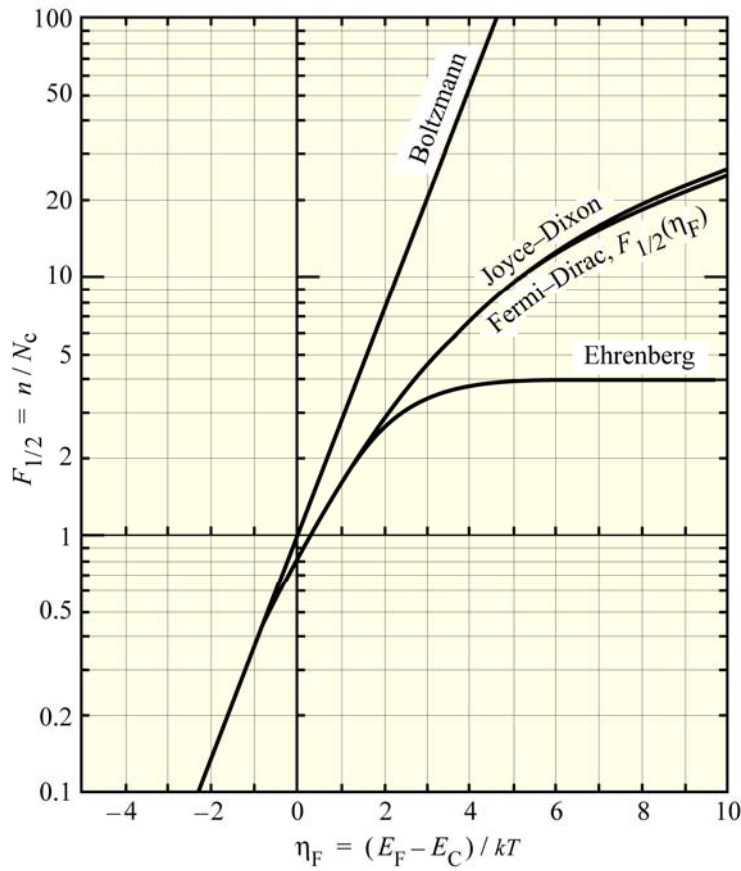
Fig. 13.6. Fermi–Dirac integral of order 1/2 as a function of the reduced Fermi energy η_F. Also shown are the Boltzmann distribution, the Joyce–Dixon approximation and the Ehrenberg approximation.

- *Extreme non-degeneracy (3D)*

  In the case of extreme non-degeneracy (*i. e.* $E_C - E_F \gg kT$ or $F_{1/2} \ll 1$ or $n \ll N_c$) the Fermi–Dirac distribution approaches the Boltzmann distribution. One obtains

  $$\eta_F = -\frac{E_C - E_F}{kT} \approx \ln \frac{n}{N_c} \tag{13.65}$$

  which is shown in *Fig.* 13.7. This approximation is good when the Fermi energy is $2\,kT$ or more below the bottom of the conduction band. Rearrangement of the equation yields the carrier concentration as a function of the Fermi energy in the non-degenerate limit

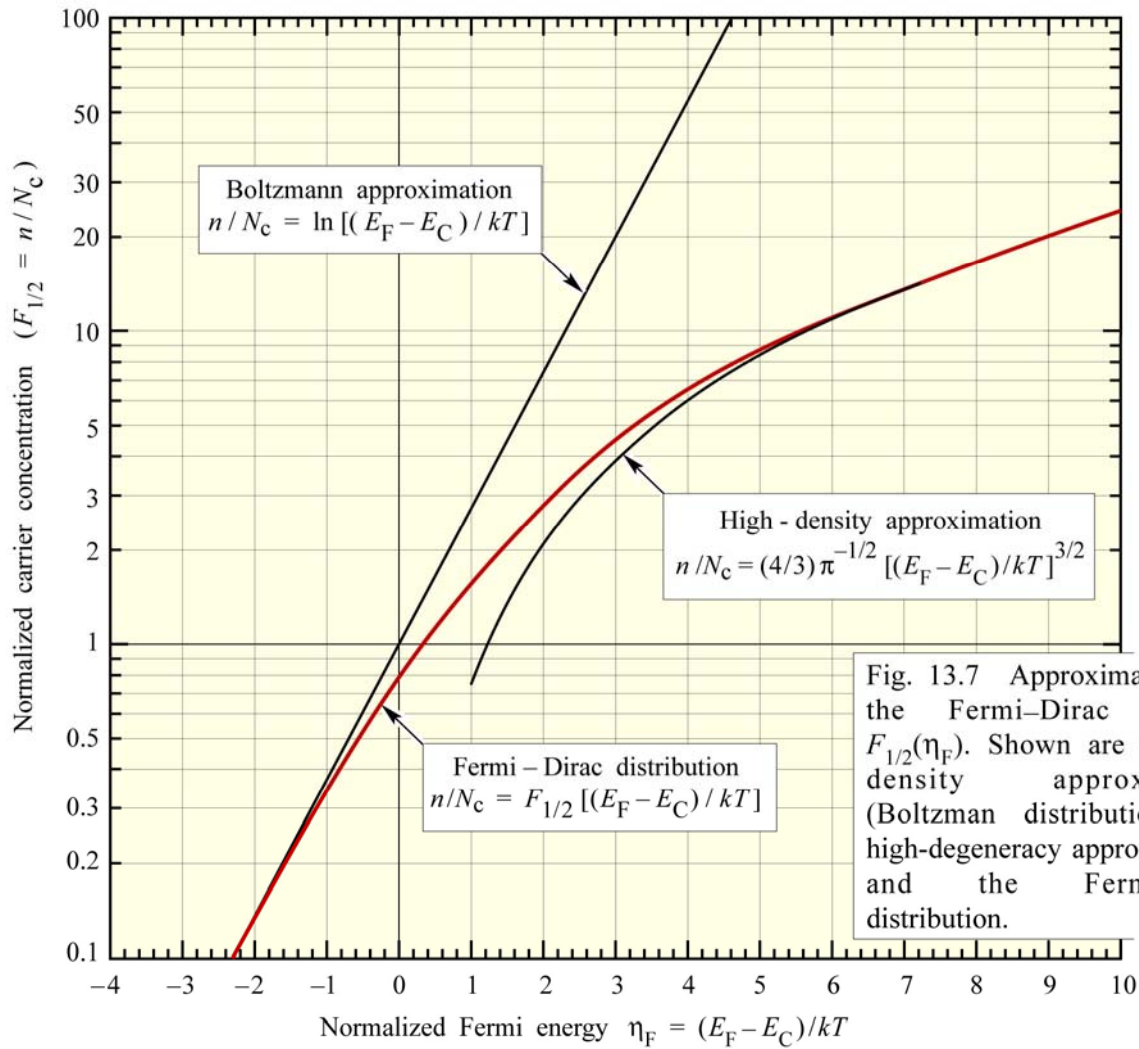 $$n = N_c \exp\left(-\frac{E_C - E_F}{kT}\right) \tag{13.66}$$

Fig. 13.7 Approximations for the Fermi–Dirac integral $F_{1/2}(\eta_F)$. Shown are the low-density approximation (Boltzman distribution), the high-degeneracy approximation, and the Fermi–Dirac distribution.

- ***Extreme degeneracy (3D)***
  In the case of extreme degeneracy (*i. e.* $(E_F - E_C) \gg kT$ or $F_{1/2} \gg 1$ or $n \gg N_c$) the Fermi–Dirac integral reduces to

$$\eta_F = -\frac{E_C - E_F}{kT} \approx \left[\frac{3}{2} \Gamma\left(\frac{3}{2}\right) \frac{n}{N_c} \right]^{2/3} \approx \left(\frac{3}{4} \sqrt{\pi} \; \frac{n}{N_c} \right)^{2/3} \tag{13.67}$$

which is shown in ***Fig***. 13.7. The range of validity for this approximation is $E_F - E_C > 10\,kT$, *i. e.* when the Fermi energy is well within the conduction band. Rearrangement of the equation and using the effective density of states (N_c) yields the carrier concentration as a function of the Fermi energy in the degenerate limit

$$n = \frac{1}{3\pi^2} \left(\frac{2\,m^*\left(E_F - E_C\right)}{\hbar^2} \right)^{3/2} \tag{13.68}$$

- ***The Ehrenberg Approximation (3D)***
  This approximation (Ehrenberg, 1950) was developed for weak degeneracy and is shown in ***Fig***. 13.6. The approximation is given by

$$\eta_F = -\frac{E_C - E_F}{kT} \approx \ln\frac{n}{N_c} - \ln\left(1 - \frac{1}{4}\frac{n}{N_c}\right). \tag{13.69}$$

For small n the second logarithm term approaches zero, that is the Boltzmann distribution is recovered. The range of validity of the approximation is limited to $E_F - E_C \leq 2\ kT$, *i. e.* to weak degeneracy.

- ***The Joyce – Dixon approximation (3D)***
  An approximation valid for a wider range of degeneracy was developed by Joyce and Dixon (Joyce and Dixon, 1977; Joyce, 1978). This approximation expresses the reduced Fermi energy as a sum of the Boltzmann term and a polynomial, *i. e.*

$$\eta_F = -\frac{E_C - E_F}{kT} \approx \ln\frac{n}{N_c} + \sum_{m=1}^{4} A_m \left(\frac{n}{N_c}\right)^m \tag{13.70}$$

where the first four coefficients A_m are given by

$$A_1 = \sqrt{2}/4 = 3.53553 \times 10^{-1},$$

$$A_2 = -4.95009 \times 10^{-3},$$

$$A_3 = 1.48386 \times 10^{-4}, \tag{13.71}$$

$$A_4 = -4.42563 \times 10^{-6}.$$

The Joyce – Dixon approximation given here is shown in ***Fig***. 13.6 and can be used for degeneracies of $E_F - E_C \approx 8\ kT$. Inclusion of higher terms in the power series ($m > 4$) allows one to extend the Joyce – Dixon approximation to higher degrees of degeneracy.

- ***The Chang–Izabelle Approximation (3D)***
  The Chang–Izabelle approximation (Chang and Izabelle, 1989) is a full-range approximation which is valid for non-degenerate as well as degenerate semiconductors. The approximation is motivated by the fact that low-density and high-density approximations are available (see Eqs. 13.66 and 13.68) which are the exact solutions in the two extremes. The Chang–Izabelle approximation represents the construction of a function, which approaches the low-density solution and the high-density solution of the Fermi–Dirac integral as shown in ***Fig***. 13.7. The reduced Fermi energy is then given by

$$\eta_F = \frac{E_C - E_F}{kT} \approx \ln\frac{n}{N_c + n} \left[\frac{3}{2}\Gamma\left(\tfrac{3}{2}\right)\right]^{2/3} \frac{n/N_c}{(A + n/N_c)^{1/3}} \tag{13.72}$$

where

$$n/N_c = F_{1/2}, \tag{13.73}$$

$$\frac{3}{2}\Gamma\left(\tfrac{3}{2}\right) = \frac{3}{2}\frac{\sqrt{\pi}}{2} = 1.32934, \tag{13.74}$$

$$A = \frac{[(3/2)\,\Gamma\,(3/2)]^2\ (n_0/N_c)^3}{[\ln\,(1 + N_c/n_0)]^3} - \frac{n_0}{N_c}\ , \tag{13.75}$$

$$\frac{n_0}{N_c} = \frac{n(E_F = E_C)}{N_c} = F_{1/2}(\eta_F = 0) = 0.76515\ . \tag{13.76}$$

One can easily verify that Eq. (13.72) recovers the low-density approximation and the high-density approximation for $n \ll N_c$ and $n \gg N_c$, respectively. Furthermore, the approximation yields an exact solution for $\eta_F = 0$, *i. e.* when the Fermi energy touches the bottom of the conduction band. The largest relative error of η_F is 1 % in the Chang–Izabelle approximation. Chang and Izabelle (1989) showed that the relative error can be further reduced by a weighting function and a polynomial function. Using these functions, the maximum relative error is reduced to 0.033%.

- ***The Nilsson approximation (3D)***
  The Nilsson approximation (Nilsson, 1973) is valid for the entire range of Fermi energies. It is given by

$$\eta_F = -\frac{\ln\,(n/N_c)}{n/N_c - 1} + \left(\frac{3}{4}\,\sqrt{\pi}\,\frac{n}{N_c}\right)^{2/3} + \frac{(3/2)\,\sqrt{\pi}\,(n/N_c)}{\left[3 + (3/4)\,\sqrt{\pi}\,(n/N_c)\right]^2}\ . \tag{13.77}$$

The maximum relative error of the approximation is 1.1%.

13.7 The Fermi–Dirac integral of order $j = 0$ (2D semiconductors)

The Fermi–Dirac integral of order $j = 0$ allows one to calculate the free carrier density in a two-dimensional (2D) semiconductor. For semiconductor structures with only two degrees of spatial freedom, the Fermi–Dirac integral is obtained from Eq. (13.60) by insertion of the two-dimensional density of states. One obtains for the 2D carrier density

$$n^{2D} = \int_{E_C}^{E_{top}} \rho_{DOS}^{2D}(E)\ f_F(E)\ dE = \frac{m^*\,kT}{\pi\,\hbar^2} \int_0^\infty \left[1 + \exp\,(\eta - \eta_F)\right]^{-1}\ d\eta \tag{13.78}$$

where $\eta = E/kT$ and $\eta_F = (E_F - E_C)/kT$ are reduced energies. The integral can be written as the Fermi–Dirac integral of zero ($j = 0$) order

$$F_{j=0}(\eta_F) = \frac{1}{\Gamma(1)} \int_0^\infty \left[1 + \exp\,(\eta - \eta_F)\right]^{-1}\ d\eta \tag{13.79}$$

where $\Gamma(1) = 1$ is the Gamma-function. The two-dimensional carrier density can be written by using the effective density of states of a 2D system (N_c^{2D}). One obtains

$$n^{2D} = N_c^{2D}\ F_0(\eta_F) \tag{13.80}$$

which is formally similar to the corresponding equation in three dimensions (Eq. 13.63). The Fermi–Dirac integral of zero order ($j = 0$) can be solved analytically. Using the integral formula

$$\int \frac{dx}{1 + e^x} = -\ln(1 + e^{-x}) \,, \tag{13.81}$$

one obtains

$$F_0(\eta_F) = \ln(1 + e^{\eta_F}) \,. \tag{13.82}$$

Thus, the two-dimensional carrier density depends on the reduced Fermi energy according to

$$\frac{n^{2D}}{N_c^{2D}} = \ln(1 + e^{\eta_F}) \,. \tag{13.83}$$

Rearrangement of the equation yields the Fermi energy as a function of the carrier density

$$\boxed{\eta_F = -\frac{E_C - E_F}{kT} = \ln\left[\exp\left(\frac{n^{2D}}{N_c^{2D}}\right) - 1\right]} \tag{13.84}$$

- **Extreme non-degeneracy (2D)**
  Approximation for the low-density regime ($n^{2D} \ll N_c^{2D}$) and the high-density regime ($n^{2D} \gg N_c^{2D}$) can be easily obtained from Eqs. (13.83) and (13.84). In the low-density regime one obtains

$$\boxed{\eta_F = -\frac{E_C - E_F}{kT} = \ln\frac{n^{2D}}{N_c^{2D}}} \tag{13.85}$$

  which is valid if the Fermi energy is much below the bottom of the conduction subband. Rearrangement of the equation yields the two-dimensional carrier density as a function of the Fermi energy in the non-degenerate limit

$$n^{2D} = N_c^{2D} \exp\left(-\frac{E_C - E_F}{kT}\right) \,. \tag{13.86}$$

- **Extreme degeneracy (2D)**
  In the high-density regime one obtains

$$\boxed{\eta_F = -\frac{E_C - E_F}{kT} = \frac{n^{2D}}{N_c^{2D}}} \tag{13.87}$$

Rearrangement of the equation and insertion of the explicit expression for N_c^{2D} yields

$$n^{2D} = \frac{m^*}{\pi \hbar^2}(E_F - E_C) \tag{13.88}$$

that is the Fermi energy and the two-dimensional density follow a linear relation for two-dimensional structures.

13.8 The Fermi–Dirac integral of order $j = -1/2$ (1D semiconductors)

The Fermi–Dirac integral of order $j = -1/2$ allows one to calculate the free carrier density (per unit length) in a one-dimensional (1D) semiconductor. In semiconductor structures with only one degree of spatial freedom, the Fermi–Dirac integral is obtained from Eq. (13.60) by insertion of the 1D density of states. One obtains

$$
n^{1D} = \int_{E_C}^{E_{top}} \rho_{DOS}^{1D}(E)\, f_F(E)\, dE = \frac{kT}{\pi \hbar} \sqrt{\frac{m^*}{2\,kT}} \int_0^\infty \frac{\eta^{-1/2}}{1 + \exp(\eta - \eta_F)}\, d\eta \quad (13.89)
$$

where $\eta = E/kT$ and $\eta_F = -(E_C - E_F)/kT$ are reduced energies. The integral can be written as the Fermi–Dirac integral of order $j = -1/2$

$$
F_{-1/2}(\eta_F) = \frac{1}{\Gamma(1/2)} \int_0^\infty \frac{\eta^{-1/2}}{1 + \exp(\eta - \eta_F)} \quad (13.90)
$$

where $\Gamma(1/2) = \pi^{1/2}$ is the Gamma-function. Using the effective density of states of a one-dimensional system (N_c^{1D}), the one-dimensional density can be written as

$$
n^{1D} = N_c^{1D}\, F_{-1/2}(\eta_F) \quad (13.91)
$$

which is similar to the corresponding equations in three (Eq. 13.63) and two (Eq. 13.80) dimensions. The Fermi–Dirac integral of order $j = -1/2$ can only be obtained by numerical integration or by approximate solutions which will be discussed in the following sections. The $j = -1/2$ Fermi–Dirac integral has asymptotic solutions for the regimes of non-degeneracy and high degeneracy.

- **Extreme non-degeneracy (1D)**
  In the regime of extreme non-degeneracy ($n^{1D} \ll N_c^{1D}$) the Fermi–Dirac integral of order $j = -1/2$ approaches the Boltzmann distribution. One obtains

$$
\boxed{\eta_F = -\frac{E_C - E_F}{kT} = \ln \frac{n^{1D}}{N_c^{1D}}} \quad (13.92)
$$

  This approximation is good for $E_F - E_C \leq 2\,kT$, i.e. when the Fermi energy is at least $2\,kT$ below the bottom of the conduction subband. Rearrangement of the equation yields the one-dimensional carrier density as a function of the Fermi energy in the non-degenerate limit

$$
n^{1D} = N_c^{1D} \exp\left(-\frac{E_C - E_F}{kT}\right). \quad (13.93)
$$

- **Extreme degeneracy (1D)**
  In the case of extreme degeneracy ($n^{1D} \gg N_c^{1D}$) the Fermi–Dirac integral of order $j = -1/2$ reduces to

$$\eta_F = -\frac{E_C - E_F}{kT} \approx \frac{1}{4}\left[\Gamma\left(\tfrac{1}{2}\right)\right]^2 \left(\frac{n^{1D}}{N_c^{1D}}\right)^2 \approx \frac{\pi}{4}\left(\frac{n^{1D}}{N_c^{1D}}\right)^2 \qquad (13.94)$$

The range of validity of the approximation is $E_F - E_C > 10\,kT$, *i. e.* when the Fermi energy is well within the conduction band.