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Fermi–Dirac Statistics

There are two possible outcomes: If the result confirms the hypothesis, then you've made a measurement. If the result is contrary to the hypothesis, then you've made a discovery.

Enrico Fermi

In the previous chapter we investigated the properties of bosons, based on the general equations for quantum gases derived in Chapter 27. The same equations—with a positive sign in the denominator—govern fermions. Nevertheless, the properties of fermions are dramatically different from those of bosons. In particular, fermions do not exhibit any phase transition that might correspond to the Bose–Einstein condensation.

The most important fermions are electrons, and understanding the properties of electrons is central to understanding the properties of all materials. In this chapter we will study the ideal Fermi gas, which turns out to explain many of the properties of electrons in metals. In Chapter 30, we will see how Fermi–Dirac statistics also explains the basic features of insulators and semiconductors.

We will begin in the next section with the fundamental equations for fermions.

29.1 Basic Equations for Fermions

The Fermi–Dirac equations for N and U , taken from eqs. (27.55) and (27.56), are given below,

$$N = \sum_{\alpha} \langle n_{\epsilon_{\alpha}} \rangle = \sum_{\alpha} (\exp[\beta(\epsilon_{\alpha} - \mu)] + 1)^{-1} \quad (29.1)$$

$$U = \sum_{\alpha} \epsilon_{\alpha} \langle n_{\epsilon_{\alpha}} \rangle = \sum_{\alpha} \epsilon_{\alpha} (\exp[\beta(\epsilon_{\alpha} - \mu)] + 1)^{-1}. \quad (29.2)$$

To find solutions to these equations, we follow the same basic procedure as we did for bosons in the previous chapter by finding $N = N(T, \mu)$ from eq. (29.1), and then inverting the equation to obtain the chemical potential, $\mu = \mu(T, N)$. However, both the

mathematical methods and the physical results for fermions are quite different than what they are for bosons.

29.2 The Fermi Function and the Fermi Energy

The average occupation number, $\langle n_\epsilon \rangle$, for fermions in an eigenstate with energy ϵ was calculated in eq. (27.53). It is called the Fermi function, and it is written as

$$f_{FD}(\epsilon) = \langle n_\epsilon \rangle = (\exp[\beta(\epsilon - \mu)] + 1)^{-1}. \quad (29.3)$$

To solve for the properties of a Fermi gas, it is extremely helpful to have a clear idea of the form of the Fermi function, which is shown for a moderately low temperature in Fig. 29.1.

For lower temperatures (higher $\beta = 1/k_B T$), the Fermi function becomes steeper at $\epsilon = \mu$. The derivative of the Fermi function is given by

$$\frac{\partial f_{FD}(\epsilon)}{\partial \epsilon} = f'_{FD}(\epsilon) = -\beta \exp[\beta(\epsilon - \mu)] (\exp[\beta(\epsilon - \mu)] + 1)^{-2}. \quad (29.4)$$

Evaluating the derivative at $\epsilon = \mu$ gives the maximum value of the slope,

$$f'_{FD}(\mu) = -\frac{\beta}{4} = -\frac{1}{4k_B T}. \quad (29.5)$$

It is clear from the form of the function that the width of the non-constant part of the function near $\epsilon = \mu$ is of the order of $2k_B T$. As the temperature is lowered, the Fermi

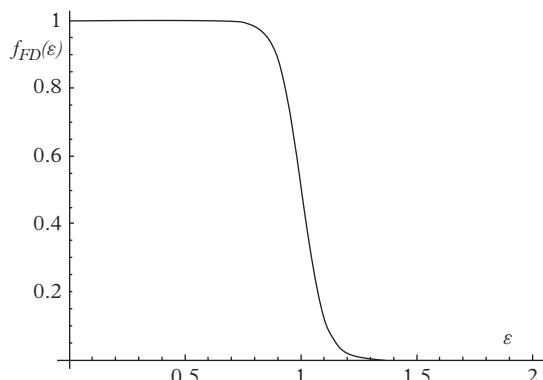


Fig. 29.1 The form of the Fermi function. The units of energy have been chosen such that $\mu = 1$, and $\beta = 10$ in this figure.

function approaches a step function. At $T = 0$, the Fermi function is equal to 1 for $\epsilon < \mu$, 0 for $\epsilon > \mu$, and $1/2$ for $\epsilon = \mu$.

For most problems of interest, $k_B T \ll \mu$, so that treating the Fermi function as a step function is a very good first approximation. Indeed, the Fermi function for most materials of common interest at room temperature is much closer to a step function than the curve shown in Fig. 29.1.

As mentioned above, the total number of particles, N , is fixed in any system we will discuss, so that the chemical potential is a function of N and the temperature T . However, as we will see later, the chemical potential is a rather weak function of temperature, so that its zero-temperature limit usually provides a very good approximation to its value at non-zero temperatures. This limit is so important that it has a name, the Fermi energy, and is denoted by ϵ_F ,

$$\epsilon_F = \lim_{T \rightarrow 0} \mu(T, N). \quad (29.6)$$

Because the Fermi function becomes a step function at $T = 0$, the Fermi energy must always lie between the energy of the highest occupied state and that of the lowest unoccupied state. In fact, as the problems in this section will show, it always lies *exactly* half way between the energies of the highest occupied state and the lowest unoccupied state. This gives a simple rule for finding the Fermi energy that greatly simplifies fermion calculations.

The definition in eq. (29.6) agrees with that of Landau (Lev Davidovich Landau, Russian physicist, 1908–1968) and Lifshitz (Evgeny Mikhailovich Lifshitz, Russian physicist, 1915–1985) in their classic book on statistical mechanics. Unfortunately, many textbooks give a different definition (the location of the highest occupied state at $T = 0$), which only agrees with the Landau–Lifshitz definition when energy levels are quasi-continuous. The alternative definition loses the connection between the Fermi energy and the chemical potential for systems with a discrete energy spectrum, or for insulators and semiconductors. This is a serious handicap in solving problems. Using the definition of ϵ_F given in eq. (29.6) makes it much easier to understand the behavior of such systems. The rule of thumb that the Fermi energy lies exactly half way between energies of the highest occupied state and the lowest unoccupied state is easy to remember and use in calculations. Finding ϵ_F should always be the first step in solving a fermion problem.

29.3 A Useful Identity

The following identity is very useful in calculations with fermions:

$$(\exp[\beta(\epsilon - \mu)] + 1)^{-1} = 1 - (\exp[-\beta(\epsilon - \mu)] + 1)^{-1}. \quad (29.7)$$

The left side of eq. (29.7) is, of course, the Fermi function, f_{FD} . On the right side, the second term gives the deviation of the Fermi function from 1.

It is easy to prove the identity in eq. (29.7), and I strongly recommend that you do so yourself. It might be easier to prove it again during an examination than to remember it. [Hint: First prove $(x + 1)^{-1} + (1/x + 1)^{-1} = 1$.]

For energies more than a couple of factors of $k_B T$ above the chemical potential μ , the Fermi function is very small, and can be approximated well by neglecting the ‘+1’ in the denominator,

$$f_{FD} = (\exp[\beta(\epsilon - \mu)] + 1)^{-1} \approx \exp[-\beta(\epsilon - \mu)]. \quad (29.8)$$

For energies more than a couple of factors of $k_B T$ below the chemical potential μ , the Fermi function is close to 1, and the second term on the right side of eq. (29.7) can be approximated well by neglecting the ‘+1’ in its denominator,

$$f_{FD} = 1 - (\exp[-\beta(\epsilon - \mu)] + 1)^{-1} \approx 1 - \exp[\beta(\epsilon - \mu)]. \quad (29.9)$$

These simple approximations are the key to solving fermion problems with a discrete spectrum or a gap in a continuous spectrum.

Up to this point we have been discussing the effects of Fermi statistics on the occupation number as a function of the energy of a given state. Now we will investigate how Fermi statistics affect the properties of systems with different distributions of energy levels.

29.4 Systems with a Discrete Energy Spectrum

We will first consider systems with a discrete spectrum, like that of the hydrogen atom. Much of the early work on the properties of fermions dealt with electronic behavior in atoms, and built on the exact quantum solution for the hydrogen atom to construct approximations in which electrons were taken to be subject to the field of the nucleus, but otherwise non-interacting. Since the electrons were orbiting the nucleus, the single-particle eigenstates were called orbitals—a name that has stuck, even for systems in which the electrons are not orbiting anything.

The problems at the end of the chapter contain several examples of fermion systems with discrete energy levels. One very simple example includes just two energy levels and a single particle. The lower level (energy 0) is non-degenerate and the upper level (energy ϵ) is two-fold degenerate. Find the chemical potential as a function of temperature.

The only equation needed is eq. (29.1), which for this problem becomes

$$\begin{aligned} N &= 1 = \sum_{\alpha} (\exp[\beta(\epsilon_{\alpha} - \mu)] + 1)^{-1} \\ &= (\exp[\beta(0 - \mu)] + 1)^{-1} + 2(\exp[\beta(\epsilon - \mu)] + 1)^{-1}. \end{aligned} \quad (29.10)$$

We expect the Fermi energy, ϵ_F , to be $\epsilon/2$, which we must check in the final solution. Assuming that $\epsilon_F = \epsilon/2$, at low temperatures we should have $\mu \approx \epsilon_F$, $-\beta\mu \ll -1$, and $\beta(\epsilon - \mu) \gg 1$. This implies that

$$1 = (1 - \exp[\beta(-\mu)]) + 2 \exp[-\beta(\epsilon - \mu)]. \quad (29.11)$$

This can be easily solved to find

$$\mu = \frac{1}{2}\epsilon - \frac{k_B T}{2} \ln 2. \quad (29.12)$$

As $T \rightarrow 0$, $\mu \rightarrow \epsilon_F = \epsilon/2$, as expected.

It is so much more valuable to work out the properties of systems with discrete spectra yourself than to see somebody else's solutions, that I am not going to present any more examples at all—just problems at the end of the chapter.

29.5 Systems with Continuous Energy Spectra

For systems with a continuous energy spectrum, we can use the integral forms in eqs. (27.61) and (27.62) to calculate the properties of the system. For fermions, these equations take the following form:

$$N = \int_0^{\infty} D_{FD}(\epsilon) (\exp[\beta(\epsilon - \mu)] + 1)^{-1} d\epsilon \quad (29.13)$$

$$U = \int_0^{\infty} D_{FD}(\epsilon) \epsilon (\exp[\beta(\epsilon - \mu)] + 1)^{-1} d\epsilon. \quad (29.14)$$

The Fermi energy is given by the zero-temperature limit of the chemical potential, as shown in eq. (29.6). In that limit, the Fermi function becomes a step function, and N is determined by the equation

$$N = \int_0^{\epsilon_F} D_{FD}(\epsilon) d\epsilon. \quad (29.15)$$

If we know the density of states, $D(\epsilon)$, we can solve eq. (29.15) for the Fermi energy ϵ_F . In the following sections we will carry this out explicitly for an ideal Fermi gas.

29.6 Ideal Fermi Gas

The case of an ideal gas of fermions in three dimensions is extremely important. This might seem surprising, since electrons certainly interact through the Coulomb force, and that interaction might be expected to dominate the behavior in a macroscopic object. Fortunately, for reasons that go well beyond the scope of this book, electrons in a solid behave as if they were very nearly independent. You will understand why this is true when you take a course in many-body quantum mechanics. In the meantime, just regard it as a stroke of good luck that simplifies your life.

We have already derived the single-particle density of states for particles in a box in eq. (27.13). To apply it to electrons we need only multiply it by 2 to take into account the spin of the electron, which takes on two eigenvalues,

$$D_{FD}(\epsilon) = \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \epsilon^{1/2}. \quad (29.16)$$

29.7 Fermi Energy

Since the Fermi energy will prove to be a good first approximation to the chemical potential, we will begin by calculating it from the density of states.

In the limit of zero temperature, the Fermi function becomes a step function, and we use eq. (29.15) for the number of particles to find an equation for ϵ_F ,

$$N = \int_0^{\epsilon_F} D_{FD}(\epsilon) d\epsilon = \int_0^{\epsilon_F} \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \epsilon^{1/2} d\epsilon = \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \frac{2}{3} \epsilon_F^{3/2}. \quad (29.17)$$

This equation can then be inverted to find ϵ_F as a function of N ,

$$\epsilon_F = \frac{\hbar^2}{2m} \left(\frac{3\pi^2 N}{V} \right)^{2/3}. \quad (29.18)$$

Note that the Fermi energy depends on the two-thirds power of the number density N/V , and inversely on the particle mass.

Because of the frequency with which the product $\beta\epsilon_F$ appears in calculations, the Fermi energy is often expressed in terms of the Fermi temperature, T_F ,

$$\epsilon_F = k_B T_F \quad (29.19)$$

$$\beta \epsilon_F = \frac{T_F}{T}. \quad (29.20)$$

Fermi temperatures turn out to be remarkably high. T_F for most metals ranges from about $2 \times 10^4 K$ to $15 \times 10^4 K$. For comparison, the temperature of the surface of the sun is only about $6 \times 10^3 K$. For experiments at room temperature ($300 K$), this means that $T/T_F \approx 0.01$, justifying the statement made in Section 29.2 that the Fermi function is very close to a step function for real systems of interest. Again for comparison, Fig. 29.1 was drawn for the case of $T/T_F \approx 0.1$.

Once we have the Fermi energy, the total energy of the system at $T = 0$ can be obtained from eq. (29.14), using the step function that is the zero-temperature limit of the Fermi function,

$$U = \int_0^{\epsilon_F} D_{FD}(\epsilon) \epsilon d\epsilon = \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \int_0^{\epsilon_F} \epsilon^{3/2} d\epsilon = \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \frac{2}{5} \epsilon_F^{5/2}. \quad (29.21)$$

Combining eq. (29.17) with eq. (29.21), we find that the energy per particle takes on a particularly simple form

$$\frac{U}{N} = \frac{3}{5} \epsilon_F. \quad (29.22)$$

The proportionality of U/N to ϵ_F is quite general, but the factor of $3/5$ depends on the dimension of the system.

29.8 Compressibility of Metals

Metals are hard to compress. They also contain electrons that are fairly well described by the ideal gas of fermions we have been discussing. Perhaps surprisingly, these two facts are closely related.

If we approximate the energy of an ideal gas of fermions by the Fermi energy in eq. (29.22) and insert the expression for the Fermi energy from eq. (29.18), we find an expression for the energy as a function of the volume V ,

$$\frac{U}{N} = \frac{3}{5} \frac{\hbar^2}{2m} \left(\frac{3\pi^2 N}{V} \right)^{2/3}. \quad (29.23)$$

Recalling the definition of the pressure as a derivative of the energy,

$$P = -\frac{\partial U}{\partial V}, \quad (29.24)$$

we find

$$P = -N \frac{3}{5} \frac{\hbar^2}{2m} \left(3\pi^2 N \right)^{2/3} \frac{\partial}{\partial V} V^{-2/3} = -N \frac{3}{5} \frac{\hbar^2}{2m} \left(\pi^2 N \right)^{2/3} \left(\frac{-2}{3} \right) V^{-5/3}, \quad (29.25)$$

or

$$P = \frac{2}{5} \frac{\hbar^2}{2m} \pi^{4/3} \left(\frac{N}{V}\right)^{5/3}. \quad (29.26)$$

Recalling the definition of the compressibility from eq. (14.14),

$$\kappa_T = -\frac{1}{V} \left(\frac{\partial V}{\partial P}\right)_{T,N} = -1 \left/ \left[V \left(\frac{\partial P}{\partial V}\right)_{T,N} \right] \right., \quad (29.27)$$

we find that

$$\kappa_T = \frac{3m}{\hbar^2} \pi^{-4/3} \left(\frac{V}{N}\right)^{5/3}. \quad (29.28)$$

This can also be written in terms of the bulk modulus,

$$B = \frac{1}{\kappa_T} = -V \left(\frac{\partial P}{\partial V}\right)_{T,N} = \frac{\hbar^2}{3m} \pi^{4/3} \left(\frac{N}{V}\right)^{5/3}. \quad (29.29)$$

Comparing eq. (29.29) with the expression for the Fermi energy in eq. (29.18)

$$\epsilon_F = \frac{\hbar^2}{2m} \left(\frac{3\pi^2 N}{V}\right)^{2/3} \quad (29.30)$$

we find a surprisingly simple result,

$$B = \frac{1}{\kappa_T} = \frac{5}{3} P = \frac{2}{3} \frac{N}{V} \epsilon_F. \quad (29.31)$$

The numerical predictions of eq. (29.31) turn out to be within roughly a factor of 2 of the experimental results for metals, even though the model ignores the lattice structure entirely. This is remarkably good agreement for a very simple model of a metal. It shows that the quantum effects of Fermi–Dirac statistics are responsible for a major part of the bulk modulus of metals.

29.9 Sommerfeld Expansion

While we have obtained important information about Fermi gases from the zero-temperature limit of the Fermi function in the previous section, the behavior at non-zero temperatures is even more interesting. The difficulty in doing calculations for

$T \neq 0$ is that the temperature dependence of the integrals in eqs. (29.13) and (29.14) is not trivial to extract.

The problem was solved by the German physicist Arnold Sommerfeld (1868–1951). His solution is known today as the Sommerfeld expansion, and it is the topic of the current section. The results obtained from the Sommerfeld expansion are essential for understanding the properties of metals.

First note that both eq. (29.13) and eq. (29.14) can be written in the form,

$$\mathcal{I} = \int_0^\infty \phi(\epsilon) f_F(\epsilon) d\epsilon = \int_0^\infty \phi(\epsilon) (\exp[\beta(\epsilon - \mu)] + 1)^{-1} d\epsilon \quad (29.32)$$

where $\phi(\epsilon) = D_{FD}(\epsilon)$ to calculate N , and $\phi(\epsilon) = \epsilon D_{FD}(\epsilon)$ to calculate U .

Break the integral in eq. (29.32) into two parts, and use the identity in eq. (29.7) to rewrite the integrand for $\epsilon < \mu$,

$$\begin{aligned} \mathcal{I} &= \int_0^\mu \phi(\epsilon) (\exp[\beta(\epsilon - \mu)] + 1)^{-1} d\epsilon \\ &\quad + \int_\mu^\infty \phi(\epsilon) (\exp[\beta(\epsilon - \mu)] + 1)^{-1} d\epsilon \\ &= \int_0^\mu \phi(\epsilon) \left[1 - (\exp[-\beta(\epsilon - \mu)] + 1)^{-1} \right] d\epsilon \\ &\quad + \int_\mu^\infty \phi(\epsilon) (\exp[\beta(\epsilon - \mu)] + 1)^{-1} d\epsilon \\ &= \int_0^\mu \phi(\epsilon) d\epsilon - \int_0^\mu \phi(\epsilon) (\exp[-\beta(\epsilon - \mu)] + 1)^{-1} d\epsilon \\ &\quad + \int_\mu^\infty \phi(\epsilon) (\exp[\beta(\epsilon - \mu)] + 1)^{-1}. \end{aligned} \quad (29.33)$$

In the last line of this equation, the first integral represents the contributions of a step function, while the second and third integrals represent the deviations of the Fermi function from the step function.

The next step is to substitute the dimensionless integration variable $z = -\beta(\epsilon - \mu)$ in the second integral, and $z = \beta(\epsilon - \mu)$ in the third integral,

$$\begin{aligned} \mathcal{I} &= \int_0^\mu \phi(\epsilon) d\epsilon - \beta^{-1} \int_0^{\beta\mu} \phi(\mu - \beta^{-1}z) (e^z + 1)^{-1} dz \\ &\quad + \beta^{-1} \int_0^\infty \phi(\mu + \beta^{-1}z) (e^z + 1)^{-1} dz. \end{aligned} \quad (29.34)$$

At low temperatures, $\beta\mu \approx \beta\epsilon_F = T_F/T \gg 1$. Since the upper limit in the second integral in eq. (29.34) is large and the integrand goes to zero exponentially rapidly as $z \rightarrow \infty$, replacing the upper limit by infinity should be a good approximation,

$$\begin{aligned}\mathcal{I} &\approx \int_0^\mu \phi(\epsilon) d\epsilon \\ &+ \beta^{-1} \int_0^\infty \left[\phi(\mu + \beta^{-1}z) - \phi(\mu - \beta^{-1}z) \right] (e^z + 1)^{-1} dz.\end{aligned}\quad (29.35)$$

Note that while the replacement of the upper limit of $\beta\mu$ in eq. (29.34) by infinity is almost always an excellent approximation, it is not exact.

For the next step we will assume that the integrand in eq. (29.35) is analytic in some region around $z = 0$ (or $\epsilon = \mu$), so that we can expand the function $\phi(\mu + \beta^{-1}z)$ in powers of z ,

$$\phi(\mu + \beta^{-1}z) = \sum_{j=0}^{\infty} \frac{1}{j!} \phi^{(j)}(\mu) \beta^{-j} z^j. \quad (29.36)$$

The assumption of analyticity is essential to the Sommerfeld expansion. While the density of states $D_{FD}(\epsilon)$ is generally analytic in some region around the Fermi energy, it is not analytic everywhere. This means that there are always small corrections to the Sommerfeld expansion, in addition to the one that comes from the extension of the upper limit of the integral in eq. (29.34) to infinity. These corrections are so small that they are often not even mentioned in textbooks. However, if the density of states is zero at $\epsilon = \mu$, all terms in the Sommerfeld expansion vanish, and only the non-analytic corrections are left.

Inserting eq. (29.36) in eq. (29.35), we find

$$\begin{aligned}\mathcal{I} &= \int_0^\mu \phi(\epsilon) d\epsilon \\ &+ \beta^{-1} \sum_{j=0}^{\infty} \frac{1}{j!} \phi^{(j)}(\mu) \beta^{-j} \int_0^\infty \left[z^j - (-z)^j \right] (e^z + 1)^{-1} dz \\ &= \int_0^\mu \phi(\epsilon) d\epsilon \\ &+ 2 \sum_{n=0}^{\infty} \frac{1}{(2n+1)!} \phi^{(2n+1)}(\mu) \beta^{-2n-2} \int_0^\infty z^{2n+1} (e^z + 1)^{-1} dz.\end{aligned}\quad (29.37)$$

The integrals on the first line of eq. (29.37) vanish for even values of j , which led us to define $n = (j-1)/2$ for odd values of j and rewrite the sum as shown in the second line.

The dimensionless integrals in eq. (29.37) can be evaluated exactly (with a little effort) to obtain the first few terms of the Sommerfeld expansion,

$$\mathcal{I} = \int_0^\mu \phi(\epsilon) d\epsilon + \frac{\pi^2}{6} \phi^{(1)}(\mu) (k_B T)^2 + \frac{7\pi^4}{360} \phi^{(3)}(\mu) (k_B T)^4 + \dots \quad (29.38)$$

In eq. (29.38), $\phi^{(1)}(\mu)$ denotes the first derivative of $\phi(\epsilon)$, evaluated at μ , and $\phi^{(3)}(\mu)$ denotes the corresponding third derivative.

As we will see in the next section, the Sommerfeld expansion converges rapidly for low temperatures.

29.10 General Fermi Gas at Low Temperatures

As discussed in Section 27.16 of the previous chapter, the first step in calculating the properties of a Fermi gas is to use eq. (29.13) to find N as a function of T and μ , and then invert the equation to obtain $\mu = \mu(T, N)$. Using the Sommerfeld expansion, eq. (29.38), derived in the previous section, we can expand eq. (29.13) to find N as a power series in T ,

$$\begin{aligned} N &= \int_0^\infty D_{FD}(\epsilon) (\exp[\beta(\epsilon - \mu)] + 1)^{-1} d\epsilon \\ &= \int_0^\mu D_{FD}(\epsilon) d\epsilon + \frac{\pi^2}{6} D_{FD}^{(1)}(\mu) (k_B T)^2 + \frac{7\pi^4}{360} D_{FD}^{(3)}(\mu) (k_B T)^4 + \dots \end{aligned} \quad (29.39)$$

Recall from eq. (29.15) that the Fermi energy is defined as the zero-temperature limit of the chemical potential,

$$N = \int_0^{\epsilon_F} D_{FD}(\epsilon) d\epsilon. \quad (29.40)$$

Since $\mu - \epsilon_F$ is small at low temperatures, we can approximate the integral in eq. (29.39) as

$$\int_0^\mu D_{FD}(\epsilon) d\epsilon \approx \int_0^{\epsilon_F} D_{FD}(\epsilon) d\epsilon + (\mu - \epsilon_F) D_{FD}(\epsilon_F). \quad (29.41)$$

Putting this approximation into eq. (29.39), we find an equation for the leading term in $\mu - \epsilon_F$,

$$\mu - \epsilon_F = -\frac{\pi^2}{6} (k_B T)^2 D_{FD}^{(1)}(\mu) / D_{FD}(\epsilon_F) + \dots \quad (29.42)$$

We see that the deviation of the chemical potential from the Fermi energy goes to zero as T^2 for low temperatures, justifying our earlier assertion that ϵ_F is a good approximation for μ at low temperatures.

The next step is to use eq. (29.42) to find a low-temperature expansion for the energy. Defining the zero-temperature energy of the system to be

$$U_0 = \int_0^{\epsilon_F} D_{FD}(\epsilon) \epsilon d\epsilon, \quad (29.43)$$

the Sommerfeld expansion of eq. (29.14) can be written as

$$\begin{aligned} U &= U_0 + (\mu - \epsilon_F) \epsilon_F D_{FD}(\epsilon_F) \\ &\quad + \frac{\pi^2}{6} [D_{FD}(\epsilon_F) + \epsilon_F D_{FD}^{(1)}(\epsilon_F)] (k_B T)^2 + \dots \end{aligned} \quad (29.44)$$

Inserting eq. (29.42) for $\mu - \epsilon_F$, this becomes

$$\begin{aligned} U &= U_0 - \frac{\pi^2}{6} (k_B T)^2 \epsilon_F D_{FD}^{(1)}(\epsilon_F) \\ &\quad + \frac{\pi^2}{6} [D_{FD}(\epsilon_F) + \epsilon_F D_{FD}^{(1)}(\epsilon_F)] (k_B T)^2 + \dots \\ &= U_0 + \frac{\pi^2}{6} D_{FD}(\epsilon_F) (k_B T)^2 + \dots \end{aligned} \quad (29.45)$$

The heat capacity at constant volume is found by differentiating of eq. (29.45) with respect to temperature,

$$C_V = \left(\frac{\partial U}{\partial T} \right)_{N,V} = \frac{\pi^2}{3} D_{FD}(\epsilon_F) k_B^2 T + \dots \quad (29.46)$$

Eq. (29.46) has very interesting properties. First, it shows that as long as $D_{FD}(\epsilon_F)$ does not vanish, the low-temperature heat capacity is proportional to the temperature T . Since the low-temperature contributions of the phonons to the heat capacity have a T^3 temperature-dependence, we can clearly separate the contributions of the phonons and electrons experimentally.

Next, we have answered the question of why the heat capacity of materials does not have a contribution of $3k_B/2$ from every particle, whether electrons or nuclei, which would be expected from classical theory. We will see this again below in eq. (29.54).

Finally, eq. (29.46) shows that the only thing we need to know to calculate the low-temperature heat capacity is the density of states at the Fermi energy. Or, turning the equation around, by measuring the low-temperature heat capacity we can determine the density of states at the Fermi energy from experiment.

29.11 Ideal Fermi Gas at Low Temperatures

While the equations for the specific heat derived so far in this chapter apply to a system of fermions with any density of states, it is particularly instructive to look at the special case of an ideal Fermi gas.

Recall that the density of states for an ideal gas of electrons was given in eq. (29.16),

$$D_{FD}(\epsilon) = \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \epsilon^{1/2} = A \epsilon^{1/2}. \quad (29.47)$$

In eq. (29.47) we defined a constant

$$A = \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2}, \quad (29.48)$$

to simplify further calculations.

Eq. (29.39) for N becomes

$$\begin{aligned} N &= \int_0^\mu A \epsilon^{1/2} d\epsilon + \frac{\pi^2}{6} A \frac{1}{2} \mu^{-1/2} (k_B T)^2 + \frac{7\pi^4}{360} A \frac{3}{8} \mu^{-5/2} (k_B T)^4 + \dots \\ &= \frac{2}{3} A \mu^{3/2} + \frac{\pi^2}{12} A \mu^{-1/2} (k_B T)^2 + \frac{7\pi^4}{960} A \mu^{-5/2} (k_B T)^4 + \dots \\ &= \frac{2}{3} A \mu^{3/2} \left[1 + \frac{\pi^2}{8} \left(\frac{k_B T}{\mu} \right)^2 + \frac{7\pi^4}{640} \left(\frac{k_B T}{\mu} \right)^4 + \dots \right]. \end{aligned} \quad (29.49)$$

Since

$$N = \frac{2}{3} A \epsilon_F^{3/2}, \quad (29.50)$$

Eq. (29.49) gives an equation for ϵ_F in terms of μ ,

$$\epsilon_F^{3/2} \approx \mu^{3/2} \left[1 + \frac{\pi^2}{8} \left(\frac{k_B T}{\mu} \right)^2 + \frac{7\pi^4}{640} \left(\frac{k_B T}{\mu} \right)^4 \right]. \quad (29.51)$$

Rewriting this for μ in terms of ϵ_F , we find

$$\mu \approx \epsilon_F \left[1 + \frac{\pi^2}{8} \left(\frac{k_B T}{\mu} \right)^2 + \frac{7\pi^4}{640} \left(\frac{k_B T}{\mu} \right)^4 \right]^{-2/3} \quad (29.52)$$

$$\approx \epsilon_F \left[1 - \frac{\pi^2}{12} \left(\frac{k_B T}{\epsilon_F} \right)^2 \right] = \epsilon_F \left[1 - \frac{\pi^2}{12} \left(\frac{T}{T_F} \right)^2 \right].$$

Since a typical value of T_F is of the order of $6 \times 10^4 K$, the T^2 -term in eq. (29.52) is of the order of 10^{-4} at room temperature, confirming that the chemical potential is very close to the Fermi energy at low temperatures. This also justifies the omission of the next term in the expansion, which is of order $(T/T_F)^4 \approx 10^{-8}$.

The heat capacity can be obtained by inserting eq. (29.47) into eq. (29.46),

$$C_V = \frac{\pi^2}{2} N k_B \left(\frac{T}{T_F} \right). \quad (29.53)$$

This equation can be rewritten in a form that shows the effect of Fermi statistics on the heat capacity,

$$C_V = \frac{3}{2} N k_B \left(\frac{\pi^2}{3} \frac{T}{T_F} \right). \quad (29.54)$$

The factor in parentheses is the quantum correction, which shows explicitly that the Fermi heat capacity at low temperatures is much smaller than that of a classical ideal gas, as claimed in the previous section.

We have seen in Chapter 26 that the specific heat due to lattice vibrations has a T^3 -behavior at low temperatures. Eq. (29.54) shows that when the density of states at the Fermi energy, $D(\epsilon_F)$, is non-zero, there is an additional T -dependence, which dominates at very low temperatures. This is indeed observed experimentally for metals. However, it is not observed for insulators or semiconductors, for reasons we will discuss in the next chapter.

29.12 Problems

PROBLEM 29.1

Numerical Fermi–Dirac Quantum Gas Problem: μ and n_0 and n_1 for a small number of particles

Using the programs that you've written for quantum gases, carry out the following calculations for Fermi–Dirac statistics.

- For the extreme cases of $N = 1, 2, 3$, and 4 , compute the chemical potential μ and the occupations of the two lowest energy states as functions of the temperature.

Don't include temperatures below $T = 0.1$ in your computations. There are numerical difficulties at very low temperatures that are not worth worrying about for this assignment.

- Go up to about $T = 3.0$ for $N = 1$, $T = 5.0$ for $N = 2$ and 3, and $T = 7.0$ for $N = 4$.
2. Are the Fermi energies you found in your computations consistent with what you had expected? Explain.
 3. Explain the occupation number you found in your computations at low temperatures for a state with energy $\epsilon = 6A$ for $N = 2$ and $N = 3$.

PROBLEM 29.2

Fermi–Dirac Quantum Gas Problem 2: Specific heat

Using the programs that you've written for quantum gases, carry out the following calculations for Fermi–Dirac statistics.

The Fermi temperature is given by the equation

$$k_B T_F = A \left(\frac{3N}{\pi} \right)^{2/3}.$$

It is discussed in the book and will be discussed in class. For this assignment, all you need to know is that it is a characteristic temperature for an ideal gas of fermions.

For $N = 1000$ particles, make three plots of the specific heat as a function of temperature. Let the lowest temperature be $T = 0.01$ for all three plots. Let the highest temperatures be $T = T_F/100$, $T = T_F/10$ and $T = 2T_F$.

1. For $T < 0.1$, the specific heat is seen to be very small. Why is this true?
2. In a temperature range of about $T = 3.0$ to $T = 0.1T_F$, how does the specific heat behave. Explain why this is to be expected.
3. For T much larger than T_F , the specific heat seems to be going to a constant value. Derive the value of this constant. Is the value you derived consistent with your plots?

PROBLEM 29.3

Fermions in a two-level system (with degeneracy)

Consider a system of N -independent fermions.

Assume that the single-particle Hamiltonians have only two energy levels, with energies 0 and ϵ . However, the two levels have degeneracies n_0 and n_1 , which are, of course, both integers.

1. First take the simple case of $n_0 = n_1 = 1$, with $N = 1$. Find the chemical potential, μ , as a function of temperature. What is the Fermi energy, $\epsilon_F = \mu(T = 0)$?
2. Now make it more interesting by taking arbitrary values of n_0 and n_1 , but specifying that $N = n_0$. Again find the chemical potential, μ , as a function of temperature *for low temperatures*. That is, assume that $\beta\epsilon \gg 1$. What is the Fermi energy?
3. Keep arbitrary values of n_0 and n_1 , but consider the case of $N < n_0$. Again find the chemical potential, μ , as a function of temperature *for low temperatures*. That is, assume that $\beta\epsilon \gg 1$. What is the Fermi energy?

4. Keep arbitrary values of n_0 and n_1 , but consider the case of $N > n_0$. Again find the chemical potential, μ , as a function of temperature *for low temperatures*. That is, assume that $\beta\epsilon \gg 1$. What is the Fermi energy?

PROBLEM 29.4

Fermions in a *three-level system* (with degeneracy)

Consider a system of N -independent fermions.

Assume that the single-particle Hamiltonians have three energy levels, with energies ϵ_1, ϵ_2 , and ϵ_3 , where $\epsilon_1 < \epsilon_2 < \epsilon_3$. The three energy levels have degeneracies n_1, n_2 , and n_3 , which are, of course, integers. The values of the n_j s are to be left arbitrary.

1. First take the case of $N = n_1$. Find the chemical potential, μ , for low temperatures. What is the Fermi energy, $\epsilon_F = \mu(T = 0)$?
2. Now take the case of $N = n_1 + n_2$. Find the chemical potential, μ , for low temperatures. What is the Fermi energy, $\epsilon_F = \mu(T = 0)$?
3. Next, consider the situation with $n_2 \geq 2$ and $N = n_1 + 1$. Find the chemical potential, μ , for low temperatures. What is the Fermi energy, $\epsilon_F = \mu(T = 0)$?

PROBLEM 29.5

Ideal Fermi gas in two dimensions

Consider an ideal Fermi gas in two dimensions. It is contained in an area of dimensions $L \times L$. The particle mass is m .

1. Calculate the density of states.
2. Using your result for the density of states, calculate the number of particles as a function of the chemical potential at zero temperature. ($\mu(T = 0) = \epsilon_F$, the Fermi energy.)
3. Calculate the Fermi energy as a function of the number of particles.
4. Again using your result for the density of states, calculate the total energy of the system at zero temperature as a function of the Fermi energy, ϵ_F .
5. Calculate the energy per particle as a function of the Fermi energy ϵ_F .

PROBLEM 29.6

More fun with the ideal Fermi gas in two dimensions

Consider the same two-dimensional, ideal Fermi gas that you dealt with in the previous assignment. You will need the result of that assignment to do this one.

1. Calculate the average number of particles as a function of μ *exactly*. (This is one of the few problems for which this can be done.)
2. Calculate μ as a function of N and T . Then find the high- and low-temperature behavior of μ .

PROBLEM 29.7**The specific heat of the Maxwell–Boltzmann quantum gas**

Using the programs that you've written for quantum gases, carry out the following calculations for Maxwell–Boltzmann statistics.

1. For both $N = 1$ and $N = 10$ particles, plot c_N as a function of temperature for T between $T = 0.1$ and $T = 8.0$.

What differences do you see between the two plots? Explain.

2. For a number of particles of your choice, plot c_N vs. T between $T = 2.0$ and $T = 50.0$.
3. What was the basis for your choice of N in the previous problem?
4. For large values of T , the specific heat seems to be going to a constant. Find the value of the constant, and compare it to the corresponding constant for Fermi–Dirac statistics.

PROBLEM 29.8**An artificial model of a density of states with a gap in the energy spectrum**

Consider a system with the following density of states

$$\mathcal{D}(\epsilon) = \begin{cases} 0 & 0 > \epsilon \\ A(\epsilon_1 - \epsilon) & \epsilon_1 > \epsilon > 0 \\ 0 & \epsilon_2 > \epsilon > \epsilon_1 \\ A(\epsilon - \epsilon_2) & \epsilon > \epsilon_2 \end{cases}$$

where A is a constant, and $\epsilon_2 > \epsilon_1 > 0$.

1. Find the Fermi energy $\epsilon_F = \mu(T = 0)$ for the following three values of the total number of particles, N .
 - (a) $N = A\epsilon_1^2/4$
 - (b) $N = A\epsilon_1^2/2$
 - (c) $N = 3A\epsilon_1^2/4$
2. For each of the three cases, find the specific heat at low temperatures from the Sommerfeld expansion.
3. For one of the cases studied above, the Sommerfeld expansion for the specific heat can be summed exactly to all orders. *And the answer is wrong!* Explain which case is being referred to, and why the Sommerfeld expansion has failed.

PROBLEM 29.9**An artificial model of a density of states with a gap in the energy spectrum—continued**

Again consider a system with the following density of states:

$$\mathcal{D}(\epsilon) = \begin{cases} 0 & 0 > \epsilon \\ A(\epsilon_1 - \epsilon) & \epsilon_1 > \epsilon > 0 \\ 0 & \epsilon_2 > \epsilon > \epsilon_1 \\ A(\epsilon - \epsilon_2) & \epsilon > \epsilon_2 \end{cases}$$

where A is a constant, and $\epsilon_2 > \epsilon_1 > 0$. The number of particles is given by $N = A\epsilon_1^2/2$, so the Fermi energy is $\epsilon_F = (\epsilon_1 + \epsilon_2)/2$.

In the last assignment we found that the Sommerfeld expansion gives incorrect results for this model. In this assignment we will calculate the low-temperature behavior correctly.

1. Show that if $\epsilon_1 \gg k_B T$, that $\mu = \epsilon_F$ is a very good approximation, even if $k_B T \approx \epsilon_2 - \epsilon_1$.
 2. Calculate the energy of this model as a function of temperature for low temperatures. Assume that $\epsilon_1 \gg \epsilon_2 - \epsilon_1 \gg k_B T$.
 3. Calculate the heat capacity of this model as a function of temperature for low temperatures from your answer to the previous question. Assume that $\epsilon_1 \gg \epsilon_2 - \epsilon_1 \gg k_B T$.
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