Many-particle Systems, 6

Fermion gas at low temperature

At low temperature the identical, noninteracting fermion average occupation number is

$$\overline{N}_{\sigma} = \frac{1}{\exp\left[(\varepsilon_{\sigma} - \varepsilon_F)/k_B T\right] + 1}.$$

The Fermi energy ε_F is one of the most important quantities in solid-state physics. To calculate it, assume there are *N* identical fermions in a cubical box (3D infinite well). As for the photon gas a single-particle quantum state consists of 3 quantum numbers n_x, n_y, n_z that take values 1,

2, 3, \ldots . Suppose that the fermions (such as electrons) have spin states $\pm 1/2.\,$ The single-particle energy is

$$\varepsilon_{\sigma} = \frac{\pi^2 \hbar^2}{2mL^2} \left(n_x^2 + n_y^2 + n_z^2 \right) = \frac{\pi^2 \hbar^2}{2mL^2} n^2.$$

Note that the energy for massive particles varies like n^2 not like n as for photons. At low temperature all states are occupied up to ε_F . This suggests there is a maximum value of n^2 , i.e., n_E^2 , such that

$$\varepsilon_F = \frac{\pi^2 \hbar^2}{2mL^2} n_F^2.$$

To determine n_F add all states up to n s that satisfy $n_F^2 = n_x^2 + n_y^2 + n_z^2$ (and convert the sum to an integral as for photons, discussed in Mn5):

$$N = 2\frac{4\pi}{8}\int_{0}^{n_{F}} n^{2} dn = \frac{\pi}{3}n_{F}^{3}.$$

Inserting into the expression for ε_{F} gives

$$\varepsilon_F = \frac{\pi^2 \hbar^2}{2m} \left(\frac{3}{\pi} \frac{N}{L^3}\right)^{2/3} = \frac{\pi^2 (\hbar c)^2}{2mc^2} \left(\frac{3}{\pi}\right)^{2/3} \rho^{2/3}$$
(1)

where ρ is the number density (number/volume) of the identical fermions in the system. (Notice that the L^2 in the original expression for ε_F becomes L^3 in (1) when it's raised to the 2/3 power. L^3 is the container volume.) The quantity multiplying $\rho^{2/3}$ has the numerical value 0.36 eV-nm² for electrons.

Example: What is the number density of atoms in solid gold? Solution: Start with mass density for gold: 19 gm/cm³. The atomic mass of gold is 197. A sample of gold with mass 197 gm would consist of an Avogadro's number worth of atoms, i.e., $6x10^{23}$ atoms. Thus, 19 gm of gold = (19/197)6x10^{23} = 5.79x10^{22} gold atoms. Consequently, $\rho = 5.79 \times 10^{22}$ cm⁻³ ≈ 58 nm⁻³.

<u>Example</u>: Suppose one electron per atom is shared among all of the atoms in a chunk of gold. Treating these shared electrons as noninteracting fermions in a 3D well what is the associated Fermi energy?

<u>Solution</u>: Using the number density found in the previous example, $\rho = 58 \text{ nm}^{-3}$; $\rho^{2/3} = 15 \text{ nm}^{-2}$ and $\varepsilon_F = (0.36 \text{ eV-nm}^2)(15 \text{ nm}^{-2}) = 5.5 \text{ eV}$.

<u>Example</u>: A neutron star consists mostly of neutrons packed at nuclear density. What is the Fermi energy for (noninteracting) neutrons in a neutron star ("cubical" infinite well)? <u>Solution</u>: Nuclear density is about 0.12 n/fm³ = 1.2×10^{17} n/nm³. The numerical factor multiplying $\rho^{2/3}$ for this case has to be modified because the neutron rest energy is about 940x10⁶ eV (not 0.5 MeV as for electrons). When this is done, $\varepsilon_F = 4.8 \times 10^7$ eV = 48 MeV.

The *total* energy of the *N*-fermion system at T = 0 is given by

$$E = \sum_{\sigma} \varepsilon_{\sigma} = \sum_{n_{x}, n_{y}, n_{z}} 2 \frac{\hbar^{2} \pi^{2}}{2mL^{2}} \left(n_{x}^{2} + n_{y}^{2} + n_{z}^{2} \right) = 2 \frac{4\pi}{8} \frac{\hbar^{2} \pi^{2}}{2mL^{2}} \int_{0}^{n_{F}} n^{4} dn = \frac{\pi}{5} \frac{\hbar^{2} \pi^{2}}{2mL^{2}} n_{F}^{5}$$

One of the profound consequences of the Fermi energy is associated with "pressure:" $P = -\partial E / \partial V$. Remembering that L^2 in the denominator above is really $V^{2/3}$, it is straightforward to show that

$$P_{F} = \frac{2\pi}{15} \frac{\hbar^{2} \pi^{2}}{2mV^{5/3}} n_{F}^{5} = \frac{2\pi}{15} \left(\frac{3}{\pi}\right)^{5/3} \frac{(\hbar c)^{2} \pi^{2}}{2mc^{2}} \rho^{5/3} = \frac{2}{5} \varepsilon_{F} \rho.$$

You can think of this quantity as the external pressure needed to appreciably compress the fermion ideal gas.

<u>Example</u>: What is P_F for the conduction electrons in gold? <u>Solution</u>: Again, using $\rho = 58 \text{ nm}^{-3}$, we find $P_F = 128 \text{ eV/nm}^3$. The latter is not as directly informative as expressing P_F in macroscopic units—i.e., converting eV to J and nm to m. When this is done we find $P_F = 2 \times 10^{10} \text{ N/m}^2$. As 1 atm = 10^5 N/m^2 , we see that $P_F = 2 \times 10^5 \text{ atm}!$ No wonder solids are hard. You *can't squeeze the electrons* (very much). (Recall Mn3, p3.)

<u>Example</u>: What is P_F for a neutron star?

<u>Solution</u>: Substituting neutron mass and neutron star density produces $P_F = 4 \times 10^{27}$ atm, so it's really difficult to squeeze a neutron star. But, of course, the star's gravity is trying to do just that. If the inward "gravitational pressure" of the star's mass exceeds its Fermi outward pressure then nothing can hold the star up from collapsing further, and a black hole results.

High temperatures, low densities

The two previous examples calculate Fermi pressures at T = 0 for systems at temperatures of 300 K and about 10^8 K! Why would T = 0 values have any relevance for such systems? The answer lies in how low temperature quantum statistics becomes high temperature quantum statistics. The critical point is that there are few excitations at low temperatures. As a result, the strong negative correlation between occupied states for fermions and the strong positive correlation for bosons are very important at low temperatures. At high temperatures there are many excitations, many different states are occupied, and correlations are much less important.

The diminishing of correlation at high temperatures is captured by the fact that the chemical potential μ is a function of temperature. As temperature is increased, μ decreases. For massive fermions at T = 0 chemical potential is positive; for massive bosons it is always negative. As temperature increases chemical potential becomes negative for both and at sufficiently high temperature the average occupation number for any single-particle state is very small and becomes

$$\bar{N}_{\sigma} = \frac{1}{\exp[(\varepsilon_{\sigma} - \mu)/k_{B}T]}$$

for both fermions and bosons. That is, in the high temperature (low density) limit it doesn't matter if the system's particles are bosons or fermions. At high temperature almost no state is occupied very much. In the high temperature limit, it is straightforward to calculate μ :

$$N = \sum_{\sigma} \overline{N}_{\sigma} = \exp(\mu/k_{B}T) \sum_{\sigma} \exp(-\varepsilon_{\sigma}/k_{B}T)$$

so that

$$\mu = k_{B}T \ln \left[\frac{N}{\sum_{\sigma} \exp(-\varepsilon_{\sigma}/k_{B}T)}\right].$$

Once again, assume that the particles are contained in a cubical box with hard walls so that

$$\sum_{\sigma} \dots = g_s \iint_{n_x} \iint_{n_y} \iint_{n_z} \dots dn_x dn_y dn_z = g_s \frac{1}{8} 4\pi \iint_{n_z} \dots n^2 dn$$

where g_s is the spin degeneracy (2 for spin-1/2, 1 for spin-0, etc.). Inserting the single-particle energy $\varepsilon_{\sigma} = \pi^2 \hbar^2 n^2 / 2mL^2$ and integrating yields

$$\mu = k_B T \ln\left(\frac{\rho}{\rho_Q}\right) \tag{2}$$

where, as above, ρ is the number density and

$$\rho_{\underline{O}} = g_s \left[\frac{mc^2 k_B T}{2\pi (\hbar c)^2} \right]^{3/2}$$

 ρ_{ϱ} is the **quantum number density**. The high temperature (or low density) limit is valid when ρ/ρ_{ϱ} is << 1. If ρ/ρ_{ϱ} is >> 1 the system is "cold" (or "dense").

<u>Example</u>: Using the electron rest energy and T = 300 K (and $g_s = 2$), we find $\rho_Q = 0.02$ nm⁻³. But for gold $\rho = 58$ nm⁻³. Consequently, $\rho/\rho_Q >> 1$, and *electrons in gold are exceedingly cold* even though T = 300 K. This justifies the Fermi pressure calculation done above.

<u>Example</u>: Using the neutron rest energy and $T = 10^8$ K (and $g_s = 2$), we find $\rho_Q = 3.7 \times 10^{11}$ nm⁻³. But for a neutron star $\rho = 1.2 \times 10^{17}$ nm⁻³. So, $\rho/\rho_Q >> 1$. **Despite their high thermal temperature, the neutrons in a neutron star are phenomenally cold!**

<u>Example</u>: Suppose the system is liquid water at 300 K. The mass density of liquid water is 1 gm/cm^3 , which is equivalent to 1/18 mole/cm³ = 33 nm⁻³. The rest energy of a water molecule is

18x(940x10⁶ eV) (and $g_s = 1$, i.e., total spin = 0); the quantum density for water at 300 K is 7.3x10⁴ nm⁻³. As a result, $\rho/\rho_Q << 1$. Water at room temperature is hot!

<u>Example</u>: For liquid helium ($g_s = 1$) at 2.17 K, $\rho/\rho_Q = 4$. This intermediate value coincides with the observation that liquid helium at this temperature is partly ordinary ("hot") liquid and partly superfluid ("cold").

Maxwellian speed distribution

Like photons, massive particles at finite temperature have a distribution of energies. This is often quantified by a speed distribution for particles at high temperature. The total number of particles (in a cubical box) is

$$N = \sum_{\sigma} N_{\sigma} = g_s \frac{4\pi}{8} \exp(\mu/k_B T) \int_{0}^{\infty} \exp(-\hbar^2 \pi^2 n^2 / 2mL^2 k_B T) n^2 dn$$

Inside the box, the particles only have kinetic energy, so

$$\hbar^2 \pi^2 n^2 / 2mL^2 = mv^2 / 2.$$

As a result,

$$\int_{0}^{\infty} \exp(-\hbar^{2}\pi^{2}n^{2}/(2mL^{2}k_{B}T)n^{2}dn = (mL/\hbar\pi)^{3}\int_{0}^{\infty} \exp(-\frac{1}{2}mv^{2}/k_{B}T)v^{2}dv.$$

From the previous section

$$\exp(\mu/k_B T) = \rho/\rho_Q = \frac{N}{g_s L^3} \left(\frac{2\pi\hbar^2}{mk_B T}\right)^{3/2}$$

Putting these pieces together we find

$$N = N \int_{0}^{\infty} 4\pi \left(\frac{m}{2\pi k_{B}T}\right)^{3/2} \exp(-\frac{1}{2}mv^{2}/k_{B}T)v^{2}dv.$$

If we divide both sides of this expression by N (producing 1 on the left-hand side) we can interpret the integral as a probability. That allows us to define a speed probability density (probability/speed), P(v), as

$$P(v) = 4\pi \left(\frac{m}{2\pi k_{B}T}\right)^{3/2} v^{2} \exp(-\frac{1}{2}mv^{2}/k_{B}T).$$
 (3)

Notice that the \hbar s have disappeared. At least in terms of speed distribution the particles (at high temperature) act like *classical* B-Bs (that is, no \hbar). This distribution is the **Maxwellian speed distribution**.

<u>Example</u>: The mean speed is calculated by $\overline{v} = \int_{0}^{\infty} vP(v) dv = (8k_BT/\pi m)^{1/2}$. For air at 300 K, \overline{v} is about 467 m/s.

<u>Example</u>: The mean kinetic energy is $\overline{K} = \int_{0}^{\infty} \frac{1}{2}mv^2 P(v)dv = \frac{3}{2}k_BT$ ($\frac{1}{2}k_BT$ for each way the particle can move). At 300 K, the mean kinetic energy is about 0.075 eV.