Ground State of Fermi Gas in Three Dimensions

Let the system be a cube of side L and volume $V = L^3$. The orbitals have the form of (3.58) and their energy is given by (3.59). The Fermi energy ε_F is the energy of the highest filled orbital at absolute zero; it is determined by the requirement that the system in the ground state hold N electrons, with each orbital filled with one electron up to the energy

$$\varepsilon_F = \frac{\hbar^2}{2m}\left(\frac{\pi n_F}{L}\right)^2 . \tag{5}$$

$\left[\varepsilon_n = \frac{\hbar^2}{2m}\left(\frac{\pi}{L}\right)^2 n^2 \quad n^2 = n_x^2 + n_y^2 + n_z^2 \right]$

Here n_F is the radius of a sphere (in the space of the integers n_x, n_y, n_z) that separates filled and empty orbitals. For the system to hold N electrons the orbitals must be filled up to n_F determined by

$$N = \boxed{2} \times \boxed{\tfrac{1}{8}} \times \boxed{\frac{4\pi}{3} n_F{}^3} = \frac{\pi}{3} n_F{}^3 ; \qquad n_F = (3N/\pi)^{1/3} . \tag{6}$$

The factor 2 arises because an electron has two possible spin orientations. The factor $\frac{1}{8}$ arises because only triplets n_x, n_y, n_z in the positive octant of the sphere in n space are to be counted. The volume of the sphere is $4\pi n_F{}^3/3$. We may then write (5) as

(5) + (6)

$$\varepsilon_F = \frac{\hbar^2}{2m}\left(\frac{3\pi^2 N}{V}\right)^{2/3} = \frac{\hbar^2}{2m}(3\pi^2 n)^{2/3} \equiv \tau_F . \tag{7}$$

This relates the Fermi energy to the electron concentration $N/V \equiv n$. The so-called "Fermi temperature" τ_F is defined as $\tau_F \equiv \varepsilon_F$.

The total energy of the system in the ground state is

$$U_0 = 2\sum_{n \le n_F} \varepsilon_{\mathbf{n}} = 2 \times \tfrac{1}{8} \times 4\pi \int_0^{n_F} dn\, n^2 \varepsilon_{\mathbf{n}} = \frac{\pi^3}{2m}\left(\frac{\hbar}{L}\right)^2 \int_0^{n_F} dn\, n^4 , \tag{8}$$

with $\varepsilon_{\mathbf{n}} = (\hbar^2/2m)(\pi n/L)^2$. In (8) and (9), n is an integer and is not N/V. Consistent with (6), we have let

$$2\sum_{\mathbf{n}} (\cdots) \to 2(\tfrac{1}{8})(4\pi) \int dn\, n^2 (\cdots) \tag{9}$$

in the conversion of the sum into an integral. Integration of (8) gives the total ground state kinetic energy:

$$U_0 = \frac{\pi^3}{10m}\left(\frac{\hbar}{L}\right)^2 n_F{}^5 = \frac{3\hbar^2}{10m}\left(\frac{\pi n_F}{L}\right)^2 N = \tfrac{3}{5} N \varepsilon_F , \tag{10}$$