Physics 112
Variation of the chemical potential with T for free electrons in three-dimensions

Peter Young
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As shown in class and a handout [1], the density of single particle states of non-interacting (i.e. free) electrons in three dimensions is

$$\rho(\epsilon) = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} \epsilon^{1/2} . \tag{1}$$

At $T = 0$, all states are occupied up to the "Fermi energy", which is the zero temperature limit of the chemical potential. This is determined from

$$N = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} \int_0^{\epsilon_F} \epsilon^{1/2}\, d\epsilon = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} \frac{2}{3}\epsilon_F^{3/2} , \tag{2}$$

where N is the number of particles, which gives

$$\epsilon_F = \frac{\hbar^2}{2m}\left(3\pi^2 n\right)^{2/3} , \tag{3}$$

where $n = N/V$. Associated with the Fermi energy is a corresponding Fermi temperature $T_F = \epsilon_F/k_B$ given by

$$\boxed{T_F = \frac{\hbar^2}{mk_B}\,\frac{1}{2}\left(3\pi^2\right)^{2/3} n^{2/3}.} \tag{4}$$

At finite temperature, each single-particle state has a mean number of particles given by the Fermi-Dirac distribution. Hence the total number of particles N can also be written as

$$N = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} \int_0^{\infty} \frac{\epsilon^{1/2}}{e^{\beta(\epsilon-\mu)}+1}\, d\epsilon . \tag{5}$$

Equating Eqs. (2) and (5) gives

$$\frac{2}{3}\epsilon_F^{3/2} = \int_0^{\infty} \frac{\epsilon^{1/2}}{e^{\beta(\epsilon-\mu)}+1}\, d\epsilon . \tag{6}$$

From Eq. (6) one determines $\mu(T)$ as a function of T. However, it is not possible to give a closed form analytical expression for $\mu(T)$ so we will determine it numerically. First, it is convenient to write Eq. (6) in dimensionless form by defining

$$\widetilde{\mu} = \frac{\mu}{\epsilon_F}, \quad \widetilde{T} = \frac{T}{T_F} . \tag{7}$$

In terms of the dimensionless "tilde" variables, Eq. (6) can be written

$$\boxed{\frac{2}{3} = \int_0^{\infty} \frac{x^{1/2}}{e^{(x-\widetilde{\mu})/\widetilde{T}}+1}\, dx .} \tag{8}$$

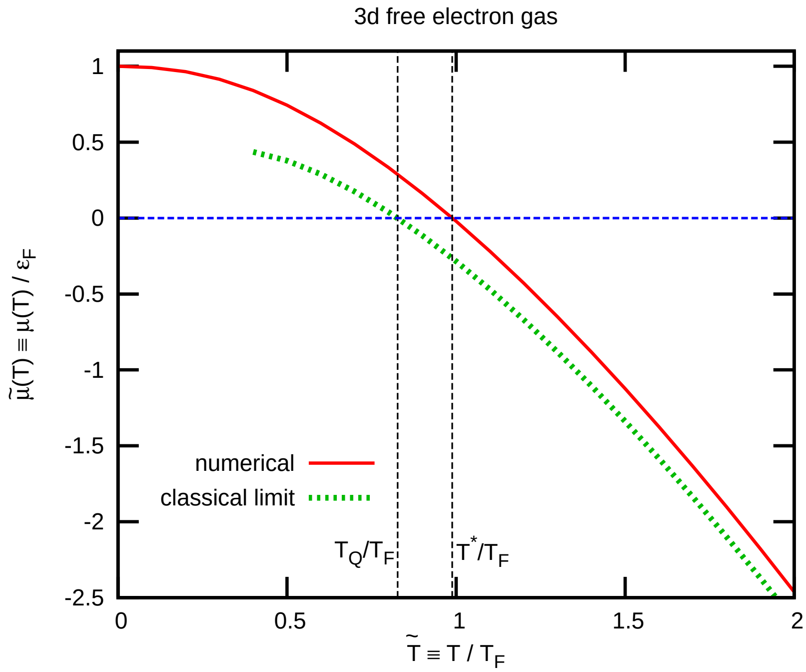

FIG. 1: The solid (red) curve shows $\widetilde{\mu}(T) \equiv \mu(T)/\epsilon_F$ against $\widetilde{T} \equiv T/T_F$, determined numerically from Eq. (8). The value of $\mu(T)$ is found to vanish at $T = T^\star$ where $T^\star/T_F = 0.9887$. This is indicated by one of the dashed vertical lines. In the classical (high-temperature) limit, $\widetilde{\mu}(T)$ is given by Eq. (14). This is shown by the dotted (green) curve. The classical result vanishes at $T = T_Q$ where T_Q is given by Eq. (13) and indicated by the other vertical dashed line. At high temperatures, the numerically calculated curve and the curve for the classical limit approach each other.

I have used Eq. (8) to determine $\widetilde{\mu} \equiv \mu/\epsilon_F$ *numerically* as a function of $\widetilde{T} \equiv T/T_F$ and show the results in Fig. 1. It is found that $\mu(T)$ changes sign at $T = T^\star$ where

$$\boxed{\frac{T^\star}{T_F} = 0.9887\,.} \tag{9}$$

In one of the handouts [2] we determined $\mu(T)$ in the classical, i.e. high-temperature, limit for spinless particles. Incorporating the spin degeneracy of 2 (this is a trivial example of an “internal” partition function discussed in class and a homework assignment [3]) we have

$$\mu_{\text{class}}(T) = -\frac{3}{2} k_B T \log\left(\frac{T}{T_Q}\right), \tag{10}$$

where here

$$\boxed{T_Q = \frac{\hbar^2}{m k_B}\, 2\pi \left(\frac{n}{2}\right)^{2/3}.} \tag{11}$$

The spin degeneracy appears through the replacement of n in the expression for T_Q for spinless particles [2] by $n/2$, i.e. the (number) density of particles *per spin species*.

Equation (10) can also be obtained from Eq. (5) by neglecting the factor of +1 in the denominator (which is justified in this limit since μ is large and negative so the exponential dominates). One can then extract $e^{\beta\mu}$ out of the integral. Evaluating the integral over ϵ using $\int_0^\infty x^{1/2} e^{-x}\, dx = \Gamma(3/2) = \sqrt{\pi}/2$, gives Eq. (10) with T_Q given by Eq. (11).

Comparing Eq. (11) with (4) we see that

$$T_Q = \frac{4\pi}{(6\pi^2)^{2/3}}\, T_F = 0.8271\, T_F\,, \tag{12}$$

so

$$\boxed{\widetilde{T}_Q \equiv \frac{T_Q}{T_F} = 0.8271\,.} \tag{13}$$

Writing $\widetilde{\mu}_{\rm class} = \mu_{\rm class}/\epsilon_F$, we can express Eq. (10) as

$$\boxed{\widetilde{\mu}_{\rm class} = -\frac{3}{2}\widetilde{T}\log\left(\frac{\widetilde{T}}{\widetilde{T}_Q}\right)\,,} \tag{14}$$

which is shown by the dotted (green) line in Fig. 1.

For electrons at metallic densities, T_F is typically several tens of thousand Kelvin, far higher than room temperature. In this limit, $T \ll T_F$ so μ is extremely close to its low temperature limit ϵ_F (which is, of course, positive). As part of the course, we have also studied the classical ideal gas, which corresponds to the opposite, very high temperature, limit, in which μ, given by Eq. (10), is large in magnitude but *negative*. The main purpose of this handout, as summarized by Fig. 1, is to show how these two limits are connected.

Another purpose is to point out that the different temperature scales, $T_F, T^\star$ and T_Q all depend on parameters of the system and fundamental constants in the same way, i.e.

$$\boxed{T_i = c_i\, \frac{\hbar^2}{m k_B}\, n^{2/3}\,,} \tag{15}$$

where "i" refers to "F", "Q", or "$\star$", and c_i is a (dimensionless) numerical constant with values

$$c_F = \frac{1}{2}\left(3\pi^2\right)^{2/3} = 4.7854, \quad c^\star = 0.9887\, c_F = 4.7312, \quad c_Q = 2^{1/3}\pi = 3.9582\,, \tag{16}$$

obtained from Eqs. (4), (9) and (11) respectively.

This handout has discussed fermions. Later, when we discuss bosons, we will find a "Bose-Einstein condensation" temperature, T_{BE} which will also vary with parameters of the system and fundamental constants in the same way as in Eq. (15), but with yet another numerical constant c_{BE}.

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[1] Physics 112 handout: *"Single particle density of states"*, `http://physics.ucsc.edu/~peter/112/dos.pdf`.
[2] Physics 112 handout: *The "classical" ideal gas*, `http://physics.ucsc.edu/~peter/112/ideal.pdf`.
[3] The correction due to spin degeneracy can be obtained from the solution to Qu. (4) in HW 5 with $\Delta = 0$, see `http://physics.ucsc.edu/~peter/112/sols/solutions5.pdf`.