

NOTES ON THE SOMMERFELD EXPANSION, APPLIED TO “ N ”

Start with the relation

$$N = \int_0^\infty D(\varepsilon) f_{FD}(\varepsilon) d\varepsilon \tag{1.1}$$

where f_{FD} , which I’ll simply write f below, is the **Fermi-Dirac** distribution and D is the density of states, which simply states that the integral of the distribution for our fermion system must equal the total number of particles, N . As noted earlier, we can use this to determine the chemical potential of the system, since f depends on μ . Let’s do this, at low but nonzero temperature.

For 3D non-relativistic fermions,

$$D(\varepsilon) = \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \varepsilon^{1/2} = D_0 \varepsilon^{1/2} \tag{1.2}$$

defining $D_0 = \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2}$. Note also that $D_0 = \frac{3}{2} \frac{N}{\varepsilon_F^{3/2}}$, using the previously-derived

$$\varepsilon_F = \frac{\hbar^2}{2m} \left(3\pi^2 \frac{N}{V} \right)^{2/3}. \text{ Therefore}$$

$$N = \int_0^\infty D_0 \varepsilon^{1/2} f(\varepsilon) d\varepsilon. \tag{1.3}$$

The “interesting” region is near $\varepsilon = \mu$, since this is the region whose shape changes appreciably with temperature, as discussed in class. Let’s focus on this by integrating by parts. Using “ $u = f$ ” and “ $dv = \varepsilon^{1/2} d\varepsilon$ ”, we write:

$$N = \frac{2}{3} D_0 \varepsilon^{3/2} f(\varepsilon) \Big|_0^\infty - \frac{2}{3} D_0 \int_0^\infty \varepsilon^{3/2} \frac{df}{d\varepsilon} d\varepsilon \tag{1.4}$$

The first term is zero at both limits (since $\varepsilon = 0$ at the left limit and $f = 0$ at the right).

The derivative $\frac{df}{d\varepsilon} = \frac{d}{d\varepsilon} \left[\exp\left(\frac{\varepsilon - \mu}{\tau}\right) + 1 \right]^{-1} = -\frac{1}{\tau} \frac{e^x}{(e^x + 1)^2}$, where $x \equiv (\varepsilon - \mu)/\tau$. Therefore

$$N = \frac{2}{3} D_0 \frac{1}{\tau} \int_0^\infty \frac{e^x}{(e^x + 1)^2} \varepsilon^{3/2} d\varepsilon \tag{1.5}$$

$$N = \frac{2}{3} D_0 \int_{-\mu/\tau}^\infty \frac{e^x}{(e^x + 1)^2} \varepsilon^{3/2} dx \tag{1.6}$$

Equations 1.6 and 1.7 are exact – we have not yet made any approximations. For negative x (i.e. $\varepsilon < \mu$) the integrand is very small. Therefore:

Approximation 1: Consider the lower limit of integration in Eq. 1.7 to be $-\infty$. (This is also the same as saying $\tau \ll \mu$, and also therefore that $\tau \ll \varepsilon_F$ - why?). This makes the integral look more "symmetric."

Approximation 2: Taylor expand $\varepsilon^{3/2}$ about $\varepsilon = \mu$ and keep only the first few terms.

$$\begin{aligned} \varepsilon^{3/2} &= \mu^{3/2} + (\varepsilon - \mu) \frac{d}{d\varepsilon} \varepsilon^{3/2} \Big|_{\varepsilon = \mu} + \frac{1}{2} (\varepsilon - \mu)^2 \frac{d^2}{d\varepsilon^2} \varepsilon^{3/2} \Big|_{\varepsilon = \mu} + \dots \\ &= \mu^{3/2} + \frac{3}{2} (\varepsilon - \mu) \mu^{1/2} + \frac{3}{8} (\varepsilon - \mu)^2 \mu^{-1/2} + \dots \\ \Rightarrow N &= \frac{2}{3} D_0 \int_{-\infty}^{\infty} \frac{e^x}{(e^x + 1)^2} \left[\mu^{3/2} + \frac{3}{2} x \tau \mu^{1/2} + \frac{3}{8} (x\tau)^2 \mu^{-1/2} + \dots \right] dx \\ &\text{Integrate term by term.} \end{aligned}$$

Term 1: Simply the derivative of f_{FD} , so

$$\int_{-\infty}^{\infty} \frac{e^x}{(e^x + 1)^2} dx = \int_{-\infty}^{\infty} -\frac{df_{FD}}{d\varepsilon} d\varepsilon = f_{FD}(-\infty) - f_{FD}(\infty) = 1 - 0 = 1$$

Term 2: Integrand is an odd function of x :

$$\frac{x e^x}{(e^x + 1)^2} = \frac{x}{(e^x + 1)(e^{-x} + 1)} = \text{odd}, \text{ so } \int_{-\infty}^{\infty} = 0.$$

Term 3: Can evaluate

$$\int_{-\infty}^{\infty} \frac{x^2 e^x}{(e^x + 1)^2} dx = \frac{\pi^2}{3}$$

This integral, like others we've seen, is related to Riemann Zeta functions.

$$\Rightarrow N = \frac{2}{3} D_0 \mu^{3/2} + \frac{1}{4} D_0 \tau^2 \mu^{-1/2} \frac{\pi^2}{3} + \dots$$

$$\Rightarrow N = N \left(\frac{\mu}{\varepsilon_F} \right)^{3/2} + N \frac{\pi^2}{8} \frac{\tau^2}{\varepsilon_F^{3/2} \mu^{1/2}} + \dots$$

$$\text{using } D_0 = \frac{3}{2} N / \varepsilon_F^{3/2} \text{ etc.}$$

Note that we used the expression for D_0 that followed Eq. 1.2. Canceling N 's:

$$1 = \left(\frac{\mu}{\varepsilon_F} \right)^{3/2} + \text{correction}, \text{ where the "correction" for nonzero temperature is small since } \tau \ll \mu \text{ and}$$

$\tau \ll \varepsilon_F$. This means that we can replace μ by ε_F in the correction term. Therefore:

$$\frac{\mu}{\varepsilon_F} = \left(1 - \frac{\pi^2}{8} \left(\frac{\tau}{\varepsilon_F} \right)^2 + \dots \right)^{2/3} \quad (1.7)$$

and, using the Taylor expansion $(1+x)^a = 1+ax+\dots$,

$$\frac{\mu}{\varepsilon_F} = 1 - \frac{\pi^2}{12} \left(\frac{\tau}{\varepsilon_F} \right)^2 + \dots \quad (1.8)$$

We now have an expression for the temperature dependence of the chemical potential of the Fermion gas. Note that the chemical potential drops from its zero-temperature value, ε_F , as the temperature rises; you can think about this "graphically" in the context of the integral in Equation 1.1.

The same method of Sommerfeld expansion can be used to determine the temperature dependence of the system's energy, U , as you'll see in the homework, as well as all sorts of other physical properties (electrical conductivity, magnetic susceptibility, etc.). The above expression for μ is useful in all of these calculations.