8.8 Supplement: Density of states & Sommerfeld expansion

In Eq. 103 we found that the average internal energy of a non-relativistic fermion gas becomes independent of the temperature in the limit $T \to 0$. This means that its heat capacity,

$$c_v = \frac{\partial}{\partial T} \langle E \rangle \bigg|_{N,V}, \to 0$$

vanishes in this limit, which we could also see by considering the fluctuation–dissipation relation $c_v = \beta^2 \left\langle (E - \langle E \rangle)^2 \right\rangle$ with only a single micro-state.

To derive the non-trivial heat capacity for a gas with a small but non-zero temperature, we need to move beyond approximating the Fermi function

$$F(E) = \frac{1}{e^{\beta(E-\mu)} + 1}$$

as a step function, and return to the full Eq. 99 for the average particle number,

$$\langle N \rangle_{\mathsf{f}} = V \frac{\sqrt{2m^3}}{\pi^2 \hbar^3} \int_0^\infty F(E) \sqrt{E}\, dE \equiv \int_0^\infty g(E)\, F(E)\, dE. \tag{107}$$

Here we have defined the **density of states**

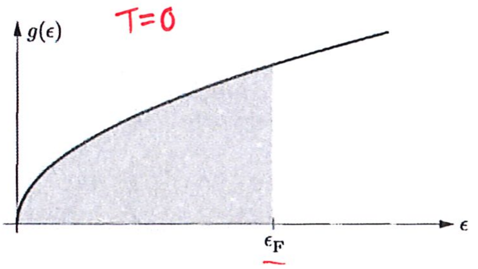
$$g(E) \equiv V \frac{\sqrt{2m^3}}{\pi^2 \hbar^3} \sqrt{E} \equiv g_0 \sqrt{E}$$

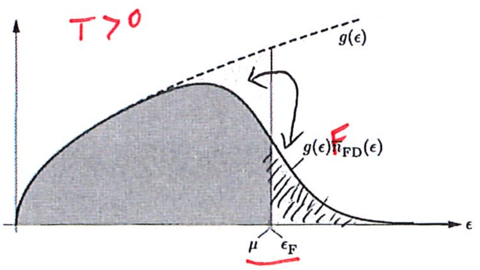
as the number of single-particle energy levels per unit energy. We can read Eq. 107 as saying that the total number of particles is given by integrating over the single-particle energy levels, $g(E)$, times the probability $F(E)$ that each of these energy levels is occupied.

The figures below, from Schroeder's *Introduction to Thermal Physics*, illustrate this integral in the case of $T = 0$ (left) and $T > 0$ (right). As we have already seen, when $T \to 0$ all energy levels with $E < E_F$ are occupied while all those with $E > E_F$ are unoccupied. With $T > 0$, there is an exponentially suppressed probability for some energy levels with $E > E_F$ to be occupied. Because the Fermi energy is set by the number of particles,

$$E_F = \frac{\hbar^2}{2m} \left(\frac{3\pi^2 \langle N \rangle_{\mathsf{f}}}{V} \right)^{2/3},$$

having some of these particles occupy energy levels with $E > E_F$ requires that an equal number of energy levels with $E < E_F$ be unoccupied.





$\int u\,dv = uv - \int v\,du$

Note that $E = \mu$ is the point where the Fermi function $F(E) = \frac{1}{2}$. We will see below that $\mu \le E_F$, as shown in the right figure above, with equality when $T = 0$.

In order to determine the particle number and internal energy, we need to evaluate the integrals

$$\langle N \rangle_{\mathsf{f}} = g_0 \int_0^\infty F(E)\sqrt{E}\,dE \qquad\qquad \langle E \rangle_{\mathsf{f}} = g_0 \int_0^\infty E\,F(E)\sqrt{E}\,dE \tag{108}$$

without approximating the Fermi function as a step function. For $T \ll E_F$, we can do this through a **Sommerfeld expansion**. Let's begin by considering the particle number. The first step in the Sommerfeld expansion is integrating by parts:

$$\int_0^\infty E^{1/2}\,F(E)\,dE = \frac{2}{3}E^{3/2}F(E)\Big|_0^\infty - \frac{2}{3}\int_0^\infty E^{3/2}\left(\frac{dF}{dE}\right)dE = \frac{2}{3}\int_0^\infty\left(\frac{-dF}{dE}\right)E^{3/2}\,dE$$

0

$u = F(E)$

$dv = E^{1/2}\,dE$

$v = \frac{2}{3}E^{3/2}$

$$-\frac{d}{dE}\left(e^{\beta(E-\mu)}+1\right)^{-1} = \frac{\beta e^{\beta(E-\mu)}}{\left(e^{\beta(E-\mu)}+1\right)^2} = \frac{\beta e^x}{(e^x+1)^2}$$

$x = \beta(E-\mu)$

$$\frac{2}{3}\int_0^\infty \frac{e^x}{(e^x+1)^2}E^{3/2}\,d(\beta E) = \frac{2}{3}\int_{-\beta\mu}^\infty \frac{e^x}{(e^x+1)^2}E^{3/2}\,dx$$

Changing variables to $x \equiv \beta(E - \mu)$, you should find

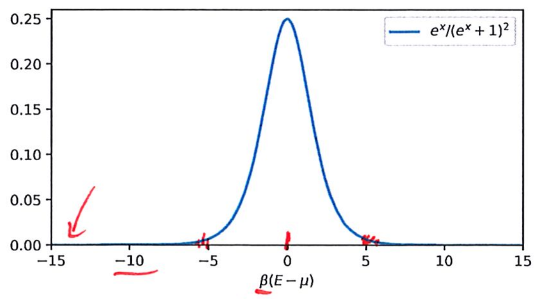
$$\langle N \rangle_{\mathsf{f}} = \frac{2}{3}g_0 \int_{-\beta\mu}^\infty \frac{e^x}{(e^x+1)^2} E^{3/2}\,dx.$$

This is not obviously simpler than the expression we started with, but has the benefit of being exponentially suppressed for *both*

$$x \gg 1 \qquad \Longrightarrow \qquad \frac{e^x}{(e^x+1)^2} \approx \frac{e^x}{e^{2x}} = \frac{1}{e^x}$$

$$\text{and} \quad x \ll -1 \qquad \Longrightarrow \qquad \frac{e^x}{(e^x+1)^2} \approx \frac{e^x}{1} = \frac{1}{e^{-x}}.$$

The additional $E^{3/2}$ factor is far too mild to overcome this exponential suppression. In other words, non-negligible contributions to the integral as a whole come only from a region centered at $E = \mu$, which becomes narrower in E as the temperature decreases (corresponding to larger $\beta = 1/T$). This is illustrated by the plot below, which shows the exponential suppression setting in when $|E - \mu|$ is larger than a few times the temperature, and certainly for $|E - \mu| \gtrsim 5/\beta = 5T$.



These considerations justify two low-temperature approximations. First, recalling $\mu > 0$ at low temperatures, for large β we are free to extend the lower limit of the integral to obtain a more convenient domain of integration,

$$\langle N \rangle_{\mathsf{f}} = \frac{2}{3} g_0 \int_{-\beta\mu}^{\infty} \frac{e^x}{(e^x+1)^2} E^{3/2}\, dx \approx \frac{2}{3} g_0 \int_{-\infty}^{\infty} \frac{e^x}{(e^x+1)^2} E^{3/2}\, dx.$$

Second, we can expand $E^{3/2}$ in a Taylor series around $E = \mu$, and truncate after the first few terms:

$$\begin{aligned} E^{3/2} &\approx \mu^{3/2} + (E-\mu) \left.\frac{\partial}{\partial E} E^{3/2}\right|_{E=\mu} + \frac{1}{2}(E-\mu)^2 \left.\frac{\partial^2}{\partial E^2} E^{3/2}\right|_{E=\mu} \\ &= \mu^{3/2} + \frac{3}{2}(E-\mu)\mu^{1/2} + \frac{3}{8}(E-\mu)^2 \mu^{-1/2} = \mu^{3/2} + \frac{3}{2}\frac{x\mu^{1/2}}{\beta} + \frac{3}{8}\frac{x^2\mu^{-1/2}}{\beta^2}. \end{aligned}$$

$x = \beta(E-\mu)$

Switching to work with $T = 1/\beta$, the Sommerfeld expansion has given us a series of manageable integrals we can consider one by one:

$$\langle N \rangle_{\mathsf{f}} \approx \frac{2}{3} g_0 \mu^{3/2} \underbrace{\mathbb{I}_1}_{1} + \underbrace{g_0 T \mu^{1/2} \mathbb{I}_2}_{0} + \frac{g_0 T^2}{4\mu^{1/2}} \mathbb{I}_3.$$

$$\mathbb{I}_1 = \int_{-\infty}^{\infty} \frac{e^x}{(e^x+1)^2}\, dx = -\int_{-\infty}^{\infty} \frac{dF}{dE}\, dE = -F(E)\Big|_{-\infty}^{\infty} = -0+1 = 1$$

$$\mathbb{I}_2 = \int_{-\infty}^{\infty} \frac{x e^x}{(e^x+1)^2}\, dx = \int_{-\infty}^{\infty} \frac{x e^x}{(e^x+1)(e^x+1)}\, dx = \int_{-\infty}^{\infty} \frac{x}{(e^x+1)(1+e^{-x})}\, dx = 0$$

$$\mathbb{I}_3 = \int_{-\infty}^{\infty} \frac{x^2 e^x}{(e^x+1)^2}\, dx = 2\int_0^{\infty} \frac{x^2 e^x}{(e^x+1)^2}\, dx = \underbrace{\cancel{\frac{-2x^2}{e^x+1}\Big|_0^{\infty}}}_{0} + 2\int_0^{\infty} \frac{2x}{e^x+1}\, dx$$

$u = x^2$

$dv = \frac{e^x}{(e^x+1)^2}\, dx$

$v = \frac{-1}{e^x+1}$

$$= 4\left(1-\frac{1}{2}\right)\Gamma(2)\zeta(2)$$

$$= 2\frac{\pi^2}{6} = \frac{\pi^2}{3}$$

Collecting the results and restoring $g_0 = V\frac{\sqrt{2m^3}}{\pi^2\hbar^3}$, you should find

$$\langle N\rangle_{\mathsf{f}} \approx \frac{2}{3}g_0\mu^{3/2} + g_0\frac{\pi^2T^2}{12\mu^{1/2}} = V\frac{(2m\mu)^{3/2}}{3\pi^2\hbar^3} + V\frac{\sqrt{2m^3}}{12\hbar^3\mu^{1/2}}T^2.$$

The first term reproduces what we found with the step-function approximation in Section 8.5, while the second term provides the promised temperature dependence, at leading order in the Sommerfeld expansion. This becomes more interesting if we rearrange Eq. 101 to work in terms of the Fermi energy:

$$E_F = \frac{\hbar^2}{2m}\left(\frac{3\pi^2\langle N\rangle_{\mathsf{f}}}{V}\right)^{2/3} \implies E_F^{3/2} = \frac{\hbar^3(3\pi^2)}{\cancel{4}2\sqrt{2m^3}}\frac{\langle N\rangle_f}{V} = \frac{3\langle N\rangle_f}{2g_0}$$

$$\langle N\rangle_f = \langle N\rangle_f\left(\frac{\mu}{E_F}\right)^{3/2} + \langle N\rangle_f\frac{\pi^2T^2}{8E_F^{3/2}\mu^{1/2}}$$

$$\frac{\mu}{E_F} = \left[1 - \frac{\pi^2T^2}{8E_F^{3/2}\mu^{1/2}}\right]^{2/3}$$

The result

$$\frac{\mu}{E_F} \approx \left[1 - \frac{\pi^2T^2}{8E_F^{3/2}\mu^{1/2}}\right]^{2/3}$$

can be simplified through one final low-temperature approximation. Because T is small, just in the second term above we can set $E_F \approx \mu$ (the zero-temperature relation). Then

$$\frac{\mu}{E_F} \approx 1 - \frac{\pi^2T^2}{12E_F^2}, \tag{109}$$

which confirms our earlier claim $\mu \le E_F$, and reveals that the leading correction to the zero-temperature relation is quadratic in T.

The calculation is essentially the same for the internal energy from Eq. 108. With $E^{3/2}$ in place of $E^{1/2}$, integrating by parts just gives

$$\langle E\rangle_{\mathsf{f}} = g_0\int_0^\infty \frac{E^{3/2}}{e^{\beta(E-\mu)}+1}dE \approx \frac{2}{5}g_0\int_{-\infty}^\infty \frac{e^x}{(e^x+1)^2}E^{5/2}\,dx$$

with the same $x = \beta(E-\mu)$ and extended lower limit of integration. The Taylor expansion

$$E^{5/2} \approx \mu^{5/2} + \frac{5}{2}(E-\mu)\mu^{3/2} + \frac{15}{8}(E-\mu)^2\mu^{1/2} = \mu^{5/2} + \frac{5}{2}\frac{x\mu^{3/2}}{\beta} + \frac{15}{8}\frac{x^2\mu^{1/2}}{\beta^2}$$

also produces the same integrals, with different coefficients:

$$\langle E\rangle_{\mathsf{f}} \approx \frac{2}{5}g_0\mu^{5/2}\underbrace{\mathbb{I}_1}_{1} + g_0T\mu^{3/2}\underbrace{\mathbb{I}_2}_{0} + \frac{3}{4}g_0T^2\mu^{1/2}\underbrace{\mathbb{I}_3}_{\pi^2/3} = \frac{2}{5}g_0\mu^{5/2} + \frac{1}{4}g_0\pi^2T^2\mu^{1/2}.$$

Inserting $g_0 = \frac{3\langle N\rangle_\mathsf{f}}{2E_F^{3/2}}$, we have

$$\langle E\rangle_\mathsf{f} \approx \frac{3}{5}\langle N\rangle_\mathsf{f}\frac{\mu^{5/2}}{E_F^{3/2}} + \frac{3}{8}\langle N\rangle_\mathsf{f}\,\pi^2T^2\frac{\mu^{1/2}}{E_F^{3/2}},$$

which we can simplify by applying Eq. 109 and dropping $\mathcal{O}(T^3)$ terms:

$$\mu^{5/2} \approx E_F^{5/2}\left(1 - \frac{\pi^2T^2}{12E_F^2}\right)^{5/2} = E_F^{5/2} - \frac{5}{24}\pi^2T^2E_F^{1/2}$$

$$\langle E\rangle_f = \frac{3}{5}\langle N\rangle_f E_F - \frac{1}{8}\langle N\rangle_f \pi^2\frac{T^2}{E_F} + \frac{3}{8}\langle N\rangle_f \pi^2\frac{T^2}{E_F}$$

$$= \frac{3}{5}\langle N\rangle_f E_F + \frac{\pi^2}{4}\langle N\rangle_f\frac{T^2}{E_F}$$

From your result you should obtain the heat capacity

$$c_v = \frac{\partial}{\partial T}\langle E\rangle\bigg|_{N,V} \approx \frac{\pi^2}{2}\frac{\langle N\rangle_\mathsf{f}}{E_F}T.$$

This low-temperature linear dependence on T agrees with experimental heat capacity measurements, as we will see in the next tutorial.

As a final comment in this supplement, let's consider what would happen to $\langle N\rangle_\mathsf{f}$ at higher temperatures $T^2 \sim E_F^2$, for which the two terms in Eq. 109 would cancel out, leaving $\mathcal{O}(T^4/E_F^4)$ effects non-negligible. In this regime, there's no guarantee that the low-temperature Sommerfeld expansion would even converge, so we need to work with the full integral from Eq. 108. Fortunately, it is not hard to numerically evaluate this integral, which is done by this Python code. For the purpose of numerical analysis, it's best to express everything in terms of dimensionless ratios, such as

$$t \equiv \frac{T}{E_F} \qquad\qquad c \equiv \frac{\mu}{E_F} \qquad\qquad x \equiv \frac{E}{T} = \beta E.$$

Also inserting $g_0 = \frac{3\langle N\rangle_\mathsf{f}}{2E_F^{3/2}}$, we have

$$\cancel{\langle N\rangle}_\mathsf{f} = \frac{3\langle N\rangle_\mathsf{f}}{2E_F^{3/2}}\int_0^\infty \frac{\sqrt{E}}{e^{\beta(E-\mu)}+1}dE = \frac{3\cancel{\langle N\rangle}_\mathsf{f}}{2}t^{3/2}\int_0^\infty \frac{\sqrt{x}e^{-x}}{e^{-c/t}+e^{-x}}dx,$$

working with small $e^{-\beta E} = e^{-x}$ rather than large e^x to avoid numerical overflow.

As in Eq. 109, $\langle N\rangle_\mathsf{f}$ drops out, and we end up with the consistency condition

$$1 \overset{?}{=} \frac{3}{2}t^{3/2}\int_0^\infty \frac{\sqrt{x}e^{-x}}{e^{-c/t}+e^{-x}}dx. \tag{110}$$

If we fix the temperature $t = T/E_F$ in units of the Fermi energy, by repeatedly evaluating this integral with different values of $c = \mu/E_F$ we can determine the self-consistent value of the chemical potential, also in units of the Fermi energy. The red $\times$'s in the figure below are results of such work for eleven temperatures $0.1 \le t \le 2$, compared to the $\mathcal{O}(t^2)$ result from the Sommerfeld expansion, Eq. 109. This leading-order Sommerfeld expansion clearly deviates from the full results by the time $T \sim E_F$. The more interesting result is that the chemical potential continues to decrease as the temperature increases, becoming negative for $T \gtrsim E_F$ and approaching the expected high-temperature classical limit.