1 Low temperature compressibility of a non-interacting Fermi gas

We can obtain the thermodynamic properties of the non-interacting Fermi gas starting from the basic formulation of the equation of state:

$$U/V = \int g(\varepsilon) f(\varepsilon)\,\mathrm{d}\varepsilon \tag{1}$$

$$n = \int g(\varepsilon)\,\mathrm{d}\varepsilon \tag{2}$$

where $g(\varepsilon)$ is the density of states per unit volume, and $f(\varepsilon) = \frac{1}{\exp\beta(\varepsilon-\mu)+1}$ is the fermionic occupation number for a single particle state of energy ε. At low temperatures we take advantage of the step-function profile of the occupation and use a Sommerfed expansion, for example we have for the density

$$n \simeq \underbrace{\int_0^{E_F} g(\varepsilon)\,\mathrm{d}\varepsilon}_{\approx n} + (\mu - E_F) g(E_F) + \frac{\pi^2}{6}(k_\mathrm{B}T)^2 g'(E_F) + \mathcal{O}\left(\frac{k_\mathrm{B}T}{E_F}\right)^4 \tag{3}$$

and therefore the chemical potential is given by

$$\mu = E_F - \frac{\pi^2}{6}(k_\mathrm{B}T)^2 \frac{g'(E_F)}{g(E_F)} \tag{4}$$

For a 3D gas of fermions with spin S and $s \equiv 2S+1$ internal states we have

$$E_F = \frac{\hbar^2}{2m}\left(\frac{6\pi^2 n}{s}\right)^{2/3} \qquad g(\varepsilon) = \frac{s}{4\pi}\frac{(2m)^{2/3}}{\hbar^3}\sqrt{\varepsilon} \qquad g'(\varepsilon) = \frac{s}{4\pi}\frac{(2m)^{2/3}}{\hbar^3}\frac{1}{2\sqrt{\varepsilon}} \tag{5}$$

$$\frac{g'(E_F)}{g(E_F)} = \frac{m}{\hbar^2}\left(\frac{s}{6\pi^2 n}\right)^{2/3} \tag{6}$$

and so

$$\mu = \frac{\hbar^2}{2m}\left(\frac{6\pi^2 n}{s}\right)^{2/3} - \frac{\pi^2}{6}(k_\mathrm{B}T)^2 \frac{m}{\hbar^2}\left(\frac{s}{6\pi^2 n}\right)^{2/3} \tag{7}$$

1.1 Compressibility for free fermions

The isothermal compressibility of the Fermi gas is defined as

$$\kappa_T = \frac{1}{n^2}\frac{\partial n}{\partial \mu} \tag{8}$$

or equivalently

$$\frac{1}{\kappa_T} = n^2 \frac{\partial \mu}{\partial n} \tag{9}$$

Using the result above we obtain for the 3D gas with s spin states

$$\frac{1}{\kappa_T} \simeq \frac{2}{3} n E_F \left[1 + \frac{\pi^2}{12} \left(\frac{k_B T}{E_F} \right)^2 \right] \tag{10}$$

or equivalently

$$\kappa_T \simeq \frac{3}{2 n E_F} \left[1 - \frac{\pi^2}{12} \left(\frac{k_B T}{E_F} \right)^2 \right] \tag{11}$$

At $T = 0$ we have the exact result

$$\kappa_T^0 = \frac{3}{2 n E_F} = \frac{3m}{\hbar^2} \frac{s^{2/3}}{(6\pi^2)^{2/3}} \frac{n^{1/3}}{n^2} \tag{12}$$

1.2 Compressibility for fermions in a lattice

We consider a single-band model of non-interacting fermions in a lattice. For deep enough lattices ($V_0 \gtrsim 5E_r$) the tight-binding approximation is valid and the dispersion relation takes the form of a cosine. In 3D:

$$E(q_x, q_y, q_z) = -2t \left[\cos(q_x a) + \cos(q_y a) + \cos(q_z a) \right] \tag{13}$$

In 3D, it is not possible to write down an analytical form for the Fermi energy or the density of states as a function of the density. To find the isothermal compressibility, one can numerically find this quantities and perform a Sommerfeld low temperature analysis of the system as was shown in the last section for the free fermion gas. For example, the density of states for this system obtained numerically is shown below in Fig. 1.

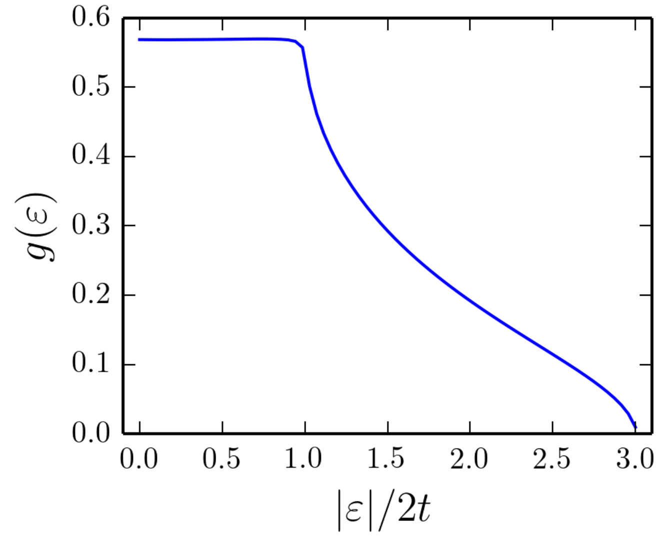

Figure 1: Density of states for the 3D tight-binding dispersion relation. The zero of energy has been chosen to be at the center of the band.

This approach is cumbersome, and furthermore is limited because it only works for non-interacting systems. In our case we can take advantage of the results of more sophisticated techniques that are at our disposal, namely the hight-temperature series expansion (HTSE) and the DQMC and NLCE solutions for the thermodynamics of the Hubbard model. All of these three methods provide values of the density as a function of chemical potentia, from which the compressibility is obtained as a first derivative.

1.3 Normalization of the compressibility

The results from the different thermodynamic treatments of the Hubbard model give us the density (in units of a^{-3}) as a function of μ/t, the ratio of the chemical potential to the tunneling energy. We use n' to represent the density in units of a^{-3}, $n' \equiv na^3$. We have for the isothermal compressibility:

$$\begin{aligned}\kappa_T(n') &= \frac{1}{n^2}\frac{\partial n}{\partial \mu} \\ &= -\frac{\partial(1/n')}{\partial(\mu/t)}\frac{a^3}{t}\end{aligned} \tag{14}$$

from where we can get the unitless quantity

$$\kappa_T(n')\frac{t}{a^3} = -\frac{\partial(1/n')}{\partial(\mu/t)} \tag{15}$$

To normalize this quantity we propose using the $T = 0$ compressibility for a non-interacting free fermion gas, multiplied by the tunneling matrix element in the limit of zero lattice depth:

$$t(V_0 \to 0\,E_r) \equiv t_0 \;=\; \frac{2}{\pi^2}E_r \;=\; 0.203\,E_r \tag{16}$$

$$\begin{aligned} \text{Normalization}: \quad \kappa_T^0(n')\frac{t_0}{a^3} &= \frac{1}{(n')^{5/3}}\frac{3s^{2/3}}{(6\pi^2)^{2/3}}\frac{\pi^2}{2}\frac{t_0}{E_r} \\ &= \frac{1}{(n')^{5/3}}\frac{3s^{2/3}}{(6\pi^2)^{2/3}} \end{aligned} \tag{17}$$

We define the normalized compressibility κ' as

$$\kappa'(n') = \frac{\kappa_T(n')\,t}{\kappa_T^0(n')\,t_0} \tag{18}$$

and obtain

$$\begin{aligned} \kappa'(n') &= -\frac{\partial(1/n')}{\partial(\mu/t)}n'^{5/3}\frac{(6\pi^2)^{2/3}}{3s^{2/3}} \\ &= \frac{1}{n'^{1/3}}\frac{\partial n'}{\partial(\mu/t)}\frac{(6\pi^2)^{2/3}}{3s^{2/3}} \\ &= \frac{\partial(n'^{2/3})}{\partial(\mu/t)}\frac{3}{2}\frac{(6\pi^2)^{2/3}}{3s^{2/3}} \\ &= \frac{\partial(n'^{2/3})}{\partial(\mu/t)}\frac{(6\pi^2)^{2/3}}{2s^{2/3}} \\ &= 4.79\frac{\partial(n'^{2/3})}{\partial(\mu/t)} \\ &= 4.79\frac{\partial(n'^{2/3})}{\partial r}\frac{\partial r}{\partial(\mu/t)} \\ &= 4.79\frac{\partial(n'^{2/3})}{\partial r}\left(\frac{\partial(\mu/t)}{\partial r}\right)^{-1} \end{aligned} \tag{19}$$