Problem Set 1
The ideal fermion gas

Let us consider a gas of $N \gg 1$ noninteracting, nonrelativistic fermions with mass m and spin s confined in a cubic box of volume $V = L^3$, with L the length of the sides. The gas is maintained at a fixed temperature T. Fermions are half-integer spin particles, so they obey the Fermi–Dirac statistics. The average occupancy of a quantum state λ with energy ε_λ is then given, in the grand-canonical ensemble, by the Fermi–Dirac distribution

$$f(\varepsilon_\lambda) = \langle n_\lambda \rangle = \frac{1}{\mathrm{e}^{\beta(\varepsilon_\lambda - \mu)} + 1}, \tag{1}$$

where $\beta = 1/k_\mathrm{B}T$ and with μ the chemical potential.

Note that some useful definite integrals are given at the end of the text.

1 General results for noninteracting fermions

(a) If A_λ is the (eigen)value of a single-particle observable A in the quantum state λ, show that

$$\sum_\lambda A_\lambda \langle n_\lambda \rangle = \int_0^\infty \mathrm{d}\varepsilon\, \rho(\varepsilon) A(\varepsilon) f(\varepsilon), \tag{2}$$

where the sum runs over quantum states λ with energy ε_λ (note that the ground state energy has been chosen to be zero), and

$$\rho(\varepsilon) \equiv \sum_\lambda \delta(\varepsilon - \varepsilon_\lambda) \tag{3}$$

is the density of states. In Eq. (2), $A(\varepsilon)$ is the value of A_λ for $\varepsilon = \varepsilon_\lambda$ [assuming for the sake of simplicity that $\forall(\lambda, \lambda')$, $\varepsilon_\lambda = \varepsilon_{\lambda'} \Rightarrow A_\lambda = A_{\lambda'}$], and $\delta(\varepsilon)$ is the Dirac delta function. What is the physical interpretation of the quantity in Eq. (2) (consider for instance the energy)?

(b) By solving the stationary Schrödinger equation (using periodic boundary conditions), show that the possible energy levels of the particles are given by

$$\varepsilon_\mathbf{k} = \frac{\hbar^2 |\mathbf{k}|^2}{2m}, \qquad \mathbf{k} = \frac{2\pi}{L}\left(n_x, n_y, n_z\right),$$

where the three quantum numbers $(n_x, n_y, n_z) \in \mathbb{Z}$.

(c) Give the spin degeneracy g_s of each eigenstate as a function of s.

(d) Show that the density of states (3) is given, in the limit $V \to \infty$, by

$$\rho(\varepsilon) = KV\sqrt{\varepsilon}\,\Theta(\varepsilon) \qquad \text{with} \qquad K = \frac{g_s}{4\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2},$$

and where $\Theta(\varepsilon)$ is the Heaviside step function. What is the ε-dependence of $\rho(\varepsilon)$ in 2d? In 1d?

(e) Sketch the Fermi–Dirac distribution (1) as a function of the single-particle energy ε_λ for (i) $T = 0$ and (ii) $T \neq 0$.

(f) Carefully demonstrate that the grand-canonical partition function for noninteracting fermions is given by

$$\Xi = \prod_\lambda \left[1 + \mathrm{e}^{-\beta(\varepsilon_\lambda - \mu)}\right].$$

(g) Deduce from the previous result that the general expression of the grand potential for noninteracting fermionic particles is given by

$$\Omega = -k_{\mathrm{B}}T \sum_{\lambda} \ln\left(1 + \mathrm{e}^{-\beta(\varepsilon_\lambda - \mu)}\right). \tag{4}$$

2 Chemical potential

In the canonical ensemble, the number of particles N is fixed, and the chemical potential μ adjusts itself to N. In the grand-canonical ensemble, μ is fixed and the number of particles fluctuates. However, in the thermodynamic limit, both ensembles are equivalent, since the fluctuations, that go as $1/\sqrt{N}$, become negligible.

The realistic system which we consider here has a fixed number N of particles. Therefore, the appropriate, "physical" statistical ensemble would be the canonical one. However, it is (very) difficult to impose the constraint $N =$ constant when computing the thermodynamic properties of the system from the canonical partition function Z. The strategy to obtain the chemical potential is then to calculate in the grand-canonical ensemble the average number of particles for a fixed μ, $\langle N\rangle(\mu)$, and then, using the equivalence between ensembles when $N \to \infty$, to invert the obtained relation to get $\mu(N)$.

(a) By using Question 1(a), express in the grand-canonical ensemble $\langle N\rangle$ in terms of $\rho(\varepsilon)$ and $f(\varepsilon)$.

(b) Introducing the fugacity $\varphi = \mathrm{e}^{\beta\mu}$, show that the chemical potential is solution of the equation

$$\frac{n}{K(k_{\mathrm{B}}T)^{3/2}} = g(\varphi) \tag{5}$$

with $n = N/V$ the density, and where

$$g(\varphi) = \int_0^\infty \mathrm{d}x \, \frac{\sqrt{x}}{\mathrm{e}^x/\varphi + 1}. \tag{6}$$

(c) Sketch the function $g(\varphi)$ defined in Eq. (6), and convince yourself from a graphical solution of Eq. (5) that (i) it has a solution for any temperature T and/or density n and (ii) μ is a decreasing function of T.

3 Equation of state

3.1 General results

(a) Show that the energy of the system is given by

$$E = KV \int_0^\infty \mathrm{d}\varepsilon \, \frac{\varepsilon^{3/2}}{\mathrm{e}^{\beta(\varepsilon-\mu)} + 1}, \qquad \text{with } \mu \text{ solution of Eq. (5).} \tag{7}$$

(b) Using Eqs. (4) and (7), demonstrate that

$$\Omega = -\frac{2}{3}E.$$

(c) Deduce from the two previous questions that the pressure of the gas is given by

$$P = \frac{2}{3}\frac{E}{V}.$$

Then, calculating the pressure P amounts to evaluate Eq. (7), which, for an arbitrary temperature, is not possible analytically. In what follows, we will thus consider various limiting cases.

3.2 Zero-temperature limit

Let us first consider the zero-temperature case $T = 0$.

(a) Demonstrate that the Fermi energy, defined as $\varepsilon_{\rm F} = \mu(T = 0)$, is given in terms of the density n by

$$\varepsilon_{\rm F} = \left(\frac{3n}{2K}\right)^{2/3}. \tag{8}$$

Hint: Calculate first the (average) number of particles N at $T = 0$.

(b) Deduce from the above considerations that the pressure at $T = 0$ is given by

$$P(T=0) = \frac{2}{15}\left(\frac{4\pi^2}{g_s}\right)^{2/3}\frac{\hbar^2}{m}\left(\frac{3n}{2}\right)^{5/3}. \tag{9}$$

What is the physical interperation of this result? How does it compare to the pressure of an ideal classical gas?

3.3 Low-temperature expansion

We now aim at obtaining the equation of state in the so-called degenerate limit, that is, when $T \ll T_{\rm F}$, where $T_{\rm F} = \varepsilon_{\rm F}/k_{\rm B}$ is the Fermi temperature.

3.3.1 Sommerfeld expansion

Consider an integral of the type

$$I = \int_{-\infty}^{+\infty} \mathrm{d}\varepsilon\, h(\varepsilon) f(\varepsilon), \tag{10}$$

where $h(\varepsilon)$ is some regular function which is integrable and (infinitely) differentiable around the chemical potential μ, and where $f(\varepsilon)$ is the Fermi–Dirac distribution from Eq. (1).

(a) Introducing

$$H(\varepsilon) = \int_{-\infty}^{\varepsilon} \mathrm{d}\varepsilon'\, h(\varepsilon'),$$

show that the integral (10) can be written as

$$I = \int_{-\infty}^{+\infty} \mathrm{d}\varepsilon\, H(\varepsilon)\left(-\frac{\partial f}{\partial \varepsilon}\right).$$

(b) Sketch $-\partial f/\partial\varepsilon$ and convince yourself that (i) in the limit $T \to 0$, $-\partial f/\partial \varepsilon = \delta(\varepsilon - \mu)$ and (ii) it is a very peaked function around μ of width $\sim k_{\rm B}T$ when $T \ll T_{\rm F}$.

(c) By Taylor-expanding the function $H(\varepsilon)$ up to second order close to μ, show that in the limit $T \ll T_{\rm F}$, the integral (10) can be approximated by

$$I \simeq H(\mu) + \frac{\pi^2}{6}\left(k_{\rm B}T\right)^2 H''(\mu). \tag{11}$$

(d) As we learned from Part 2 of this Problem Set, the chemical potential depends itself on temperature (in the canonical ensemble). To get the full low-temperature expansion of Eq. (11), we must thus determine $\mu(T)$ in such a limit. Using the Sommerfeld expansion (11) to calculate the (average) number of particles in the system, show that for $T \ll T_{\rm F}$,

$$\mu(T) \simeq \varepsilon_{\rm F}\left[1 - \frac{\pi^2}{12}\left(\frac{T}{T_{\rm F}}\right)^2\right], \tag{12}$$

with $\varepsilon_{\rm F}$ the Fermi energy defined in Eq. (8).

3.3.2 Low-temperature pressure

Using a Sommerfeld expansion, show that the low-temperature pressure of the degenerate fermionic gas is given by

$$P(T \ll T_{\mathrm{F}}) \simeq P(T=0)\left[1+\frac{5\pi^2}{12}\left(\frac{T}{T_{\mathrm{F}}}\right)^2\right],$$

with $P(T=0)$ the zero-temperature pressure given in Eq. (9).

3.4 High-temperature limit

(a) In the high-temperature, nondegenerate limit $T \gg T_{\mathrm{F}}$, show from Eq. (5) that the fugacity is given by

$$\varphi = \frac{2n}{\sqrt{\pi}K(k_{\mathrm{B}}T)^{3/2}}.$$

(b) In the same limit, show from Eq. (7) that the equation of state is that of an ideal classical gas, i.e.,

$$P(T \gg T_{\mathrm{F}}) = n\,k_{\mathrm{B}}T.$$

4 Heat capacity

From the considerations above, argue that the low-temperature heat capacity is linear in T. How does this result compare with the high-temperature, classical case?

A few integrals

$$\begin{aligned}
\int_0^{+\infty} \mathrm{d}x\, x^{1/2}\, \mathrm{e}^{-x} &= \frac{\sqrt{\pi}}{2} \\
\int_0^{+\infty} \mathrm{d}x\, x^{3/2}\, \mathrm{e}^{-x} &= \frac{3\sqrt{\pi}}{4} \\
\int_{-\infty}^{+\infty} \mathrm{d}x\, \frac{x^2\,\mathrm{e}^{x}}{(\mathrm{e}^{x}+1)^2} &= \frac{\pi^2}{3}
\end{aligned}$$