

Exercise 1. Ideal fermionic quantum gas in a harmonic trap

In this exercise we study the fermionic spinless ideal gas confined in a three-dimensional harmonic potential and compare it with the classical case (see Exercise Sheet 3). The eigenenergies of the gas are given by

$$\varepsilon_{\mathbf{a}} = \hbar\omega(a_x + a_y + a_z), \quad (1)$$

where $\mathbf{a} = (a_x, a_y, a_z)$, with $a_i \in \{0, 1, 2, \dots\}$, labels the states and the zero point energy $\varepsilon_0 = 3\hbar\omega/2$ was omitted. The occupation number corresponding to state \mathbf{a} is given by $n_{\mathbf{a}}$.

- (a) Consider the high-temperature, low-density limit ($z \ll 1$). Derive the grand canonical partition function \mathcal{Z}_f of this system and compute the grand potential Ω_f . Show that

$$\Omega_f \propto f_4(z), \quad (2)$$

where the function $f_s(z)$ is defined as

$$f_s(z) = - \sum_{l=1}^{\infty} (-1)^l \frac{z^l}{l^s}. \quad (3)$$

Solution. We begin with the general definition of the grand canonical partition function within the occupation number formalism (chapter 3 of the lecture notes) and find

$$\mathcal{Z}_f = \prod_{\mathbf{a}} \sum_{n_{\mathbf{a}}} \left(z e^{-\beta\varepsilon_{\mathbf{a}}} \right)^{n_{\mathbf{a}}} = \prod_{\mathbf{a}} (1 + z e^{-\beta\varepsilon_{\mathbf{a}}}). \quad (S.1)$$

In order to compute the grand potential $\Omega = -1/\beta \log \mathcal{Z}$, we use the series expansion

$$\log(1+x) = - \sum_{l=1}^{\infty} \frac{(-x)^l}{l} \quad \text{for } -1 < x \leq 1. \quad (S.2)$$

This expansion is applicable to the logarithm of the partition function in (S.1) if $z e^{-\beta\varepsilon_{\mathbf{a}}} \leq 1$ (it is always positive) in the high-temperature, low density limit $z \ll 1$.

We find

$$\begin{aligned} \log \mathcal{Z}_f &= \sum_{\mathbf{a}} \log(1 + z e^{-\beta\varepsilon_{\mathbf{a}}}) = - \sum_{\mathbf{a}} \sum_{l=1}^{\infty} (-1)^l \frac{z^l}{l} e^{-l\beta\varepsilon_{\mathbf{a}}} = - \sum_{l=1}^{\infty} (-1)^l \frac{z^l}{l} \left(\sum_{\mathbf{a}} e^{-l\beta\varepsilon_{\mathbf{a}}} \right)^3 \\ &= - \sum_{l=1}^{\infty} (-1)^l \frac{z^l}{l} \left(\frac{1}{1 - e^{-l\beta\hbar\omega}} \right)^3 = - \begin{cases} - \sum_{l=1}^{\infty} (-1)^l \frac{z^l}{l} \frac{1}{(l\beta\hbar\omega)^3} & \text{if } \beta \rightarrow 0 \\ - \sum_{l=1}^{\infty} (-1)^l \frac{z^l}{l} & \text{if } \beta \rightarrow \infty \end{cases} \\ &= \begin{cases} \frac{1}{(\beta\hbar\omega)^3} f_4(z) & \text{if } \beta \rightarrow 0 \\ f_1(z) & \text{if } \beta \rightarrow \infty \end{cases}, \end{aligned} \quad (S.3)$$

and obtained both the high and the low temperature limits (in either case $z \ll 1$ must be given).

Alternatively, for the high temperature limit, with the help of the Euler-Maclaurin formula (see, e.g., Exercise Sheet 4), we can approximate the sum over the oscillator modes by an integral and find in leading order

$$\log \mathcal{Z}_f = - \sum_{l=1}^{\infty} (-1)^l \frac{z^l}{l} \left(\sum_{a=0}^{\infty} e^{-l\beta\hbar\omega a} \right)^3 \quad (S.4)$$

$$\begin{aligned} &\approx - \sum_{l=1}^{\infty} (-1)^l \frac{z^l}{l} \left(\int_0^{\infty} da e^{-l\beta\hbar\omega a} \right)^3 = - \sum_{l=1}^{\infty} (-1)^l \frac{z^l}{l} \left(\int_0^{\infty} da e^{-l\beta\hbar\omega a} \right)^3 \\ &= - \frac{1}{(\beta\hbar\omega)^3} \sum_{l=1}^{\infty} \left[(-1)^l \frac{z^l}{l^4} \right] = \frac{1}{(\beta\hbar\omega)^3} f_4(z) \end{aligned} \quad (S.5)$$

Either way, the high temperature expansion results in the grand potential

$$\Omega_f = -\frac{1}{\beta} \frac{1}{(\beta\hbar\omega)^3} f_4(z). \quad (\text{S.6})$$

- (b) Calculate the particle number $\langle N \rangle$ and the internal energy U as a function of N . In order to get U in terms of N (instead of dealing with the chemical potential), introduce the parameter

$$\rho \equiv \left(\frac{\hbar\omega \langle N \rangle^{1/3}}{k_B T} \right)^3 \quad (4)$$

and relate it to z using the high-temperature, low-density expansion of $\langle N \rangle$ (up to $\mathcal{O}(z^2)$). Interpret the condition $\rho \ll 1$.

Finally, expand U up to second order in ρ , relating it to N .

Solution. First, we compute the internal energy of the system,

$$U_f = \left. \frac{\partial(\beta\Omega_f)}{\partial\beta} \right|_z, \quad (\text{S.7})$$

where the derivative has to be taken at constant fugacity $z = e^{\beta\mu}$. Starting from (S.6) we find

$$U_f = \frac{3}{\beta} \frac{1}{(\beta\hbar\omega)^3} f_4(z), \quad (\text{S.8})$$

which shows that the internal energy is proportional to the grand potential, $U_f = -3\Omega_f$.

The average particle number can be computed in a similar way,

$$\langle N_f \rangle = z \frac{\partial}{\partial z} \log \mathcal{Z}_f. \quad (\text{S.9})$$

We have

$$\langle N_f \rangle = z \frac{\partial}{\partial z} \frac{1}{(\beta\hbar\omega)^3} f_4(z) = \frac{1}{(\beta\hbar\omega)^3} f_3(z), \quad (\text{S.10})$$

where we used

$$z \frac{\partial}{\partial z} f_4(z) = f_3(z). \quad (\text{S.11})$$

In order to relate the internal energy to the particle number, we start with the high-temperature, low-density expansion of the total particle number,

$$\langle N_f \rangle = \frac{1}{(\beta\hbar\omega)^3} f_3(z) \approx \frac{1}{(\beta\hbar\omega)^3} \left(z - \frac{z^2}{8} \right). \quad (\text{S.12})$$

Rewriting this equation using the parameter ρ leads to

$$\rho = z - \frac{z^2}{8}. \quad (\text{S.13})$$

The condition $z \ll 1$ therefore implies $\rho \ll 1$. Solving this equation for z , we obtain $z = 4 \pm 2\sqrt{4 - 2\rho}$. Choosing the relevant solution and expanding $\sqrt{1+x} \approx 1 + \frac{x}{2} - \frac{x^2}{8}$ we find

$$z = \rho + \frac{\rho^2}{8}. \quad (\text{S.14})$$

Expanding in ρ allows us to deal with the particle number instead of the chemical potential.

To interpret the condition $\rho \ll 1$ we first note that for this system, the Fermi energy follows $\epsilon_F = 3\hbar\omega a_{\max}$, while the number of occupied states is proportional to a_{\max}^3 . The characteristic energy scale is thus given by $3\hbar\omega N^{1/3}$. Therefore, this condition requires that the characteristic energy scale is much smaller than

the thermal energy $k_B T$ (*high-temperature* limit). This means that we consider temperatures at which the average occupation of the states is much smaller than one (*low-density* limit).

We write the internal energy up to second order in ρ as

$$\begin{aligned} U &= \frac{3}{\beta} \frac{1}{(\beta\hbar\omega)^3} f_4(z) = \frac{3}{\beta} \frac{1}{(\beta\hbar\omega)^3} \left(z - \frac{z^2}{16} \right) \\ &= \frac{3}{\beta} \frac{1}{(\beta\hbar\omega)^3} \left(\rho + \frac{\rho^2}{16} \right) \\ &= \frac{3}{\beta} \left(N + N^2 (\beta\hbar\omega)^3 \frac{1}{16} \right) = 3Nk_B T \left(1 + N \left(\frac{\hbar\omega}{k_B T} \right)^3 \frac{1}{16} \right), \end{aligned} \quad (\text{S.15})$$

where we recover the equipartition law in leading order and the positive first order quantum corrections $\propto N(\hbar\omega/k_B T)^3 \ll 1$ distinguishing the fermions from the classical ideal gas.

- (c) Compute the heat capacity C . Which quantity has to be fixed in order to do this?

Solution. Since our system does not have a volume as thermodynamic variable we have to compute the specific heat C_N by fixing the number of particles. Hence, as a starting point we use the expression (S.15) for the inner energy, where we can keep N fixed:

$$C_N = \left(\frac{\partial U}{\partial T} \right)_N = 3Nk_B \left(1 - \frac{1}{8} N \left(\frac{\hbar\omega}{k_B T} \right)^3 \right). \quad (\text{S.16})$$

- (d) Compute the isothermal compressibility κ_T .

Solution. By definition

$$\kappa_T = \frac{v}{N} \left(\frac{\partial N}{\partial \mu} \right)_T, \quad (\text{S.17})$$

where $v = \frac{V}{N}$. Therefore,

$$\kappa_T = \frac{v}{\langle N \rangle} \left(\frac{\partial z}{\partial \mu} \frac{\partial N}{\partial z} \right)_T = \frac{v}{N} \beta z \frac{1}{(\beta\hbar\omega)^3} \frac{\partial f_3(z)}{\partial z} = v \beta \frac{f_2(z)}{f_3(z)} \approx \frac{N}{V k_B T} \left(1 - \frac{1}{8} N \left(\frac{\hbar\omega}{k_B T} \right)^3 \right). \quad (\text{S.18})$$

- (e) Interpret your results for U , C , and κ_T by comparing them with the corresponding results for the classical Boltzmann gas. How do the quantum corrections influence the fermionic system?

Solution. In summary we have found up to first order in ρ :

$$U = 3Nk_B T \left(1 + N \left(\frac{\hbar\omega}{k_B T} \right)^3 \frac{1}{16} \right), \quad (\text{S.19})$$

$$C_N = 3Nk_B \left(1 - \frac{1}{8} N \left(\frac{\hbar\omega}{k_B T} \right)^3 \right), \quad (\text{S.20})$$

$$\kappa_T = \frac{N}{V k_B T} \left(1 - \frac{1}{8} N \left(\frac{\hbar\omega}{k_B T} \right)^3 \right), \quad (\text{S.21})$$

These results as a function of temperature are plotted in Fig. 1; each for the classical and the fermionic case. Note that our expansions up to second order in ρ are strictly speaking only valid for $\rho \ll 1$, while the plots extend to larger values of ρ to emphasize the trends.

We see that

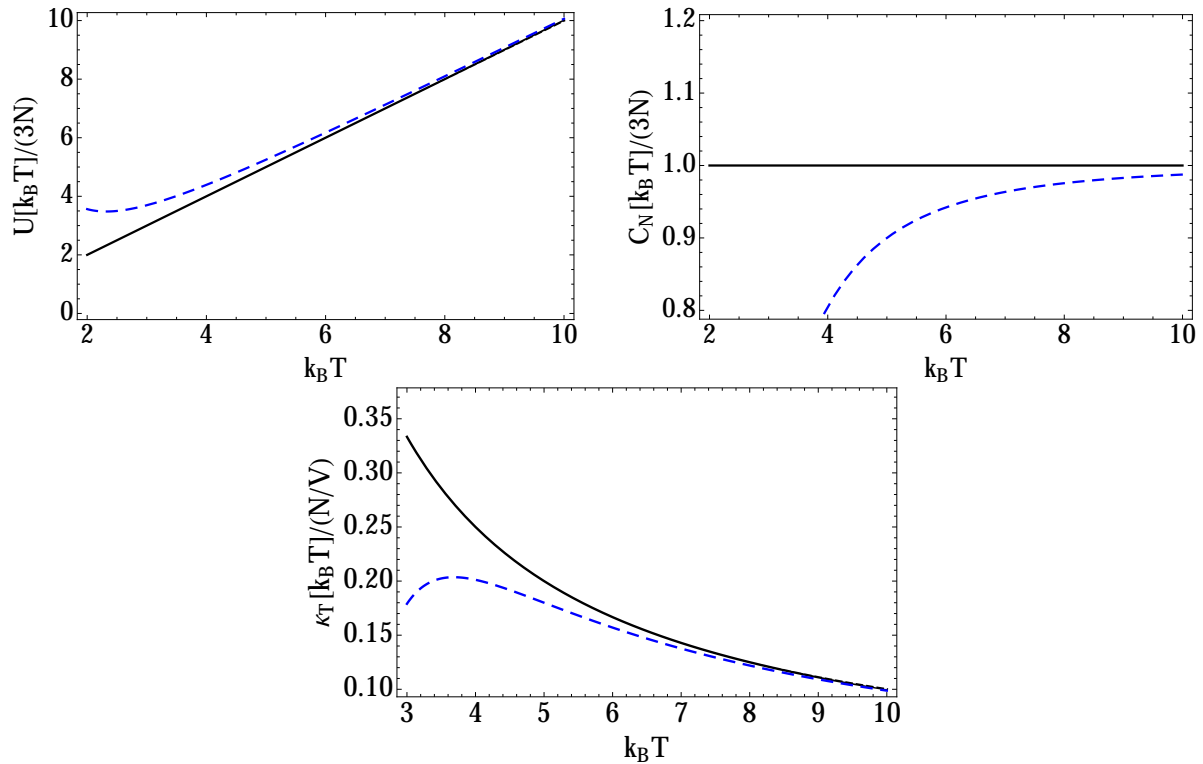


Figure 1: Thermodynamics of the fermionic gas (dashed, blue) compared to the classical gas (solid, black). Note that these quantities are computed within the high-temperature, low-density approximation and are therefore not exact results. Still, they can be used to observe trends. We set $N(\hbar\omega)^3 = 100$.

- In first order in ρ the results for the classical (Boltzmann) gas in a harmonic trap are recovered (cf. Exercise Sheet 3).
- Due to quantum corrections, the internal energy U for fermions is higher than the classical ideal gas. This can be understood by taking quantum statistics into account. Fermions are not allowed to occupy the same state multiply (Pauli). Lowering the temperature, the system tends to occupy low energy states with growing probability. While the classical system does not care about multiple occupancies, in the fermionic system the double occupancy is forbidden and occupation of low-energy states is thus reduced, increasing the inner energy U_f compared to the classical gas.

Exercise 2. Sommerfeld expansion and density of states

Consider a thermally equilibrated system of non-interacting fermions with single particle states labeled by the quantum numbers ν and corresponding energies ε_ν .

- (a) Work in the grand canonical ensemble and write the particle and energy densities in the form

$$n = \frac{1}{V} \sum_{\nu} f(\varepsilon_\nu) = \int d\varepsilon g(\varepsilon) f(\varepsilon), \quad (5)$$

$$u = \frac{1}{V} \sum_{\nu} \varepsilon_\nu f(\varepsilon_\nu) = \int d\varepsilon \varepsilon g(\varepsilon) f(\varepsilon), \quad (6)$$

where $f(\varepsilon)$ is the Fermi-Dirac distribution function. What is $g(\varepsilon)$?

Solution. In thermal equilibrium, the occupation probability of a particular state with energy ε is given by the Fermi-Dirac distribution

$$f(\varepsilon) = \frac{1}{e^{(\varepsilon-\mu)/k_B T} + 1}, \quad (S.22)$$

and we find from the definition of n and u

$$n = \frac{1}{V} \sum_{\nu} f(\varepsilon_\nu) = \int d\varepsilon f(\varepsilon) \frac{1}{V} \sum_{\nu} \delta(\varepsilon - \varepsilon_\nu) = \int d\varepsilon g(\varepsilon) f(\varepsilon), \quad (S.23)$$

$$u = \frac{1}{V} \sum_{\nu} \varepsilon_\nu f(\varepsilon_\nu) = \int d\varepsilon \varepsilon f(\varepsilon) \frac{1}{V} \sum_{\nu} \delta(\varepsilon - \varepsilon_\nu) = \int d\varepsilon \varepsilon g(\varepsilon) f(\varepsilon), \quad (S.24)$$

with

$$g(\varepsilon) = \frac{1}{V} \sum_{\nu} \delta(\varepsilon - \varepsilon_\nu) = \frac{1}{V} \omega(\varepsilon), \quad (S.25)$$

and $\omega(\varepsilon)$ as in the lecture notes.

That is, $g(\varepsilon)$ is the density of energy levels divided by the volume.

- (b) The above expressions for n and u are of the form

$$\int_{-\infty}^{\infty} d\varepsilon H(\varepsilon) f(\varepsilon). \quad (7)$$

For temperatures $T \ll \frac{\varepsilon_F}{k_B}$ (which is typically the case for metals), $H(\varepsilon)$ is slowly varying in the region where $\frac{df}{d\varepsilon} \neq 0$ significantly and the Sommerfeld expansion¹

$$\int_{-\infty}^{\infty} d\varepsilon H(\varepsilon) f(\varepsilon) = \int_{-\infty}^{\mu} d\varepsilon H(\varepsilon) + \frac{\pi^2}{6} (k_B T)^2 H'(\mu) + \frac{7\pi^4}{360} (k_B T)^4 H'''(\mu) + \mathcal{O}\left(\frac{k_B T}{\mu}\right)^6 \quad (8)$$

becomes handy. Make use of this expansion up to $\mathcal{O}\left(\frac{k_B T}{\mu}\right)^2$ to expand n and u in T .

Hint: Use (in a self-consistent way) that $\mu - \varepsilon_F \propto T^2$ in leading order in T and expand

$$\int_{-\infty}^{\mu} d\varepsilon H(\varepsilon) \approx \int_{-\infty}^{\varepsilon_F} d\varepsilon H(\varepsilon) + (\mu - \varepsilon_F) H(\varepsilon_F). \quad (9)$$

¹For a reference on the Sommerfeld expansion see, e.g., Ashcroft, N. W. and Mermin N. D., *Solid State Physics*, Holt, Rinehart and Winston, 1976.

Solution. From the Sommerfeld expansion we obtain

$$n = \int_{-\infty}^{\mu} d\varepsilon g(\varepsilon) + \frac{\pi^2}{6} (k_B T)^2 g'(\varepsilon) + \mathcal{O}\left(\frac{k_B T}{\mu}\right)^4 \quad (\text{S.26})$$

$$u = \int_{-\infty}^{\mu} d\varepsilon \varepsilon g(\varepsilon) + \frac{\pi^2}{6} (k_B T)^2 [\mu g'(\varepsilon) + g(\mu)] + \mathcal{O}\left(\frac{k_B T}{\mu}\right)^4. \quad (\text{S.27})$$

As we know that $\lim_{T \rightarrow 0} \mu = \varepsilon_F$, the remaining integrals can be expanded around the chemical potential (see hint):

$$n \approx \int_{-\infty}^{\varepsilon_F} d\varepsilon g(\varepsilon) + \left[(\mu - \varepsilon_F) g(\varepsilon_F) + \frac{\pi^2}{6} (k_B T)^2 g'(\varepsilon_F) \right], \quad (\text{S.28})$$

$$u \approx \int_{-\infty}^{\varepsilon_F} d\varepsilon \varepsilon g(\varepsilon) + \varepsilon_F \left[(\mu - \varepsilon_F) g(\varepsilon_F) + \frac{\pi^2}{6} (k_B T)^2 g'(\varepsilon_F) \right] + \frac{\pi^2}{6} (k_B T)^2 g(\varepsilon_F). \quad (\text{S.29})$$

For this to be self-consistent, we need to check that the chemical potential $\mu = \varepsilon_F + \alpha T^2 + \mathcal{O}(T^3)$, which we see next.

- (c) Find the chemical potential μ and the specific heat c_v at constant density n .

Solution. As the density is constant and we have at $T = 0$ that

$$n = \int d\varepsilon g(\varepsilon) f(\varepsilon) = \int_{-\infty}^{\varepsilon_F} d\varepsilon g(\varepsilon), \quad (\text{S.30})$$

it follows, from Eq. (S.28), that

$$\mu = \varepsilon_F - \frac{\pi^2}{6} (k_B T)^2 \frac{g'(\varepsilon_F)}{g(\varepsilon_F)}. \quad (\text{S.31})$$

Similarly,

$$u = u_0 + \frac{\pi^2}{6} (k_B T)^2 g(\varepsilon_F), \quad (\text{S.32})$$

and therefore

$$c_v = \left(\frac{\partial u}{\partial T} \right)_n = \frac{\pi^2}{3} k_B^2 T g(\varepsilon_F). \quad (\text{S.33})$$

From this we see the important results that i) the chemical potential varies with respect to temperature in dependence of $g'(\varepsilon)$ and ii) that heat measurements are a tool to access the density of states at the Fermi energy.

- (d) Determine $g(\varepsilon)$ for the case of a free Fermi gas and calculate its chemical potential and specific heat from the previous results. Compare your result for the specific heat with the one for a classical gas.

Solution. For free fermions, the label ν corresponds to the momentum of the particles \mathbf{k} and the energies ε are given by the dispersion relation

$$\varepsilon_{\mathbf{k}} = \frac{\hbar^2 \mathbf{k}^2}{2m}. \quad (\text{S.34})$$

With the help of the step function Θ , the density of states can be written as (cf. lecture notes)

$$g(\varepsilon) = \frac{1}{4\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \varepsilon^{1/2} \Theta(\varepsilon), \quad (\text{S.35})$$

or alternatively

$$g(\varepsilon) = \frac{3}{2} \frac{n}{\varepsilon_F} \left(\frac{\varepsilon}{\varepsilon_F} \right)^{1/2} \Theta(\varepsilon). \quad (\text{S.36})$$

Using this result we obtain (as for the low-temperature, high-density limit in the lecture)

$$\mu = \varepsilon_f \left[1 - \frac{\pi^2}{12} \left(\frac{k_B T}{\varepsilon_F} \right)^2 \right], \quad (\text{S.37})$$

$$c_v = \frac{\pi^2}{2} \left(\frac{k_B T}{\varepsilon_F} \right) n k_B. \quad (\text{S.38})$$

For a classical ideal gas (Maxwell-Boltzmann distribution) we find

$$c_v = \frac{3}{2} n k_B, \quad (\text{S.39})$$

which means that in the fermionic case the specific heat is suppressed by a factor

$$\frac{\pi^2}{2} \frac{k_B T}{\varepsilon_F}. \quad (\text{S.40})$$

The origin of this suppression lies in the Fermi-Dirac distribution and the Pauli principle. For low temperatures $k_B T \ll \varepsilon_F$ (note that this can easily be several hundred Kelvin for electrons in metals) only a fraction of all the fermions, namely the ones around the Fermi energy, get thermally excited and contribute to the heat capacity, whereas for a classical gas all the particles can contribute.

- (e) For the free Fermi gas $g'(\varepsilon_F) > 0$. This does not need to be the true in more complex systems such as solids (cf., e.g., semiconductors). What are the consequences of $g'(\varepsilon_F) \leq 0$?

Solution. The sign of the density of states determines whether the chemical potential increases, decreases or stays constant with respect to the temperature. A negative sign would lead to an increase in the chemical potential by increasing temperature.