Oblig04 - Alternative A — Fys2160 — 2016

Exercise 0.4. Relativistic Fermi Gas

For relativistic electrons - that is for electrons where $\varepsilon \gg mc^2$ - the energy is given as $\varepsilon \simeq pc$, where p is the momentum. For a particle in a square box of size $L \times L \times L$, the momentum is

$$p = \frac{\pi\hbar}{L}\left(n_x^2 + n_y^2 + n_z^2\right)^{1/2} ,\tag{0.25}$$

just as for non-relativistic electrons.

a) Show that the density of states has the form

$$D(\varepsilon) = \frac{\pi}{a^3}\varepsilon^2 ,\tag{0.26}$$

where $a = c\pi\hbar/L$.

b) Show that the Fermi energy of a gas of N electrons is

$$\varepsilon_F = \hbar c\pi \left(3n/\pi\right)^{1/3} ,\tag{0.27}$$

where $n = N/V$.

c) Show that the total energy when $T = 0$ is

$$U_0 = \frac{3}{4}N\varepsilon_F .\tag{0.28}$$

Exercise 0.5. Chemical potential in a Fermi Gas

For a Fermi-gas with N particles and volume V we can define the chemical potential μ by solving the following equation with respect to μ:

$$N = \int_0^\infty D(\varepsilon)f(\varepsilon,\mu,T)\,d\varepsilon ,\tag{0.29}$$

where the density of states, $D(\varepsilon)$ for particles with spinn 1/2 is given as

$$D(\varepsilon) = \frac{3N}{2\varepsilon_F^{3/2}}\varepsilon^{1/2} = \frac{4V}{\sqrt{\pi}}\left(\frac{2\pi m}{h^2}\right)^{3/2}\varepsilon^{1/2} ,\tag{0.30}$$

and f is given as

$$f(\varepsilon,\mu,T) = \frac{1}{1 + \exp\left(\frac{\varepsilon-\mu}{kT}\right)} .\tag{0.31}$$

Eq. (0.29) can be solved numerically to find $\mu(T)$, and we will here show how to proceed to do this.

In order to solve the equations numerically, it is useful to non-dimensionalize the equations. We do this by introducing a characteristic energy, ε_F, corresponding to the Fermi energy:

$$\varepsilon_F = \frac{h^2}{8m} \left(\frac{3N}{\pi V} \right)^{2/3} . \tag{0.32}$$

Based on this energy, we introduce new dimensionless variables $t = kT/\varepsilon_F$, $c = \mu/\varepsilon_F$ and $x = \varepsilon/\varepsilon_F$.

a) Show that (0.29) can be written as

$$1 = \frac{3}{2} \int_0^\infty \frac{x^{1/2}}{\exp((x-c)/t)+1} \, dx , \tag{0.33}$$

using the dimensionless variables.

b) What happens when $t = 0$? What is c in this case? Explain.

c) Now we will find $c(t)$ numerically by varying c while holding t fixed until the integral gives the desired value. You should do this for t in the range from 0.1 to 2 and plot the results. (Hint: You can use the function `integral(F,0,Inf)` to find the integral of the function for a given set of values for t and c. You then need to adjust c until the integral becomes $2/3$. The function `F` is formulated as an alpha-function. For example, the function $F(x) = 2cx^2$ is formulated as `F = @(x)2*c*x.^2;`).

d) Use your calculated values for $\mu(T)$ to find the energy $U(T)$ numerically for temperatures up to $t = 2$. Plot the result.

e) Find the heat capacity as a function of temperature from your numerical calculation of the energy as a function of temperature.

f) Plot the distribution function $f(\varepsilon, \mu(T), T)$ as a function of ε for a range of values of T using your calculated values for $\mu(T)$. Comment on the results.

g) (For discussion in class) Explain graphically why the initial curvature of $\mu(T)$ is upward in 1d and downward in 3d. (Hint: Use the integral for N and use the graphs to consider the behavior of the integrand from $T = 0$ to a finite temperature. You have found the density of states in 1d previously.)

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Exercise 0.6. Lattice gas

Learning outcomes. In this project you will learn how to address interactions in a gas. Focus will be on the partition function, its relation to free energy and free-energy minimization.

Model system. In this exercise we will study a simplified model for a gas of interacting particles. We assumed that the gas consists of a volume V of M celles, each with a volume b. Each cell can either be empty or occupied by a single particles. The system is in contact with a reservoir with constant temperature T and the number of particles, N, of the system is constant. This means that N, V, T for the system is given. In this model we want to address the interactions between the particles. The energy of the system is therefore assumed only to depend on how the particles are located relative to each other. The energy of two particles next to each other is $-\varepsilon$. The figure illustrates the energy of two possible configurations of 4 particles in 8 cells.

Simplified model. We start by studying a small system with only $M = 4$ cells on a line along the x-axis as illustrated in the Fig. **??**
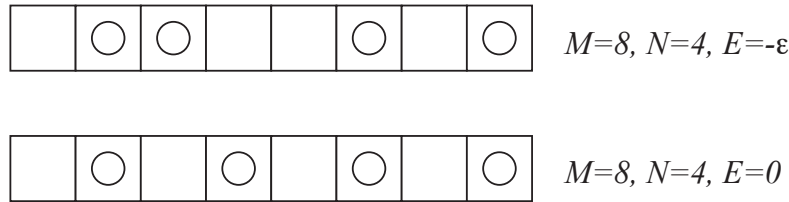

$M{=}8,\ N{=}4,\ E{=}{-}\varepsilon$

$M{=}8,\ N{=}4,\ E{=}0$

Fig. 0.1 Plots of $\hat{g}(\hat{\rho})$, for $\hat{T} = 0.9$ for a set of values of $\hat{\rho}$ from 0.4 to 0.8 in 10 steps.

a) Find the partition function for the system when $N = 1$ and $M = 4$.

b) Find an expression for the partition function when $N = 2$ and $M = 4$.

c) What is the probability that the particles are next to each other when $N = 2$ and $M = 4$?

d) What is the energy, $E = E(N, V, T)$, of the system when $N = 2$ and $M = 4$?

   We will now study a numerical simulation of a three-dimensional system. Assume that a state of system can be described by a matrix m. You have been provided a function `energy(m)` that returns the energy of a state described by m, and you have been provided a function, $m = $ `rndstate()` that return a random state m.

e) Sketch a program to that finds an approximate value for the partition function of the average energy of a system based on 10000 randomly generated states for a given temperature T.

We will now make a simplified model for this system. In the simplified model, we assume that the energy of a system of N particles is

$$E = -\frac{6\varepsilon}{2}\left(\frac{N}{M}\right)N = -3\,\varepsilon\bar{n}N\,, \tag{0.34}$$

where $\bar{n} = N/M = n/n_0$, where $n = N/V$ and $n_0 = 1/b$, and ε is the interaction energy between two particles that are next to each other.

f) Show that the entropy of a system with $M = V/b$ positions and N atoms is approximately equal to

$$S = -Nk\bar{n}^{-1}\left(\bar{n}\ln\bar{n} + (1-\bar{n})\ln(1-\bar{n})\right)\,. \tag{0.35}$$

g) Show that Gibb's free energy per particles can be written as:

$$g = G/N = -3\varepsilon\bar{n} + kT\bar{n}^{-1}\left(\bar{n}\ln\bar{n} + (1-\bar{n})\ln(1-\bar{n})\right) + pb\bar{n}^{-1}\,. \tag{0.36}$$

h) The figure shows $g(\bar{n})$ for a constant p as three different temperatures $T_1 < T_2 < T_3$. Explain what the figure tells you about the system.
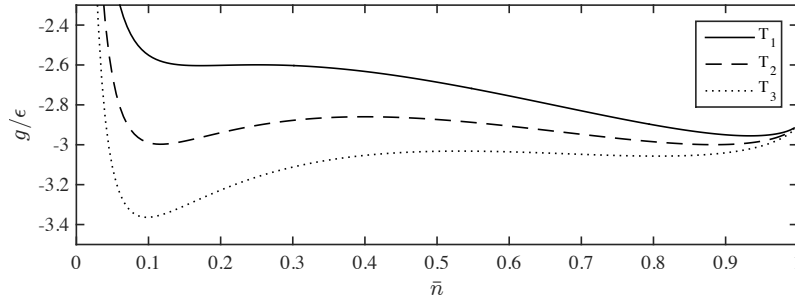

Fig. 0.2 Plot of $g(\bar{n})$ for a constant p and at three different temperatures $T_1 < T_2 < T_3$.

Exercise 0.7. Ideal gas in electrical field

The Helmholtz free energy for an ideal gas is

$$F = -kT\ln\frac{Z_1^N}{N!}\,, \tag{0.37}$$

where the partition function for a single particle is:

$$Z_1 = n_Q(T)V\,. \tag{0.38}$$

Here, V is the volume of the gas, N is the number of particles in the gas, T is the temperature, and $n_Q(T) = \left(2\pi mkT/h^2\right)^{3/2}$.

a) Show that the chemical potential of the gas is:

$$\mu = kT \ln \frac{n}{n_Q} . \tag{0.39}$$

Assume that the gas consists of charged particles that can move freely along the x-axis. You can still assume that the gas is dilute, so that the particles do not interact with each other. But they are in a uniform electrical field along the x-axis. The energy of a particles in the electric field is $e(x) = qUx$, where q is the charge of the particles, and U is the electrical field. You can assumed that the temperature is constant throughout the gas.

b) Find Helmholtz free energy as a function of x for the ideal gas of charged particles in an electrical field U.

c) Find the chemcial potential of the gas as a function of x in the electrical field.

d) Find the density of the gas as a function of x for a gas in diffusive equilibrium and with constant temperature.