Oblig01 — Fys2160 — 2016

Exercise 0.1. Micro- and Macrostates

Learning outcomes. In this project you will learn how to make simplified models of macroscopic systems and to count the microstates in these models. You will learn to find the multiplicity of a single, isolated system, and an isolated, compound system consisting of two system in thermal contact. You will learn how to use Boltzmann's formula to connect the multiplicity of a macrostate with the entropy of the system, and how to find the termperature of the system. Thus, you will learn how to find macroscopic properties of a system from a simplified, microscopic model of the system. The idea is that we will use a general method to go from the microscopic model to a macroscopic property such as temperature, and that this method is the same even though the systems we study vary.

Model systems. We will introduce two model systems: The Einstein crystal and the spin system. These model systems can be considered to represent a specific system: The Einstein crystal could represent a Silicon crystal, and the spin system could represent a system of magnetic diopoles in an external magnetic field. However, these systems also represents basic models that you will use as building blocks for more advanced models later — the harmonic oscillator of statistical mechanics if you want.

Part 1: The Einstein crystal. A real crystal consists of a set of atoms in a periodic configurations interacting through interatomic interactions that include both short range and longer ranged forces. As a result, individual atoms will oscillate around an equilibrium position while interacting mostly with its nearest neighbors. As a simplified model for this system we consider each atom, i, to behave like an independent harmonic oscillator with a potential energy U_i:

$$U_i(\mathbf{r}_i) = \frac{1}{2}k_x(x_i - x_{i,eq})^2 + \frac{1}{2}k_y(y_i - y_{i,eq})^2 + \frac{1}{2}k_z(z_i - z_{i,eq})^2 \ , \tag{0.1}$$

From quantum mechanics, we know that the energy of a harmoic oscillator i is

$$\varepsilon_i = n_i \Delta\varepsilon \ , \tag{0.2}$$

where n_i is an integer describing the state of oscillator i. We can therefore describe the state of a crystal with N independent (meaning non-interacting) oscillators by the states n_i for $i = 1, \ldots, N$. The total energy of the crystal in this simplified model is then:

$$U = \sum_{i=1}^{N} \varepsilon\, n_i \ . \tag{0.3}$$

For simplicity we will measure energy in units of ε:

$$q = \frac{U}{\varepsilon} = \sum_{i=1}^{N} n_i \; . \tag{0.4}$$

This means that for an isolated system with a given total energy, the sum of all the n_i is constant, but we can still change how the energy is distributed in the system. We can think of the energy a given number of energy units that we are free to distribute between the oscillators. Any distribution is allowed as long as we do not change the total energy.

This simple model for a crystal, called the *Einstein crystal*, captures surprisingly many of the important features of the statistical physics of a crystal.

We describe a microstate of this system by the numbers n_i for each oscillator:

$$\{n_1, n_2, \ldots, n_N\} \tag{0.5}$$

For example, for a system with $N = 4$ and $q = 4$, a possible microstate is $\{1,0,2,1\}$, that is $n_1 = 1$, $n_2 = 0$, $n_3 = 2$, and $n_4 = 1$.

Unstructured problem formulation. For a system of two Einstein crystals in thermal contact, find the probabilities for all possible partitionings of energy between the systems and visualize and discuss the results. Find expressions for the entropy and the temperature of an isolated Einsten crystal as a function of relevant macroscopic variables.

Structured problem formulation. We will first count the microstates of a single Einstein crystal, then address two Einstein crystals in contact, develop a computer program to find the number of microstates for a given partitioning of energy, and use this find the probabilities of the corresponding macrostates.

a) First, we familiarize ourselves with the microstates. For a system with $N = 3$ oscillators and $q = 3$ list all the possible microstates.

The general formula for the number of microstates for N oscillators with q units of energy is:

$$\Omega(N,q) = \binom{q+N-1}{q} = \frac{(q+N-1)!}{q!(N-1)!} \; . \tag{0.6}$$

b) Check that the results you found above are consistent with this formula.

We are now ready to discuss a system consisting of two isolated Einstein crystals, system A with N_A oscillators and energy q_A and system B with N_B oscillators and energy q_B.

c) For a system consisting of subsystem A with $N_A = 2$ and $q_A = 5$ and subsystem B with $N_B = 2$ and $q_B = 1$ list all possible microstates of the system.

The two systems are put in *thermal* contact. This means that they can exchange energy, but that the number of particles and the volume of each subsystem does not change. The total energy $q = q_A + q_B = 6$ is constant, but the energy can now be distributed between the two systems. Let us now count the number of possible microstates for each possible value of q_A and q_B. We call a state with a given q_A (and therefore also a given $q_B = q - q_A$) a *macrostate* of the system.

d) For $N_A = 2$, $N_B = 2$, and $q = 6$ what are the possible values of q_A and q_B?

e) For each possible macrostate q_A find the number of compatible microstates. Write a program to calculate the number of microstates as a function of q_A, N_A and N_B and check that it produces the right results for the $N_A = 2$, $N_B = 2$ system from above. Assume that all microstates are equally probably and find the probabilities of each macrostate.

f) Compare the total number of microstates available to the system before and after the systems came in thermal contact. Comment on the result. What aspects of this result do you think is general?

g) Plot the probability $P(q_A)$ as a function of q_A for all possible values of q_A for a system with $N_A = 50$, $N_B = 50$ and $q = q_A + q_B = 100$. What is the most probable macrostate and how probably is this state?

Finding thermodynamic properties. We will now apply Boltzmann's formula to connect the microscopic model to macroscopic properties. The multiplicity of the Einstein model can be simplified to

$$\Omega(N,q) = \binom{q+N-1}{q} = \frac{(q+N-1)!}{q!(N-1)!} \ . \tag{0.7}$$

h) Show that the multiplicity can be simplified to

$$\ln \Omega(N,q) \simeq N\left(\ln(q/N) + 1\right) \ , \tag{0.8}$$

using Stirling's approximation $\ln x! = x \ln x - x$, that $N/q \ll 1$, and that $N \gg 1$.

i) Find an expression for the entropy of the Einstein crystal.

j) Find an expression for the temperature of the Einstein crystal. Comment on the results.

Part 2: The spin system. We will now addres a different system using a similar approach. In a paramagnetic system with binary spins, each particle can be in two possible states, $S = +1$ or $S = -1$. We call such a "particle" a spin — since it is only the spin we are interested in. The energy of a single spin depends on the orientation of the spin relative to an external magnetic field B. If the spin is parallell (or antiparallell) to the external field, the energy is $E = -S\mu B$, where $S = +1$ corresponds to a spin parallell to the field and $S = -1$ corresponds to a spin antiparallell to the field.

The simplest system we can consider consists of N independent spins, S_i. (Independent here means that the spins do not interact, just like for an ideal gas or an Einstein crystal).

Unstructured problem formulation. Illustrate the spin model by simulations of random microstates. Find the multiplicity of the spin system as a function of relevant variables. Use this to find the entropy and the temperature, and comment on and illustrate the results.

Structured problem formulation. We will start by characterizing the microstates in the spin system.

k) How can you enumerate the microstates in the system and how many microstates are there in an N-spin system?

We introduce S_+ as the number of spins with value $+1$ and S_- as the number of spins with value -1. The macrostate can be described by S_+ or alternatively by $2s = S_+ - S_-$, where s is called the net spin.

l) Find an expression of the total energy E as a function of the net spin, s.

m) Generate $M = 10000$ microstates for a $N = 50$ system randomly — assuming that all microstates are equally likely — and plot the energies, E, of the system. Plot a histogram of the energies using for example `hist` in matlab.

n) Show that the multiplicity of a macrostate S_+ is

$$\Omega(N, S_+) = \frac{N!}{S_+! S_-!} \ . \tag{0.9}$$

o) Show that the multiplicity can be written as a function of the net spin, s, on the following form:

$$\Omega(N, s) = \frac{N!}{\left(\frac{N}{2} + s\right)! \left(\frac{N}{2} - s\right)!} \ , \tag{0.10}$$

p) By mapping this problem onto a problem you already know the solution to, show that the multiplicity can be written as

$$\Omega(N, s) = \Omega(N, 0) \exp(-2s^2/N) \ , \tag{0.11}$$

where $\Omega(N, 0)$ is a constant. You may assume that $N \gg 1$ and that $s \ll N$.

q) Compare your analytical result with the histogram you generated of the microstates and comment on the results.

We will now return to describing the system using the exact, and not the approximate, multiplicity.

r) Find the entropy as a function of N and S_+.

s) Find an expression for the temperature of the system.
(Hint: $\partial S/\partial U = (\partial S/\partial S_+)(\partial S_+/\partial U) = (\partial S/\partial S_+)(\partial S_+/\partial U)$.)