
Problem Sheet 3

for the lecture “Statistical Physics”, Master course “Computational Science”, year 2007/08

due date: Tuesday, November 20, 2007

Problem 1

2.5 points

A very raw model of an elastic material is the following: let’s consider a 1D chain made of N segments. Each segment can be in two different states A or B . A segment in the state A has a length l_A and energy ϵ_A , whereas it has a length l_B and energy ϵ_B when it is in the state B .

1. Find an expression that relates the energy E of the chain, and its length L .
2. Find the number of microstates $\Omega(a, b)$ available for a chain with n_A segments in the state A and n_B segments in the state B .
3. In statistical mechanics, the entropy of a system is $S \equiv k_B \ln(\Omega)$, where k_B is the Boltzmann constant. What is the entropy of the chain in terms of a and b .
4. The entropy defined in statistical mechanics is observed to agree with the thermodynamic entropy. Our system can be viewed as a thermodynamic system being at a certain temperature T , and subject to an external tension χ . The use of thermodynamic relations, leads us to the following relationship

$$T \cdot dS = dE - \chi \cdot dL \quad (1)$$

derive an expression for the tension χ in terms of ϵ_A , ϵ_B , L , a , and b .

5. Deduce the length of the chain in equilibrium L_{eq} (i.e. when $\chi = 0$).
6. Show that for small deviations of the length of the chain respect L_{eq} , it is possible to recover the famous *Hooke law*. [**hint**: expand χ with respect to L using *Taylor*].
7. What is the spring constant of the chain in the Hooke-regime?

Problem 2

2.5 points

Let’s calculate the entropy S as a function of the classic ideal gas made of N particles inside a volume V , with a total energy E ,

$$S(E) \approx N k_B \left[\ln \left(\frac{V}{N h^3} \left(\frac{4 \pi m E}{3 N} \right)^{3/2} \right) + \frac{5}{2} \right] \quad (2)$$

The previous expression can be calculated from the following Boltzmann relation

$$S(E) \approx k_B \ln \left(\frac{\Sigma(E)}{h^f N!} \right) \quad (3)$$

where f is the number of degrees of freedom ($f = 3N$ if only translations are taken into account), and $\Sigma(E)$ is the number of states with an energy smaller or equal to E , namely

$$\Sigma(E) = \int \dots \int_{\sum_i p_i^2/2m \leq E} dq_1 \dots dq_f dp_1 \dots dp_f \quad (4)$$

where q represent position coordinates, and p momentum coordinates of the phase space.

1. Derive an analytical expression for $\Sigma(E)$. Take into account that the volume of a D dimensional sphere of radius r (where $r^2 = x_1^2 + x_2^2 + \dots + x_D^2$) is

$$V_D(r) = \frac{\pi^{D/2}}{(D/2)!} r^D \quad (5)$$

2. Derive equation 2 using Stirling approximation ($N \gg 1$), and disregarding the terms of the order of $o(\ln(N))$ or smaller respect the terms of order $o(N)$.
3. Obtain an expression for the energy in terms of the entropy, V and N , i.e. $E = E(S, V, N)$.
4. Calculate the specific heat at constant volume C_V . [**hint:** use the relations, $T = \left(\frac{\partial E}{\partial S}\right)_{N,V}$, and $C_V = \left(\frac{\partial E}{\partial T}\right)_{N,V}$].
5. Calculate the pressure P of the gas through the relation $P = -\left(\frac{\partial E}{\partial V}\right)_{N,S}$. Which conclusions can you get?.
6. [**Optional Bonus:**] Proof the relation given in equation 5 by comparing the values of the integral

$$\int_{\mathbb{R}^D} \exp \left[-\sum_{i=1}^D x_i^2 \right] dx_1 \dots dx_D \quad (6)$$

in cartesian and in polar coordinate systems [**hint:** Suppose that $V_D(r) = C_D R^D$, and therefore in polar coordinates: $dV = C_D D R^{D-1} dR$; furthermore, remember that

$$\int_{-\infty}^{+\infty} e^{-x^2} dx = \pi^{1/2}$$

, and

$$\int_0^{+\infty} e^{-x^2} x^{D-1} dx = \frac{1}{2} \left(\frac{D}{2} + 1 \right)!$$

].

Problem 3

2.5 points

Consider a three dimensional lattice with $V = L \times L \times L$ sites, each of which can be either occupied by one (and only one) particle or be free. This is a simple model for a gas in a box (it is actually called “lattice gas”), in which the positional degrees of freedom are discrete, and so we can quite directly “count” the microstates.

1. Define the multiplicity function $g(V, N)$, which counts the number of ways in which you can put N particles inside the box, when it has V occupiable sites. Give an expression for $g(V, N)$.
2. The entropy of the lattice gas is $\sigma(V, N) = \ln g(V, N)$. Since V and N are going to be big, it is quite appropriate to use Stirling's approximation. What approximate expression for $\sigma(V, N)$ does this give?
3. We will soon see that the pressure of a system can be calculated once we know the entropy as a function of volume. We'll derive in the lecture the equation

$$p = T \left(\frac{\partial S}{\partial V} \right)_{T, N}$$

Using this equation, what is the pressure of the lattice gas? Write your answer also in terms of the density ρ of particles in the box, $\rho = N/V$.

4. If the density ρ is small, you can approximate the pressure which you obtained above by once more using the expansion of the logarithm $\ln(1 - x) \approx -x$. Which approximate pressure do you get? Do you recognize the equation you've just derived?

Problem 4

2.5 points

Let's revisit the spin system discussed in the lecture. An important question one might ask is the following: How does the average magnetization per spin depend on the temperature in thermal equilibrium? This is how the question can be answered:

1. Let $g(N, s)$ be the multiplicity function, which counts, in how many ways we can get a spin excess of $2s$ for N spins. By using the Gaussian approximation discussed in [Problem 1, sheet 2], show that the entropy can then approximately be written as

$$\sigma(N, s) = \sigma_0 - \frac{2s^2}{N},$$

where σ_0 is some constant that does not depend on s .

2. Rewrite $\sigma(N, s)$ as $\sigma(N, U)$, where $U = -2smB$ is the energy of the spin system, m the magnetic moment of each spin, and B the externally applied magnetic field. After making this substitution, show that when you thermally couple the spin system to a reservoir at temperature τ , the average energy is

$$U(\tau) = -\frac{Nm^2B^2}{\tau}.$$

3. Since the total magnetization M is given by $M = 2sm$, show that when the system is at temperature τ , the average magnetization per spin is given by

$$\frac{M}{N} = \frac{m^2B}{\tau}.$$

This equation is known as "Curie's law".

