
Problem Sheet 2

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

due date: Tuesday, November 13, 2007

Problem 1

2 points

The multiplicity function $g(N, s) = \binom{N}{k}$, $k = \frac{N}{2} - s$ was defined in the lecture. N characterizes the total number of particles and s the spin excess. It was claimed that for large N the Gauss (or: “normal”) distribution is a proper approximation. To proof this, do the following calculations:

1. Take the logarithm of the multiplicity function $g(N, s)$ and show that using the simple version of the Stirling approximation $\ln N! \cong N \ln N - N$ you can write it as

$$\ln \binom{N}{k} \cong -N \left[\left(\frac{k}{N} \right) \ln \left(\frac{k}{N} \right) + \left(1 - \frac{k}{N} \right) \ln \left(1 - \frac{k}{N} \right) \right]. \quad (1)$$

2. Now substitute $k = \frac{N}{2} - s$ and approximate the logarithm by using its (quadratic Taylor-) expansion $\ln(1+x) \approx x - \frac{1}{2}x^2$. Show that you will obtain

$$\binom{N}{k} \cong 2^N e^{-\frac{2s^2}{N}}$$

3. From now on we are going to treat s as a *continuous* variable ranging from $-\infty$ to $+\infty$ (i.e. $s \in \mathbb{R}$ rather than $s \in \{-\frac{N}{2}, -\frac{N}{2} + 1, \dots, \frac{N}{2}\}$). Unfortunately, this and the fact that we used the simple Stirling approximation means that $g(N, s)$ is not properly normalized. What we want is the following normalization:

$$\int_{-\infty}^{+\infty} ds g(N, s) = 2^N,$$

since 2^N is the total number of spin configurations. With what prefactor do we additionally have to multiply our $g(N, s)$ in order to satisfy this normalization?

Hint: You will need the Gaussian integral

$$\int_{-\infty}^{+\infty} dx e^{-ax^2} = \sqrt{\frac{\pi}{a}}.$$

4. The probability distribution for s is now given by $\frac{g(N, s)}{2^N}$ (where $g(N, s)$ is the *correctly normalized* multiplicity!). Compare your result with the general Gauss probability distribution with mean μ and variance σ^2 , given by

$$\mathcal{G}(x; \mu, \sigma) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}.$$

What, therefore, is in our case the mean value μ and the standard derivation σ ?

Problem 2

2 points

Let's suppose a society A in which E_A coins of 1 euro are distributed among its N_A citizens.

1. How many ways Ω_A do we have to distribute the E_A coins in this society ?
2. Let's define the following two magnitudes: the *entropy of a society* S and the *temperature of a society* T , as $S \equiv \ln(\Omega)$, and $\frac{1}{T} \equiv \left(\frac{\partial S}{\partial E}\right)_N$ respectively. Derive expressions for the entropy and the temperature of this society A. Furthermore, show that the following expression

$$E_A = \frac{N_A}{\exp(\frac{1}{T}) - 1} \quad (2)$$

holds.

3. Show that the probability of finding one member of this society having E_n coins is given by

$$P(E_n) = (1 - e^{-1/T}) e^{-E_n/T} \quad (3)$$

when $E_A, N_A \gg 1$ and $E_A, N_A \gg E_n$. [**hint:** how many ways there are of distributing $E_A - E_n$ coins between $N - 1$ citizens? Make use of eq. 2 after simplifying factorial terms in the numerator and the denominator.]

Consider now a second society B, which has E_B coins of 1 euro distributed among its N_B citizens. Suppose that we now put in contact both societies A and B, such that they can exchange coins among them.

1. Derive an expression for the equilibrium condition of this two societies, i.e., find which will be the new values of E_A and E_B after we allow the societies to be in contact for long time. Are the previously defined magnitudes T and S useful to explain the relations between both societies? Justify your answer.
2. Show that the entropy of the society AB is larger than the sum of the entropies of the societies A and B when they are isolated one from the other.

Problem 3

2 points

Given an alloy $A_{(1-x)}B_x$ consisting of a lattice with N positions occupied by $N - b$ atoms of type A, and $x \equiv b/N$ atoms of type B,

1. Calculate how many possible rearrangements $\Omega(N, b)$ of the atoms are possible in this lattice.
2. If we define the entropy as $S \equiv \ln(\Omega(N, b))$. Show that the entropy of this system is given by $S(N, b) = -(N - b) \ln(1 - b/N) - b \ln(b/N)$
3. Plot S versus x , and show for which mixture of A and B we will have a maximum value of the entropy.
4. If we put side by side two pure crystals made of A and B respectively. What do you think will happen? Justify the answer. Aside of entropy, is there any other consideration to take into account?

Problem 4

2 points

Show that the probability of finding n of the N molecules of an ideal gas in a volume V_1 when the container has a volume V ,

$$W_N(n) = \frac{N!}{n!(N-n)!} p^n (1-p)^{N-n} \quad (4)$$

where $p = V_1/V$,

1. has a maximum value for $n = \langle n \rangle = Np$.
2. can be rewritten as a Gaussian of the form

$$W_N(n) = W_N(\langle n \rangle) \exp \left[\frac{-1}{2} \frac{(n - \langle n \rangle)^2}{Np(1-p)} \right] \quad (5)$$

[**hint:** Use Stirling, and perform a Taylor-expansion up to second order of the function $\ln(W_N(n))$.]

Problem 5

2 points

For a classical ideal gas of atoms in thermal equilibrium the Cartesian components of the velocity are statistically independent. In three dimensions the probability density function is,

$$p(v_x, v_y, v_z) = (2\pi\sigma^2)^{-3/2} \exp \left[-\frac{v_x^2 + v_y^2 + v_z^2}{2\sigma^2} \right] \quad (6)$$

where $\sigma^2 = k_B T/m$. The energy of an atom is $E_i = m|\vec{v}|^2/2$. Find the probability density function $p(E_i)$ for the energy of an atom in a 3D, 2D and 1D gas. Plot schematically the three $p(E)$, and compute for the three cases the expected value $\langle E \rangle$ of the energy of an atom as a function of the temperature T of the system. [**hint:** compute first the cumulative probability function by integrating over the velocity space all cases with energy smaller or equal to E , the use of spherical coordinates is more than advisable, and then, derive from the cumulative function the density function].

