

Problem sheet 4

Please hand in your solutions before the lecture on Wednesday, 11th of November.

Problem I - Mixing Entropy

Suppose we have a box which is divided into two chambers with volumes V_1 and V_2 , which are connected by a closed door. The first chamber is filled with an ideal gas of sort A consisting of N particles with energy E .

- Write down the entropy $S_i = S_i(N, V_1, E)$ as a function of the number of particles N , the occupied volume V_1 and the energy E . (1 point)
- Now we open the door. What is the entropy change ΔS_1 , when the gas has also filled the second chamber completely? (1 point)
- Suppose the second chamber was filled with N ideal gas particles of sort B at the beginning. Calculate the entropy before and after opening the door and its change ΔS_2 . Is there any realistic situation where $\Delta S_1 > \Delta S_2$? (2 points)

Problem II - Magnetization Part II

On the last problem sheet we introduced the magnetization of a two level system. The microcanonical partition function of N spins is given by

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

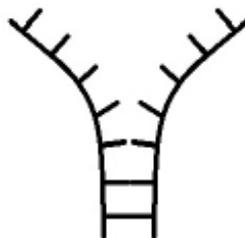
where m denotes the magnetization of the system.

- Assuming that magnetization is small ($N \gg |m|$), once again calculate the entropy $S(m)$, now using the Stirling formula $\ln(n!) \approx n \ln n - n$. (1 point)
- Calculate the temperature $T(E)$ at constant number of spins N , when we define the energy as $E = -\mu_0 B m$, with the magnetic field B . Plot $k_B T / (\mu_0 B)$ as a function of the normalized energy $E / (N \mu_0 B)$. What happens to the temperature if E approaches zero? (3 points)
Hint: You can plot $T(E)$ either with the help of a computer program of your choice or draw it by hand.
- Calculate the energy as a function of the temperature $E(T)$. (2 points)

Problem III - DNA molecule

The microstates of a double-strand molecule are defined as follows:

Each strand has B binding sites and which can only bind with the counterpart when they have the same number, meaning binding site one of strand one can only bind to binding site one of strand two and so forth. A binding can only open if all bindings with lower numbers are open. An open binding has the energy ϵ , a closed one has the energy 0.



- (a) We start a system consisting of $K = 2$ distinguishable molecules. Write down the total energy E of this system as a function of open binding sites N_1, N_2 , where the subscript denotes the molecules. Calculate the microcanonical partition sum $\Omega(E)$ as a function of the total energy $E = M\epsilon$ with $M \in \mathbb{N}$. (1 point)
- (b) Calculate the entropy $S(E)$ and the temperature $T(E)$. What is the asymptotic behaviour of T for $E \gg \epsilon$? (3 points)
- (c) Now assume we put those **two** molecules into a heat bath. Calculate the canonical partition sum as a function of the temperature T . Also, determine the mean energy $\langle E \rangle$. Hint: Use $x = e^{-\beta\epsilon}$. (3 points)
- (d) Expand the exponential function $x = e^{-\beta\epsilon}$ up to first order for $\beta\epsilon \ll 1$ in your result for $\langle E \rangle$. What relation between $\langle E(T) \rangle$ and T do you obtain for $k_B T \gg \epsilon$? (2 points)
- (e) We now add one molecule to the system. For this system of $K = 3$ molecules, repeat your calculation of the asymptotic behaviour for $T(E)$ for $E \gg \epsilon$ in the microcanonical ensemble and the $\langle E(T) \rangle$ for $k_B T \gg \epsilon$ in the canonical ensemble. (9 points)
- (f) Now compare the relations you obtained for both systems in the microcanonical and canonical ensemble. How do they change by adding one molecule? What do you assume would happen to the differences between the microcanonical and the canonical if we now consider a system of large number ($K \gg 1$) of such molecules? How is this limiting case called? (2 points)