Statistical Physics I
WS 2015/16, FUB

Problem sheet 7

Please hand in your solutions before the lecture on Wednesday, 2th of December.

Problem I - Ising Modell

Consider a system of N Spins which can take the values $\sigma_i = \pm 1$. Further assume that those spins are arranged on a periodic chain, i.e., $\sigma_{N+1} = \sigma_1$. The Hamiltonian of the system $\boldsymbol{\sigma}$ is given by

$$H(\boldsymbol{\sigma}) = -J \sum_{i=1}^{N} \sigma_i \sigma_{i+1} - \mu_0 B \sum_{i=1}^{N} \sigma_i \, ,$$

with a coupling constant J and the an external magnetic field B.

(a) Write down the canonical partition sum of the system. Show that this partition sum can be written as

$$Z = \sum_{\sigma_1=\pm 1} \cdots \sum_{\sigma_N=\pm 1} T(\sigma_1, \sigma_2) T(\sigma_2, \sigma_3) \ldots T(\sigma_N, \sigma_1) = \sum_{\{\boldsymbol{\sigma}\}} \prod_{i=1}^{N} T(\sigma_i, \sigma_{i+1}) \, ,$$

where $T(\sigma_i, \sigma_{i+1})$ is a function which is symmetric in its arguments. *(1 point)*

(b) We now transform the function $T(\sigma_i, \sigma_{i+1})$ into a matrix $\mathbb{T}$ which is independent of σ_i and σ_{i+1}. Show that with this matrix the partition function can then be rewritten as $Z = \mathrm{Tr}\left(\mathbb{T}^N\right)$. Give an explicit expression of the transfer matrix $\mathbb{T}$.
Hint: Introduce two orthogonal vectors $|\sigma_i = 1\rangle$ and $|\sigma_i = -1\rangle$ and transform the matrix $\mathbb{T}$ into the function T by using $|\sigma_i\rangle$ and $|\sigma_{i+1}\rangle$.
(3 point)

(c) Use a invariance proberty of the trace and an appropriate transformation of $\mathbb{T}$ to show that the partition sum can now be calculated explicitly and has the form $Z = \lambda_1^N + \lambda_2^N$. Determine λ_1 and λ_2. *(3 points)*

(d) Now we apply the thermodynamic limit. Neglect all terms of the form x^N with $x < 1$ to calculate the free energy.
Result: $A = -NJ - Nk_BT \ln\left(\cosh(\beta\mu_0 B) + \sqrt{\sinh^2(\beta\mu_0 B) + \mathrm{e}^{-4\beta J}}\right)$
(2 points)

(e) We begin with the case without any external magnetic field B. Calculate the entropy S and the heat capacity C. What happens to the entropy if $T = 0$?. What is the asymptotic behavior of the heat capacity for $k_BT \ll J$ and $k_BT \gg J$. *(5 points)*

(f) In case of a non-vanishing magnetic field, calculate the free energy for $T \to 0$ and $J > 0$. Which quantities control the alignment of the spins in this case? *(2 points)*

(g) Calculate the free energy for $T \to 0$ and $J < 0$ with $|J| > \mu_0 B/2$. Which quantities control the alignment of the spins now? *(2 points)*

(h) Calculate the free energy for $k_BT \gg |J|$ (zeroth order). Which system does your result resemble then? *(2 points)*

Problem II - Gas-Solid Interface

Consider non-interacting molecules coexisting in gas-solid phases (N_g gas molecules in $V_g \approx V$, and N_s solid molecules in V_s) in a three dimensional system. Molecules in the solid phase can sublime into the gas phase and gas molecules can resublime onto the solid.

(a) Express $\langle N_g \rangle$ in terms of z_g and z_s. Here, z_g and z_s are single-molecule canonical partition functions for the gas and solid phases, respectively. Assume the thermodynamic limit and that gas molecules are indistinguishable while solid molecules are distinguishable. Further assume that $\mu_s < -k_B T \ln z_s$ and chemical equilibrium.
Hint: Show that in the thermodynamic limit you obtain a relation between z_s and $\beta\mu_s$ independent of $\langle N_s \rangle$. *(4 points)*

(b) Assuming that the gas is an ideal gas and the solid is a harmonic oscillator with frequency ω, calculate the density of gas molecules $\rho = \langle N_g \rangle / V$. At 273 K the density of an ideal gas is approximately $2.69 \cdot 10^{25}$ m^{-3} and assume we are dealing with helium atoms, what would be the wavelength of the photons oscillations in the solid neglecting quantum effects? *(3 points)*

Summary Statistical physics

For each of the four ensembles you have been introduced to in the lecture, give the 3 quantities that are defining the ensemble. Also, write down the most general form of the partition function for those ensembles. Finally, for each ensemble give a physically motivated example where those should be used. Be creative! ;) *(3 points)*