

Assignment 6

Handout 11.12.2020 – Return 17./18.12.2020 – Discussion 14./15.01.2020

Exercise 6.1 [4 points]: Entropic polymer elasticity: canonical ensemble

In the lecture, the force-length relation of a 1D polymer was calculated using the microcanonical ensemble.

1. Now do the calculation in the canonical ensemble. (2 points)

HINT: Consider again a chain of N monomers of size a with $x_i = +a$ or $-a$ and $X = \sum_i x_i$ the total length of the polymer (for the given configuration). Note that the polymer is “ideal”, i.e. the distribution of bonds does not change the energy of the chain in the force free case; in turn, under an external force F the energy of this system is given by $E = -FX$.

2. Show that your result is identical to the one in the lecture. Discuss the limits $Fa \ll k_B T$ and $Fa \gg k_B T$. (2 points)

Exercise 6.2 [8 points]: Debye model

Consider the Debye model for the specific heat of a crystal as discussed in the lecture.

1. *Corrections to classical limit:* In the lecture it was shown that the Debye model yields $E = 3Nk_B T$ in the classical limit as expected. Calculate the first two corrections from a Taylor expansion in T_D/T of the integrand of the energy formula and discuss the resulting heat capacity. (4 points)
2. *Number of phonons:* Write the mean number of phonons $\langle N \rangle$ in the Debye-model as an integral (similar but different to the integral formula for the energy) and evaluate it for low and high temperatures. (4 points)

Exercise 6.3 [3 points]: Molecular zipper

Consider a zipper consisting of N units. Each unit can either be in the closed state with energy 0 or in the open state with energy $\epsilon > 0$. The zipper can open only from the left, that is, a given unit can only switch to the open state, when all units to its left are already open.

1. Calculate the canonical partition sum. (1 point)
2. Determine the average number of open units. Discuss the limit $\beta\epsilon \gg 1$. (2 points)