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Thermische Fysica 2 (NS-335B)
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Opgave 1. Energy, entropy and free energy

Consider a linear lattice of 5 sites, on which 0, 1, 2 or 3 particles are located. The size of the particles prevents two oi them to occupy neighboring sites. Consequently, the phase space of this system consists of 13 states.
To each state, we now assign an energy given by the hamiltonian

$$H = \mu N,$$

where N is the number of particles and μ is the chemical potential.

a) Draw the ground state for $\mu > 0$ and $\mu < 0$.

b) Determine the entropy of the ground state if $\mu = 0$.

c) Determine the expectation value for the number of particles, $\langle N \rangle$, as well as the expectation value of the squared number of particles, in the limit of high temperature (i.e., $\beta\mu \approx 0$).

d) Use linear response to predict how the expected number of particles in the system reacts to the introduction of a small chemical potential, at high temperatures.

Opgave 2. Polymers

Consider a polymer in two dimensions, which is modeled as a string of N segments, each with length l. The positions of the ends of the segments are $\vec{x}_i$, with $i = 0, \ldots, N$; here, $\vec{x}_i$ and $\vec{x}_N$ are the ends of the polymers, and the remaing positions are the points where two segments are connected: $\vec{x}_i$ is the location where segments i and $i + 1$ are connected.

a) Compute the expectation value of the squared end-to-end length:

$$R_{ee}^2 \equiv \langle |\vec{x}_N - \vec{x}_0|^2 \rangle,$$

as a function of N and l, assuming that the orientation of connected seg- ments is arbitrary.
At the 'hinges', we now introduce a harmonic potential which favors two connected segments to take the same orientation:

$$E = -\frac{\epsilon}{l^2} \sum_{i=1}^{N-1} \vec{\sigma}_i \cdot \vec{\sigma}_{i-1}.$$

b) Determine the ground-state energy of the polymer.

c) At low temperatures, the angle θ between connected segments will be small. Show that in that case, this angle θ is drawn from a gaussian distribu- tion with a standard deviation characterized by $\sqrt{\langle \theta^2 \rangle} = \sqrt{\frac{A}{\beta\epsilon}}$; and determine the prefactor A.

d) The expectation value for the correlation in orientation between segments i and $i + j$ can be written as

$$\langle \vec{x}_i \cdot \vec{x}_{i+j} \rangle \approx l^2 \exp -jB$$

Determine B. Here you can use the approximations

$$\langle \cos\theta \rangle \approx \langle 1 - \theta/2 \rangle = 1 - \langle \theta^2 \rangle/2 \approx \exp -\langle \theta \rangle/2$$

e) Compute the expectation value of the squared end-to-end length, based on the result presented in d). here you can make the approximation that g the polymer is long $N \gg 1/B$.