Physics 6311: Statistical Mechanics - Homework 6

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due date: Tuesday, October 3, 2023

Problem 1: Quantum harmonic oscillator (10 points)

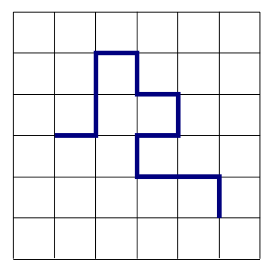
Consider a quantum harmonic oscillator given by the Hamilton operator

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m}{2}\omega^2 \hat{x}^2$$

where m is the mass and ω is the oscillator frequency. The oscillator is in contact with a heat bath at temperature T.

a) Using the canonical ensemble, compute the partition function of the oscillator.
b) Find the average energy and the specific heat as functions of temperature. Compare with the results of the classical oscillator discussed in class.
c) Find the entropy and show that it fulfills the third law of thermodynamics.

Problem 2: Polymer on a lattice (10 points)



A polymer can be modeled as a path of $N+1$ identical segments on a square lattice (see picture). At each of the N joints (lattice sites), the polymer can either go straight, or it can bend by 90 degrees left or right. (Different segments do not interact with each other, i.e., the path can intersect itself.) A straight joint has zero energy while a right-angle joint has energy ϵ. Assume that one end of the polymer is fixed at the origin of the coordinate system.

a) Using the canonical ensemble, find the partition function and the Helmholtz free energy of this polymer as functions of temperature T and the number of joints N.
b) Calculate the internal energy of the polymer and its specific heat.
c) Find the average number N_{st} of straight joints as a function of temperature T and the total number of joints N.
d) How does N_{st} behave for $T \to 0$ and $T \to \infty$?

Problem 3: Two interacting magnetic moments (10 points)

Consider two classical magnetic moments represented by three-dimensional unit vectors $\mathbf{S}_1$ and $\mathbf{S}_2$. They interact via an exchange interaction with the Hamiltonian $H = -J\ \mathbf{S}_1 \cdot \mathbf{S}_2$ where J is a positive constant.

a) In the ground state, what do you expect the relative orientation of the two moments to be?

b) Use the canonical ensemble to calculate the partition function and the Helmholtz free energy.

c) Determine average energy and heat capacity as functions of temperature.

d) At low temperatures, what is the average angle between the moments, and what is its standard deviation?

Problem 4: Model of DNA (10 points)

A simple model of the DNA double helix molecule is analogous to a zipper: a chain of N links each of which can be open or closed. A closed link has energy ϵ_0, and an open link has energy $\epsilon_1 > \epsilon_0$. Replication of the DNA starts with the opening of the "zipper". Assume that it can only open from one end (say the left), i.e., a link can only be open if all links left of it are also open.

a) Calculate the partition function for this DNA model.

b) Find the average number of open links n as a function of N and temperature T .

c) Discuss the behavior of n in the limits of high and low temperatures.