

Physics 6311: Test Prep Homework 7

due date: Tuesday, March 12, 2018

Problem 1: Three-dimensional rotor (8 points)

A random rotor $\vec{S} = (\sin \Theta \cos \phi, \sin \Theta \sin \phi, \cos \Theta)$ is a three-dimensional unit vector pointing in a random direction. The probability density of the usual Euler angles Θ and ϕ reads

$$P_{\Theta, \phi}(\Theta, \phi) = \begin{cases} \sin(\Theta)/(4\pi) & 0 \leq \Theta < \pi, 0 \leq \phi < 2\pi \\ 0 & \text{otherwise} \end{cases}.$$

- Calculate the averages of $\langle S_x \rangle$, $\langle S_y \rangle$, and $\langle S_z \rangle$ of the rotor components.
- Compute the second moment and the variance of S_z .
- Find the probability density $P_{S_z}(S_z)$ of the z component of the rotor.

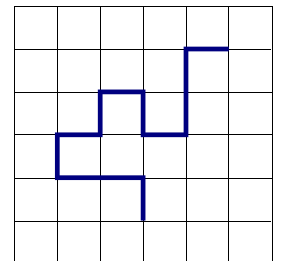
Problem 2: Schottky peak in two-level system (8 points)

Consider a system with two energy levels ϵ_1 and ϵ_2 . The system is in contact with a heat bath a temperature T .

- Calculate the partition and the average energy.
- Calculate the heat capacity and discuss its behavior for $T \rightarrow 0$ and $T \rightarrow \infty$.
- Calculate at what temperature T_S the heat capacity is maximum. This peak in the heat capacity is called the Schottky peak.

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.



- 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 .
- 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 $T \rightarrow 0$ and $T \rightarrow \infty$?

Problem 4: Adsorbed atoms in equilibrium with ideal gas (14 points)

- a) Consider a classical ideal gas of $N \gg 1$ atoms (mass m) in a volume V . Use the canonical ensemble to calculate its chemical potential μ_{gas} as a function of temperature T and particle number density N/V .
- b) Rewrite μ_{gas} as a function of pressure and temperature.
- c) Now consider a single adsorption site on a solid surface. It can either be empty (energy 0) or occupied by a gas atom (energy $-\epsilon$ with $\epsilon > 0$). Use the grand-canonical ensemble to calculate the grand partition function of the adsorption site as a function of temperature T and chemical potential μ_{sf} .
- d) Calculate the average number of atoms on the adsorption site as a function of temperature T , and chemical potential μ_{sf} .
- e) The gas and surface are brought into thermal and chemical equilibrium. Find the average number of atoms on the adsorption site as a function of the pressure of the ideal gas and the temperature. Discuss the limits of vanishing and infinite pressure. (Hint: In chemical equilibrium the chemical potentials of the adsorbed atoms and the gas atoms are equal.)