Course on "Advanced Statistical Physics"
Spring Semester (2016)
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Homework #5: Canonical and Grand Canonical Ensembles Due: May 2, 2016

Note: *References from which some of the following problems have been taken are available upon request.*

1: Consider an ideal classical diatomic gas whose molecules have an electric dipole moment $\boldsymbol{\mu}$. The system is contained in a box of volume V, with a uniform applied electric field $\mathbf{E}$. Ignoring interactions between molecules,

(i) find the electric polarization $\mathbf{P}$ as a function of temperature (T),

(ii) plot the polarization function as a function of $\boldsymbol{\mu}\cdot\mathbf{E}/k_BT$. Interpret the behavior shown by the plot.

(iii) Finally calculate the dielectric constant of the gas in the low-field limit $\boldsymbol{\mu}\cdot\mathbf{E} \ll k_BT$.

2: The potential energy between the atoms of a hydrogen molecule can be modelled by means of the Morse potential

$$V(r) = V_0\left[e^{-2(r-r_0)/a} - 2e^{-(r-r_0)/a}\right] \tag{1}$$

where $V_0 = 7\times10^{12}$ erg, $r_0 = 8\times10^{-9}$ cm and $a = 5\times10^{-9}$ cm. Using the results from quantum mechanics for energy levels of a rigid rotor and also for an oscillator:

(i) Find the lowest angular frequency of rotational motion and the frequency of small-amplitude vibrations.

(ii) Estimate the temperatures T_{rot} and T_{vib} at which rotations and vibrations respectively begin to contribute significantly to the internal energy. Which one is higher and why?

3: Consider a system of identical but distinguishable particles, each of which has two states, with energies ε and $-\varepsilon$ available to it. Use the microcanonical, canonical and grand canonical ensembles to calculate the mean entropy per particle as a function of the mean energy per particle in the limit of a very large system. Verify that all three ensembles yield identical results in this limit.

4: *Electron trapping in a solid.* Consider a solid with A identical and independent sites each of which is capable of trapping at most one electron. We use for the magnetic moment of the electrons an Ising spin model: the electron spin magnetic moment can only take the two values $\boldsymbol{\mu} = \pm\tilde{\mu}\hat{z}$ corresponding to the two states($\pm$). In the presence of an external magnetic field $\mathbf{B} = B\hat{z}$, the energy of a trapped electron depends on the orientation of the magnetic moment:

$$\varepsilon_\pm = -u_0 \pm \tilde{\mu}B \tag{2}$$

in which u_0 is the rest of the energy of a trapped electron independent of spin.

(i) Consider first the case where the number of trapped electrons is fixed at N ($N \le A$). Calculate $Z_N(T, A)$, the partition function of the system of N trapped electrons. Calculate E, the average energy of the system, and $\overline{N}_+$, the average number of electrons with a magnetic moment in the state (+) state.

(ii) Calculate the chemical potential μ_e of the trapped electrons. Give the expression for N in terms of μ_e.

(iii) We now consider the grand canonical case. We assume the solid is in equilibrium with a gas of electrons that we consider to be ideal and classical. This imposes a chemical potential μ_e. Calculate the grand partition function of the system $Q(T, A, \mu_e)$,

(a) by using the partition function Z_N explicitly,

(b) by first calculating the grand partition function of a single trap $\xi(T, A, \mu)$.

(iv) Use ξ to calculate the probabilities p_+ and p_- for a trap to be occupied by an electron with a magnetic moment parallel and antiparallel to B. Find the expressions for $\overline{N}_+$, $\overline{N}_-$ and N. Verify that the expressions for E obtained in the canonical and grand canonical ensembles are identical if we take $N = \overline{N}$.

5: A one-dimensional lattice consists of $N+1$ equally spaced Ising spins (Fig. 1) coupled by nearest-neighbor exchange interactions. The Hamiltonian of the system is

$$H = -J\sum_{j=1}^{N} S_j S_{j+1} \tag{3}$$

Figure 1. See Problem 5.

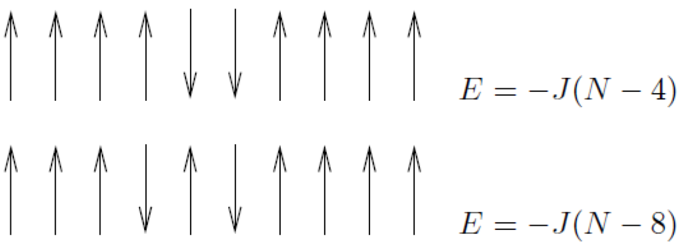

Figure 2. Two configurations with the same number of flipped spins but with different energies.

where J is a positive constant. We can see from Fig. 2 that, in this problem, flipping two neighboring spins and flipping two distant spins generates configurations with different energies. The energy of a configuration is determined by the number of nearest-neighbor pairs of antiparallel spins, called kinks. To obtain an elementary kink, one flips all spins to the left (or right) of a chosen site (Fig. 3).

(i) Prove that a configuration with m kinks has the energy:

$$E_m = -NJ + 2mJ \tag{4}$$

(ii) Represent schematically the configurations corresponding respectively to the states of minimum and maximum energy E_{min} and E_{max}. Give the number of kinks and the degeneracies associated with these two states.

We fix the number of kinks to $m = n$ and, therefore, the energy is fixed at $E = E_n$.

(iii) Calculate Ω_n, the number of states with n kinks and find the expression for the corresponding entropy $S(n, N)$ assuming n, $N \gg 1$. Calculate the equilibrium temperature $\beta = 1/k_BT$ as a function of n and N.

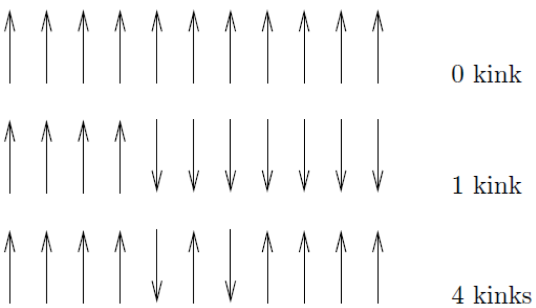

Figure 3. See Problem 5.

Verify that it can also be written as:

$$\beta = -\frac{1}{J} \tanh^{-1}\left(\frac{E}{NJ}\right) \tag{5}$$

It seems natural to associate high temperature with high energy. Is this confirmed for this spin lattice? If no, why?

(iv) Calculate the probability p that two neighboring spins are antiparallel.

We now consider the problem in the canonical ensemble. The temperature is fixed but the energy is known only on average.

(v) Compare the changes in the entropy and energy when the system goes from no kinks to one kink. Verify that, for $T = 0$, there is no spontaneous magnetization in this one-dimensional system.

(vi) Show that the partition function of the one-dimensional Ising model may be written as:

$$Z = 2^{(N+1)} \left(\cosh \beta J\right)^{N} \tag{6}$$

Can one make an analogy with paramagnetism and explain why the solution of the one-dimensional Ising model is trivial?