PHY-602: Statistical Physics, UMass Amherst, Problem Set #10

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Due: Wednesday, Nov 29. (Late homework receives 50% credit.)

I. PHASE TRANSITION IN DNA ZIPPER MODEL

Consider a simplified theory for the unwinding of two-stranded DNA molecules models the system as a zipper that has N links, each of which has two states: closed (energy 0) and open (energy $\epsilon > 0$). The DNA molecule ("zipper") can only unzip from its left end, and link s can only open if all the links to the left of it are already open. We already encountered this model, but we will now suppose that there are g orientations which each open link can assume (with g a positive integer). In other words, the open state of a link is g-fold degenerate, corresponding to the rotational freedom of a link.

1. What is the free energy of such a zipper with N links in contact with a thermal reservoir at temperature T?
2. Find the average ratio of open links in the limit $N \to \infty$. Show that for $g > 1$, the system undergoes a first order phase transition at a temperature that you will identify.

II. ONE-DIMENSIONAL SPIN-1 ISING MODEL

Write down the transfer matrix $\mathbf{T}$ for a one-dimensional spin-1 Ising model in zero field and periodic boundary conditions, described by the energy function ("Hamiltonian")

$$\mathcal{H}(\{S_i\}) = -J \sum_i S_i S_{i+1},$$

with $S_i = -1,0,+1$ and $J > 0$. Deduce the exact expression of the free energy in the thermodynamic limit, and compute its low- and high-temperature limits.

III. ISING MODEL ON A COMPLETE GRAPH

Consider an Ising model with infinite range interactions: each spin interacts with the same strength with all the other spins in the lattice with N sites. The Hamiltonian reads

$$\mathcal{H} = -\frac{J}{2N} \sum_{i,j=1}^{N} S_i S_j - h \sum_{i=1}^{N} S_i,$$

with $S_i = \pm 1$ and where the i,j sums run over all spins. The factor of N is front of the interaction term is chosen to get a sensible thermodynamic limit.

1. Show that $\mathcal{H}$ can be expressed in terms of the total spin $S = \sum_i S_i$ only.
2. Show the identity

$$e^{\frac{\beta J}{2N} S^2} = \sqrt{\frac{N\beta J}{2\pi}} \int_{-\infty}^{\infty} dm e^{-\frac{N\beta J}{2} m^2 + \beta J S m},$$

   and use it to perform the sum over the spins $\sum_{\{S_i\}}$ in the partition function. Express the partition function as

$$Z = \sqrt{\frac{N\beta J}{2\pi}} \int_{-\infty}^{\infty} dm e^{-N\beta f(m)} \text{ with } f(m) = \frac{Jm^2}{2} - k_B T \ln(2\cosh[\beta(Jm+h)]).$$

3. Deduce the free energy per spin and the mean magnetization per spin $\langle s \rangle$ in the thermodynamic limit $N \to \infty$. Compare with the mean-field solution of the Ising model discussed in class.

Note: the trick used in question 2 is a powerful formal technique known as the Hubbard-Stratonovich transformation. It is very useful in statistical mechanics, condensed matter physics, and quantum field theory.