Physics 504: Statistical Mechanics
Department of Physics, UIUC
Spring Semester 2013
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Problem Set No. 6:
Phase Transitions
Due Date: April 28, 2013

1 The One-Dimensional Classical Ising Model

Consider a classical Ising model of a magnetic a chain of N sites and that there is an Ising degree of freedom $\sigma_n = \pm 1$ on each site $n = 1, \ldots, N$. We will assume that the chain is closed into a ring, *i.e.* that the $N+1$st site coincides with the 1st site. We will further assume that the energy of a configuration $E[\sigma]$ of this magnet involves only interactions among nearest-neighboring sites

$$E[\sigma] = -J \sum_{n=1}^{N} \sigma_n \sigma_{n+1} - H \sum_{n=1}^{N} \sigma_n$$

where J is the exchange interaction and H is the external magnetic field. We will assume that $J > 0$ (ferromagnetic).

1. Show that the partition function of this Ising chain (with periodic boundary conditions) is equal to the trace of the Nth power a 2×2 transfer matrix $\mathcal{T}$
$$Z = \text{tr}\ \mathcal{T}^N$$
Find an explicit expression of the matrix elements of the transfer matrix in terms of the exchange interaction J, the magnetic field H and the temperature T.

2. Find an explicit expression of the two eigenvalues $t_\pm$ of the transfer matrix in terms of the exchange interaction J, the magnetic field H and the temperature T.

3. Find an explicit expression for the free energy $F_N(T, J, H)$ for a chain of N sites as a function of the exchange interaction J, the magnetic field H and the temperature T.

4. Find the expression of the free energy *in the thermodynamic limit*, $F_\infty = \lim_{N\to\infty} F_N(T, J, H)$. Which eigenvalue of the transfer matrix determines the expression of the free energy in the thermodynamic limit? Show that in the thermodynamic limit the free energy is *extensive* and determine its

explicit form as a function of T, J and H. Show that, in the thermodynamic limit and in the limit $H \to 0$, the free energy is continuous and at least twice differentiable function of T for all $T > 0$ and that, as a consequence, that the classical Ising chain does not have any finite temperature phase transition.

5. Use the thermodynamic free energy $F_\infty(T, J, H)$ to find explicit expressions for

   (a) The local magnetization $m(T, J, H)$
   (b) The magnetic susceptibility $\chi(T, J, H)$
   (c) The entropy $S(T, J, H)$
   (d) The specific heat $c(T, J, H)$

   Determine the behavior of all four thermodynamic quantities as functions of T, J and H, in the limits of a) low tempertature and b) high temperature. (Low and high relative to what?). Discuss in particular the behavior of the magnetization in the limits $H \to 0$ and $T \to 0$.

2 Mean-Field Theory

In this problem we will consider a variant of the Ising model within the mean field approximation. Let us consider an *antiferromagnetic* 2D Ising model on a square lattice with N sites in the presence of an *uniform* magnetic field h. Since the square lattice is *bipartite* we will denote by $[\mathbf{r}_A]$ the sites on the A sublattice and by $[\mathbf{r}_B]$ the sites of the B sublattice. That the lattice is bipartite means that the four nearest-neighboring sites of every site of the A sublattice belong to the B sublattice (and vice versa). Upon flipping the spins on one sublattice (say B) this problem is the same as an Ising *ferromagnet* in a *staggered* magnetic field (which takes opposite values on the sites of the two sublattices). The Hamiltonian of a configuration $[\sigma]$ now is

$$H[\sigma] = -J \sum_{\langle \mathbf{r}_A, \mathbf{r}_B \rangle} \sigma(\mathbf{r}_A)\sigma(\mathbf{r}_B) - h \sum_{\mathbf{r}_A} \sigma(\mathbf{r}_A) + h \sum_{\mathbf{r}_B} \sigma(\mathbf{r}_B)$$

where $J > 0$ and $H > 0$, and $\langle \mathbf{r}_A, \mathbf{r}_B \rangle$ denotes nearest-neighboring sites.

You will examine this problem using the *variational* principle discussed in class. Let us denote by H_0 the Hamiltonian of our variational ansatz. The variational principle states that the free energy F of the exact problem has the upper bound $\widetilde{F}$

$$F \le \widetilde{F} = F_0 + \langle H - H_0 \rangle_0$$

where F_0 is the free energy for the Gibbs ensemble of H_0, and $\langle \mathcal{O} \rangle_0$ denotes the expectation value of the observable $\mathcal{O}$ in the Gibbs ensemble of H_0. Since we have a problem in with two sublattices we will use the following mean-field H_0

$$H_0 = -h_A \sum_{\mathbf{r}_A} \sigma(\mathbf{r}_A) - h_B \sum_{\mathbf{r}_B} \sigma(\mathbf{r}_B)$$

where h_A and h_B are two variational parameters.

1. Show that the magnetic field h does not break the $\mathbb{Z}_2$ symmetry of flipping all spins simultaneously.

2. Consider the full Hamiltonian H at zero temperature. Show that there is a ground state phase transition as a function of the magnetic field h from the antiferromagnetic state (which in the language of the Hamiltonian H is the uniform state) to a ferromagnetic configuration (which in the language of the Hamiltonian H is a staggered configuration). Find the value of the critical field h_c at which this phase transition at $T = 0$ takes place. In the following sections you will study the extension of this phase transition for $T > 0$ using mean-field theory.

3. Show that the variational free energy $\widetilde{F}$ has the following expression

$$\begin{aligned}\widetilde{F} = & F_0(\beta h_A, \beta h_B) - 4NJ\langle\sigma_A\rangle_0\langle\sigma_B\rangle_0 \\ & - \frac{1}{2}Nh\Big(\langle\sigma_A\rangle_0 - \langle\sigma_B\rangle_0\Big) + \frac{1}{2}N\Big(h_A\langle\sigma_A\rangle_0 + \langle\sigma_B\rangle_0\Big)\end{aligned}$$

   where $\beta = 1/(kT)$. Here

$$\langle\sigma_A\rangle_0 \equiv m_A = m + n, \quad \langle\sigma_B\rangle_0 \equiv m_B = m - n$$

   are the magnetizations of the two sublattices in the Gibbs ensemble of H_0. We will identify m with the order parameter of this phase transition.

4. Show that the mean-field equations for the variational parameters h_A and h_B for this problem, obtained by requiring that $\widetilde{F}$ be as small as possible, are

$$\begin{aligned} m_A &= \tanh(\beta h - 4\beta J m_B)) \\ m_B &= \tanh(-\beta h + 4\beta J m_A) \end{aligned}$$

5. Use the mean field equations of the preceding section to show that there is a continuous phase transition from a state with $m = 0$ to a state with $m \neq 0$. Find the an expression for the phase boundary $H_c(T_c)$ where the antiferromagnetic order parameter m first appears.

6. Expand the free energy $\widetilde{F}$ in powers of the order parameter m of the form

$$\widetilde{F} = A + Bm^2 + Cm^4 + O(m^6)$$

   and find explicit expressions for the coefficients A, B and C as functions of n, T and h. Show that the coefficient B of the quadratic term in this expansion changes sign along the phase boundary of the previous section.