Statistical Mechanics 2011–12 — Problem Set 6

due: February 2, 2012

6.1 Spin 1 Ising model

(a) Consider the mean-field Hamiltonian of a spin 1 Ising model

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

where $S_i = 0, \pm 1$. Calculate the partition function and the free energy using the Hubbard-Stratonovich transformation. Find the equation for the magnetization per spin $m \equiv \langle S_i \rangle$ and the critical temperature T_c for the ferromagnetic phase transition when $H = 0$.

(b) Find the critical exponents β and γ and compare with those of the regular (spin $1/2$) mean field Ising model. Reminder: these exponents are defined by

$$|m| \propto (-t)^{\beta} \quad \text{for} \quad T < T_c \tag{2}$$

and

$$\chi_0 \propto t^{-\gamma} \quad \text{for} \quad T > T_c. \tag{3}$$

Here, $t \equiv (T - T_c)/T_c \ll 1$ and $\chi_0 = \frac{\partial m}{\partial H}\big|_{H\to 0}$.

(c) Now consider a one-dimensional system. The Hamiltonian for the one-dimensional spin 1 chain with periodic boundary conditions and zero external field is

$$\mathcal{H} = -J\sum_{i=1}^{N} S_i S_{i+1}, \tag{4}$$

where $S_{N+1} = S_1$. Write down the transfer matrix $T_{S,S'}$ explicitly and diagonalize it. Obtain the expression for the free energy per site and show that there is no phase transition at any finite temperature. Hint: the eigenvectors of T may be guessed from the symmetry properties of the matrix.

(d) Use the transfer matrix to calculate the correlation length ξ associated with the correlation function $\langle S_i S_{i+j} \rangle$. How does ξ behave in the limit of zero temperature $T \to 0$?

6.2 An anisotropic XY model

A system of magnetic moments in d-dimensions is described by the Hamiltonian

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j \tag{5}$$

where each spin $\vec{S}_i$ can take one of the following 4 values:

$$(1, 0) \quad , \quad (-1, 0) \quad , \quad (0, 1) \quad , \quad (0, -1). \tag{6}$$

(a) Derive an equation for the average magnetization $\vec{m} = \langle \vec{S}_i \rangle$ within the mean-field approximation and discuss the solution: Is there a phase transition at a finite temperature? What is the nature of the phases below and above the transition?

(b) Show that for small $\vec{m}$ the solution to the above equation is obtained as a minimum of a Landau free energy of the form

$$\Phi = A|\vec{m}|^2 + B|\vec{m}|^4 + C(m_x^4 + m_y^4) + \dots \tag{7}$$

Express the coefficients A, B, C as functions of the temperature and J.

(c) In case there is a transition, find the transition temperature and the order parameter (magnitude and direction) near the transition.

(d) Calculate the zero-field susceptibility tensor $\chi_{ij} = \frac{\partial m_i}{\partial H_j}$ for $T > T_c$.

6.3 Scaling and critical exponents

Assuming that the singular part of the free energy $f(T, H)$ is a generalized homogeneous function in the limit $(T - T_c)/T_c \to 0$, $H \to 0$,

(a) show that the critical exponents obey the scaling relation

$$\gamma = \beta(\delta - 1). \tag{8}$$

(b) Define the critical exponent φ as the one controlling the behavior of the specific heat C_H of a magnet as a function of H in the $H \to 0$ limit at $T = T_c$:

$$C_H \sim H^{-\varphi} \sim M^{-\varphi\delta} \qquad (T = T_C). \tag{9}$$

Use the scaling hypothesis to show that

$$\varphi\beta\delta = \alpha. \tag{10}$$

6.4 Ginzburg criterion and upper critical dimension

Consider a magnetic system whose Landau free energy has the form

$$F[m] = \int d^d x \Big[\frac{\gamma}{2} (\nabla m)^2 + atm^2 + um^n - Hm \Big]. \tag{11}$$

Use the Ginzburg criterion to find the upper critical dimension of this system.

6.5 Bonus question (optional): Monte Carlo study of the 2-d Ising model

This question will explore the two-dimensional Ising model using the Metropolis Monte Carlo algorithm. The Hamiltonian of the system is given by

$$\mathcal{H} = -J \sum_{\langle ij \rangle} S_i S_j - H \sum_i S_i, \tag{12}$$

where $S_i = \pm 1$. We will consider the case of zeros external field, i.e., $H = 0$. The lattice has $N = L^2$ sites, where L is its linear size, and periodic boundary conditions. For this model, the exact critical temperature (in the limit $L \to \infty$) is known to be $k_B T_c = 2J/\ln(1+\sqrt{2}) \approx 2.27J$.

The goal of this question is to estimate numerically the mean magnetization and to study how the configuration of spins typically looks like at different temperatures. With most programming languages it should be possible to carry out the Metropolis algorithm estimation for systems of size $L = 100 \sim 200$. If you only know how to program in Matlab, see instructions below.

(a) Implement the Metropolis algorithm and use it to simulate the two dimensional Ising model at several temperatures above and below T_c. Evaluate the equilibration time τ_{eq} at a few temperatures. After the systems has equilibrated, collect sufficient statistics and calculate the mean magnitude of the magnetization per site, $m(T) \equiv \frac{1}{N} \sum_i \langle |S_i| \rangle$, as a function of the temperature. Repeat the measurement for several different system sizes (e.g., $L = 25, 50, 100, 200$), and plot the results in a single figure. Note that the equilibration time τ_{eq} increases sharply close to T_c.

(b) For your largest system size, plot a representative equilibrium configuration of the lattice for a few different temperatures around the critical temperature, (e.g., $T = 2.1, 2.2, 2.3, 2.4, 2.5$). Observe that close to T_c there are correlations nearly at all length scales (no need to do any calculations).

Please attach your code to your answer.

If you can only program in Matlab: Write your own Matlab code for the simulations of this question and carry out the simulations for a system of size $L = 5$. In addition, a C++ program compiled for use in Matlab will be available on the course tutorials website. Use this program to repeat the question for systems of larger sizes. Instructions on the use of the this program will be posted on the website.