Statistical Mechanics 2012/2013 Problem Set 4

Submission date: 31.12.12

1.1 Ising anti-ferromagnet (26 points)

Consider the nearest-neighbor anti-ferromagnet with the Hamiltonian

$$\mathcal{H} = J \sum_{\langle i,j \rangle} S_i S_j - H \sum_i S_i \ , \tag{1}$$

where $J > 0$, and $S_i = \pm 1$. Here at a zero field spins prefer to be anti-parallel.

(a) Develop the mean field theory of this system, by dividing it into two sub-lattices of nonzero net magnetization in the ground state. What is the order parameter here?

(b) What is the transition temperature as a function of magnetic field for small H ?

(c) How does the zero field magnetic susceptibility behave as one approaches $T_c(H = 0)$?

1.2 XY model in one dimension (27 points)

In this problem we will demonstrate that the transfer matrix method can be applied to problems with continuous variables. To this end we will consider two component unit spins $\vec{S}_i = (\cos\theta_i, \sin\theta_i)$ in one dimension with periodic boundary conditions. The energy is given by the nearest neighbor interactions described by $\mathcal{H} = -J \sum_{i=1}^{N} \vec{S}_i \cdot \vec{S}_{i+1}$.

(a) Write down the (infinite dimensional) transfer matrix $T_{\theta,\theta'}$. Show that it can be diagonalized with eigenvectors $f_m(\theta) \propto e^{im\theta}$ for integer m, and find the corresponding eigenvalues.

(b) Now consider an *open* linear chain with free boundary conditions (i.e., there is no boundary energy for the first and last spins). Show that in the thermodynamic limit, the free energy of the open chain is the same as that of the periodic chain. **This conclusion is true for any one-dimensional model with short-range interactions.**

(c) In the limit $T \to 0$, calculate the free energy per site and the heat capacity. Use the leading order behaviour of the eigenvalues in small T. Compare with the heat capacity of that of the one-dimensional Ising model, using the expression for its free energy obtained in class. Explain shortly explain the differences in terms the number of available states each system exhibits in the limit $T \to 0$.

1.3 Correlations in the spin 1 Ising model (27 points)

Consider the zero-field spin 1 Ising model with periodic boundary conditions given by the Hamiltonian

$$\mathcal{H} = -J \sum_{i=1}^{N} S_i S_{i+1}, \tag{2}$$

where $S_i = 0, \pm 1$.

(a) Compute the eigenvalues of the transfer matrix, λ_i. You can do that by guessing one of the eigenvectors from symmetry considerations.

(b) Use the transfer matrix method to calculate the correlation length associated with the correlation function $C(j) = \langle S_i S_{i+j} \rangle - \langle S_i \rangle \langle S_{i+j} \rangle$. You can do that by demonstrating that this model exhibits the same scaling behaviour that we saw in class for the Ising model, whereby the correlation length given by

$$\xi = \frac{1}{\ln(\lambda_1/\lambda_2)}, \tag{3}$$

where λ_1 and λ_2 are the largest and next-to-largest eigenvalues, respectively. In order to obtain this, express the $C(j)$ as a trace over a symmetric matrix and the diagonal matrix,

$$D = \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix}. \tag{4}$$

Use a general form of a symmetric matrix to obtain the two leading order terms in $C(j)$. This will tell you which entries you need to compute in this matrix. Demonstrate that the leading order term vanishes and you are left with the term that yields eq. (3). **This equation can in fact be proven to be true in general for any one dimensional model with short-range interactions.**

(c) How does the correlation function behave at large distances j ?

(d) How does the correlation function in the limit of zero temperature $T \to 0$? What is the physical interpretation of this behaviour ?

1.4 Monte Carlo study of the 2D Ising model (20 points)

In this question you will use your Monte Carlo simulation of the 2D Ising model, written for exercise 1, to observe the phase transition in the 2D Ising model.

(a) Simulate the system for several temperatures above and below T_c. After the systems has equilibrated, collect sufficient statistics and calculate the mean magnitude of the magnetization per site,

$$m(T) = \frac{1}{L^2} \sum_{i=1}^{L^2} |\langle S_i \rangle| \,, \tag{5}$$

as a function of the temperature. Repeat the measure- ment 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 eq increases sharply close to T_c. This phenomenon, known as **critical slowing down**, is very common in numerical simulations of systems close the critical point.

(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).

1.5 Anisotropic 2D Ising model (6 bonus points)

Consider the anisotropic Ising model on a square lattice with periodic boundary conditions defined by the following Hamiltonian

$$H = -\sum_{k,l} \left(J_x \sigma_{k,l} \sigma_{k+1,l} + J_y \sigma_{k,l} \sigma_{k,l+1} \right). \tag{6}$$

(a) By following the derivation presented in class calculate the free energy of the model. You do not have to write down every step in the derivation. Simply sketch how the different steps in the derivation are modified due to the anisotropy.

(b) Find the critical boundary in the (J_x, J_y) plane. Show the critical point coincides with the expression we obtained in class in the Isotropic case.