Statistical Mechanics Fall 2014 — Problem Set 2

due: Wednesday, December 3, 2014

2.1 XY model in one dimension (35 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 briefly the differences in terms the number of available states each system exhibits in the limit $T \to 0$.

2.2 Correlations in the spin 1 Ising model (35 points)

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

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

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

$$\xi = \frac{1}{\ln(\lambda_1/\lambda_2)}, \tag{2}$$

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,

$$D = \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix}. \tag{3}$$

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. (2). **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 ?

2.3 Monte Carlo study of the 2D Ising model (30 points)

In this question we will use Monte Carlo simulation to observe the phase transition in the 2D Ising model. If you did not implement the 2D Ising Monte Carlo simulation, see instruction in ex1 and in the website (you can still submit the bonus question in ex1!).

(a) For a system of moderate size (e.g. L=50), simulate the system for several temperatures above and below T_c. Observe the dynamics of the magnetization over a long time course. Attach plots of the magnetization as function of time above T_c, at T_c and below T_c.

(b) After the systems has equilibrated, collect sufficient statistics and calculate the variance of the magnetization per site,

$$Var(M) = \left\langle \left[\frac{1}{L^2} \sum_{i=1}^{L^2} (S_i - \langle S_i \rangle) \right]^2 \right\rangle, \tag{4}$$

as a function of the temperature. Repeat the measurement for several different system sizes (e.g., L = 25, 50, 100), and plot the results in a single figure. Discuss the result in relation with the expected behavior of the magnetic susceptibility at the transition. Note that the equilibration time 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.

(c) 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).