Phase Transitions

Homework Sheet 3
Due 10am Mon Feb 27 2017, in the 563 box.

Please attempt these problems without referring to textbooks, although you may use your notes. The most efficient way to learn is to attempt a question and then if you are stuck, read the relevant section of the notes, then close the notes and try again.

Question 3–1.
This question is an exercise in the use of the transfer matrix method. In the first parts of the question, we deal with the $d = 1$ Ising model with periodic boundary conditions.

(a) Construct the matrix $\mathbf{S}$ which diagonalises the transfer matrix $\mathbf{T}$: that is, $\mathbf{T}' = \mathbf{S}^{-1}\mathbf{T}\mathbf{S}$ is diagonal. You will find it helpful to write down the matrix elements in terms of the variable ϕ given by

$$\cot(2\phi) = e^{2K}\sinh(h).$$

(b) Check that you understand why

$$\langle S_i \rangle = \frac{\mathrm{Tr}\,(\mathbf{S}^{-1}\sigma_z\mathbf{S}(\mathbf{T}')^N)}{Z_N}$$

and use your answer to part (a) to show that $\langle S_i \rangle = \cos(2\phi)$ as $N \to \infty$. In a similar fashion calculate $\langle S_i S_j \rangle$ and hence show that in the thermodynamic limit

$$G(i, i+j) \equiv \langle S_i S_j \rangle - \langle S_i \rangle \langle S_j \rangle = \sin^2(2\phi)\left(\frac{\lambda_2}{\lambda_1}\right)^j.$$

(c) Calculate the isothermal susceptibility χ_T. Verify explicitly that $\chi_T = \sum_j G(i, i+j)/k_B T$. (Caution: In the thermodynamic limit, the sum runs over $-\infty$ to $+\infty$.)

(d) Now we will examine what happens when the system has boundaries. Consider the partition function with free boundary conditions:

$$Z_N(h, K) = \sum_{S_1} \cdots \sum_{S_N} e^{h(S_1+\cdots+S_N)+K(S_1S_2+\cdots+S_{N-1}S_N)}.$$

In this case, the partition function is not simply $\mathrm{Tr}(\mathbf{T}')^N$. Work out what the correct expression is (you will need to introduce a new matrix in addition to T), and show that the free energy F_N is given by

$$F_N = Nf_b(h, K) + f_s(h, K) + F_{fs}(N, h, K)$$

where f_b is the bulk free energy, f_s is the surface free energy due to the boundaries, and $F_{fs}(N, h, K)$ is an intrinsically finite size contribution which depends on the system size as $e^{-C(h,K)N}$, where C is a function of h and K.

(e) Check that in the case $h = 0$ and $N \to \infty$ your result for the surface free energy agrees with that obtained from $\lim_{N\to\infty} F_N^{free} - F_N^{periodic}$ (notation should be obvious).

Question 3–2.

This question invites you to generalise the transfer matrix formalism to the two dimensional Ising model on a square lattice. Suppose that there are N rows parallel to the x axis and M rows parallel to the y axis. We will require that $N \to \infty$ whilst we will calculate the transfer matrix for $M = 1$ and $M = 2$. Periodic boundary conditions apply in both directions, so that our system has the topology of a torus. The Hamiltonian H_Ω is given by

$$-\beta H_\Omega = K \sum_{n=1}^{N} \sum_{m=1}^{M} S_{mn} S_{m+1n} + S_{mn} S_{mn+1}$$

(a) For the case $M = 1$ show that the transfer matrix is a 2×2 matrix, and show that its eigenvalues are

$$\lambda_1 = 1 + x^2 \qquad \lambda_2 = x^2 - 1$$

where

$$x \equiv e^K.$$

(b) Now consider the case $M = 2$. We need to extend the transfer matrix formalism. Consider the vector

$$\mathbf{v}_n = (S_{1n} S_{2n} \ldots S_{mn}).$$

This vector gives the configuration of a row n. Show that

$$H_\Omega = \sum_{n=1}^{N} E_1(\mathbf{v}_n, \mathbf{v}_{n+1}) + E_2(\mathbf{v}_n)$$

where E_1 is the energy of interaction between neighbouring rows and E_2 is the energy of a single row. Hence show that

$$Z = \sum_{\mathbf{v}_1 \cdots \mathbf{v}_N} T_{\mathbf{v}_1 \mathbf{v}_2} T_{\mathbf{v}_2 \mathbf{v}_3} \cdots T_{\mathbf{v}_N \mathbf{v}_1}$$

where T is a transfer matrix of dimensions $2^M \times 2^M$, whose form you should give.

(c) Calculate T for the case $M = 2$.

(d) Show that the two largest eigenvalues are

$$\lambda_1 = \left(x^4 + 2 + x^{-4} + \sqrt{x^8 + x^{-8} + 14}\right)/2$$

and

$$\lambda_2 = x^4 - 1.$$