

Phase Transitions

Homework Sheet 3

Due 5pm Fri 22 Feb 2008, 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

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

and use your answer to part (a) to show that $\langle S_i \rangle = \cos(2\phi)$ as $N \rightarrow \infty$. 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:

$$Z_N(h, K) = \sum_{S_1} \dots \sum_{S_N} e^{h(S_1 + \dots + S_N) + K(S_1 S_2 + \dots + S_{N-1} S_N)}.$$

In this case, the partition function is not simply $\text{Tr}(\mathbf{T}')^N$. 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

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

where f_b is the bulk free energy, f_s is the surface free energy due to the boundaries, and $F_{f_s}(N, h, K)$ 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 $N \rightarrow \infty$ your result for the surface free energy agrees with that obtained from $\lim_{N \rightarrow \infty} F_N^{free} - F_N^{periodic}$ (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 $N \rightarrow \infty$ 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

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

where

$$x \equiv e^K.$$

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

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

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

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

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

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

Question 3–3.

Consider the following simple model of a β -brass binary alloy. Equal numbers of copper and zinc atoms reside on the sites of a body-centred cubic lattice. At high temperatures, each site is occupied at random by either copper or zinc. At $T = T_c$, it is found that there is a continuous phase transition to a state of order where each atomic species is found

preferentially on one of the two sub-lattices of the b.c.c. lattice. The order parameter for this transition may be chosen to be the difference between the expected number of copper and zinc atoms on a chosen sub-lattice. Let the variable $S_i = +1$ if site i is occupied by a copper atom and $S_i = -1$ if it is occupied by a zinc atom. Assume that the interaction between all types of atom is nearest neighbour (i.e. define energies J_{CuCu} , J_{CuZn} etc), write down an appropriate Hamiltonian for a lattice gas model of this alloy. Show that it reduces to the nearest neighbour Ising model Hamiltonian, with an exchange interaction

$$J = \frac{1}{4}(J_{CuCu} + J_{ZnZn} - 2J_{CuZn}).$$

Your result shows that this system is in the same universality class as the Ising ferromagnetic transition. Is there any analogue of the external magnetic field for the alloy system? If so, what would the phase diagram be expected to be?