Homework 6, Statistical Mechanics: Concepts and applications
2019/20 ICFP Master (first year)

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With solutions. Please contact Botao Li if you find the exercise or the solution unclear or wrong.

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In lecture 06 (Ising model: from Ising to Onsager) we treated the question of spontaneous symmetry breaking in the 2d Ising model, following Peierls (1936), but also in the one-dimensional Ising model with $1/r^2$ interactions, following D. J. Thouless' (1969) in the paper that was the beginning of the Kosterlitz-Thouless story leading up to the 2016 Nobel prize (see Kosterlitz 2016 for a partly historical yet mostly scientific account). We then moved on to discuss the transfer-matrix solution of the two-dimensional Ising model, following Onsager (1944) and Schultz et al (1964), approximately halfway through the papers.

I. AN INTEGRAL IN THE ONE-DIMENSIONAL ISING MODEL WITH LONG-RANGE INTERACTIONS

The Ising model with long-range interaction is defined by the energy

$$E(i,j) = -J\frac{\sigma_i\sigma_j}{|r_i - r_j|^2}, \tag{1}$$

where the $\sigma = \pm 1$ are Ising spins. Suppose that the spins are on a line of length L, and that they are separated by a lattice spacing $a \ll L$. Suppose that there is a domain wall at position $L/2$ (with nearest lattice sites at $L/2 - a/2$ and at $L/2 + a/2$). All the spins left of the interface are equal to -1 and all the spins to the right are equal to $+1$. The excitation energy of the interface is given by:

$$E = J' \int_0^{L/2-a/2} \int_{L/2+a/2}^{L} \frac{dx dy}{(x-y)^2} \tag{2}$$

- Justify eq. (2).... Why is this a good formula, and why do we install a microscopic lengthscale a

Assuming the domain wall appears at the center of the system, the difference of energy between the ground state and the configuration with the domain wall is

$$\sum_{i=1}^{N/2} \sum_{j=N/2+1}^{N} \frac{2J}{(r_i - r_j)^2}$$

where $N \sim L/a$ is the number of spins in the system. All the possible pairs, which contain one site to the left of the domain wall and one site to the right of the domain wall, contribute to the excitation energy. In the limit $a \ll L$,

$$\begin{aligned}\sum_{i=1}^{N/2}\sum_{j=N/2+1}^{N}\frac{2J}{(r_i-r_j)^2} &= \sum_{i=1}^{N/2}a\sum_{j=N/2+1}^{N}a\frac{2J}{a^2(r_i-r_j)^2}\\ &\approx \int_0^{L/2-a/2}dx\int_{L/2+a/2}^{L}dy\frac{2J}{a^2(x-y)^2}\\ &= J'\int_0^{L/2-a/2}\int_{L/2+a/2}^{L}\frac{dxdy}{(x-y)^2}\end{aligned}$$

where $J' = 2J/a^2$. Due to the presence of the distance between two sites, the excitation energy is finite. In order to make the excitation energy finite in the continuous limit, there is a little gap, of length a, between the two intervals of the integrals.

- Actually compute this integral.

$$\begin{aligned}J'\int_0^{L/2-a/2}\int_{L/2+a/2}^{L}\frac{dxdy}{(x-y)^2} &= J'\int_{L/2+a/2}^{L}\left(\frac{1}{y}-\frac{1}{L/2-a/2-y}\right)dy\\ &= J'\ln(L/a)\end{aligned}$$

- Explain, by taking into account the entropy of the domain walls, why the one-dimensional Ising model with an energy function as in eq. (2) can be expected to have a phase transition at a finite temperature.

Since the domain wall can appear anywhere in the system, there are $N \sim L/a$ configurations which has a domain wall. The entropy given by the domain wall is $\Delta S = k\ln(L/a)$. Thus, the free energy introduced by the domain wall is

$$\Delta F = \Delta E - T\Delta S = (J' - kT)\ln(L/a)$$

When $T < J'/k$, the domain wall raises the free energy of the system. Thus the system stays in the ground state. When $T > J'/k$, the domain wall decreases the free energy of the system. Thus the system will be in the states which has a domain wall, or perhaps in other excited states. Thus, there is a phase transition as $T = J'/k$.

- What would you expect to be the phase behavior of the Ising model with interaction

$$E(i,j) = -J' \frac{\sigma_i \sigma_j}{|r_i - r_j|^{2+\epsilon}} \tag{3}$$

with $\epsilon \pm 0$?

When $\epsilon < 0$, the integral gives $\Delta E \sim (L/a)^{-\epsilon}$. The energy diverges faster than the entropy with respect to the system size. Thus the system is expected to always be ordered. When $\epsilon > 0$, ΔE almost remains constant. The system is expected to always be disordered. However, as mentioned in the lecture, domain-wall arguments are not rigorous and always have to be questioned. In the present case, there is a phase transition for $\epsilon \in$ $[-0.5, 0]$.

NB: The Thouless paper (Phys Rev 187, 732 (1969)) is only two pages long, but it contains results that are stronger than those by illustrious authors Dyson, Anderson and Ruelle, from the same period.

II. PARTITION FUNCTION OF THE 2×2 ISING MODEL WITH PERIODIC BOUNDARY CONDITIONS

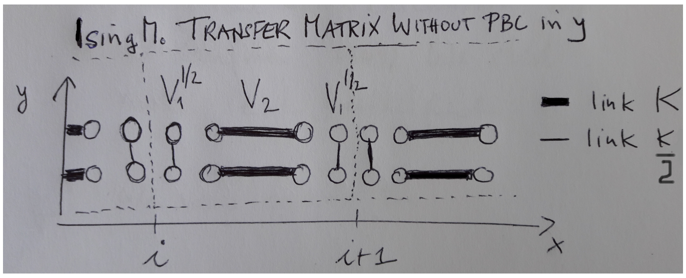

FIG. 1: Sketch of the transfer matrix for the $2 \times M$ Ising model without periodic boundary conditions in y. The matrices V_1 and V_2 can be found in the mathematica notebook file.

In the second part of lecture 06, we discussed the Ising model on a stripe of width 2, without periodic boundary conditions in y. It is given by

$$T = V_1^{1/2} V_2 V_1^{1/2} \tag{4}$$

(see Fig. 1). The precise values of V_1 and of V_2 were discussed in the lecture, but they can also be found in the mathematica notebook file on the webpage (where $V_1^{1/2}$ is called "V1sq").

- In which way do we have to modify the transfer matrix if we introduce periodic boundary conditions in y? (Note that periodic boundary conditions with two spins are somewhat artificial, as we then have two spins interact in two ways).

  Assuming that the two interaction as the same strength, the new V_1 is (using the conversion in the mathematica file)

$$diag\left(e^{2K}, e^{-2K}, e^{-2K}, e^{2K}\right)$$

  And the transfer matrix becomes

$$T = V_1^{1/2} V_2 V_1^{1/2} = \begin{pmatrix} e^{4K} & 1 & 1 & 1 \\ 1 & 1 & e^{-4K} & 1 \\ 1 & e^{-4K} & 1 & 1 \\ 1 & 1 & 1 & e^{4K} \end{pmatrix}$$

- Use this new transfer matrix to compute explicitly the partition function of the 2×2 Ising model with (artificial) periodic boundary conditions both in x and in y. Check your calculation with an (explicit) enumeration on paper of the 16 configurations of the 2×2 Ising model.

$$Z = Tr\left(T^2\right) = 2e^{8K} + 12 + 2e^{-8K}$$

- Explain how you would obtain the partition function of the 4×4 Ising model with periodic boundary conditions, but without doing any actual computation. What is the dimension of the transfer matrix?

  The transfer matrix T will be 16×16. T can still be decomposed into $V_1^{1/2} V_2 V_1^{1/2}$, where V_2 contains the interaction between two strips, and V_1, which is diagonal, contains the interactions within one strip. The partition function will be

$$Z = Tr\left(T^4\right)$$

- Explain how you would obtain the free energy per particle of the $4 \times M$ Ising model with periodic boundary conditions, for any M and in the limit $M \to \infty$, again without doing any detailed calculations.

For a $4 \times M$ system with periodic boundary condition,

$$Z = Tr\left(T^M\right) = \sum_{i=1}^{16} \lambda_i^M$$

where $\lambda_1 > \lambda_2 > ... > \lambda_{16}$ are the eigenvalues of the transfer matrix. In the limit of $M \to \infty$,

$$Z \approx \lambda_1^M$$

Then the free energy

$$F = \frac{1}{\beta}\ln(Z) \approx \frac{M}{\beta}\ln(\lambda_1)$$