Universität zu Köln Institut für Biologische Physik

## Advanced Statistical Mechanics (WS 2019/20) Problem Set 3

## Problem 3: An introduction to the 1d Ising Model.

The Ising model is, perhaps, the most studied model in statistical physics. As introduced in the lecture, it consists of a discrete set of magnetic degrees of freedom (or spins)  $s_i$ . In this case, the system is uniaxial anisotropic, which means that the spins align along an unique axis (for example the z-axis). We say then that  $s_i = \pm 1$ . In the case of a 1d system (an spins chain), the system is completely solvable (Ising 1926) and this is what we will explore in this exercise. Consider a one-dimensional Ising model with nearest-neighbor interactions, in the absence of a magnetic field. The Hamiltonian of this system is

$$H = -J \sum_{i=1}^{N} s_i s_{i+1}$$
 (1)

with  $s_i = \pm 1$  and J > 0. A given spin state consists of *domains*, i.e., contiguous stretches of up or down spins. The domains are separated by boundaries called *domain walls*, which are marked by dots in Fig. 1. The system has two ground states, in which all spins are aligned and there are no domain walls.



Figure 1: A configuration of spins (arrows) and of domain walls (dots) in the one-dimensional Ising model.

(a) Show that the energy of a spin state depends only on the number of domain walls, M, and compute the excitation energy  $\Delta E_M = E_M - E_0$ , where  $E_0$  is the ground state energy. Compute the number of states with M domain walls (note that each configuration of domain walls corresponds to exactly two spin states).

*Hint:* The computation is easier if one assumes free boundary conditions for the spins. Alternatively one can assume periodic boundary conditions (positions N + 1 and 1 are identical). This forces an even number of domain walls. The leading behavior in the thermodynamic limit  $(N \gg 1)$  will not depend on the boundary conditions.

- (b) Compute the partition function Z at inverse temperature  $\beta$  as a sum over domain wall configurations.
- (c) Compute the mean density of domain walls,  $\rho = \langle M/N \rangle$ , the mean energy density u = U/N, and the specific heat per unit length, c, at temperature  $\beta^{-1}$ . Evaluate the asymptotic behavior of these quantities in the low-temperature limit.

(d) The spin-spin correlation function is defined by

$$C(r) \equiv N^{-1} \sum_{i=1}^{N} \langle s_i s_{i+r} \rangle.$$
<sup>(2)</sup>

Using the domain wall representation, show that this correlation depends exponentially on the distance,

$$C(r) \sim \exp(-|r|/\xi),\tag{3}$$

and compute the correlation length as a function of the domain wall density,  $\xi(\rho)$ . Using the result of (c), then compute  $\xi(\beta^{-1})$  and evaluate the asymptotic behavior in the low-temperature limit. *Hint*: First convince yourself that the correlation function can be written as an inhomogeneous magnetisation with a constraint for one of the spins,  $s_k = 1$ :

$$C(r) = \langle s_{k+r} \rangle \Big|_{s_k=1} \equiv m(r).$$
(4)

Define the vector  $\mathbf{p}_r$  with two components  $p_r^+$  and  $p_r^- = 1 - p_r^+$ , which denote the probabilities of the two spin states at position r. Write down a recursion relation  $\mathbf{p}_r = \mathcal{T}\mathbf{p}_{r-1}$  with a 2x2 matrix  $\mathcal{T}$  and express the coefficients of this matrix in terms of the domain wall density  $\rho$ . Simplify to a recursion for the position-dependent magnetisation  $m(r) = p_r^+ - p_r^-$  and solve this recursion.

(e) More generally, the recursive formalism covers the entire statistics of the system. Consider the partition function  $Z_N^{\sigma,\sigma'}$  in a system of size N with constrained boundary spins,  $s_1 = \sigma$  and  $s_{N+1} = \sigma'$ . Compute the 2x2 matrix

$$\mathbf{T} = \begin{pmatrix} Z_1^{++} & Z_1^{+-} \\ Z_1^{-+} & Z_1^{--} \end{pmatrix},$$
(5)

which is called the *transfer matrix* of the system (each of these partition functions consists of a single term). By complete induction, show that the partition functions in a system of size N with constrained boundary spins are simply related to the transfer matrix,

$$\begin{pmatrix} Z_N^{++} & Z_N^{+-} \\ Z_N^{-+} & Z_N^{--} \end{pmatrix} = \mathbf{T}^N$$
(6)

(it is useful to write out the matrix product  $\mathbf{T}^N$  explicitly for, say, N = 2, 3). In particular, the partition function with periodic boundary conditions takes the form  $Z_N = \text{Tr} \mathbf{T}^N$ . Compute  $Z_N$  using the asymptotic identity  $\text{Tr} \mathbf{A}^N \simeq \lambda_1^N$ , where  $\lambda_1$  is the largest eigenvalue of  $\mathbf{A}$ , and recover the result of (b).

## Problem 4: Mean Field Theory of the XY-model

The Ising model discussed above is a particular case of a broader type of systems with many magnetic degrees of freedom, in which the spins tend to align along a particular axis, e.g the z-axis, such that  $s^z = \pm 1$ . Alternatively, unit-length spins may prefer to lay down on a plane, e.g. the xy-plane, from which follows that  $(s^x)^2 + (s^y)^2 = 1$ . This is known as the planar or XY-model, for which we discuss the mean field theory in this exercise.

(a) Starting with the Hamiltonian

$$H = -\sum_{\vec{r},\vec{r}'} J(\vec{r} - \vec{r}') \vec{s}_{\vec{r}} \cdot \vec{s}_{\vec{r}'} - \vec{h} \cdot \sum_{\vec{r}} \vec{s}_{\vec{r}}$$
(7)

and defining the magnetisation vector  $\vec{M} = (M^x, M^y)$ , expand the spin vector functions to first order around the magnetisation and rewrite the mean field hamiltonian  $H_{MF}$  in terms of the norm



Figure 2: At each site in position  $\vec{r}$  there is a spin  $\vec{s_r}$  that lies down on the xy-plane. In this figure, we define the angle between  $\vec{s_r}$  and the x-axis as  $\phi_{\vec{r}}$ . On the same plane lies the magnetisation vector  $\vec{M}$ . We define the angle between  $\vec{M}$  and the x-axis as  $\theta$ . For convenience, the external magnetic field  $\vec{h}$  lies along the x-axis.

of the magnetisation M and the corresponding angles  $\theta$  and  $\phi_{\vec{r}}$  (See the figure above). Hint: As has been done before, define  $J \equiv \sum_{\vec{r}} J(\vec{r} - \vec{r'})$ . As shown in the picture, for convenience, one can define the coordinates such that the external magnetic field lies down along the x-axis,  $\vec{h} = h\hat{x}$ .

- (b) Write the mean field partition function  $Z_{MF}$ . In particular, think about how to properly define the sum over all the configurations in this case.
- (c) Using the following integral

$$\int_{0}^{2\pi} e^{a\cos(\theta) + b\sin(\theta)} d\theta = 2\pi I_0(\sqrt{a^2 + b^2})$$
(8)

with  $I_0(x)$  the modified Bessel function of the first class, calculate the free energy of the system  $F_{MF}$ .

(d) Argue that the mean field values for the critical exponents of the XY-model are the same as those for the Ising model that were calculated in the lecture.

To be discussed on: Mon, November 11

Course information: http://www.thp.uni-koeln.de/~lassig/teaching.html