ECOLE POLYTECHNIQUE FEDERALE DE LAUSANNE

School of Computer and Communication Sciences

Handout 2 Statistical Physics for Communication and Computer Science

Homework 2 February 27, 2013

In the following problems you will solve the Ising model in one dimension: this is the simplest model for the interaction of magnetic moments of atoms in a crystal. We assume N even for simplicity and let $i \in \{-\frac{N}{2}, \cdots, \frac{N}{2}\}$ label the $N+1$ vertices of a one dimensional chain of atoms. We attach spin variables $s_i \in \{-1, +1\}$ to each site of the chain (these are the magnetic moments of atoms sitting at positions i). The Hamiltonian (or energy function, or cost function) of the one-dimensional Ising model is

$$\mathcal{H}_N = -J \sum_{i=-\frac{N}{2}}^{\frac{N}{2}-1} s_i s_{i+1} - H \sum_{i=-\frac{N}{2}}^{\frac{N}{2}} s_i \tag{1}$$

Here $J > 0$ is the interaction constant between spins (ferromagnetic case) and $H \in \mathbb{R}$ an external magnetic field. When the system is at thermal equilibrium at temperature T, the probability of a configuration $\{s_i\}$ is given by the Gibbs distribution (k is Boltzmann's constant defined such that kT has units of energy)

$$\mu(\{s_i\}) = \frac{1}{Z_N} e^{-\frac{\mathcal{H}}{kT}}, \qquad \text{where} \qquad Z_N = \sum_{\{s_i = \pm 1\}} e^{-\frac{\mathcal{H}_N}{kT}} \tag{2}$$

is the partition function (in German "Zustandssumme" which means "sum over states"). The following notation is standard: $\frac{1}{kT} = \beta$, $\beta J = K$, $\beta H = h$.

The first problem introduces the transfer matrix method, which is a general way of solving one-dimensional models. The second problem is concerned with boundary conditions. In the third one you will solve the same model thanks to the message passing approach which we will develop further in the course.

Problem 1 (Transfer matrix method)**.** In this problem we take a periodic boundary condition which leads to simpler calculations. This means that the sites $i \in \{-\frac{N}{2}, \cdots, \frac{N}{2}\}$ are arranged on a circle, and that there is an extra interaction term in (1), namely $-J s_{-\frac{N}{2}} s_{\frac{N}{2}}$ (since the two extremities of the chain have been brought next to each other). Consider the *transfer matrix*

$$T = \begin{pmatrix} e^{K+h} & e^{-K} \\ e^{-K} & e^{K-h} \end{pmatrix} \tag{3}$$

A. Show that the partition function can be expressed as

$$Z_N = tr\,(T^N). \tag{4}$$

where tr is the sum over eigenvalues.

B. Find the eigenvalues of T and show that the free energy per spin is in the thermodynamic limit

$$f(h) \equiv -\lim_{N \to +\infty} \frac{1}{\beta N} \ln Z_N = -\beta^{-1} \ln[e^K \cosh h + (e^{2K} \sinh^2 h + e^{-2K})^{1/2}]. \tag{5}$$

C. Compute the magnetization from the *thermodynamic definition*: $m = -\frac{\partial}{\partial H} f(h)$ and plot the curve m as a function of H for various values of β. Convince yourself both on the plot and from the analytic formula that there is *no sharp phase transition* for any temperature $T > 0$[1].

D. Now we want to compute the local magnetization at a fixed site i, and the correlation between two spins at sites i and j, namely

$$\langle s_i \rangle = \frac{\sum_{\{s_k=\pm 1\}} s_i e^{-\frac{\mathcal{H}}{kT}}}{Z_N}, \qquad \langle s_i s_j \rangle = \frac{\sum_{\{s_k=\pm 1\}} s_i s_j e^{-\frac{\mathcal{H}}{kT}}}{Z_N} \tag{6}$$

Introduce a matrix $S = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ and express these two quantities in terms of traces involving S and T. Noting that T can be diagonalized by an orthogonal rotation of angle ϕ, deduce that

$$\lim_{N\to+\infty} \langle s_i \rangle = \cos 2\phi, \qquad \lim_{N\to+\infty} \langle s_i s_j \rangle = \cos^2 2\phi + \sin^2 2\phi \left(\frac{\lambda_-}{\lambda_+}\right)^{|j-i|} \tag{7}$$

were $\lambda_- < \lambda_+$ are the eigenvalues of T. Check that the first formula above agrees with m found in 1.c. Interpret the second formula.

Problem 2 (Message passing method)**.** Consider the model on the open chain with free boundary conditions (no constraint on the end spins). we want to compute $\langle s_i \rangle$ for a fixed i, in the infinite size limit $N \to +\infty$, by an iterative method. For simplicity consider the middle spin $\langle s_0 \rangle$. You can convince yourself that the method works for any fixed i.

A. In the expression for $\langle s_i \rangle$ perform the sums over the end spins $s_{-\frac{N}{2}}$ and $s_{\frac{N}{2}}$. Show that this leads to a spin system with the new hamiltonian

$$\beta\mathcal{H}_N^{(1)} = -K \sum_{i=-\frac{N}{2}+1}^{\frac{N}{2}-2} s_i s_{i+1} - h \sum_{i=-\frac{N}{2}+2}^{\frac{N}{2}-2} s_i - (h + \tanh^{-1}(\tanh K \tanh h))(s_{-\frac{N}{2}+1} + s_{-\frac{N}{2}-1}) \tag{8}$$

B. Iterate to show that

$$\lim_{N\to+\infty} \langle s_0 \rangle = \tanh(h + 2\tanh^{-1}(\tanh K \tanh u)) \tag{9}$$

where u is the solution of the fixed point equation

$$u = h + \tanh^{-1}(\tanh K \tanh u) \tag{10}$$

Incidentally, show that the solution of this fixed point equation is unique so that there is no ambiguity in this result. For this point it is useful to note that if a mapping is a contraction i.e, $\sup_u |g'(u)| < 1$, then the sequence $u_{t+1} = g(u_t)$ is Cauchy.

C. Check that the result agrees with the expression for m found in the first problem. Calculations are maybe simpler if you use the identity

$$\tanh(x + y) = \frac{\tanh x + \tanh y}{1 + \tanh x \tanh y} \tag{11}$$

[1] In his 1925 PhD thesis, under Lenz's guidance, Ising mistakenly concluded from this calculation that the model would not exhibit any phase transition even when formulated on two or three dimensional square grids. It was only in 1936 that Peierls proved the existence of a phase transition at a finite temperature for dimensions greater or equal to 2.