Problem Set 2
The Ising model

1 1d Ising model: exact solution with the transfer matrix method

Let us consider a chain of N spins $s_i = \pm 1$ ($i = 0, 1, \ldots, N-1$) at the temperature T and in an external magnetic field H, with a ferromagnetic interaction J between nearest neighbors. The corresponding Hamiltonian reads

$$\mathcal{H} = -J \sum_{i=0}^{N-1} s_i s_{i+1} - H \sum_{i=0}^{N-1} s_i,$$

where we use periodic boundary conditions, that is, $s_N = s_0$.

1.1 Thermodynamical properties of the system

(a) Show that the canonical partition function of the system reads

$$Z = \sum_{s_0=\pm 1} \sum_{s_1=\pm 1} \sum_{s_2=\pm 1} \cdots \sum_{s_{N-1}=\pm 1} \mathcal{T}_{s_0 s_1} \mathcal{T}_{s_1 s_2} \ldots \mathcal{T}_{s_{N-1} s_0},$$

where the *transfer matrix* $\mathcal{T}$ (with dimensions 2×2) is defined through its matrix elements as

$$\mathcal{T}_{s_i s_{i+1}} = \exp\left(\beta J s_i s_{i+1} + \frac{\beta H}{2}[s_i + s_{i+1}]\right),$$

with $\beta = 1/k_\mathrm{B}T$, and where the rows are labelled by $s_i = +1$ and -1, and the columns by $s_{i+1} = +1$ and -1, respectively. In particular, show that

$$\mathcal{T} = \begin{pmatrix} \mathrm{e}^{\beta(J+H)} & \mathrm{e}^{-\beta J} \\ \mathrm{e}^{-\beta J} & \mathrm{e}^{\beta(J-H)} \end{pmatrix}.$$

(b) Using matrix multplication, show that

$$Z = \sum_{s_0=\pm 1} \left(\mathcal{T}^N\right)_{s_0 s_0} = \mathrm{Tr}\left\{\mathcal{T}^N\right\} = \lambda_0^N + \lambda_1^N,$$

where λ_0 and λ_1 ($|\lambda_0| > |\lambda_1|$ by convention) are the eigenvalues of $\mathcal{T}$. At the thermodynamical limit ($N \to \infty$), argue that $Z = \lambda_0^N$.

(c) Deduce from the previous result that

$$Z = \left[\mathrm{e}^{\beta J} \cosh(\beta H) + \sqrt{\mathrm{e}^{2\beta J} \sinh^2(\beta H) + \mathrm{e}^{-2\beta J}}\right]^N$$

(d) Still at the thermodynamical limit, determine the free energy of the system.

(e) Deduce from the previous question the average magnetization $M = \langle s_i \rangle$ of the system. Plot your result as a function of the applied magnetic field. What can you tell about the noninteracting case $J = 0$ and the limit $J/k_\mathrm{B}T \gg 1$ (strongly-interacting limit). Give a qualitative interpretation to your results. Is there a phase transition for the exactly-solved 1d Ising model? Compare with the mean-field solution (cf. lecture and/or Problem 2).

1.2 Correlation function

The correlation function between two spins separated by $R-1$ lattice sites is defined as

$$\Gamma_R = \langle s_0 s_R \rangle - \langle s_0 \rangle \langle s_R \rangle,$$

and the correlation length ξ by

$$\xi^{-1} = \lim_{R\to\infty} \left\{ -\frac{\ln |\Gamma_R|}{R} \right\}. \tag{1.1}$$

(a) Let us express Γ_R in terms of the transfer matrix $\mathcal{T}$ and the matrix $\mathcal{S}$ representing the spin operator. We write $\mathcal{T}$ and $\mathcal{S}$ in their diagonal form:

$$\mathcal{T} = \sum_{n=0,1} \lambda_n |u_n\rangle\langle u_n|,$$
$$\mathcal{S} = \sum_{s_i=\pm 1} s_i |s_i\rangle\langle s_i|.$$

The vectors $|s_i = +1\rangle = (1,0)$ and $|s_i = -1\rangle = (0,1)$ correspond to the two possible spin states. Using $\mathcal{T}$ and $\mathcal{S}$, show that

$$\langle s_0 \rangle = \langle s_R \rangle = \langle u_0 | \mathcal{S} | u_0 \rangle$$

in the thermodynamical limit.

(b) Then, show that

$$\langle s_0 s_R \rangle = \sum_{n=0}^{1} \left(\frac{\lambda_n}{\lambda_0} \right)^R \langle u_0 | \mathcal{S} | u_n \rangle \langle u_n | \mathcal{S} | u_0 \rangle$$

for $N \gg 1$.

(c) Deduce from the two previous questions that

$$\Gamma_R = \left(\frac{\lambda_1}{\lambda_0} \right)^R \langle u_0 | \mathcal{S} | u_1 \rangle \langle u_1 | \mathcal{S} | u_0 \rangle. \tag{1.2}$$

(d) Calculate explicitly the correlation function (1.2). It will be accepted without calculating them that the eigenvectors of the transfer matrix read $|u_0\rangle = (\alpha_+, \alpha_-)$ and $|u_1\rangle = (\alpha_-, -\alpha_+)$, with

$$\alpha_\pm = \frac{1}{\sqrt{2}} \left(1 \pm \frac{\mathrm{e}^{\beta J} \sinh(\beta H)}{\sqrt{\mathrm{e}^{2\beta J} \sinh^2(\beta H) + \mathrm{e}^{-2\beta J}}} \right)^{1/2}.$$

In particular, study the zero-magnetic field limit. In the latter case, plot the correlation function as a function of R.

(e) Calculate the correlation length (1.1) using the expression (1.2). Comment on the low- and high-temperature limits.

2 Mean-field solution of the Ising model

Consider a system of $N(\gg 1)$ atoms whose positions are fixed to the nodes of a crystalline lattice with volume V, which is in equilibrium with a thermostat at the temperature T and subject to an external magnetic field $\mathbf{B}_0$. To each atom i is associated a magnetic moment $\boldsymbol{\mu}_i = g\mu_\mathrm{B}\mathbf{S}_i$, where g is the Landé factor, μ_B the Bohr magneton, and $\mathbf{S}_i$ the spin of the i^th atom. In what follows, we assume that S_i can only take the values $\pm 1/2$ in the direction of the applied magnetic field.

2.1 Paramagnetism

Let us first neglect the interactions between the magnetic moments. The system can then be described by a Hamiltonian coupling the magnetic moments with the applied field $\mathbf{B}_0$ and which simply reads

$$\mathcal{H} = -\sum_{i=1}^{N} \boldsymbol{\mu}_i \cdot \mathbf{B}_0 = -g\mu_\mathrm{B}\sum_{i=1}^{N} \mathbf{S}_i \cdot \mathbf{B}_0.$$

(a) What is the state of the system at zero temperature (give a concise answer, without performing any calculation)? What is the effect of a temperature increase on such a state?

(b) Calculate the canonical partition function Z and the free energy F of the system.

(c) Show that the average magnetization M of the system reads

$$M = \frac{N}{V}\frac{g\mu_\mathrm{B}}{2}\tanh\left(\frac{g\mu_\mathrm{B}B_0}{2k_\mathrm{B}T}\right).$$

Plot M as a function of the applied magnetic field. Does the system showcase a phase transition?

(d) One defines the magnetic susceptibility as

$$\chi = \lim_{B_0\to 0}\frac{\partial M}{\partial B_0}. \tag{2.1}$$

Show that χ follows the Curie law

$$\chi = \frac{\mathcal{C}}{T}. \tag{2.2}$$

Give an expression of $\mathcal{C}$ as a function of the parameters of the problem. Notice that for weak magnetic fields, one has $M = \chi B_0$.

2.2 Ferromagnetism

Let us now consider a ferromagnetic interaction between nearest-neighbor magnetic moments. The Hamiltonian of the system then reads

$$\mathcal{H} = -g\mu_\mathrm{B}\sum_{i=1}^{N} \mathbf{S}_i \cdot \mathbf{B}_0 - J\sum_{\langle i,j\rangle} \mathbf{S}_i \cdot \mathbf{S}_j, \tag{2.3}$$

where $\langle i,j\rangle$ corresponds to a summation over pairs of nearest neighbors i and j on the lattice, and where J is the ferromagnetic coupling constant (what is the sign of J?).

(a) Within the mean field approximation, one neglects the correlations between the fluctuations of the spins with respect to their mean value $\langle \mathbf{S}_i\rangle$. In what follows, we assume that each atom has p nearest neighbors. Show that the effective magnetic field B_eff exerted on a lattice site i reads $B_\mathrm{eff} = B_0 + \lambda M$, where M is the magnetization of the interacting system. Give an expression of λ as a function of the parameters of the problem. Show that the Hamiltonian (2.3) reads within the mean field approximation as

$$\mathcal{H} = -g\mu_{\mathrm{B}} B_{\mathrm{eff}} \sum_{i=1}^{N} S_i + J\frac{Np}{2}\left(\frac{VM}{Ng\mu_{\mathrm{B}}}\right)^2.$$

(b) Calculate Z and F within the mean field approximation.

(c) Use the results of Part 2.1 to determine the following self-consistent equation, which determines the value(s) of the magnetization M:

$$M = \frac{N}{V}\frac{g\mu_{\mathrm{B}}}{2}\tanh\left(\frac{\beta g\mu_{\mathrm{B}}}{2}(B_0 + \lambda M)\right). \tag{2.4}$$

Rederive the above result by minimizing the free energy found at question 2.2(b) with respect to M.

2.2.1 Properties of the system at zero magnetic field

In this part of the problem, we consider a vanishing external magnetic field, i.e., $B_0 = 0$.

(a) How many solutions to the transcendental equation (2.4) can you find? (Use a graphical method.) Does the system present a phase transition? If yes, give an expression for the critical temperature T_{c}.

(b) Determine the magnetization in the low-temperature limit $T \ll T_{\mathrm{c}}$, as well as in the vicinity of T_{c} (i.e., for $0 < 1 - T/T_{\mathrm{c}} \ll 1$).

(c) Calculate the ensemble-averaged energy of the system. Deduce from your result the corresponding specific heat $\mathcal{C}$. How does the latter quantity behave as a function of temperature? In particular, what happens for $T = T_{\mathrm{c}}$?

2.2.2 Properties of the system at finite magnetic field

We now consider the system to be subject to a finite magnetic field ($B_0 \neq 0$).

(a) Solve for the self-consistent equation (2.4) graphically. Consider first the case $T > T_{\mathrm{c}}$, and then $T < T_{\mathrm{c}}$. You shall consider that the magnetic field is finite, but weak (with respect to what?)

(b) Use the previous result to calculate the magnetic susceptibility defined in Eq. (2.1). Compare to the paramagnetic case and to the Curie law (2.2).

2.2.3 Mean-field critical exponants

From your results above, deduce the mean-field critical exponants, which are defined, in the vicinity of the critical temperature, as

$$\begin{aligned} M(T, B_0 = 0) &\sim (T_{\mathrm{c}} - T)^{\beta}, \\ C(T, B_0 = 0) &\sim |T - T_{\mathrm{c}}|^{-\alpha}, \\ \chi &\sim |T - T_{\mathrm{c}}|^{-\gamma}. \end{aligned}$$

Compare these results to those of Problem Set 3.