Exam — Session 1

Duration: 2 h.

Documents, cell phones, computers, tablets, pocket calculators, etc., are not allowed.
The text contains 4 pages in total, and the 2 exercices are independent from each other.

1 The three-state Ising model: mean-field treatment

Let us consider the following variant of the usual Ising model studied during the semester: N spins on a lattice where the number of nearest neighbors of each spin is z can take the *three values* $s_i = -1$, 0, or +1. The corresponding Hamiltonian reads

$$H = -J \sum_{\langle i,j \rangle} s_i s_j - h \sum_{i=1}^{N} s_i, \tag{1.1}$$

where $J > 0$ is a ferromagnetic exchange interaction, and h the external magnetic field (in energy units). In Eq. (1.1), $\langle i, j \rangle$ denotes a summation over pairs of nearest neighbor sites i and j. The system is maintained at a temperature T. In the following, we denote $\beta = 1/k_{\mathrm{B}}T$, with k_{B} the Boltzmann constant.

(a) For $h = 0$ and $T = 0$, what are the ground states of the system? Same question for $h \to 0^+$ and $T = 0$.

(b) Let us decompose the spin $s_i = m + \delta s_i$ into its (statistical) averaged value $m = \langle s_i \rangle$ and the fluctuations δs_i around it. Let us further define the spin-spin correlation function $c_{ij} = \langle s_i s_j \rangle - \langle s_i \rangle \langle s_j \rangle$. Give an expression of c_{ij} in terms of δs_i and δs_j. What is the value of c_{ij} within the mean-field approximation (MFA)?

(c) Show that within the MFA, the Hamiltonian (1.1) takes the form

$$H \simeq \frac{zJN}{2} m^2 - (zJm + h) \sum_{i=1}^{N} s_i.$$

(d) Calculate the canonical partition function Z as well as the free energy F within the MFA.

(e) Show, by the method of your choice, that the self-consistent equation for the average magnetization $m = \langle s_i \rangle$ reads

$$m = \frac{2 \sinh(\beta[zJm + h])}{1 + 2\cosh(\beta[zJm + h])}. \tag{1.2}$$

(f) *Intermezzo:* Consider the function

$$f(x) = \frac{2\sinh x}{1 + 2\cosh x}, \qquad x \in \mathbb{R}.$$

(i) Give the value of $f(x = 0)$?

(ii) What are the two asymptotic values $\lim_{x\to\pm\infty} f(x)$?

(iii) Show that $f(x)$ is an odd function.

(iv) Show that for $x \ll 1$, $f(x) = 2x/3 - x^3/9 + \mathcal{O}(x^5)$.

(v) Sketch the function $f(x)$.

(g) *From now on, we consider the case of a vanishing external magnetic field, $h = 0$.* With the help of the self-consistent equation (1.2), show that there exists a paramagnetic-ferromagnetic phase transition at the critical temperature $k_{\mathrm{B}}T_{\mathrm{c}} = 2zJ/3$.

(h) Close to the critical instability ($T \simeq T_c$), the free energy found in Question (d) admits, for $h = 0$ and $m \ll 1$, the Landau expansion

$$\Delta F(m) = F(m) - F(m=0) \simeq \frac{a(T)}{2} m^2 + \frac{b}{4} m^4 + \mathcal{O}(m^6), \tag{1.3}$$

with $a(T) = a_0(T - T_c)$, and where $a_0 > 0$ and $b > 0$ are two positive, temperature-independent quantities. Using the above expansion, sketch ΔF as a function of m for $T > T_c$ and $T < T_c$, and discuss the stability of the solutions of the self-consistent equation found previously.

(i) Using Eq. (1.3), determine the (mean-field) critical exponent β, defined through

$$m(T) \sim (T_c - T)^{\beta},$$

with $T \to T_c^-$.

(j) Due to the fact that some neighboring spins can be zero, a given spin can see different local fields and have therefore different interaction energies despite identical values of m. Show this on a specific example (a two-dimensional square lattice will do).

2 Freely jointed chain model of a polymer chain

We consider a succession of rigid monomers of length a represented by vectors $\boldsymbol{a}_i$ ($i \in \{1, \cdots, N\}$), see Fig. 1. Once a referential $(O, \boldsymbol{e}_x, \boldsymbol{e}_y, \boldsymbol{e}_z)$ has been chosen, the orientation of $\boldsymbol{a}_i$ is given by the usual spherical angles ($\theta_i \in [0, \pi]$, $\varphi_i \in [0, 2\pi]$). The polymer chain is in solution in a solvent of volume V (such a solvent can be considered as a heat reservoir which maintains the temperature T of the system).

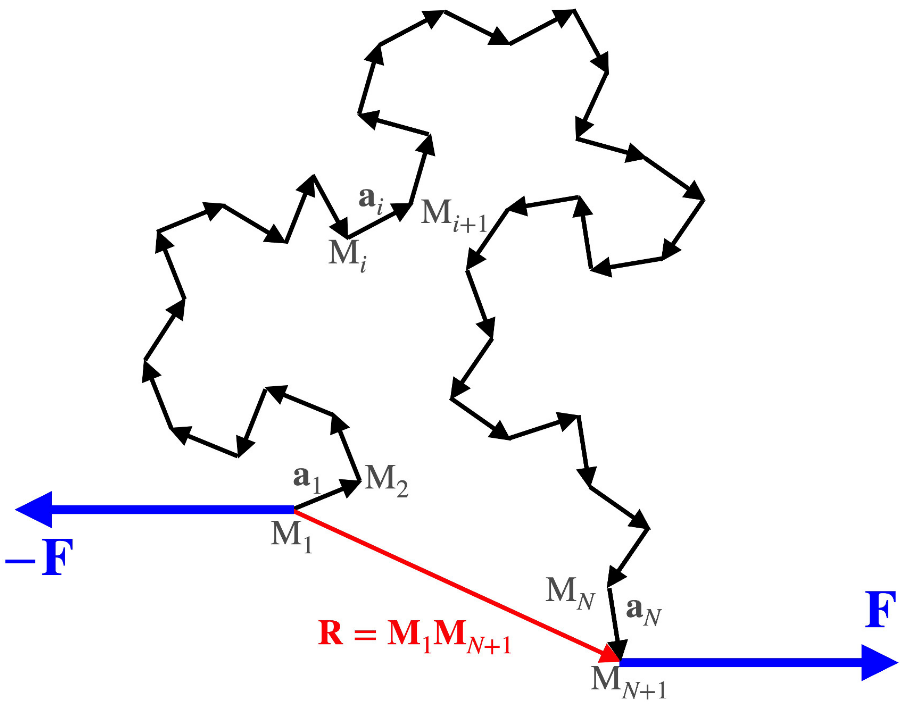

Figure 1: Sketch of a polymer chain (represented in 2d for simplicity) subject to external forces $\boldsymbol{F}$ applied at its two ends, and composed of N monomers $\boldsymbol{a}_i = \boldsymbol{M}_i\boldsymbol{M}_{i+1}$, with $|\boldsymbol{a}_i| = a$. The end-to-end vector $\boldsymbol{R} = \boldsymbol{M}_1\boldsymbol{M}_{N+1}$ is shown in red.

2.1 Derivation of the equation of state

2.1.1 Without any force ($\boldsymbol{F} = \boldsymbol{0}$)

We start by considering the case of a vanishing force, $F = 0$.

(a) Assuming that all orientations have equal probabilities, give the probability $\mathrm{d}^2P(\theta_i, \varphi_i, \mathrm{d}^2\Omega)$ of finding the monomer i in the direction (θ_i, φ_i) up to the infinitesimal solid angle $\mathrm{d}^2\Omega = \sin\theta_i\,\mathrm{d}\theta_i\mathrm{d}\varphi_i$. Deduce the probability density $\rho(\boldsymbol{a}_1, \ldots, \boldsymbol{a}_N)$ to have a given configuration $\{\boldsymbol{a}_1, \cdots, \boldsymbol{a}_N\}$ of the chain.

(b) Give (without any calculation) the average values $\langle \boldsymbol{a}_i \rangle$ and $\langle \boldsymbol{a}_i \cdot \boldsymbol{a}_j \rangle$.

(c) Calculate the (canonical) partition function Z of the chain.

(d) One defines the end-to-end vector $\boldsymbol{R} = \boldsymbol{M}_1\boldsymbol{M}_{N+1}$, where M_1 (resp. M_{N+1}) is the first (resp. the last) monomer of the chain (see Fig. 1). Calculate $\langle \boldsymbol{R} \rangle$ and $\langle \boldsymbol{R}^2 \rangle$. Give a physical interpretation of $\sqrt{\langle \boldsymbol{R}^2 \rangle}$.

2.1.2 Chain stretched by a force $\boldsymbol{F} \neq \boldsymbol{0}$

The chain is now submitted to a torque, namely a force $\boldsymbol{F}$ acting on M_{N+1} and a force $-\boldsymbol{F}$ acting on M_1 (see Fig. 1). In what follows, we assume that the tensile force $\boldsymbol{F}$ is constant and aligned towards the z direction, *i.e.*, $\boldsymbol{F} = F\boldsymbol{e}_z$.

(a) Show that after an infinitesimal displacement of all monomers $M_j \to M_j + \overrightarrow{\mathrm{d}M_j}$, the work done by the forces is $\delta W = \boldsymbol{F} \cdot \mathrm{d}\boldsymbol{R}$. Deduce that the chain can be considered as having the potential energy $U_\mathrm{p} = -\boldsymbol{F} \cdot \boldsymbol{R}$.

(b) Compute the canonical partition function Z of the chain experiencing the tensile force $\boldsymbol{F}$. Deduce an expression of $\langle \boldsymbol{R} \rangle$ as a function of $\boldsymbol{F}$ that you will express in terms of the Langevin function

$$\mathcal{L}(x) = \frac{1}{\tanh x} - \frac{1}{x} = \frac{\mathrm{e}^x + \mathrm{e}^{-x}}{\mathrm{e}^x - \mathrm{e}^{-x}} - \frac{1}{x}. \tag{2.1}$$

(c) In the limit of weak forces $\beta F a \ll 1$, with $\beta = 1/k_\mathrm{B}T$, show that $\langle \boldsymbol{R} \rangle$ has a linear behavior with $\boldsymbol{F}$. Define a "susceptibility ratio" (infinitesimal response)/(infinitesimal solicitation) for the system and compute it. Which name can be given to this quantity?

(d) In the limit of strong forces $\beta F a \gg 1$, give an expression of $\langle \boldsymbol{R} \rangle$ and comment your result.

(e) In the case of a DNA molecule with $a = 50\,\mathrm{nm}$ at room temperature, give a numerical estimate of F for which there is a transition between the weak and strong force regimes. Note that $k_\mathrm{B} \simeq 1.4 \times 10^{-23}\,\mathrm{J/K}$.

2.2 Fluctuations

The purpose of this section is to calculate the fluctuations of the end-to-end vector $\boldsymbol{R}$. We are especially interested in calculating $\Delta R^2 = \langle \boldsymbol{R}^2 \rangle - \langle \boldsymbol{R} \rangle^2$.

(a) Carefully justify the following relations:

$$\langle a_{z,i}a_{z,j} \rangle = \langle a_{z,i} \rangle \langle a_{z,j} \rangle,$$
$$\langle a_{x,i}a_{x,j} \rangle = \langle a_{y,i}a_{y,j} \rangle = \frac{1}{3}\left(a^2 - \langle a_{z,i}a_{z,j} \rangle\right)\delta_{ij},$$

where $(i, j) \in \{1, \cdots, N\}^2$ and with δ_{ij} the Kronecker delta. Note that to derive the above expressions, it might be useful to consider separately the cases $i = j$ and $i \neq j$.

(b) Deduce from the previous results that

$$\Delta R_x^2 = \Delta R_y^2 = Na^2 \, \frac{\mathcal{L}\left(\beta F a\right)}{\beta F a},$$
$$\Delta R_z^2 = Na^2 \left[1 - 2\,\frac{\mathcal{L}\left(\beta F a\right)}{\beta F a} - \mathcal{L}\left(\beta F a\right)^2\right],$$

where $\mathcal{L}\left(x\right)$ is the Langevin function defined in Eq. (2.1). Deduce the expression of ΔR^2.

(c) Give the limit of ΔR_x^2, ΔR_y^2, and ΔR_z^2 in the weak force limit and comment your result.

(d) Same question in the strong force regime.