Phase Transitions

Homework Set 1: Ising Model

Useful notation and relations

Throughout, $s_i = \pm 1$ and M denotes the total magnetisation. We use $m = \langle M \rangle / N$ for magnetisation per spin and $\langle \cdot \rangle$ for thermal averages. In the diluted model, p is the bond-occupation probability.

A. Equilibrium thermodynamics and fluctuations

Problem 1. Entropy and free energy

The entropy of a system in thermal equilibrium is defined by

$$S = -k_B \sum_r P_r \ln P_r,$$

where P_r is the probability of the microstate r, with energy E_r. In the canonical ensemble,

$$P_r = \frac{e^{-E_r/(k_B T)}}{Z}, \qquad Z = \sum_r e^{-E_r/(k_B T)}.$$

a) Use the Boltzmann distribution to show that

$$S = k_B \ln Z + \frac{\langle E \rangle}{T}.$$

b) Starting from the statistical-mechanical expression $F = -k_B T \ln Z$, establish the thermodynamic relation

$$F = \langle E \rangle - TS.$$

Problem 2. Fluctuation–dissipation theorem

For a system of N Ising spins, the susceptibility per spin $\chi = (\partial \langle M \rangle / \partial H)_T / N$ is related to magnetisation fluctuations by

$$N k_B T \, \chi = \langle M^2 \rangle - \langle M \rangle^2.$$

Using the canonical partition function and a similar derivation, prove that the specific heat per spin $c = (\partial \langle E \rangle / \partial T)_H / N$ satisfies

$$k_B T^2 c = \frac{1}{N} (\langle E^2 \rangle - \langle E \rangle^2).$$

B. Critical exponents

Problem 3. Inequality between critical exponents

The heat capacities at fixed external magnetic field and at fixed total magnetisation are, respectively,

$$C_H = T\left(\frac{\partial S}{\partial T}\right)_H, \qquad C_M = T\left(\frac{\partial S}{\partial T}\right)_M.$$

Here S and M are the total entropy and magnetisation, and $\chi_{\mathrm{tot}} = (\partial M/\,\partial H)_T$ is the total magnetic susceptibility. You are given the thermodynamic identity

$$\chi_{\mathrm{tot}}(C_H - C_M) = T\left(\frac{\partial M}{\partial T}\right)_H^2.$$

Assuming $C_M \geq 0$, establish the inequality

$$\alpha + 2\beta + \gamma \geq 2,$$

where, near the critical temperature in zero field, $C_H \propto |T - T_c|^{-\alpha}$, $M_0 \propto (T_c - T)^{\beta}$ for $T < T_c$, and $\chi_{\mathrm{tot}} \propto |T - T_c|^{-\gamma}$.

C. Diluted Ising model and percolation

Consider the bond-diluted Ising model on a regular lattice in zero external field,

$$E = -\sum_{\langle ij \rangle} J_{ij}\, s_i s_j, \qquad s_i = \pm 1,$$

where the independent nearest-neighbour couplings are distributed according to

$$J_{ij} = \begin{cases} J > 0, & \text{with probability } p, \\ 0, & \text{with probability } 1 - p. \end{cases}$$

Let p_c denote the bond-percolation threshold.

Problem 4. Percolation clusters and magnetic order

a) Explain how the diluted Ising model is related to bond percolation.

For the remaining parts, assume $T = 0$ and $H = 0$.

b) Describe the ground-state configurations of the diluted Ising model. Explain the role of the connected clusters of non-zero bonds.

c) Show that the spin–spin correlation function satisfies

$$\langle s_i s_j \rangle = \begin{cases} 1, & \text{if } i \text{ and } j \text{ belong to the same cluster,} \\ 0, & \text{otherwise,} \end{cases}$$

when the orientations of different disconnected clusters are averaged independently.

d) Explain why the spontaneous magnetisation per spin $m_0(p)$ vanishes for $p \leq p_c$. Express $m_0(p)$ for $p > p_c$ in terms of the percolation order parameter $P_\infty(p)$, the fraction of sites belonging to the infinite cluster.

Problem 5. Magnetisation and susceptibility of the diluted Ising model

At low temperatures, $k_B T \ll J$, and for a small non-zero external field H, take the magnetisation per spin to be

$$m(p,H) = \pm P_\infty(p) + \sum_{s=1}^{\infty} s\ n(s,p) \tanh\left(\frac{sH}{k_B T}\right),$$

where $n(s,p)$ is the number of finite clusters of size s per lattice site and $P_\infty(p)$ is the fraction of sites in the infinite cluster. The sign of the first term corresponds to the orientation selected by the external field.

a) Interpret physically the contribution $P_\infty(p)$. Determine the spontaneous magnetisation per spin $m_0(p)$ in the limit $H \to 0^{\pm}$.

b) Define the zero-field isothermal susceptibility per spin χ_T for $p < p_c$. Assuming $|H| \ll k_B T$, express χ_T in terms of the cluster-size distribution $n(s,p)$. Explain why it diverges as $p \to p_c$.