https://www2.physik.uni-muenchen.de/lehre/vorlesungen/sose_24/t_m1_advanced-statistical-physics/index.html

Sheet 3:

Hand-out: Friday, May. 03, 2024; Hand-in: Sunday, May. 12, 2024, 11:59 pm

Problem 1 The one-dimensional Ising model – **(solution: Central Exercise)**

In this problem, we consider the 1D Ising model described by the Hamiltonian

$$\mathcal{H} = -J \sum_{j=1}^{N-1} s_{j+1} s_j, \qquad s_j = \pm 1, \tag{1}$$

assuming open boundary conditions and $J > 0$.

Starting from (one of the two) lowest energy state(s), flipping a pair of spins on neighboring lattice sites costs an energy $\Delta E = 4J$. In contrast, flipping two spins independently at a certain distance $d > 1$ costs energy $\Delta E = 8J$. With this in mind, we can describe the system, and its energy, in terms of the locations of kinks (also called domain walls) across which the orientation of the spins changes. To obtain a single kink in the system on the link $\langle j+1, j \rangle$ between sites j and $j+1$, all spins to the left (or right) of j have to be flipped.

Thus, the energy of a configuration with n kinks is (neglecting edge effects):

$$E(N, n) = -NJ + 2nJ. \tag{2}$$

(1.a) (**2 Points**) Describe the two lowest energy spin configurations, and explain how the expression for $E(N, n)$ in Eq. (2) is obtained.

(1.b) (**3 Points**) Calculate the number of states Ω_n with exactly n kinks, at the energy $E(N, n)$, assuming $n, N \gg 1$. Calculate the corresponding entropy $S(N, n)$ of the ensemble formed by these states.

(1.c) (**3 Points**) Using the result derived in (1.b), calculate the equilibrium temperature $T = 1/k_B\beta$ of the ensemble as a function of n and N and verify that

$$\beta = -\frac{1}{J} \operatorname{artanh}\left(\frac{E}{NJ}\right). \tag{3}$$

Typically we associate high energy with high entropy – is this still the case here? If not, explain why!

(1.d) (**4 Points**) Use the formula $F(T, N, n) = E(N, n) - TS(N, n)$ for the free energy to show that for any infinitesimal $T > 0$ the system does not spontaneously magnetize.
Hint: Consider the ground states with zero kinks, and excited states with exactly one kink. Compare the resulting free energies and argue why no spontaneous magnetization is possible in the thermodynamic limit.

Problem 2 Negative temperatures – (solution: Tutorials)

In some physical systems (e.g. nuclear paramagnets), for a short period of time, the nuclear spins and underlying crystalline lattice can separately reach thermodynamic equilibrium. The necessary condition for this is that the spin-lattice relaxation time is long compared to both the individual spin and lattice relaxation times. If the system is in global equilibrium and an external parameter is suddenly changed, this can result in a transient period where the two subsystems are isolated from each other and reach equilibrium independently, characterized by different temperatures, and even a *negative* temperature for the spin lattice.

Consider the Ising spin model of a paramagnetic crystal, i.e. a system of N quantized spins in a magnetic field $\boldsymbol{B} = B\boldsymbol{e}_z$ at temperature $T = 1/k_B\beta$, described by the Hamiltonian:

$$\mathcal{H} = -\mu B \sum_{j=1}^{N} s_j, \qquad s_j = \pm 1, \tag{4}$$

where μ is the magnetic moment.

(2.a) (**2 Points**) Calculate the canonical partition function $Z(\beta, B)$ for a single spin. Give the probability $p_\uparrow$ ($p_\downarrow$) that a spin is in the "up" ("down") state with energy $\epsilon_\uparrow = -\mu B$ ($\epsilon_\downarrow = \mu B$) and the corresponding average number of spins $N_\uparrow$, $N_\downarrow$ in each state. Also determine an expression for the energy E.

(2.b) (**2 Points**) Calculate the corresponding partition function for a system of N spins $Z_N(\beta, B)$ (consider using arguments at fixed $N_\uparrow$). Use this result to confirm your previous expression for E derived in (2.a).

(2.c) (**2 Points**) Define $m = p_\uparrow - p_\downarrow$ and show that

$$\beta\mu B = \mathrm{artanh}(m) = \frac{1}{2}\ln\left(\frac{1+m}{1-m}\right). \tag{5}$$

Verify that the entropy per spin can be written in the form

$$\frac{S}{k_B N} = -\left[\left(\frac{1+m}{2}\right)\ln\left(\frac{1+m}{2}\right) + \left(\frac{1-m}{2}\right)\ln\left(\frac{1-m}{2}\right)\right]. \tag{6}$$

(2.d) (**2 Points**) Fixing the energy, plot S/k_B as a function of $E/N\mu B$ and show that there is a region of negative temperature $T < 0$. Plot $M = Nm\mu$ as a function of $\beta\mu B$ and verify that negative temperatures correspond to negative magnetizations.

(2.e) (**2 Points**) Calculate the equilibrium temperature of the spin system, and verify that it can be written as

$$\beta(E) = \frac{1}{k_B T(E)} = -\frac{1}{\mu B}\,\mathrm{artanh}\left(\frac{E}{N\mu B}\right). \tag{7}$$

(Bonus) Consider having two paramagnetic crystals (i.e. as above), such that $N_1\mu_1 > N_2\mu_2$. The two crystals are isolated from one another and independently at equilibrium, with equilibrium temperatures $\beta_1(E_1)$ and $\beta_2(E_2)$ respectively. They are then put into thermal contact – show that if entropy is maximized and if we define the "hotter" system as the one which is giving up heat to the "colder" system, then in this sense negative temperatures are "hotter" than positive temperatures.

Problem 3 Concavity of the free energy – **(solution: Central Exercise)**

In thermodynamics, one can show that it is a prerequisite for the stability of matter that thermodynamic potentials have certain convexity/concavity properties (see Chapter 2 of the lecture notes on stability conditions).

One such stability condition states that the Gibbs free energy $G = -k_B T \ln Z$ in the presence of a magnetic field H must be concave, more precisely

$$\left(\frac{\partial^2 G}{\partial H^2}\right)_T \leq 0. \tag{8}$$

(3.a) (**10 Points**) *Verify that Eq.* (8) *holds for one of our key Hamiltonians, the Ising Hamiltonian.* It is defined on a hyper cubic lattice in d dimensions (i.e. on a chain, square lattice, cubic lattice etc.) by the following Hamiltonian:

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} s_i s_j - H \sum_i s_i, \tag{9}$$

where i and j label the sites of the lattice; the first sum is over all pairs of nearest neighbor lattice sites, denoted $\langle i, j\rangle$. The spins s_i can take values $s_i = \pm 1$.

The partition function is then given by $Z = \mathrm{tr}\, \mathrm{e}^{-\beta\mathcal{H}} = \sum_{\{s\}} \mathrm{e}^{-\beta\mathcal{H}}$, where the sum is over the set of 2^N spin configurations $\{s\} = \{(s_1, s_2, \ldots, s_N)\}$, if the lattice has N sites.

Advice: Do *not* attempt to evaluate Z explicitly, unless you want to win the Nobel prize: no one has been able to do that for $d > 1$ for almost the last 100 years. Rather use that the concavity condition, Eq. (8), can also be written as

$$G(\alpha_1 H_1 + \alpha_2 H_2) \geq \alpha_1 G(H_1) + \alpha_2 G(H_2) \tag{10}$$

for $0 \leq \alpha_{1,2} \leq 1$ and $\alpha_1 + \alpha_2 = 1$ and the Hölder inequality, which can be stated as: given two sequences $\{g_k\}$, $\{h_k\}$ with $g_k, h_k \geq 0$ for all k, and two real numbers $0 \leq \alpha, \beta \leq 1$ with $\alpha + \beta = 1$, then

$$\sum_k g_k^\alpha \cdot h_k^\beta \leq \left(\sum_k g_k\right)^\alpha \cdot \left(\sum_k h_k\right)^\beta ; \tag{11}$$

you have to figure out how best to apply this result to the partition function.