Exercise set 2

AI

1 Clock model

The Hamiltonian for the M state ($\mathbb{Z}_M$) clock model reads

$$H = -J \sum_{\langle ij \rangle} \cos[(n_i - n_j)2\pi/M]; \qquad n_i = 0, \dots M-1, \tag{1}$$

corresponding to N planar rotors that can point along M directions on a plane. The case $M = 2$ corresponds to the Ising Hamiltonian.

1.1 $M = 3$

Consider the case $M = 3$ and use your favourite mean field approach to characterize the phase transition of the system, i.e. find the critical temperature and the order parameter at such a temperature. Is the transition first or second order? Discuss the approximations introduced and their validity.

Hint: for this planar system you can introduce the complex order parameter

$$\sigma \mathrm{e}^{\mathbb{i}\psi} = \frac{1}{N} \sum_i \mathrm{e}^{\mathbb{i} n_i 2\pi/M}, \tag{2}$$

where N is the total number of spins. Since all the ground states are equivalent, in the previous equation you can choose $\psi = 0$ corresponding to condensation in the state with all $n_i = 0$.

1.2 $M = 4$

Repeat the previous calculations with $M = 4$, and discuss the differences with the previous point.

2 Ising magnet in a fluctuating magnetic field

This exercise is characterized by a substantial higher level of difficulty. Give it a try, we then discuss it in class.

Consider a one-dimensional Ising model with N spins in a fluctuating magnetic field. The field h is Gaussian-distributed, with variance $\sigma^2/(N\beta)$ and zero mean.

Show that the system exhibits an order-disorder phase transition at finite temperature, and determine such a temperature.

Hints: Write first the partition function, keeping in mind that you know its expression when h is fixed.
In the thermodynamic limit, the distribution of h is very narrow, so it is safe to assume small values of h in your calculations.
As usual, for N large, integrals of the type $\mathrm{e}^{Nf(x)}$ can be solved with the saddle point approximation.

You might find useful the following Taylor expansion in h

$$\sqrt{e^{2\beta J}\sinh^2(\beta h) + e^{-2\beta J}} + e^{\beta J}\cosh(\beta h)$$
$$\simeq \ln(x + 1/x) + \frac{\beta^2 h^2 x}{2} - \frac{1}{24}\beta^4 h^4 x\left(3x^2 - 1\right); \qquad \text{with } x = \mathrm{e}^{2\beta J}$$

3 Detailed balance

A system has two energy levels with energy difference ϵ. Write the master equation for the continuous time Markov chain, in terms of the transition rates between the two energy levels. Find the eigenvalues and the eigenvectors of the corresponding matrix. Assume that the rates satisfy the detailed balance condition, and identify the physically relevant eigenvector. You can express the frequencies in units of ω_0, a microscopic attempt rate.

4 Chemical reactions

Consider the chemical reaction

$$A \rightleftharpoons B,$$

described by the kinetic equations

$$\begin{aligned}
\frac{\mathrm{d}\,[A]}{\mathrm{d}t} &= k_{AB}\,[B] - k_{BA}\,[A]\,, \\
\frac{\mathrm{d}\,[B]}{\mathrm{d}t} &= -k_{AB}\,[B] + k_{BA}\,[A]\,,
\end{aligned}$$

where $[A]$ and $[B]$ are the concentration of the two species. Show that the equilibrium concentrations $\langle [A] \rangle$ and $\langle [B] \rangle$ satisfy the detailed-balance condition

$$k_{BA}\,\langle [A] \rangle = k_{AB}\,\langle [B] \rangle\,.$$

Show that the solutions to the kinetic equation yield

$$\Delta c_A(t) = [A]\,(t) - \langle [A] \rangle = \Delta c_A(0)\mathrm{e}^{-t/\tau},$$

with

$$\frac{1}{\tau} = k_{AB} + k_{BA}.$$

5 Clock model: dynamics

Consider again the clock model with $M = 3$, now with a single ($N = 1$) rotor but in an external field, with Hamiltonian

$$H = -\vec{h} \cdot \vec{s} \tag{3}$$

with $\vec{h} = (h_x, h_y)$, $\vec{s} = (\cos n\alpha, \sin n\alpha)$, $\alpha = 2\pi/M$, $n = 0,\, 1,\, 2$.

a) Consider first the case where the jumps between the states $n = 0$ and $n = 2$ are forbidden. This corresponds to a stochastic process on a linear network with 3 states: $0 \leftrightarrows 1 \leftrightarrows 2$.

Choose the external field so as the system exhibits equispaced energy levels, and write the master equation in terms of the clockwise p and counterclockwise q transition rates, after fixing their ratio p/q according to the detailed balance condition.

Find the eigenvalues and the eigenvectors of the corresponding stochastic matrix and identify the eigenvector corresponding to the leading eigenvalue.

b) Consider now the case where the rotor is allowed to "jump" between the states $n = 0$ and $n = 2$ in both directions with the corresponding rates

p and q: $0 \leftrightarrows 1 \leftrightarrows 2 \leftrightarrows 0$, i.e. a three-state network with a loop structure. Write the new stochastic matrix, find its eigenvalues and the eigenvectors. Identify the eigenvector corresponding to the leading eigenvalue. Discuss the difference with the point a).

Can you use the same stochastic matrix to describe a non-thermally activated stochastic system?

6 Three-state loop

Consider a three-state network with a loop structure, and generic transition rates $k_{nn'}$, n, $n' = 0, 1, 2$.

Show that the steady state solution to the master equation satisfies the detailed balance condition if the following condition holds

$$k_{n_0 n_3} k_{n_3 n_2} k_{n_2 n_1} k_{n_1 n_0} = k_{n_0 n_1} k_{n_1 n_2} k_{n_2 n_3} k_{n_3 n_0} \tag{4}$$