Statistical Physics of Computation 2025 - Exercises

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Week 2

2.1 Blume-Capel model

Consider the following variation of the Curie-Weiss model with spin 1:

$$H[s] = -\frac{1}{2N}\sum_{i,j} s_i s_j + \Delta \sum_i s_i^2 \tag{1}$$

where $\Delta > 0$, $s_i \in \{-1, 0, 1\}$ and $i = 1 \dots N$. In the following we will use the physics naming conventions: a configuration is a specific choice of spins $s \in \{-1, 0, 1\}^N$. A ground state is a configuration that minimizes the energy $H[s]$. A paramagnetic configuration is a configuration such that $\frac{1}{N}\sum_i s_i = 0$ (i.e. with zero magnetisation), and a ferromagnetic one is such that $\frac{1}{N}\sum_i s_i \neq 0$ (i.e. with non-zero magnetisation). Notice that contrary to the Curie-Weiss model, in the Blume-Capel model there are paramagnetic configurations in which all spins are aligned, such as $s_i = 0$ for all i.

2.1.1 Physical intuition

1. Argue that at zero temperature the Gibbs distribution concentrates on the ground states (for generic H, not necessarily the one of the exercise), i.e. it assigns the same weight to the ground state configurations and zero probability to all others.

2. Argue that at infinite temperature the spins are distributed uniformly in their domain (for generic H, not necessarily the one of the exercise).

3. Consider the $\Delta = 0$ case.

   - Compute the ground state.
   - Compute the average magnetization and energy density (energy divided by the number of spins) at zero temperature. If there are multiple configurations in the ground state, you can consider adding an infinitesimal bias for one of them, i.e. consider adding a perturbation to the Hamiltonian that lifts the degeneracy favoring one specific ground state.
   - Compute the average magnetization and energy at infinite temperature (for $N \gg 1$).
   - Draw a guess for the phase diagram as a function of the temperature, and recognize a ferromagnetic and paramagnetic phase.

4. Now consider the general $\Delta > 0$ case. Show that you can have a paramagnetic ground state at large N. How does this ground state look like? (Hint: try to compute the energy for a **special** paramagnetic state, and show it's actually lower than the two ground states you

found for $\Delta = 0$ for a certain choice of parameters). Draw a guess for the phase diagram and recognize the ferromagnetic and paramagnetic phase.

2.1.2 Phase diagram with the canonical ensemble

In this section we obtain an asymptotic description of the system in the large N limit. To do this, we compute the partition function $\mathcal{Z}$:

$$\mathcal{Z} = \sum_s e^{-\beta H[s]} \tag{2}$$

where $\beta = 1/T$ is the inverse of the temperature and $\sum_s$ is the sum **over all possible values** of $\mathbf{s}$.

1. Introduce the magnetisation using a Dirac delta and its Fourier representation to obtain the expression

$$\mathcal{Z} = \int \mathrm{d}m\, \mathrm{d}\hat{m} \sum_s \exp\left\{ \frac{N}{2}\beta m^2 + Nm\hat{m} + \sum_i \left(-\beta\Delta s_i^2 - s_i\hat{m}\right) \right\} \tag{3}$$

2. Sum over the spins to write

$$\mathcal{Z} = \int \mathrm{d}m\, \mathrm{d}\hat{m} e^{Nf(m,\hat{m})} \tag{4}$$

   where

$$f(m,\hat{m}) = \frac{\beta m^2}{2} + m\hat{m} + \log\left(1 + 2e^{-\beta\Delta}\cosh\hat{m}\right) \tag{5}$$

3. Show that in the large N limit that the magnetisation m obeys the state equation

$$\frac{2e^{-\beta\Delta}\sinh\beta m}{1 + 2e^{-\beta\Delta}\cosh\beta m} = m \tag{6}$$

4. Does the state equation admit a paramagnetic solution? At which temperatures?

5. Take $\Delta = 0.3$ and $\Delta = 0.49$ and plot numerically $f(m,\hat{m})$ as a function of the magnetisation and at the saddle point for different values of the temperature. Use the programming language / plotting software that you prefer. Which value of Δ has a second order phase transition and which has a first order one?

6. Obtain the critical temperature, i.e. the temperature at which the paramagnetic minimum at $m = 0$ of $g(m)$ changes concavity and becomes a local maximum, at $\Delta = 0$. You can assume that at $\Delta = 0$, and in a neighbourhood of it, the behaviour is qualitatively the same as the one that you observed for $\Delta = 0.3$ in the previous point. What can we say about generic Δ?

7. Use all your knowledge to make a better sketch of the phase diagram

8. Consider $\Delta > 1/2$. We know we are in a paramagnetic $m = 0$ phase. Is it the one with random spins or with $s = 0$? Study this looking at the observable q:

$$q = \frac{1}{N}\sum_i s_i^2 \tag{7}$$

   Show that q concentrates around the derivative of the free energy

$$q = -\frac{1}{\beta N \mathcal{Z}}\frac{\partial}{\partial\Delta}e^{-\beta H[s]} = \frac{2e^{-\Delta/T}}{1 + 2e^{-\Delta/T}} \tag{8}$$