Statistical Physics of Computation - Exercises

Emanuele Troiani, Vittorio Erba

September 2024

Week 2

2.1 Blume-Capel model

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

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

where $\Delta > 0$, $s_i \in \{-1, 0, 1\}$ and the model has N spins. In the following we will use the physics naming conventions: a configuration is a specific choice of spins $\mathbf{s} \in \{-1, 0, 1\}^N$. A ground state is a configurations that minimise the energy $H[\mathbf{s}]$. 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, i.e. it assigns the same weight to the ground state configurations and zero probability to all others.

   Write the partition function as

   $$\mathcal{Z} = \int \mathrm{d}E e^{-\beta E + S(E)} \tag{2}$$

   The energy is integrated over all the values of the energy that the system can achieve. If the temperature is zero, then β is infinitely large and the integral is dominated by the minima of the energy. Thus, the Gibbs distribution has non-zero probability only on the minima of the energy.

2. Argue that at infinite temperature the spins are distributed uniformly in their domain.

   One can just write the Boltzmann weights as

   $$e^{-\beta H[\mathbf{s}]} \tag{3}$$

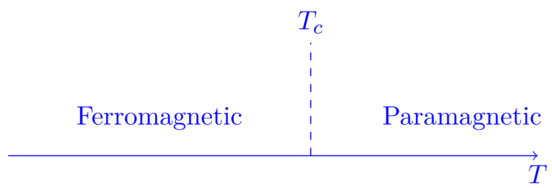
   If the temperature is infinite then $\beta = 0$, so the weights are all 1, and they are then uniform.

3. Consider the $\Delta = 0$ case. Which is the ground state? Compute the magnetisation at zero and infinite temperature in the large N limit. Draw a guess for the phase diagram and recognize the ferromagnetic and paramagnetic phase. 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.

   The ground state is the one with minimal energy, which would maximise all the couples $s_i s_j$. For this one need $s_i = s_j \neq 0$. We are thus free to take all the spins identical to 1 or -1. We choose to bias the positive spin configuration, i.e. take an infinitesimal positive external magnetic field, so the magnetisation would be $m = +1$ as the spins all have the same value $+1$. Note that the energy in this state is $-N/2$. In the high temperature limit the spins are equally distributed (as there is no interaction in the Gibbs measure), so that each spin is distributed uniformly in $\{-1, 1, 0\}$ and the magnetisation is zero. Note that the energy density is also zero

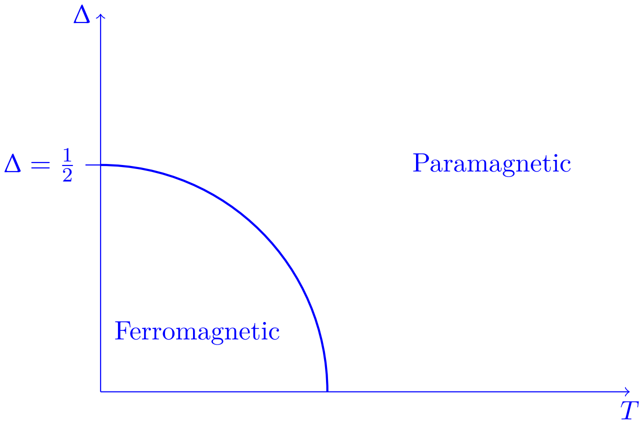
$$e = \left\langle \frac{1}{2N^2} \sum_{i,j} s_i s_j \right\rangle = \left\langle \frac{1}{2N^2} \sum_{i} s_i^2 \right\rangle \to 0 \tag{4}$$

   where the angular average is the average w.r.t. the Gibbs measure at large temperature. The phase diagram then seems to have 2 phases, a ferromagnetic phase for low temperature, and a paramagnetic phase for large temperature.



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.

   The interaction term in Δ makes it such that spins equal to 1 or -1 bring a positive energy contribution. In particular the energy of the all one (or all minus one) configuration will be $(\Delta - 1/2)N$. We now consider paramagnetic states with $\mathbf{s} = \mathbf{0}$ with energy 0. What happens at low temperature? We will be in the lowest energy state as a function of Δ, which means that for $\Delta > 1/2$ we can conjecture we will be in the paramagnetic state, and viceversa. Thus, we have a guess for the phase diagram at $T = 0$ from this point, and a guess for the phase diagram at $\Delta = 0$ from the previous point, which allows us to guess the complete phase diagram.



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 $\mathcal{Z}$:

$$\mathcal{Z} = \sum_s e^{-\beta H[\mathbf{s}]} \tag{5}$$

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

$$\mathcal{Z} = \int \mathrm{d}m\, \mathrm{d}\hat{m} \sum_s \exp\left\{ \frac{N}{2}\beta m^2 + Nm\hat{m} + \sum_i \left(-\beta\Delta s_i^2 - s_i\hat{m}\right) \right\} \tag{6}$$

One can proceed as for the Curie Weiss model. It's important to normalise the argument of the Dirac delta correctly to have it of order $\mathcal{O}(N)$.

$$\mathcal{Z} = \sum_s \exp\left\{ \frac{\beta}{2N} \sum_{i,j} s_i s_j - \beta\Delta \sum_i s_i^2 \right\} = \tag{7}$$

$$= \sum_s \exp\left\{ \frac{N}{2} \left(\frac{1}{N} \sum_i s_i \right)^2 - \beta\Delta \sum_i s_i^2 \right\} = \tag{8}$$

$$= \int \mathrm{d}m \sum_s \exp\left\{ \frac{N}{2}\beta m^2 - \beta\Delta \sum_i s_i^2 \right\} \delta\left(Nm - \sum_i s_i \right) = \tag{9}$$

$$= \int \mathrm{d}m\, \mathrm{d}\hat{m} \sum_s \exp\left\{ \frac{N}{2}\beta m^2 - \beta\Delta \sum_i s_i^2 + Nm\hat{m} - \sum_i s_i\hat{m} \right\} = \tag{10}$$

$$= \int \mathrm{d}m\, \mathrm{d}\hat{m} \sum_s \exp\left\{ \frac{N}{2}\beta m^2 + Nm\hat{m} + \sum_i \left(-\beta\Delta s_i^2 - s_i\hat{m}\right) \right\} \tag{11}$$

2. Sum over the spins to write

$$\mathcal{Z} = \int \mathrm{d}m\, \mathrm{d}\hat{m} e^{Nf(m,\hat{m})} \tag{12}$$

where

$$f(m,\hat{m}) = \frac{\beta m^2}{2} + m\hat{m} + \log\left(1 + 2e^{-\beta\Delta}\cosh\hat{m}\right) \tag{13}$$

One really just needs to sum over the values of the spin. The key idea here is to show that the different spins are decoupled.

$$\mathcal{Z} = \int \mathrm{d}m\, \mathrm{d}\hat{m} \sum_s \exp\left\{\frac{N}{2}\beta m^2 + Nm\hat{m} + \sum_i \left(-\beta\Delta s_i^2 - s_i\hat{m}\right)\right\} = \tag{14}$$

$$= \int \mathrm{d}m\, \mathrm{d}\hat{m} \exp\left\{\frac{N}{2}\beta m^2 + Nm\hat{m}\right\} \sum_s \exp\left\{\sum_i \left(-\beta\Delta s_i^2 - s_i\hat{m}\right)\right\} = \tag{15}$$

$$= \int \mathrm{d}m\, \mathrm{d}\hat{m} \exp\left\{\frac{N}{2}\beta m^2 + Nm\hat{m}\right\} \left(\sum_{s_i} \exp\left\{-\beta\Delta s_i^2 - s_i\hat{m}\right\}\right)^N = \tag{16}$$

$$= \int \mathrm{d}m\, \mathrm{d}\hat{m} \exp\left\{\frac{N}{2}\beta m^2 + Nm\hat{m}\right\} \left(1 + e^{-\beta\Delta - \hat{m}} + e^{-\beta\Delta + \hat{m}}\right)^N = \tag{17}$$

$$= \int \mathrm{d}m\, \mathrm{d}\hat{m} \exp\left\{\frac{N}{2}\beta m^2 + Nm\hat{m}\right\} \left(1 + 2e^{-\beta\Delta}\cosh\hat{m}\right)^N \tag{18}$$

$$= \int \mathrm{d}m\, \mathrm{d}\hat{m} \exp\left\{\frac{N}{2}\beta m^2 + Nm\hat{m} + N\log\left(1 + 2e^{-\beta\Delta}\cosh\hat{m}\right)\right\} \tag{19}$$

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

$$\frac{2e^{-\beta\Delta}\sinh\beta m}{1 + 2e^{-\beta\Delta}\cosh\beta m} = m \tag{20}$$

We can use the saddle point method to obtain two equations for m and $\hat{m}$:

$$\frac{\partial f(m,\hat{m})}{\partial m} = 0\,, \qquad \frac{\partial f(m,\hat{m})}{\partial \hat{m}} = 0 \tag{21}$$

Doing the computation we get

$$\hat{m} = -\beta m \tag{22}$$

which we can plug back in to get

$$g(m) = f(m, -\beta m) = -\frac{\beta m^2}{2} + \log\left(1 + 2e^{-\beta\Delta}\cosh\beta m\right) \tag{23}$$

We now do another derivative to get

$$\frac{2e^{-\beta\Delta}\sinh\beta m}{1 + 2e^{-\beta\Delta}\cosh\beta m} = m \tag{24}$$

4. Find one (easy) solution of the state equation. By direct substitution $m = 0$ is always solution

5. Take $\Delta = 0.3$ and $\Delta = 0.49$ and plot numerically $g(m)$ as a function of the magnetisation 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?

   We have shown in Figures 2 and 1 the two cases. For $\Delta = 0.3$ we can see that the minimum shifts smoothly from ± 1 to 0 as one increases the temperature. This is the sign of a second order phase transition. On the other hand, for $\Delta = 0.49$ increasing the temperature makes the two ± 1 minima less deep. As soon as they are less deep than the one in 0, the magnetisation changes value abruptly, signalling a first order transition.

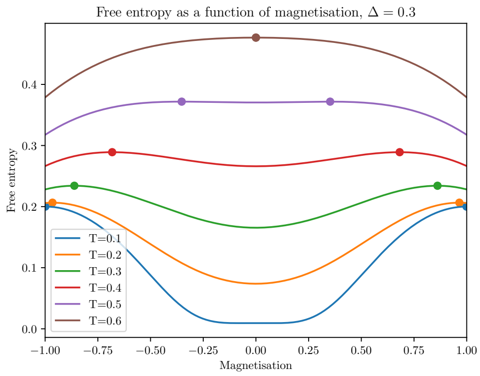


Figure 1: Second order phase transition

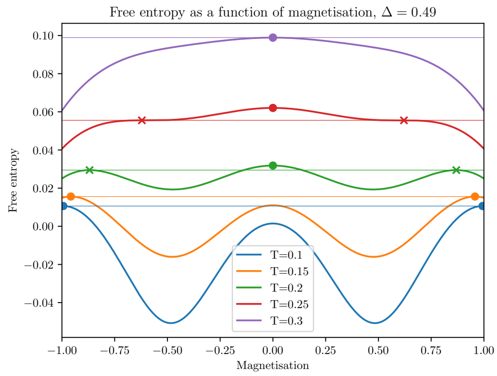


Figure 2: First order phase transition

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?

   The configuration with $m = 0$ is the dominant one if it's a maximum of the free entropy. The condition such that this is true is that $g''(0) < 0$. We thus find a condition for the critical temperature by imposing $g''(0) = 0$. After a tedious computation one can show that

$$g''(0) = \frac{2e^{-\Delta/T}}{T + 2e^{-\Delta/T}} - 1 \tag{25}$$

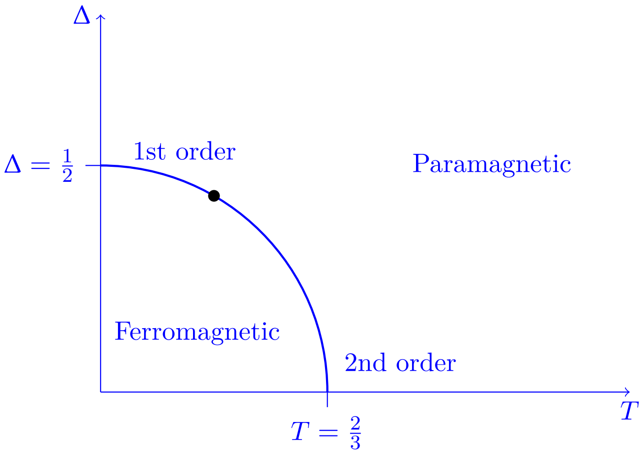
   We can just impose our condition $g''(0) = 0$ to obtain

$$e^{\Delta/T_C} = 2\left(\frac{1}{T_C} - 1\right) \tag{26}$$

   Which for $\Delta = 0$, predicts the temperature $T_C = 2/3$. Notice we don't actually need to impose $\Delta = 0$, the formula we just derived for the critical temperature is true for any value of Δ that has a second order transition (and breaks for a first order one).

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

We can add more information on the transition line: one portion close to the $T = 0$ axis is going to be the first order transition, the other is the second order transition line. For the latter we have derived a curve. In the figure we just give a qualitative display of the line.



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

$$q = \frac{1}{N} \sum_i s_i^2 \tag{27}$$

Show that q concentrates around the derivative of the free energy

$$q = -\frac{1}{\beta N \mathcal{Z}} \frac{\partial}{\partial \Delta} e^{-\beta H[\mathbf{s}]} = \frac{2e^{-\Delta/T}}{1 + 2e^{-\Delta/T}} \tag{28}$$

What we show here is a very generic way of studying an observable. First we write the definition of q in our model

$$\langle q \rangle = \frac{1}{N\mathcal{Z}} \sum_s \left(\sum_i s_i^2 \right) \exp\left\{ \frac{\beta}{2N} \sum_{i,j} s_i s_j - \beta\Delta \sum_i s_i^2 \right\} = \tag{29}$$

$$= -\frac{1}{\beta N\mathcal{Z}} \sum_s \frac{\partial}{\partial \Delta} \exp\left\{ \frac{\beta}{2N} \sum_{i,j} s_i s_j - \beta\Delta \sum_i s_i^2 \right\} = \tag{30}$$

$$= -\frac{1}{\beta N\mathcal{Z}} \frac{\partial}{\partial \Delta} \sum_s \exp\left\{ \frac{\beta}{2N} \sum_{i,j} s_i s_j - \beta\Delta \sum_i s_i^2 \right\} = \tag{31}$$

$$= -\frac{1}{\beta N\mathcal{Z}} \frac{\partial}{\partial \Delta} e^{Ng(m^*)} \tag{32}$$

$$\tag{33}$$

where in the last step we used the whole computation done in the central part of the exercise, m^* is the solution of the state equation. Now we impose $m^* = 0$, because that is the solution of the state equation in the paramagnetic phase, which means

$$g(0) = -\log\left(1 + 2e^{-\beta\Delta}\right) \tag{34}$$

Similarly, the partition function $\mathcal{Z}$ at $m^* = 0$ is

$$\mathcal{Z} = e^{Ng(0)} = \left(1 + 2e^{-\beta\Delta}\right)^N \tag{35}$$

Now we plug these two facts in

$$q = -\frac{1}{\beta N \mathcal{Z}} \frac{\partial}{\partial \Delta} e^{Ng(m^*)} = -\frac{1}{\beta N \mathcal{Z}} \frac{\partial}{\partial \Delta} \left(1 + 2e^{-\beta\Delta}\right)^N = \frac{2e^{-\beta\Delta}}{1 + 2e^{-\beta\Delta}} \tag{36}$$

Thus we have shown that at low temperatures (i.e. $\beta \to \infty$ the paramagnetic phase becomes ordered, as $q \to 1$.