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.

   Consider the Gibbs distribution
   $$p(s) \propto e^{-\beta H[s]} \,. \tag{2}$$
   Suppose that H^* is the minimum of the energy, and that s^* is one minimizer. Then
   $$p(s) = e^{-\beta(H[s]-H^*)} p(s^*) \,. \tag{3}$$
   Thus, is s is not a minimizer, it is given probability zero if $\beta \gg 1$, while if s is a minimizer, it is given the same probability as s^*, implying that the Gibbs measure is uniform over the minimizer.

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

   Consider the Gibbs distribution
   $$p(s) \propto e^{-\beta H[s]} \,. \tag{4}$$
   If the temperature is infinite then $\beta = 0$, so that all configurations are given the same probability.

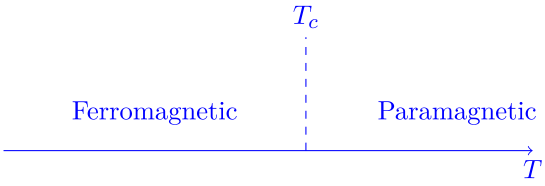
3. Consider the $\Delta = 0$ case.

- 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.

- The ground state is the configuration 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. Then the average magnetization is given by $m = +1$ as the spins all have the same value $+1$, and the average energy density is given by $e = -1/2$.
- In the high temperature limit the Gibbs measure is the uniform measure, meaning that all spins are uniformly and independently distributed are equally distributed over $\{-1, 1, 0\}$. Thus $m = 0$ and

$$e = \left\langle \frac{1}{2N^2} \sum_{i,j} s_i s_j \right\rangle = \left\langle \frac{1}{2N^2} \sum_{i} s_i^2 \right\rangle \to 0 \tag{5}$$

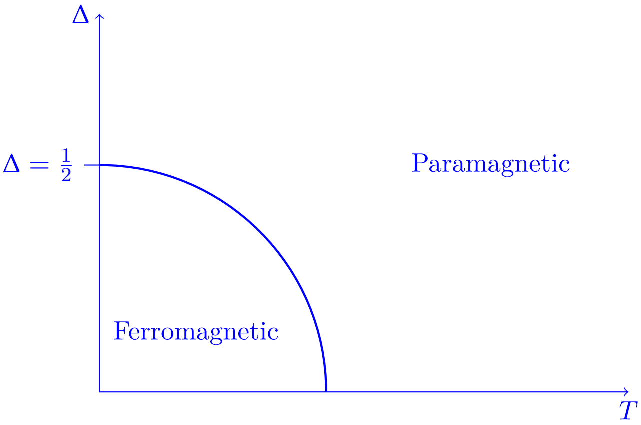
  where the limit is for large N.
- The phase diagram then seems to have 2 phases, a ferromagnetic phase for low temperature, and a paramagnetic phase for large temperature. Notice that from this analysis we do not know if there is a phase transition, of simply a smooth cross-over between the high-temperature paramagnetic phase and the low-temperature ferromagnetic phase. We also cannot guarantee that there are not other phases at intermediate values of T. To clarify this, we need to solve the model.



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 $(\Delta - 1/2)N$. On the other hand, the state $s_i = 0$ has energy 0 and is paramagnetic.

For large enough Δ, we see that this paramagnetic state not only has lower energy than the ferromagnetic ground states we found at $\Delta = 0$, but is also the only possible ground state, as any non-zero spin would increase the energy by Δ.
Thus, we have a guess for the phase diagram at $T = 0$, and a guess for the phase diagram at $\Delta = 0$ from the previous subexercise, which allows us to guess the complete phase diagram (again, only a guess, we need to compute!).



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 $\mathcal{Z}$:

$$\mathcal{Z} = \sum_s e^{-\beta H[s]} \tag{6}$$

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

$$\mathcal{Z} = \int \mathrm{d}m \, \mathrm{d}\hat{m} \sum_s \exp\left\{ \frac{N}{2}\beta m^2 + N m \hat{m} + \sum_i \left(-\beta \Delta s_i^2 - s_i \hat{m} \right) \right\} \tag{7}$$

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 $\mathcal{O}(N)$.

$$\mathcal{Z} = \sum_s \exp\left\{ \frac{\beta}{2N} \sum_{i,j} s_i s_j - \beta\Delta \sum_i s_i^2 \right\} = \tag{8}$$

$$= \sum_s \exp\left\{ \frac{N}{2} \left(\frac{1}{N} \sum_i s_i \right)^2 - \beta\Delta \sum_i s_i^2 \right\} = \tag{9}$$

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

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

$$= \int \mathrm{d}m\, \mathrm{d}\hat{m} \sum_s \exp\left\{ \frac{N}{2}\beta m^2 + Nm\hat{m} + \sum_i \left(-\beta\Delta s_i^2 - s_i \hat{m} \right) \right\} \tag{12}$$

2. Sum over the spins to write

$$\mathcal{Z} = \int \mathrm{d}m\, \mathrm{d}\hat{m} e^{Nf(m,\hat{m})} \tag{13}$$

where

$$f(m,\hat{m}) = \frac{\beta m^2}{2} + m\hat{m} + \log\left(1 + 2e^{-\beta\Delta} \cosh \hat{m} \right) \tag{14}$$

The idea here is to show that the different spins are decoupled.

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

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

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

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

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

$$= \int \mathrm{d}m\, \mathrm{d}\hat{m} \exp\left\{ \frac{N}{2}\beta m^2 + Nm\hat{m} + N \log\left(1 + 2e^{-\beta\Delta} \cosh \hat{m} \right) \right\} \tag{20}$$

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

$$\frac{2e^{-\beta\Delta} \sinh \beta m}{1 + 2e^{-\beta\Delta} \cosh \beta m} = m \tag{21}$$

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

$$\frac{\partial f(m,\hat{m})}{\partial m} = 0\,, \qquad \frac{\partial f(m,\hat{m})}{\partial \hat{m}} = 0 \tag{22}$$

Doing the computation we get

$$\hat{m} = -\beta m \tag{23}$$

which we can plug back in to get

$$g(m) = f(m, -\beta m) = -\frac{\beta m^2}{2} + \log\left(1 + 2e^{-\beta\Delta}\cosh\beta m\right) \tag{24}$$

We now do another derivative to get

$$\frac{2e^{-\beta\Delta}\sinh\beta m}{1 + 2e^{-\beta\Delta}\cosh\beta m} = m \tag{25}$$

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

   Yes, by direct substitution $m = 0$ is a solution at all 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?

   We have shown in Figures 1 and 2 the two cases. For $\Delta = 0.3$ we can see that the global maxima shift 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 local maximum at $m = 0$ grow in height, until it becomes the global maximum. As soon as the maximum on $m = 0$ becomes the global maximum, the value of magnetization associated to the global maximum changes discontinuously, signaling a first order transition.

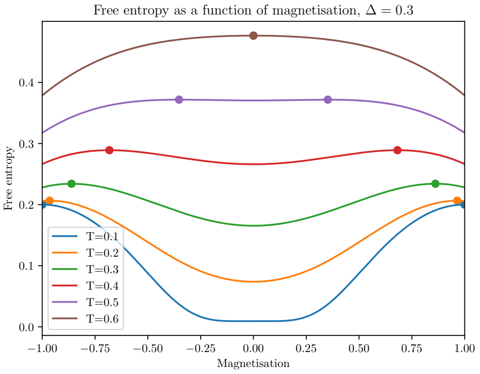


Figure 1: Second order phase transition

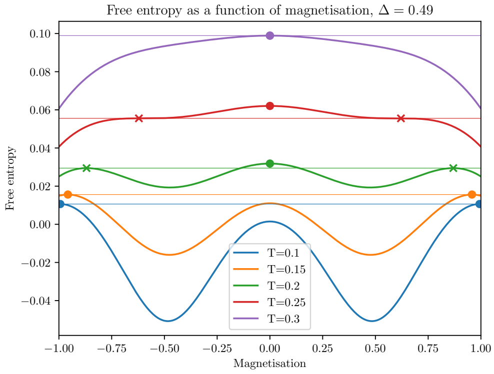


Figure 2: First order phase transition

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

   $$g''(0) = \frac{2e^{-\Delta/T}}{T + 2e^{-\Delta/T}} - 1 \tag{26}$$

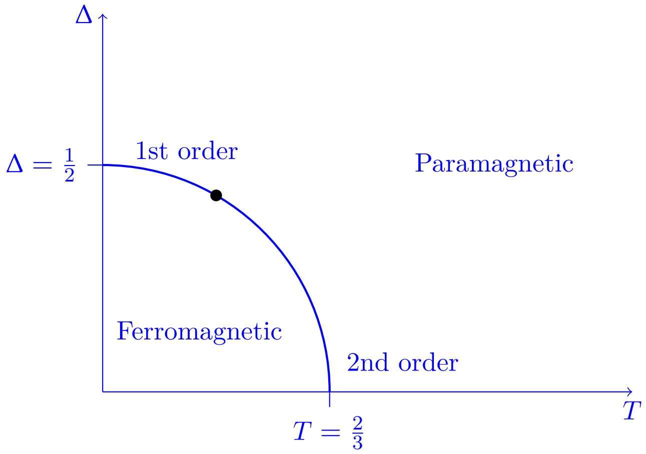
   We can just impose our condition $g''(0) = 0$ to obtain

   $$e^{\Delta/T_C} = 2\left(\frac{1}{T_C} - 1\right) \tag{27}$$

   Which for $\Delta = 0$, predicts the temperature $T_C = 2/3$. For larger Δ, the critical temperature will satisfy the same equations, provided that for that value of Δ the transition is still continuous. A thorough assessment would require the full study of f.

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. In the figure we just give a qualitative display of the transition 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 $s = 0$? Study this looking at the observable q:

   $$q = \frac{1}{N}\sum_i s_i^2 \tag{28}$$

   Show that q concentrates around the derivative of the free energy

   $$q = -\frac{1}{\beta N \mathcal{Z}}\frac{\partial}{\partial \Delta} e^{-\beta H[s]} = \frac{2e^{-\Delta/T}}{1 + 2e^{-\Delta/T}} \tag{29}$$

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

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

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

$$= -\frac{1}{\beta N \mathcal{Z}} \frac{\partial}{\partial \Delta} \sum_s \exp \left\{ \frac{\beta}{2N} \sum_{i,j} s_i s_j - \beta\Delta \sum_i s_i^2 \right\} = \tag{32}$$

$$= -\frac{1}{\beta N \mathcal{Z}} \frac{\partial}{\partial \Delta} e^{N g(m^*)} \tag{33}$$

$$\tag{34}$$

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

$$g(0) = -\log\left(1 + 2e^{-\beta\Delta}\right) \tag{35}$$

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

$$\mathcal{Z} = e^{N g(0)} = \left(1 + 2e^{-\beta\Delta}\right)^N \tag{36}$$

Now we plug these two facts in

$$q = -\frac{1}{\beta N \mathcal{Z}} \frac{\partial}{\partial \Delta} e^{N g(m^*)} = -\frac{1}{\beta N \mathcal{Z}} \frac{\partial}{\partial \Delta} \left(1 + 2e^{-\beta\Delta}\right)^N = \frac{2e^{-\beta\Delta}}{1 + 2e^{-\beta\Delta}} \tag{37}$$

Thus we have shown that at low temperatures (i.e. $\beta \to \infty$) the paramagnetic phase becomes ordered, as $q \to 0$.