

Statistical Physics

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# ISING MODEL WITH SUPER LONG-RANGE INTERACTIONS

ANALYTIC ANALYSIS AND MONTE CARLO SIMULATIONS

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# Motivation and Introduction

This project was initially conceived as an optional deliverable for my Statistical Physics course.

The main idea of the long range interaction Ising model is that spins interact with other spins that are far away, not only with their immediate neighbours. In this case, I will model a system in which all spins interact with *all* other spins with the same strength, what I call *super long-range interactions*.

The project will begin by an analytical exploration of the model. I will find general expressions for some important thermodynamical properties, like heat capacity and magnetic susceptibility, and justify the existence of a phase transition for the particular case of zero field. Next, I will present the results obtained by the Monte Carlo simulations. These will include the heat capacity and the magnetic susceptibility of the finitely sized simulations. The goal is to analyze the behaviour for finite systems and to compare the results with the analytical predictions for infinite systems.

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# 1 Analytic analysis

We consider a set of  $N$  spins, where each can point either up or down. As said in the introduction, we assume that all spins interact with *all* other spins, with the same strength. This is what we call *super long range interactions*. Additionally we consider the effect of an external constant magnetic field  $H$ . It is useful to note that due to the nature of the interactions the spatial distribution of spins is not relevant, and we can equivalently think of the system as a lattice or a chain.

We will analyze the Hamiltonian of the system, as well as some useful thermodynamic properties such as magnetization, energy, entropy and the Helmholtz free energy. Next, we will find the relationship with temperature, and after that we will find general expressions for the heat capacity and magnetic susceptibility. We will explore in detail the phase transition that occurs for the particular case of zero-field. Finally, we will qualitatively assess the behavior for the cases of non zero field.

## 1.1 Hamiltonian

Each spin is represented by a discrete variable  $s_i$  that is either 1 (up) or  $-1$  (down), and  $\{s_i\}$  defines a particular state or configuration of the system. The Hamiltonian that describes such a system is:

$$\mathcal{H}(\{s_i\}) = \frac{-J}{N} \sum_{i=1}^{N-1} \sum_{j>i}^N s_i s_j - H \sum_{i=1}^N s_i \quad (1)$$

The term  $J > 0$  represents the strength of the interaction between spins, and is always positive, characteristic of ferromagnetic interactions. Note that the  $N$  in the denominator is necessary to ensure the extensive behaviour of the energy in the thermodynamic limit.

## 1.2 Magnetization and energy

The total magnetization of the system  $M$  for a given configuration is defined as the sum of all the spins, and the mean magnetization per spin  $m$  is simply  $M/N$ :

$$M = M(\{s_i\}) = \sum_{i=1}^N s_i \quad , \quad m = M/N$$

With this definition, an important relation can now be found. Note that:

$$M^2 = \sum_{i=1}^N \sum_{j=1}^N s_i s_j = \sum_{i=1}^N s_i^2 + 2 \sum_{i=1}^{N-1} \sum_{j>i}^N s_i s_j = \sum_{i=1}^N s_i^2 - 2 \frac{N}{J} (\mathcal{H}(\{s_i\}) + HM)$$

The term summing the squared spins is simply equal to  $N$ , since each spin is either 1 or  $-1$ , and thus  $s_i^2 = 1$ . Note also that the Hamiltonian is simply the total energy  $E$  of the given configuration. We thus arrive to an extremely useful constraint:

$$E = \frac{J}{2} - HM - \frac{J}{2N} M^2 \quad (2)$$

This equation relates the total energy of the system with the total magnetization, for a given configuration of spins  $\{s_i\}$ . We will exploit this relation extensively.

We may also take the thermodynamical limit  $N \rightarrow \infty$  and write it in terms of  $m$ :

$$E \approx -NJ \left( \frac{H}{J} m + \frac{1}{2} m^2 \right) \quad (3)$$

### 1.3 Entropy

We will find the entropy through the microcanonical partition function. First, note that we can find an expression for the degeneracy for a given magnetization  $M$ . This is equivalent to counting all the configurations of the system that result in the same magnetization.

A given state of magnetization  $M$  uniquely corresponds to a number of positive spins  $N_+$  and a number of negative spins  $N_-$ . In fact:

$$M = N_+ - N_- \quad \text{and} \quad N = N_+ + N_-$$

The degeneracy of a given state of  $M$   $w(M)$  thus corresponds to the number of different ways that we can arrange the  $N_+$  spins out of the  $N$  spins (or equivalently  $N_-$  out of  $N$ ). Writing  $N_+$  in terms of  $M$  and  $N$ , this is simply:

$$w(M) = \binom{N}{N_+} = \binom{N}{N_-} = \frac{N!}{N_+!(N - N_+)!} = \frac{N!}{(\frac{N+M}{2})!(\frac{N-M}{2})!}$$

We can now find the microcanonical partition function of the system, which simply corresponds to the degeneracy of a state with energy  $E$ . Assuming that the sign of  $M$  is the same as that of  $H$ , note that due to the symmetry of the problem for every energy  $E$  there are two compatible values of  $M$ . This is also seen in 2. Using this reasoning, we arrive to the partition function:

$$\Omega(E) = 2w(M) = 2 \frac{N!}{(\frac{N+M}{2})!(\frac{N-M}{2})!}$$

The entropy of the system will then be:

$$S = k_B \ln \Omega = k_B \ln \left( \frac{2 \cdot N!}{(\frac{N+M}{2})!(\frac{N-M}{2})!} \right)$$

Taking the thermodynamic limit ( $N \rightarrow \infty$ ) and using Stirling's formula (we neglect a term  $\ln 2$ ):

$$S \approx k_B \left[ N \ln N - \frac{N+M}{2} \ln \left( \frac{N+M}{2} \right) - \frac{N-M}{2} \ln \left( \frac{N-M}{2} \right) \right]$$

Or rearranging in a more elegant manner in terms of  $m$ :

$$S(N, m) \approx -N \frac{k_B}{2} \ln \left( \frac{(1-m)^{1-m} (1+m)^{1+m}}{4} \right) \quad (4)$$

Note that as  $m \rightarrow \pm 1$ ,  $S \rightarrow 0$ .

### 1.4 Helmholtz free energy

The question of what states are stable and physical can be answered by referring to the Helmholtz potential. Systems at constant temperature (and volume) stabilize to the minima of this function:

$$A = E - TS \approx \frac{J}{2} - HM - \frac{J}{2N} M^2 - k_B T \left[ N \ln N - \frac{N+M}{2} \ln \left( \frac{N+M}{2} \right) - \frac{N-M}{2} \ln \left( \frac{N-M}{2} \right) \right]$$

We can rewrite it in terms of  $m$ , and ignoring a term  $1/N$  since we are in the context of the thermodynamic limit, we obtain:

$$A(N, m, J, T, H) \approx -NJ \left[ \frac{1}{2} m^2 + \frac{H}{J} m - \frac{T k_B}{2J} \ln \left( \frac{(1-m)^{1-m} (1+m)^{1+m}}{4} \right) \right] \quad (5)$$

Note how the domain is restricted to  $|M| \leq N$  (or  $|m| \leq 1$ ). The following is a plot of this function to gain a feeling of the minima of the potential for different values of  $H$  and  $T$ . A rigorous analysis for the particular case  $H = 0$  will be carried out in a later section.

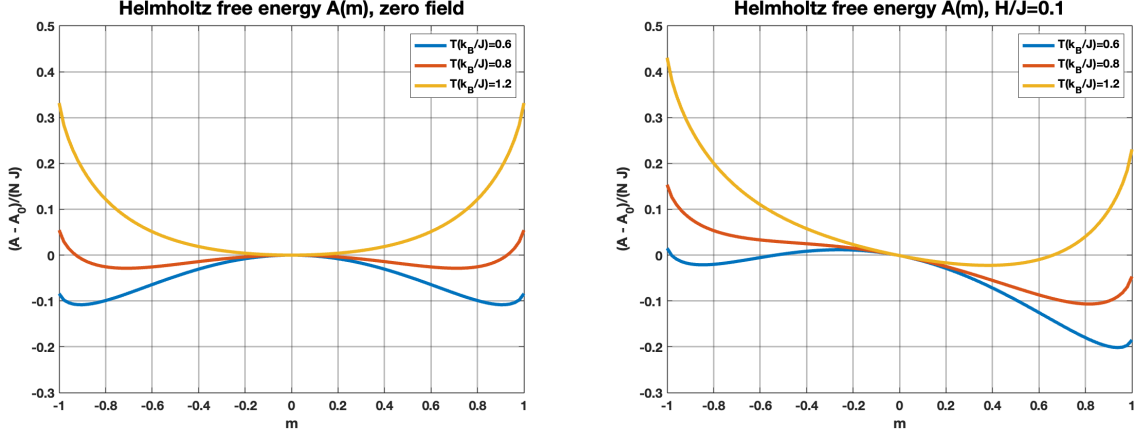


Figure 1: Helmholtz free energy

## 1.5 Relationship with temperature

Now that we have an expression for the entropy of the system, we can find a relationship between the magnetization  $M$  (or  $m$ ) and the temperature  $T$ . We may also find this same equation by looking for the minima of the Helmholtz potential, but instead we will do it through the entropy. Starting from one of the definitions of temperature, and applying the chain rule, we have:

$$\frac{1}{T} = \left. \frac{\partial S}{\partial E} \right|_N = \left. \frac{\partial S}{\partial M} \right|_N \left. \frac{\partial M}{\partial E} \right|_N$$

The first term can be computed from 1.3, and leaving out details, results in:

$$\left. \frac{\partial S}{\partial M} \right|_N = \frac{k_B}{2} \ln \left( \frac{N - M}{N + M} \right)$$

The second term can be computed from 2, assuming it defines  $M$  as a function of  $E$  implicitly, and taking taking the partial derivative with respect to  $E$  of both sides of the equation. This results in:

$$\left. \frac{\partial M}{\partial E} \right|_N = \frac{-N}{JM + NH}$$

All in all, substituting the terms and rearranging, we obtain the relation:

$$2 \frac{JM + NH}{Nk_B T} = \ln \left( \frac{N + M}{N - M} \right) \quad (6)$$

This is a transcendental equation that relates the total magnetization of the system with the temperature (and potentially a magnetic field), in the thermodynamic limit. We may rewrite it in terms of  $m$  as:

$$\frac{1 + m}{1 - m} = e^{\frac{2}{k_B T} (Jm + H)}$$

Actually, leaving out the details, this expression can be further manipulated into a more elegant form:

$$m = \tanh \left( \frac{J}{k_B T} \left( m + \frac{H}{J} \right) \right) \quad (7)$$

This is the same self-consistent equation, now in terms of the mean magnetization per spin. In fact, this is a very similar equation to that which appears when applying the mean field theory approximation to the standard Ising model. The only difference is the coordination number that appears there, that in this model can be taken equal to 1 (instead of  $N$ , due to the normalization factor of  $N$  that we have introduced to ensure extensibility).

## 1.6 Heat capacity

Recalling the definition of the specific heat capacity  $c_V$  and applying the chain rule:

$$c_V = \frac{1}{N} \left. \frac{\partial E}{\partial T} \right|_V = \frac{1}{N} \left. \frac{\partial E}{\partial M} \right|_V \left. \frac{\partial M}{\partial T} \right|_V$$

The first term can be easily calculated from (2) giving:

$$\left. \frac{\partial E}{\partial M} \right|_V = -H - \frac{JM}{N}$$

The second term is a little more complicated. We can use the self consistent equation (6) assuming that it defines implicitly  $M(T, H)$ , and taking the derivative with respect to  $T$  on both sides:

$$\frac{\partial}{\partial T} \left[ \frac{2JM}{Nk_B T} = \ln \left( \frac{N+M}{N-M} \right) \right] \implies \frac{-2JM}{Nk_B T^2} + \frac{2J}{Nk_B T} \frac{\partial M}{\partial T} = \frac{2N}{N^2 - M^2} \frac{\partial M}{\partial T}$$

From which we can obtain, after a little work:

$$\left. \frac{\partial M}{\partial T} \right|_V = \frac{M}{T} \frac{N^2 - M^2}{N^2 \left( 1 - \frac{k_B T}{J} \right) - M^2}$$

All in all, writing in terms of  $m$  (and thus now  $m(T, H)$  is implicitly defined in (7)) we get that in the thermodynamic limit:

$$c_V(T, H) = \frac{J}{T} \frac{1 - m^2}{m^2 - \left( 1 - \frac{k_B T}{J} \right)} \left( m^2 + \frac{H}{J} m \right) \quad (8)$$

The particular behavior of  $m(T, H)$  should be analyzed more carefully, by a stability analysis perhaps. But in any case, it turns out that:

In the limit  $T \rightarrow 0$ , it can be shown that  $c_V \rightarrow 0$ .

In the limit  $T \rightarrow \infty$ ,  $m \rightarrow 0$  (seen from (7)), and thus  $c_V \rightarrow 0$

## 1.7 Magnetic susceptibility

Recall that magnetic susceptibility is defined as:

$$\chi_M = \frac{1}{N} \left. \frac{\partial M}{\partial H} \right|_T$$

We can find this partial derivative by assuming (6) defines implicitly  $M(T, H)$  and differentiating with respect to  $H$  (for a fixed  $T$ ) both sides of the equation:

$$J \frac{\partial M}{\partial H} + N = \frac{N^2 k_B T}{N^2 - M^2} \frac{\partial M}{\partial H}$$

From this equation we can isolate  $\frac{\partial M}{\partial H}$ . Rewriting in terms of  $m$ , and instead assuming that (7) defines  $m$  implicitly  $m(T, H)$ , we can express  $\chi_M$  as:

$$\chi_M(T, H) = \frac{1}{J} \frac{1 - m^2}{m^2 - \left( 1 - \frac{k_B T}{J} \right)} \quad (9)$$

Once again, the particular behavior of  $m(T, H)$  should be analyzed more carefully. But in any case, it turns out that:

In the limit  $T \rightarrow 0$ , it can be shown that  $\chi_M \rightarrow 0$ .

In the limit  $T \rightarrow \infty$ , it turns out that  $m \rightarrow 0$  (seen from (7)), and thus  $\chi_M \rightarrow 0$

## 1.8 Phase transition at zero field

We will now explore the solutions of (7) for the case of zero magnetic field, as a function of temperature. When considering  $H = 0$ , the equation becomes:

$$m = \tanh\left(\frac{J}{k_B T} m\right) \quad (10)$$

Note how  $m = 0$  is a solution for all  $T$ . Actually, as  $T \rightarrow \infty$  this is the only possible solution. We can seek other solutions with  $m \neq 0$ , noting that these however do not exist for all temperatures. In fact, we can analytically find the critical temperature for which these other solutions appear. Since the onset of the transition will be characterized by  $m \approx 0$ , we approximate  $\tanh\left(\frac{J}{k_B T} m\right) \approx \frac{J}{k_B T} m$ . The equation becomes:

$$m = \tanh\left(\frac{J}{k_B T} m\right) \approx \frac{J}{k_B T} m$$

Which has a solution different from  $m = 0$  when  $T = J/k_B$ .

All in all, it is easy to show (graphically perhaps) that for  $T < J/k_B$  there exist three solutions: 0, and  $0 < m_{\pm} < 1$ . Note that  $m_{\pm}$  just have different signs. For  $T > J/k_B$ , only  $m = 0$  is a solution. Also note that when  $T \rightarrow 0$ ,  $m \rightarrow \pm 1$ .

### Stability analysis of $m(T)$

We will analyze the minima of the Helmholtz potential (5) for the case  $H = 0$ , considering it is a function of  $m$ ,  $A(m)$ , and all other variables fixed. This is because we are interested in finding the values of  $m$  that make this function a minimum for a given fixed value of  $T$ . Note how the domain is restricted to  $|m| \leq 1$ . We compute it's first and second derivatives at constant  $N$ ,  $T$ , first in the general case:

$$\begin{aligned} \left. \frac{\partial A}{\partial m} \right|_{N,T} &= -NJm - NH - N \frac{K_B T}{2} \ln\left(\frac{1-m}{1+m}\right) \\ \left. \frac{\partial^2 A}{\partial m^2} \right|_{N,T} &= NJ \left( \frac{k_B T}{J} \frac{1}{1-m^2} - 1 \right) \end{aligned}$$

Now we focus on the case  $H = 0$ . Looking for the critical points, where the first derivative becomes 0, we get the same transcendental equation as (10). This was expected. We already discussed that for  $T > J/k_B$  the only solution is  $m = 0$ , while for  $T < J/k_B$  the equation has 3 solutions, one of which includes  $m = 0$  and the other two are symmetrical  $m_{\pm}$ .

For the solution  $m = 0$  it is easily found that:

$$\left. \frac{\partial^2 A}{\partial m^2} \right|_{m=0} = \frac{N}{J} \left( \frac{k_B T}{J} - 1 \right) \implies \begin{cases} \left. \frac{\partial^2 A}{\partial m^2} \right|_{m=0} < 0 & T < \frac{J}{k_B} \\ \left. \frac{\partial^2 A}{\partial m^2} \right|_{m=0} > 0 & T > \frac{J}{k_B} \end{cases}$$

This illustrates how the solution  $m = 0$  is a local minima of the potential for  $T > \frac{J}{k_B}$  and thus a stable solution. For smaller temperatures, it is actually a local maxima, and thus an unstable state.

For the solution  $m_{\pm} \neq 0$  that only exists for  $T < \frac{J}{k_B}$ , it can be proved that it is a local minima of the function. The Taylor expansion of the Helmholtz free energy up to order 4 around  $m = 0$  (for zero field) is:

$$A(m)|_{H=0} = -2NKT - \left(1 - \frac{T}{T_C}\right) \frac{m^2}{2} + \mathcal{O}(m^4)$$

Note how for  $T \leq T_C$  and  $m \rightarrow 0$ ,  $A(m)|_{H=0} \leq A(0)|_{H=0}$ , proving that the other critical points are smaller than  $A(0)|_{H=0}$  (since the behaviour cannot change between 0 and these critical points). This means that for  $T < \frac{J}{k_B}$  the states  $m_{\pm} \neq 0$  that are a solution of (10) are stable states, for zero field. This behaviour is clearly visualized in the plots of figure 1.

## Critical temperature

In summary, this discussion implies the existence of a phase transition at the critical temperature for the system in the thermodynamic limit and at zero field, below which the system presents spontaneous magnetization:

$$T_C = \frac{J}{k_B} \quad (11)$$

The following plot shows the behaviour of the mean magnetization per spin that we have discussed (in the thermodynamic limit  $N \rightarrow \infty$ ) as a function of the reduced temperature  $T/T_C$ , obtained through numerical methods. Note how the non-zero magnetization can be either positive or negative, but we have just plotted the absolute value  $|m|$ .

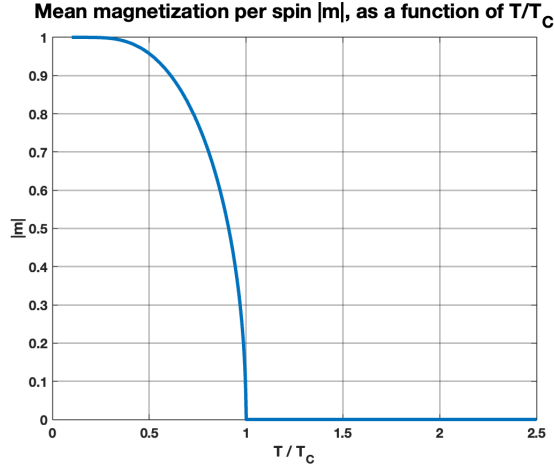


Figure 2: Mean magnetization per spin  $|m|$  for zero field.

## Critical behavior of $c_V$

Particularising the heat capacity (8) to the case  $H = 0$  and remembering that  $m(T)$  has just been defined in this case, we obtain:

$$c_V(T, H = 0) = \begin{cases} 0 & T > T_C \\ k_B \frac{T_C}{T} m^2 \frac{1-m^2}{m^2 - (1 - \frac{T}{T_C})} & T < T_C, \quad m \neq 0 \end{cases} \quad (12)$$

We observe that a discontinuity appears in  $T_C$ . We will analyze the limits:

In the limit  $T \rightarrow T_C^-$ ,  $m \rightarrow 0$  and we can expand (10):

$$m = \tanh\left(\frac{T_C}{T} m\right) \approx \frac{T_C}{T} m - \frac{1}{3} \left(\frac{T_C}{T}\right)^3 m^3 \quad \Rightarrow \quad m^2 \approx 3 \left(\frac{T}{T_C}\right)^2 \left(1 - \frac{T}{T_C}\right)$$

Substituting and taking the limit  $T \rightarrow T_C^-$  in (12):

$$c_V(T) \approx 3k_B \frac{T}{T_C} \frac{1 - 3\left(\frac{T}{T_C}\right)^2 \left(1 - \frac{T}{T_C}\right)}{3\left(\frac{T}{T_C}\right)^2 - 1} \quad \Rightarrow \quad c_V \rightarrow \frac{3}{2} k_B$$

Note how the discontinuity is finite. This behaviour is characteristic of a second order phase transition. Typically, in a second order phase transition  $E(T)$  is continuous, but its first derivative presents a discontinuity at  $T = T_C$ .



### Critical behavior of $\chi_M$

At zero field, referring again to our definition of  $m(T)$ , equation (9) results in:

$$\chi_M(T, H = 0) = \begin{cases} \frac{1}{k_B T_C} \frac{1}{\frac{T}{T_C} - 1} & T > T_C \\ \frac{1}{k_B T_C} \frac{1 - m^2}{m^2 - (1 - \frac{T}{T_C})} & T < T_C, \quad m \neq 0 \end{cases} \quad (13)$$

Once again we observe how there appears to be a discontinuity in  $T_C$ . Analyzing the limits:

For the limit  $T \rightarrow T_C^+$  we have that:  $\chi_M \rightarrow \infty$

For the limit  $T \rightarrow T_C^-$  we can once again use  $m^2 \approx 3 \left( \frac{T}{T_C} \right)^2 \left( 1 - \frac{T}{T_C} \right)$ :  $\chi_M \rightarrow \infty$

Note how in contrast to the heat capacity  $c_V$ , the discontinuity in  $\chi_M$  is infinite, it's a divergence. This is also observed in second order phase transitions. Physically, this suggests that near the critical temperature the system is "infinitely" reactive to changes in the magnetic field.

I suspect the rate of divergence is different in both limits however, and a more detailed analysis might reveal exactly the critical exponents and factors.

The following is a plot of the specific heat capacity obtained numerically from (8) and the specific magnetic susceptibility obtained numerically from (9), where we can visualize our predictions for the case of zero field:

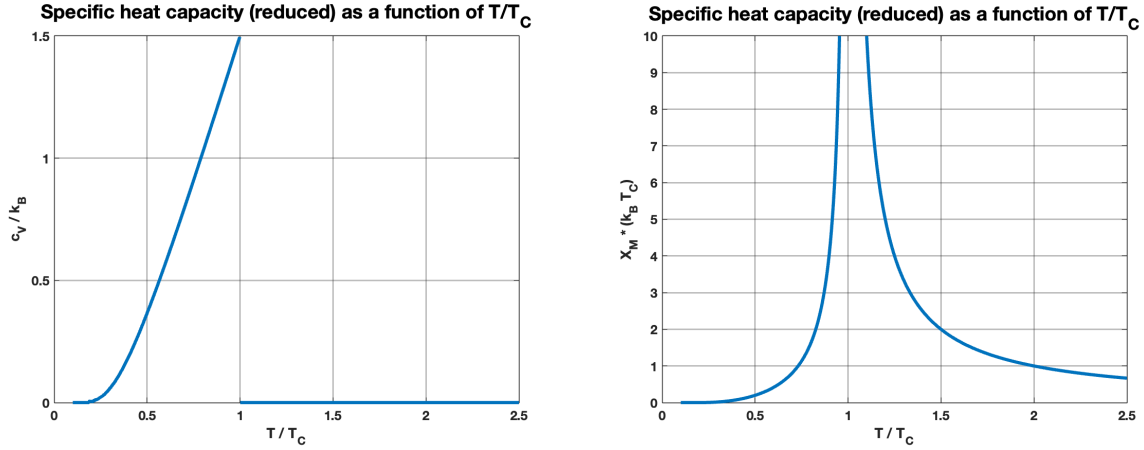


Figure 3: Heat capacity and magnetic susceptibility for zero field

## 1.9 Behavior for non-zero field

In this section we will explore briefly the behavior for  $H \neq 0$ . Note that in this case, one of the two symmetric solutions  $m_{\pm}$  of the self-consistency equation has a lower Helmholtz potential and will thus be the most stable. This most-stable solution is the one that has been used in the following plots. However, the other solution is still physical and explains the concept of Hysteresis. The following is a plot of the surfaces  $E(T, H)$  (3),  $m(T, H)$  (7),  $cv(T, H)$  (8) and  $\chi_M(T, H)$  (9):

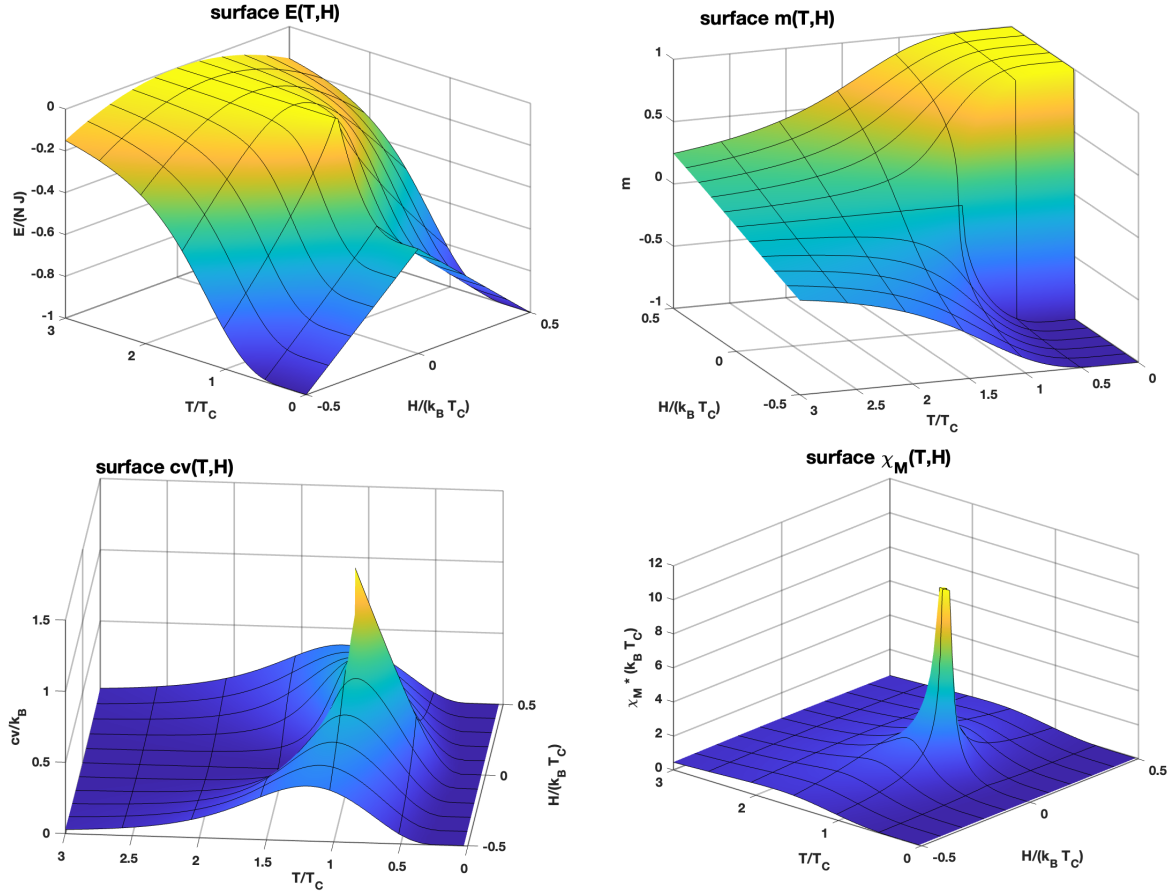


Figure 4: Important thermodynamic properties as a function of  $T$  and  $H$

Note how the discontinuity in the behavior of  $c_V$  only seems to happen for  $H = 0, T = T_C$ . The same happens for the divergence in  $\chi_M$  at  $T = T_C$ .

However, we now observe the existence of a discontinuity in  $m$  that is only apparent for  $T < T_C$  as we vary  $H$ . This is due to the fact that one of the minima of  $A(m)$  is lower than the other for  $H > 0$ , and the other way around for  $H < 0$ . Note that if we started on any of the minima and decreased the temperature gradually, we would not observe the sudden jump at  $H = 0$ , but at a lower (or higher) value of  $H$ . This is because the minima is still a local minima, even if the other one is lower, and we will not "fall" to the other value until this stops being a local minima. This is the effect of hysteresis.

## 2 Monte Carlo simulations

In this section I will explain the setup for the simulations, and present the results. The goal is to compare the results for a finite sized system with the predictions of the previous section.

I will not explain in detail the frame of Monte Carlo simulations, but the main idea is to sample the state space of our system  $\{s_i\}$  and then find the relevant statistics from the samples. The sampling could be completely random, but in order to be more efficient we will use the method of *importance sampling* by implementing a Metropolis algorithm.

### 2.1 Setup

Recall that this project was developed to this extent because I wanted to revisit the code. So I tried to do my best to exploit Python's object oriented mindset, creating classes that include a *State* with its corresponding spins and Hamiltonian, as well as an *ensemble*, which is simply a collection of states used for sampling. I will not dive into detail in the implementation here, feel free to check my GitHub, but I just want to note that the function to compute the Hamiltonian had to be precompiled in order to improve efficiency. Still, Python is not the most efficient language and there is a lot of room for improvement.

#### Collection of samples

After sampling the configuration space, we end up with what I call an ensemble or a collection. Suppose we make  $N_s$  samples:

$$\text{collection} = \{\{s_i\}_k\} \quad k = 1, \dots, N_s$$

Where  $\{s_i\}_k$  is just the particular configuration of spins of sample  $k$ .

#### Statistics

The basic thermodynamical quantities we will compute from the samples are:

$$\begin{aligned} \langle E \rangle &= \frac{1}{N_s} \sum_{k=1}^{N_s} E(\{s_i\}_k) \\ \langle M \rangle &= \frac{1}{N_s} \sum_{k=1}^{N_s} M(\{s_i\}_k) \quad , \quad \langle m \rangle = \frac{1}{N} \langle M \rangle \end{aligned}$$

We will exploit a basic result arising from the canonical ensemble in order to compute  $c_V$  and  $\chi_M$  from the statistical fluctuations of the samples:

$$\begin{aligned} c_V &= \frac{1}{N} k_B \beta^2 (\langle E^2 \rangle - \langle E \rangle^2) \\ \chi_M &= \frac{1}{N} \beta (\langle M^2 \rangle - \langle M \rangle^2) \end{aligned}$$

Where obviously,  $\langle E^2 \rangle = \frac{1}{N_s} \sum_{k=1}^{N_s} E(\{s_i\}_k)^2$  and  $\langle M^2 \rangle = \frac{1}{N_s} \sum_{k=1}^{N_s} M(\{s_i\}_k)^2$ .

### Metropolis step

A Metropolis step is simply the following algorithm to “move” in state space:

1. Start from state  $\mu = \{s_i\}_\mu$  with energy  $E_\mu$ .
2. Choose a random spin and change it's state. That is,  $s_i \rightarrow -s_i$ . This generates a new state  $\nu = \{s_i\}_\nu$  with energy  $E_\nu$ .
3. Compute the difference in energies:  $\Delta E = E_\mu - E_\nu$ .
  - (a) If  $\Delta E < 0$  we accept the move into state  $\nu$ .
  - (b) If  $\Delta E > 0$  we generate a random number  $x$  uniform(0, 1):
    - i. If  $x \leq \exp(-\beta\Delta E)$  we accept the move into state  $\nu$ .
    - ii. If  $x > \exp(-\beta\Delta E)$  we stay in state  $\mu$ .

This algorithm stems from the Metropolis choice of importance sampling particularised for a system in equilibrium at constant temperature that follows a Canonical distribution. This ensures that the sampling is optimal and that we give more “importance” to the more probable states following the distribution.

### Monte Carlo step

What I define as a Monte Carlo step is simply the iteration of  $N$  metropolis steps.

My sampling criteria will be to store each Monte Carlo step as a new sample. This could be different, and for example I might choose to do bigger steps before saving a new sample. But I wanted to keep things simple.

Starting from the last recorded state, we perform the remaining Monte Carlo steps until we have the desired number of samples.

## 2.2 Scheduling

The idea is to simulate the system for the case of zero field, for a range of temperatures. I chose  $0.1 < T < 2.5$  with 50 equidistant steps. For each temperature, I start the simulation in a random state and perform 10000 Monte Carlo steps. I store each of the samples to visualize their evolution to detect and discard any potential transition states, and later calculate the thermodynamic properties.

## 2.3 Results

### Evolution of samples

In the following plots we see the evolution of the moving average of  $m$  and  $E$  over the past 100 samples, defined as:

$$\langle m(s) \rangle_{100}^j = \frac{1}{100} \sum_{k=j-99}^{k=j} m(\{s_i\}_k)$$

$$\langle E(s) \rangle_{100}^j = \frac{1}{N} \frac{1}{100} \sum_{k=j-99}^{k=j} E(\{s_i\}_k)$$

If sample  $j$  does not have at least 99 previous samples, we simply average over the available number samples. The goal of plotting this moving average is to reduce some noise but still gain insight into the correlations of the different MC steps. Note that each temperature is a different color, and that the 3 cases of  $N = 50$ ,  $N = 100$ ,  $N = 500$  are plotted in each case.

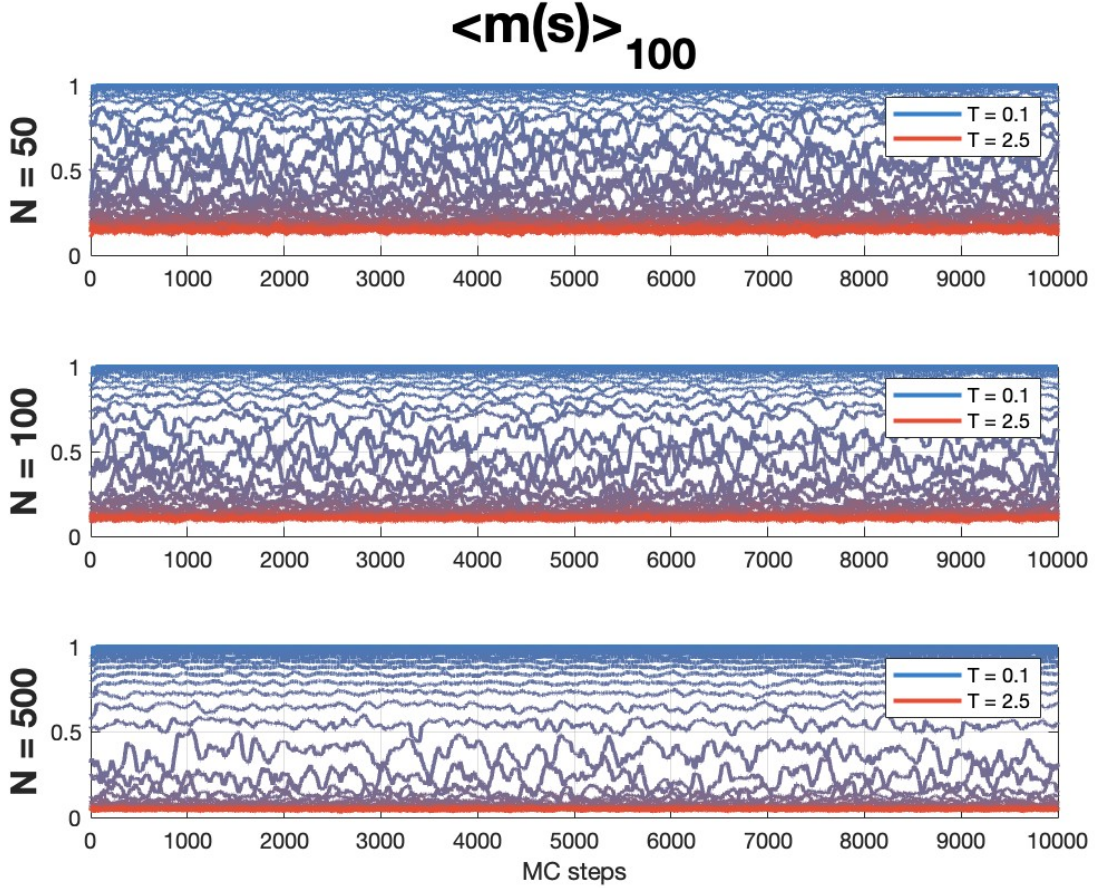


Figure 5: Moving average of 100 samples of  $m$  for different temperatures and sizes.

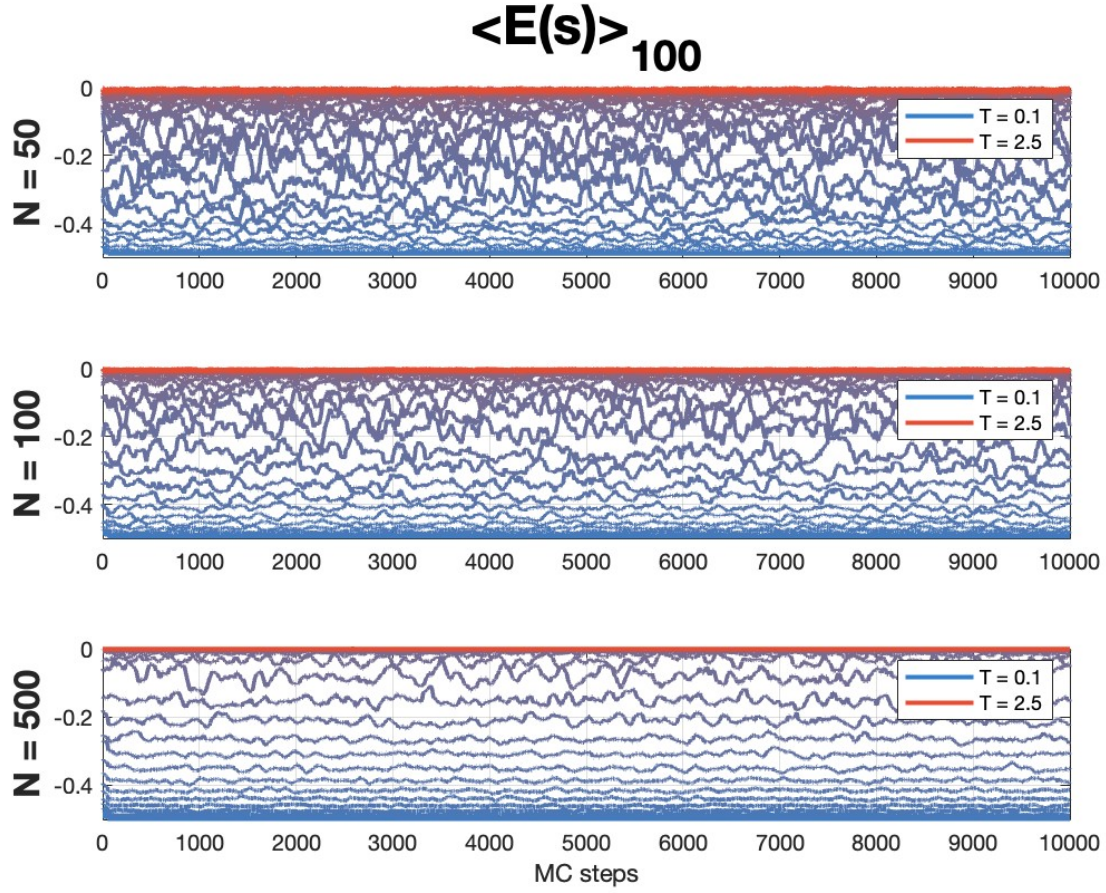


Figure 6: Moving average of 100 samples of  $E/N$  for different temperatures and sizes.

From the previous plots it is interesting to observe that the relative fluctuations decrease as the system increases its size. This means that the evolution of the system becomes less noisy for the same amount of MC steps, which could be expected. As  $N$  increases, a single MC step will have less effect on  $m$  and  $E$ .

Very importantly, we don't observe the existence of a clear transient state that we should discard on any case. The steady state seems to be reached with very few MC steps, so the computed averages will indeed represent a system in equilibrium.

Also, we see that the correlation time of the fluctuations around the steady state is a lot shorter than the length of all the sampling. This means that in our averages we will include a lot of fluctuations or a lot of uncorrelated samples, which is the ultimate goal.

## Thermodynamic properties

The following figure summarizes the computed averages from the previous samples for the different temperatures and sizes, as well as comparing with the analytic results in the thermodynamic limit:

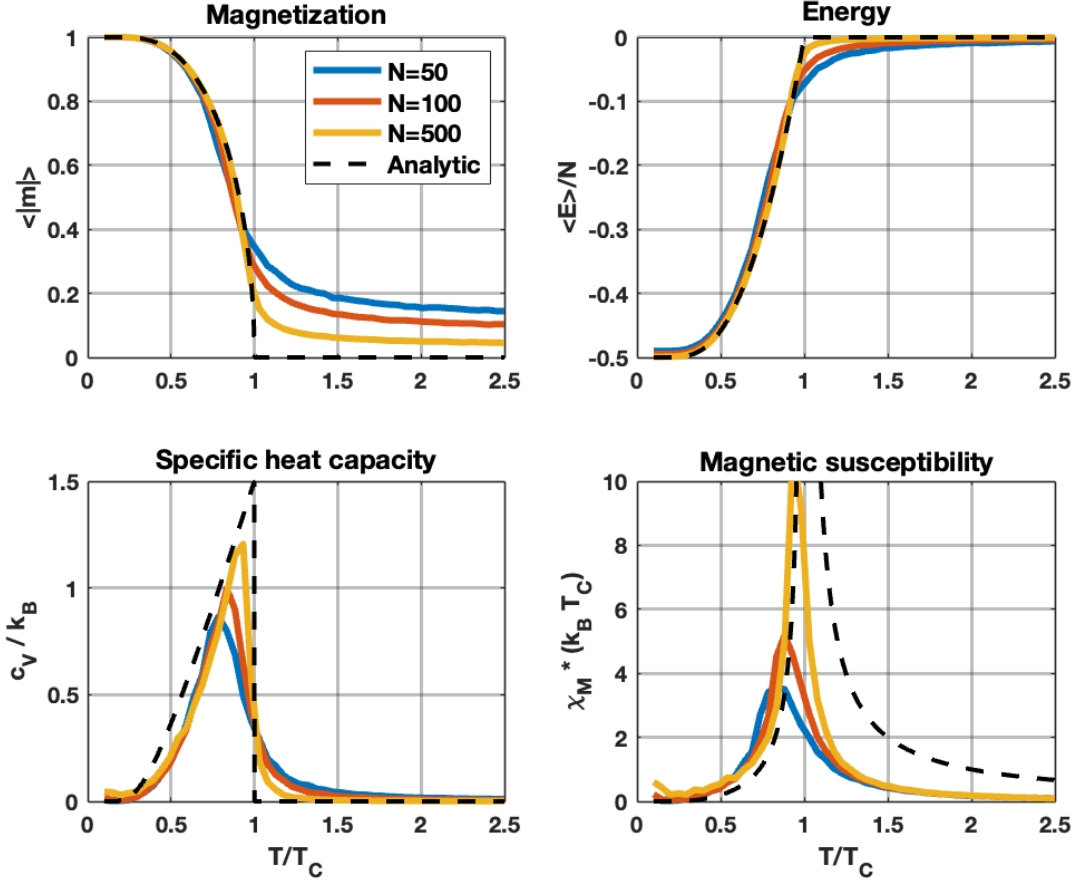


Figure 7: Results of the Monte Carlo simulations

As we can see, the smaller the system, the further it is from the analytical solution. This is because it was obtained in the thermodynamic limit  $N \rightarrow \infty$ . We also observe that for  $N = 500$  we are not that far from the predicted behavior.

As  $N$  increases, the magnetization gets closer and closer to 0 for  $T > T_C$  and the critical behavior of  $c_V$  gets closer to the predicted discontinuity. The magnetic susceptibility also increases more and more towards the predicted divergence, although the behavior for larger  $T$  is smaller than predicted.

The only apparent problem seems to be in the heat capacity for temperatures close to 0. I suspect this is due to numerical instabilities caused by dividing by values close to 0, and that this could be corrected incrementing the number of samples by a few orders.