COMPLEX SYSTEMS MODELLING
**Universidade de Aveiro**

# Phase transition in the Ising model

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## 1 ISING MODEL ON A RING

The energy of the Ising model on a ring is

$$E = -J\sum_{n=1}^{N} S_n S_{n-1} - H\sum_{n=1}^{N} S_n \tag{1.1}$$

where $S_n = \pm 1$ and $S_{N+1} \equiv S_1$. The energy of a spin $S_n$ interacting with nearest-neighbouring spins in a magnetic field $H$ is

$$E_n(S_n) = -JS_n(S_{n-1} + S_{n+1}) - HS_n \tag{1.2}$$

After performing the Metropolis algorithm steps that compute the accepted microstates, $M^{(a)}$, the final steps (step 9. and 10. in the project's assignment) allow us to get the averagesover the microstates. We have to skip the first 100 microstates because the system is far from equilibrium. $< M >$ is given by:

$$< M > = \frac{1}{m}\sum_{a=1}^{m} M^{(a)} \tag{1.3}$$

where $m$ is the total number of microstates and $M$ is the magnetization.

**Task 1:** Choose $J = 1$ as the energy unit. Analyse how $< M >$ depends on $m$. In other words, calculate $< M >$ after first 100 microstates, then after 200 microstates, and so on. Plot $< M > (k)$ versus $t = 100 \times k$. It shows how $< M >$ tends to the equilibrium state.

**Task 2:** Use the Metropolis algorithm and find the temperature dependence of the magnetization and compare with the exact solution of $M$.

Firstly, these are the chosen parameters for the simulation:

- Number of spins: $N = 1000$;
- Number of generated microstates: $m = 100000$;
- The temperature range: $T = [0.1, 10]$;
- The temperature step: $\Delta T = 0.05$;
- Magnetic field: $H = 0.1$.

**Resolution of task 1:**

After performing the Metropolis algorithm for the Ising model on a ring of atoms, we can display the resulting magnetization of the system along the microstates. The result consists on the average value of the magnetization, $< M >$, over the microstates. The average is cumulative, and jumps from 100 to 100 values of microstates, as mentioned before.

The resulting plot is shown on figure 1.1, where we have three curves for distinct temperatures (0.1, 5 and 10). For all of the cases we can denote that all the magnetizations of the system converge to a determined value, and that means that the system reached the equilibrium state. In the case of $T = 5$ and $T = 10$, the magnetization of the system converges to near zero and, on the other hand, for $T = 0.1$ it converges to 1. The next question is: Why doesn't $M$ allways converge to the same value for different temperatures? From a physics' perspective, it is because, probably, for lower temperatures the system is low on energy. Hence, there isn't forcing for spin inversion and then the magnetization can't drop too much. Also, we can see a decay of the $M_a$ convergence value from 1 (for $T = 0.1$) to 0 (for $T = 5$ and $T = 10$). This decay is of the magnetization converging is related with the results in task 2, where the magnetization decays in function of temperature, and can be explained probably by the fact that the material turns into a paramagnetic one (more details into that, in the second chapter).

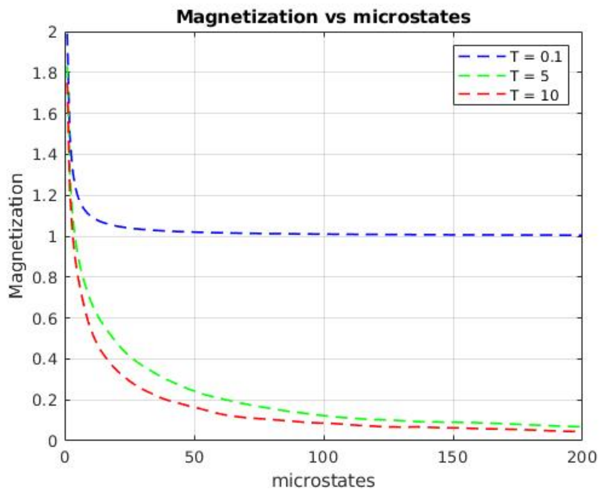



Figure 1.1: Magnetization of the accepted microstates, $M_a$ for three different temperatures.

**Resolution of task 2:**

Regarding the dependance of the magnetization with the temperature, for this system, we can see that this dependance, in fact, exists (figure 1.1), with the experimental magnetization obtained from the Metropolis Algorithm showing an exponential decrease decrease in the first two units of temperatures, especially. Then, the magnetization tends to zero as the temperature increases. Note that the initial microstate was a configuration on the ring where all spins were upwards. This decision helped on performing better results in the algorithm early on the iterations, because it is more stable.

The behavior of the resulting magnetization shows a lot of similarity with the exact result, which is given by,

$$M(T,H) = \frac{sinh(\beta H}{\sqrt{sinh^2(\beta H) + e^{-4\beta J}}} \tag{1.4}$$

where the magnetic field, $H$, is always 1. Figure 1.2 illustrates that the experimental result, for the chosen number of spins and the generated microstates, is quite good. Quantitatively, we performed some calculations to have a better idea of how accurate this solution is. Here are the statistical calculations, which can be considered evaluation metrics for accuracy and precision:

- $\sigma = 0.9106$ (standard deviation – precision);
- $MSE = 0.0025$ (mean-squared error between the theoretical function and the numerical experiment – accuracy).

From the metrics above, we can conclude that the results have a very good accuracy ($MSE$ very low), although the standard deviation is a reasonably high, showing that the magnetizations have a little too much variance. That is justifiable, even visually in the plot, where there are several spikes which are clearly visible, and this affects the precision To improve the quality of the results, we should increase $N$ and $m$, but we should be clever with the computational resources available, because too much iterations in the algorithm would be irrealistic to process.

Could we do a linear regression, with a log-scale, and plot a fit linear or polinomial model to the results? The log-log graph in figure 1.3 shows clearly that is not useful to try to represent a linear or polinomial fit to $< M >$, unless we choose a section halfway from the set of microstates, where we could fit accurately a line with a negative slope representing magnetization. Anyway, we don't perform a linear or polinomial fit, as this is a complex representation even for a log-log scale. Note that this log-scale gives a good insight of the different behaviours of the system of spins when the phase changes. Firstly the logarithm of magnetization behaved as a line with no slope, and from some temperature, theere was phase transition, and the line with a negative slope that could model the results (for higher temepratures), represents how the system behaves for the new physical phase, above a certain critical point.

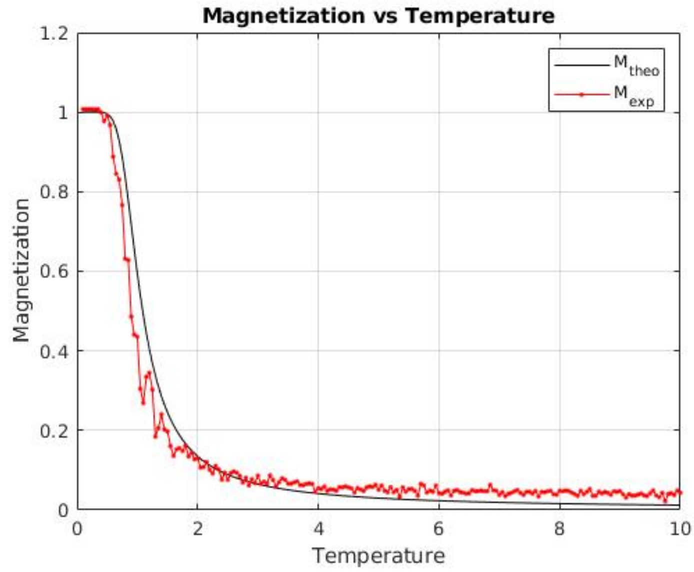



Figure 1.2: Resulting average magnetization, $< M >$, in function of temperature

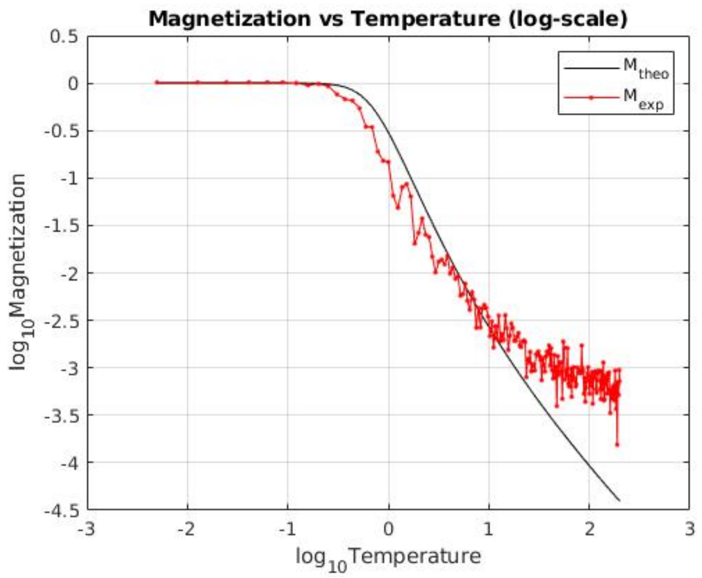



Figure 1.3: $< M >$ in function of temperature (log-scale)

# 2 Ising model with all-to-all interaction (long-ranged interaction)

The energy of the Ising model with the long-ranged interaction is

$$E = -\frac{J}{N} S_n \sum_{n=1}^{N-1} \sum_{m=n+1}^{N} S_n S_m - H \sum_{n=1}^{N} S_n \tag{2.1}$$

where $S_N = \pm 1$. The energy of the spin $S_n$ interacting with the other spins in a magnetic field $H$ is

$$E_n(S_n) = -\frac{J}{N} S_n \sum_{m=1, m\neq n} S_m - HS_n \tag{2.2}$$

Using the Metropolis algorithm, one can calculate the averaged magnetization and susceptibility:

$$< M >= \frac{1}{m} \sum_{a=1}^{m} M^{(a)} \tag{2.3}$$

$$\chi^{(a)} = \frac{N}{T} \left[ \frac{1}{m} \sum_{a=1}^{m} (M^{(a)})^2 - < M >^2 \right] \tag{2.4}$$

where $m$ is the total number of microstates.

**Task:** Choose $J = 1$ as the energy unit (same as last problem). Compare the results of simulations with the exact results for $M$ and $chi$. Plot $M$ and $\chi$ versus $T$. Analyse the temperature dependence of $M$ and $\chi$ near the critical point, $T_c = J$.

The parameters for the simulations are the following:

- Number of spins: $N = 100$;
- Number of generated microstates: $m = 50000$;
- The temperature range: $T = [0.1, 10]$;
- The temperature step: $\Delta T = 0.05$;
- Magnetic field: $H = 0$ or $H = 0.001$.

**Resolution:**

The Ising model with an all-to-all interaction should present better results, as the system is more complex and act in a more realitic and homogeneous way, with the atoms interferring more with each other in the 1D system.

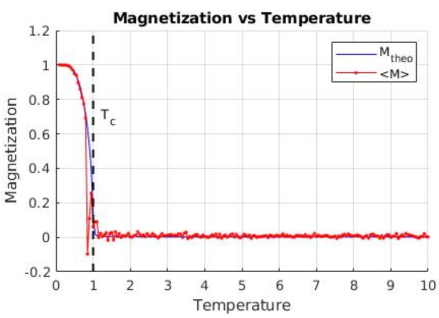
After performing the Metropolis algorithm to get the magnetization, $< M >$, and susceptibility (which is a measure of how much a material will become magnetized in an applied magnetic field), $\chi$, we can see the temperature dependency of these two variables in figures 2.1 and 2.2. Note that the results are applied to a constant magnetic field of $H = 0.001$ and $< M >$ was calculated in jumps of 100 of $k$, like exercise 1. In those figures, we can also see the behavior of $\chi$ and $< M >$ near the Curie temperature ($T_c = J$) and the theoretical prediction of the magnetization.

Starting by superfitially commenting the plot's results, we can see that, $< M >$ starts to converge to zero at approximately $T = T_c$, and that the approximation to the exact solution is relativelly good. Furthermore, for the resulting susceptibility, $\chi$, there is a clear spike (or maxima) near the Curie Temperature but not exactly there (like the exact solution), and the experimental solution seems to be fairly well approximated to the exact one.

We know that when temperature surpasses the Curie temperature, the material is paramagnetic. From the deductions done in the lecture 8 of this class, we know that when $H = 0$ and $T \gg T_c$ (paramagnetic system), then $\chi \to 0$. Here, $H$ is fairly low, almost zero, so we can say that this behavior happens to be the right one. Also, the magnetization (represented in figure 2.1) tends to be zero paramagnets do not retain any magnetization in the absence of an externally applied magnetic field (in this case, $H$ is very low) because thermal motion randomizes the spin orientations.

On the susceptibility, in our simulation, the maximum is located little bit below $T_c$, and according to the theory it should be at $T = Tc$. One explanation of that could be the limited number of repetitions used fo the Metropolis algorithm. After all, it is a stochastic method and the results present a certain error. But also we repeated the simulations (for the same number of spins and microstates) and this maximum value sits in the range of temperatures of 0.75 to 0.85, and the before mentioned explanation may not be the reason why the maximum is displaced. Other explanation is that with the all-to-all interaction doesn't solve well situations like phase transistion ($T = T_c$), and hence doesn't compute a good solution around $T_c$.

As we mentioned in the first observations before, in $T_c$ is where the convergence starts of both the magnetization and the susceptibility. In other words, for this temperature



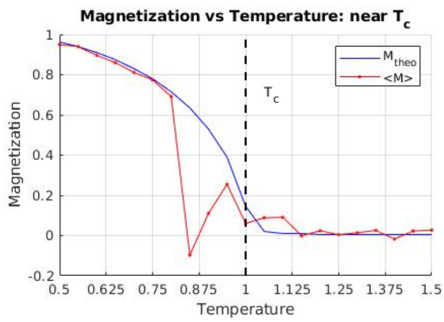




Figure 2.1: Magnetization in function of temperature

The evaluation metrics (same as before) for the results of this simulation are the following:

- Magnetization: $\sigma = 0.2419$; $MSE = 0.0045$
- Susceptibility: $\sigma = 3.8051$ ; $MSE = 17.9567$

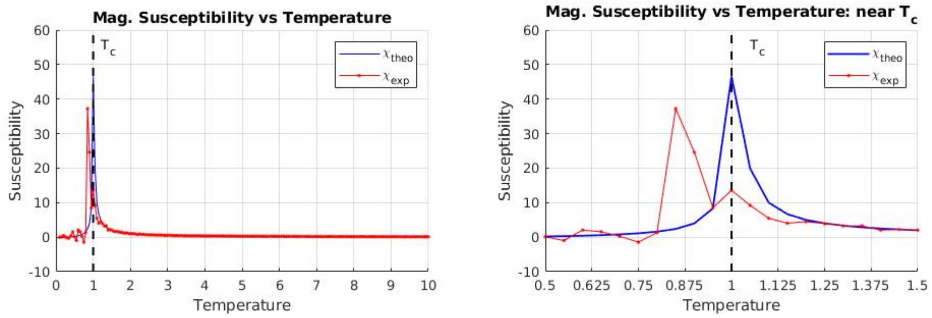



Figure 2.2: Magnetic susceptibility in function of temperature

and we can conclude that the results are relativelly good for the selected parameters, although the results for susceptibility are not normalixed (from 0 to 1) and the magnitude of MSE and $\sigma$ don't illustrate a good idea on how relativelly good the results of susceptibility are, in relation to magnetization. So, normalizing the susceptibility data, like this:

$$\chi_{norm} = \frac{\chi - \chi_{min}}{\chi_{max} - \chi_{min}}$$

we now have the following resulting metrics:

- Magnetization: $\sigma = 0.2419$; $MSE = 0.0045$
- Susceptibility (norm.): $\sigma = 0.0938$ ; $MSE = 0.0098$

which show that for this simulation, the accuracy as well as the precision is better for the magnetic susceptibility than for the magnetization. Now, as an extra to this work, we will compute the MSE and the standard-deviation for four more simulations, and the purpose of this little experiment is to conclude, with some degree confidence, what is the overall best represented variable (magnetization or susceptibility). The following table shows the results of these metrics, that include the results referred above:

| simulations | $MSE(M)$ | $\sigma(M)$ | $MSE(\chi)$ | $\sigma(\chi)$ |
|---|---|---|---|---|
| sim. 1 | 0.2419 | 0.0045 | 0.0938 | 0.0098 |
| sim. 2 | 0.2432 | 0.0104 | 0.0982 | 0.0124 |
| sim. 3 | 0.2434 | 0.0031 | 0.0856 | 0.0091 |
| sim. 4 | 0.2424 | 0.0074 | 0.0956 | 0.0119 |
| sim. 5 | 0.2433 | 0.0026 | 0.1071 | 0.0133 |

Looking at the table we understand that the values are systematically identical to the second decimal place, most of the times. So we conclude that the magnetization presents worst precision and accuracy than the susceptibility, for this algorithm, with the Ising model.