Simulation of the Ising Model in 2D

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I. Introduction

The Ising model was proposed by Wilhelm Lenz and Ernst Ising in 1920 to study the behavior of ferromagnetic materials, and today it has become one of the major paradigms of statistical mechanics. In 1944 Lars Onsager managed to find the analytical solution to the problem, but the development is arduous and cumbersome. Therefore, in this work we will analyze the behavior of this system in its 2-dimensional version through simulations. Of course, the various magnitudes obtained will have associated errors of different nature, for example due to the finitude of the systems studied.

Without further delay, let us introduce the problem. Suppose a group of N particles with two possible states, spin $+1$ and -1 ("pointing" up or down). These particles are in a square matrix whose physical meaning we will obviate, and their state will depend on the interactions with the rest of particles (specifically, local interactions). The hamiltonian of such system is,

$$H = \sum_{<i,j>} -J\sigma_i\sigma_j \tag{1}$$

where σ is the spin, J is the interaction constant, and $\sum_{<i,j>}$ denotes the sum over first neighbors. The analytical results, as already mentioned, have been known for years, so that we can compare the values of the temperature and critical exponents related to the phase transition shown in the model.

II. Methodology and results

To solve the Ising model in 2D we will follow a Monte-Carlo approach, since this kind of problems usually present certain computational difficulties as the number of logical operations necessary to simulate the evolution of the system or its thermalization. We will apply two different MC algorithms, previously explained in class: Metropolis and Wolff.

At most of the temperatures, Metropolis is applied since it is a simple algorithm and has no issues, but near the critical point Wolff is more suitable, since it's faster than Metropolis. In fact Wolff is a global algorithm, and does not present critical slowing down in the critical region. In particular, we apply Wolff in the region $T \in (2.1, 2.6)$. Notice that this temperature is a reduced one, since we take $k = J = 1$. The results obtained for 5 different lengths are shown in the following figures:

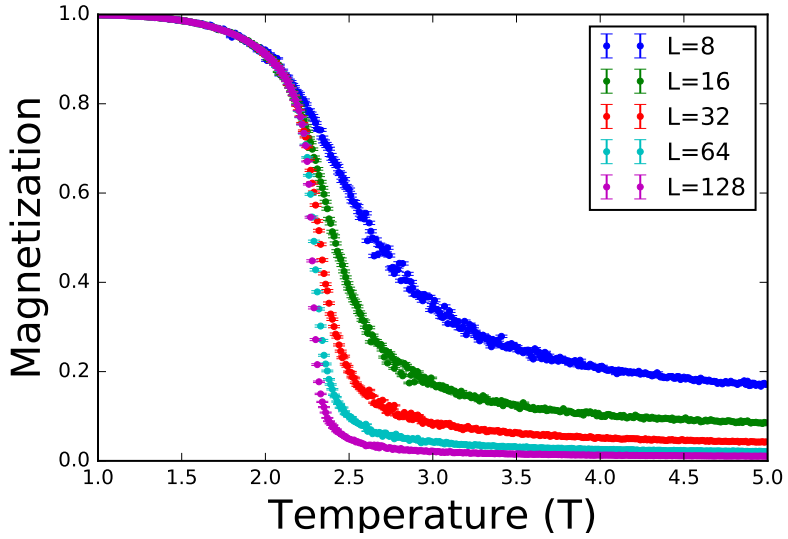

Figure 1: *Magnetization for lattices of $L = 8, 16, 32, 64$ and 124 sites. As we can see, the phase transition over 2.3 can be easily determined for bigger lattice sizes, but small ones have strong finite size effects. Error bars related to the standard deviation are so small that are very difficult to see. For small temperatures, thermal noise is not enough to induce disorder and the magnetization per site is either $M = 1$ or $M = -1$. For high temperatures the interaction between spins is not enough and the noise is so high that the average magnetization is 0. As we said before, finite size effects are very strong for small lattices, forcing the system to have a remanent magnetization at high temperatures.*

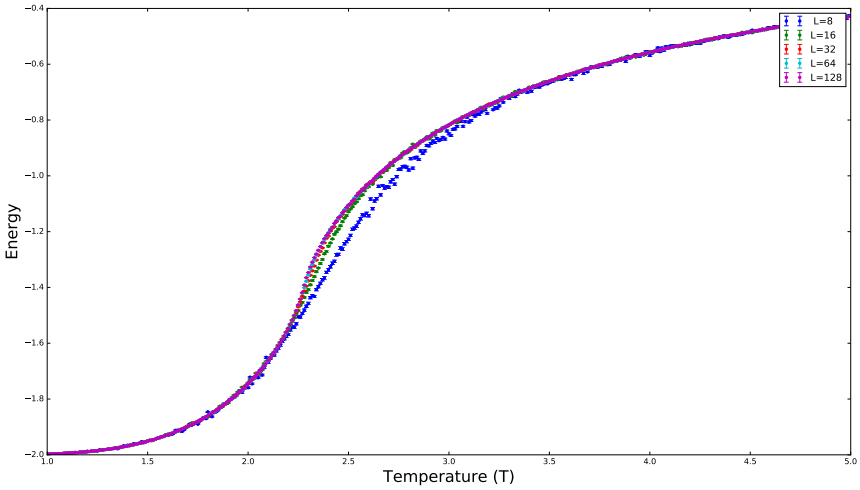

Figure 2: *Energy per site of the system for different lattice sizes. All them fall practically one on top of the other. As temperature increases, the energy approaches the 0 value (meaning that it's increasing). The shape of the energy goes as a coth as predicted theoretically.*

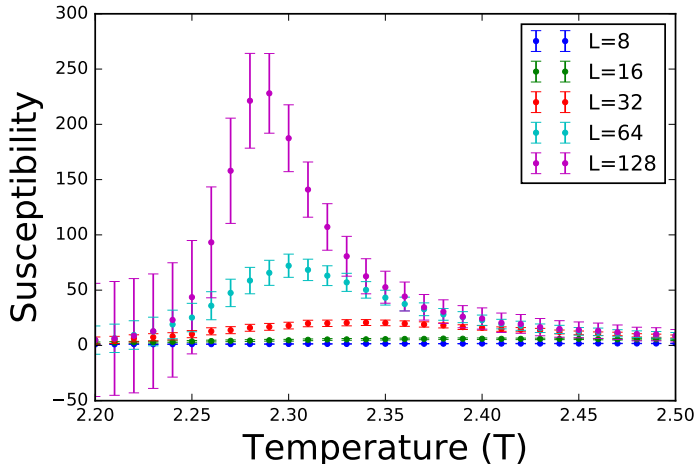

Figure 3: *Susceptibility measures for the studied lattices. Susceptibility is defined in terms of the magnetization as* $\chi = \sqrt{< M^2 > - < M >^2}/(T\sqrt{K})$*, where K is the number of measures. As we can see, bigger lattices are more pronounced and the divergence is closer to the analytical value* T_c*. Error bars have been computed by error propagation and in the approximation of independent moments,* $< M^2 >$ *and* $< M >$*. With this,* $\delta\chi = \beta\delta < M^2 > -2 < M > \delta < M >$*. We can consider the alternative approximation* $\delta\chi = \sqrt{< M^4 > - < M^2 >^2}/(T\sqrt{K})$*.*

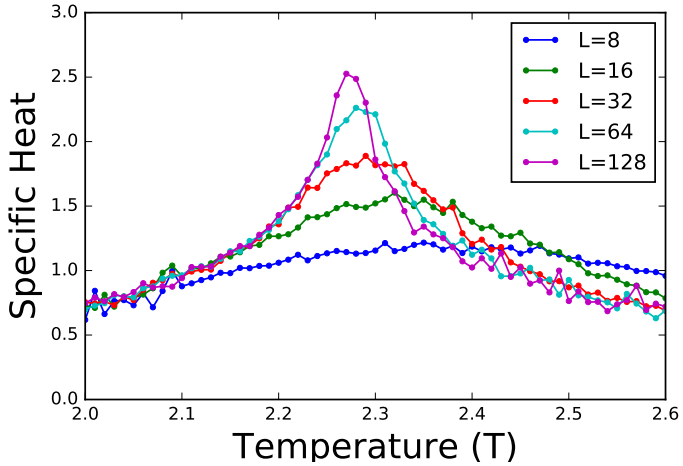

Figure 4: *Behavior of the specific heat, defined as* $C_h = \sqrt{< E^2 > - < E >^2}/(T^2\sqrt{K})$*, where K is the number of measures. As can be seen, at larger sizes the specific heat becomes more pronounced and is shifted towards the analytical value of the critical temperature. Since computing the standard deviation requires an average of averages, which is computationally expensive, error bars have been computed by error propagation and in the approximation of independent moments,* $< E^2 >$ *and* $< E >$*. With this,* $\delta C_h = \beta\delta < E^2 > -2 < E > \delta < E >$*. We can consider the alternative approximation* $\delta C_h = \sqrt{< E^4 > - < E^2 >^2}/(T^2\sqrt{K})$*. However, both errors are very large, an order of magnitude greater than the measurements, so it has been chosen not to display them for easier visualization.*

Alternatively, we will provide figures for the susceptibility and the specific heat per site in the appendix of this document.

One of the main objectives of this work is to obtain the critical temperature in which the phase transition occurs. To determine this, we have two options: either we use the fourth cumulant, or we can determine the critical temperature from the divergence of the susceptibility and then do a linear regression to know the temperature in the thermodynamic limit. We have chosen this second method for its simplicity, since the temperature obtained was good enough, but we aim the reader to try the alternative method of the fourth cumulant. From the values in Fig1 we can

Table 1: *Critical temperature values for different lattice sizes.*

T_c	L
2.64	8
2.38	16
2.3	32
2.3	64
2.26	128

do a linear regression to obtain T_c in the limit $N <\rightarrow \infty$, giving a value of,

$$T_c = 2.27 \pm 0.01 \tag{2}$$

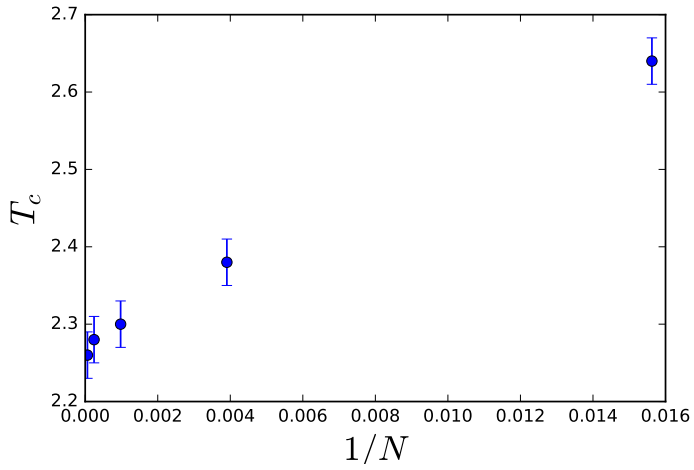

Figure 5: *Linear regression to find the critical temperature for an infinite system. As we see, the computed temperatures fit very well in a linear behavior.*

Once we have determined the critical temperature, we can compute the critical exponents. Since the behavior near T_c goes always as $\sim t^{criticalexponent}$, where t is the reduced temperature, the slope of a linear regression gives this exponent. The following procedure has been done:

1. We do a loglog plot of the magnitudes (magnetization, susceptibility and heat capacity), computing previously the reduced temperature.
2. Observing the points near the critical temperature, we choose the ones with a linear behavior (the closest ones, over 10-15 points).

3. Finally, from this values, we do a linear regression to obtain the slope, which directly gives us the critical exponent.

This has been done for the largest lattice, since is the closest to the exact solution. The values obtained from the linear regression are,

Table 2: *Critical exponents obtained from the simulations. The double values for gamma and alpha are due to the exponent being calculated by the right or left of the critical temperature. As we can see, all the values are in consonance with the theoretical values, $\beta = 0.125$, $\gamma = 1.75$ and $\alpha = 0$. Although some theoretical exponents do not fall within our values with their respective errors, they are close enough. Recall that Ising model is relatively complicated to perform in a computational way, given the character of the system and the insufficient size for the studied lattices.*

β	γ_-	γ_+	α_-	α_+
0.119 ± 0.01	1.77 ± 0.03	1.73 ± 0.02	0.02 ± 0.01	0.03 ± 0.01

To find the critical exponent ν one has to implement extra code to compute the correlation function,

$$Corr = < \sigma(0)\sigma(r) > - < \sigma > \sim e^{-r/\xi} \tag{3}$$

As an example, for a lattice of L=64 and near the critical temperature $T = 2.38$, the following behavior is shown,

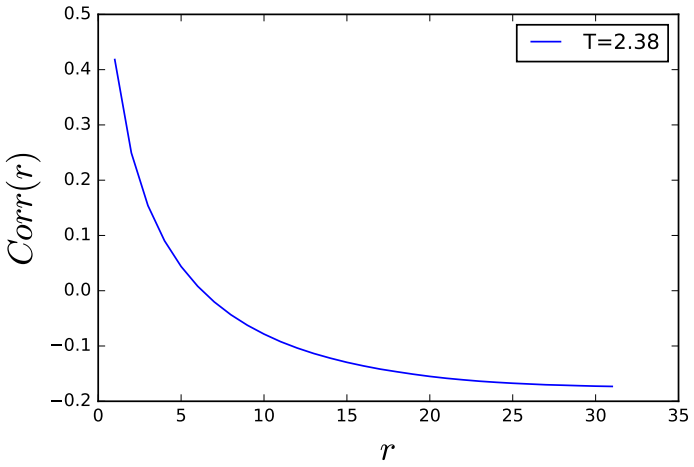

Figure 6: *Correlation function for a lattice with L=64, in terms of the distance to a certain spin. As we can see, there is an exponential decay as theory predicts.*

From the linear regression of the nearest points (the ones that have a better exponential decay) we can obtain the correlation length, $\xi \sim -r/log(Corr)$. Finding the correlation length for several temperatures near the critical region, and plotting them in terms of the reduced temperature, we can find the ν exponent, $\xi \sim |t|^{-\nu}$.

To finish our study, we willstudy de data collapse due to the correction of finite size effects. Since $\xi \sim L$ near the critical point, we can re-scale with the critical exponents,

$$ML^{\beta/\nu} = f(L^{\nu}t) \tag{4}$$

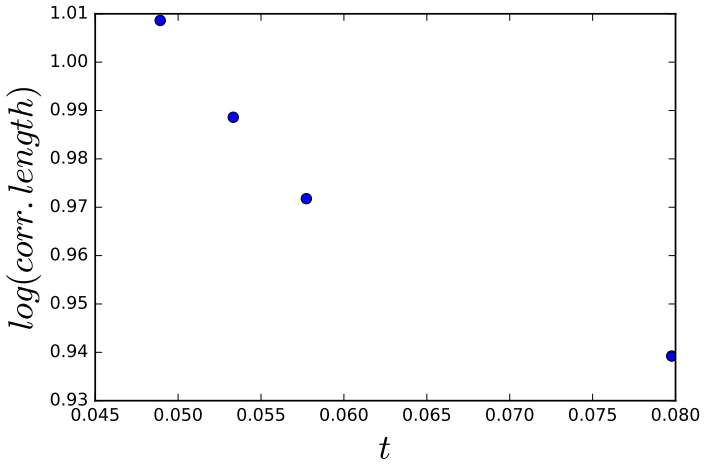

Figure 7: *Logarithm of ξ in terms of the reduced temperature near the critical threshold. As we can see the regression is negative.We obtain $\nu = 2 \pm 1$, which is consistent with the theoretical value $\nu = 1$.*

$$ML^{-\gamma/\nu} = f(L^{\nu}t) \tag{5}$$

And this should provide the collapse of the data into a single plot. Hence we obtain,

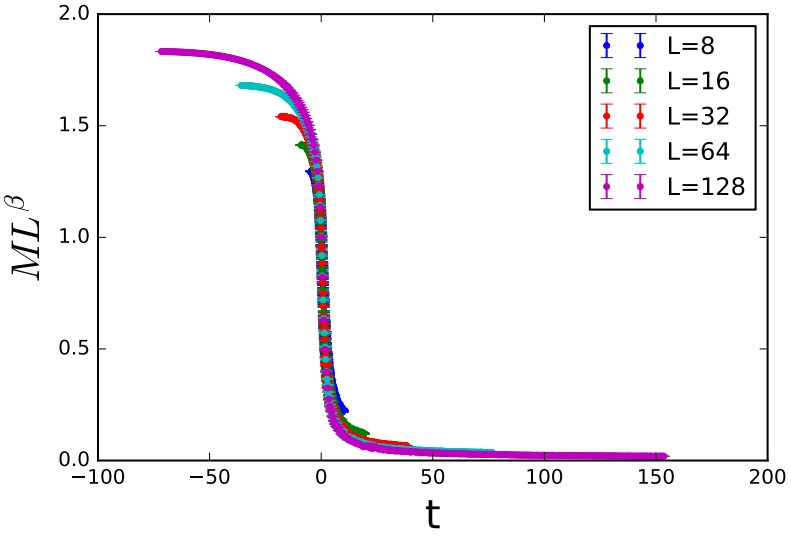

Figure 8: *Re-scaled magnetization in terms of the re-scaled reduced temperature. As we can see, all the data collapses into a single function, which is universal for any lattice size. This shows the phase transition, in which the correlation length is of the order of the system size.*

III. Appendix

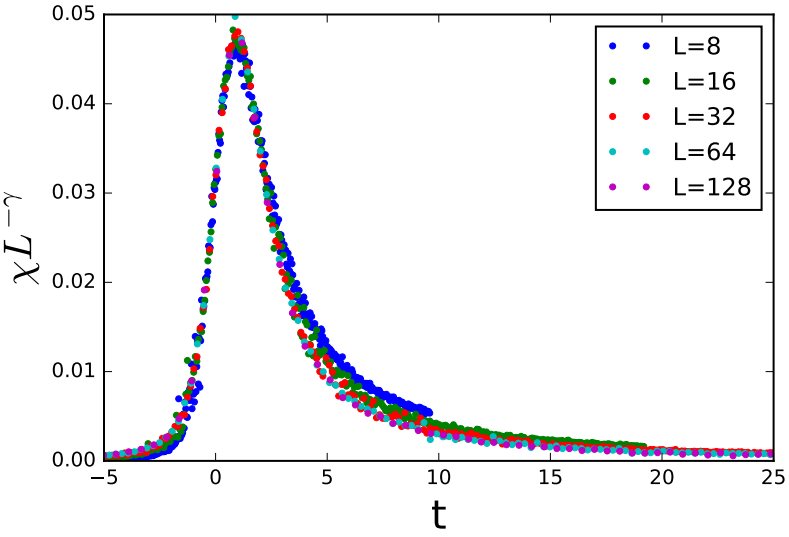

Figure 9: *Re-scaled susceptibility in terms of the re-scaled reduced temperature. Again we observe a perfect data collapse.*

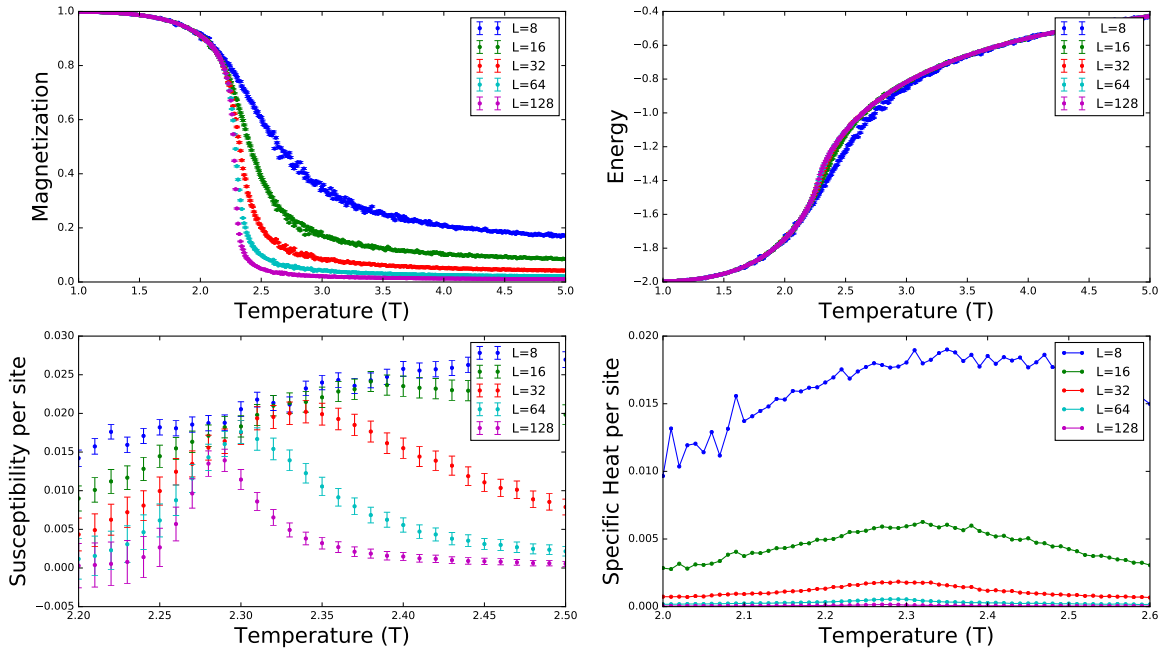

Figure 10: *Alternative plot of the magnetization, energy, susceptibility and specific heat per site.*