2D Ising Model Simulation

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I. INTRODUCTION

The main purpose of this simulation is to analyse a 2-dimensional magnetic system described by the Ising model. It consists on a square-lattice with N particles positioned on each vertex formed by the lattice. Particles are in binary spin states S (+1 or -1) and exhibit interaction with their nearest neighbours. The system's energy is described by the following Hamiltonian:

$$H = -\sum_{<i,j>} JS_iS_j. \tag{1}$$

Where J is the scale factor between spin interaction and energy. It is indeed possible to obtain the system's magnetization and to study it as a function of temperature.

The two dimension Ising model exhibit a phase transition at the so called critical temperature T_c. Using the Monte Carlo method and the Markov chain it is possible to analyse the system's energy numerically. The code developed chooses in a random fashion the value of the spin in the lattice, and it changes this value when the system's energy becomes smaller or, when it is bigger, with a specific probability that depends on the temperature. After a large number of Monte Carlo steps, the system finally stabilizes and reaches a thermic equilibrium.

Studying different variables such as the average energy, magnetization, calorific capacity and susceptibility of the system, we are able to see how the critical temperature changes in addition to determine T_c at the thermodynamical limit. Using this newly found critical temperature, it is possible to eventually compute the system's critical exponents.

Note: All temperatures used are in the form of the reduced temperature:

$$T^* = \frac{K_B T}{J}.$$

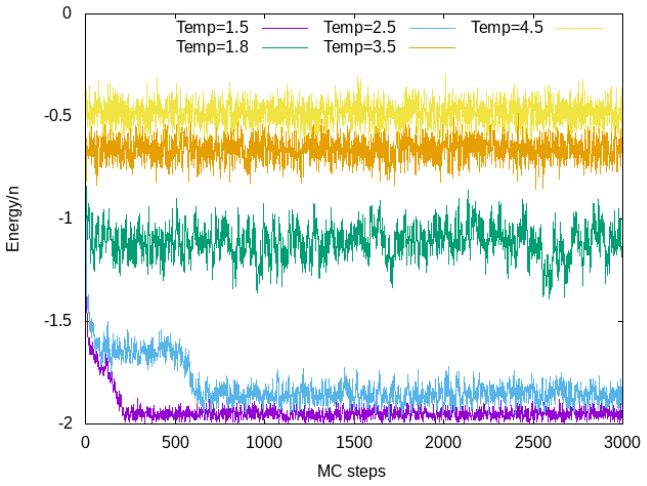

FIG. 1: Energy temporal evolution for T=1.5, 1.8, 2.5, 3.5, 4.5. 3000 Monte Carlo steps are done.

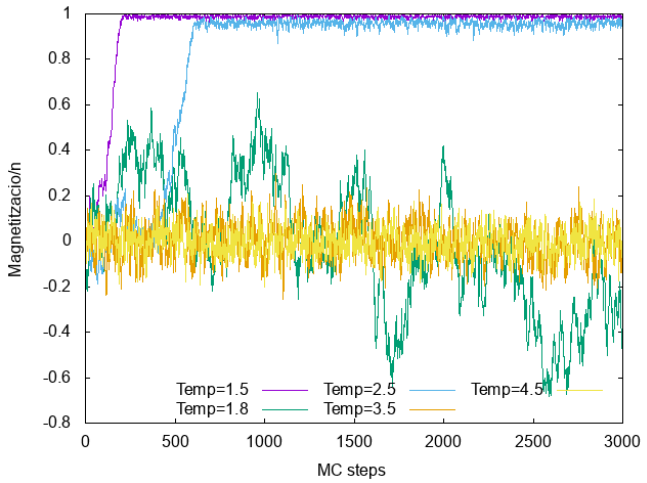

FIG. 2: Magnetization temporal evolution for T=1.5, 1.8, 2.5, 3.5, 4.5. 3000 Monte Carlo steps are done.

II. DISCUSSION OF TEMPORAL EVOLUTION

Using the Monte Carlo method we compute the energy and the magnetization for five distinct temperatures: $T = 1.5, 1.8, 2.5, 3.5, 4.5$ and for a characteristic lattice size $L = 30$. The values for each MC step are plotted in order to examine the system's time evolution, as it can be seen in Fig.(1), Fig.(2).

At the beginning of the simulation, the energy and magnetization of the system has an anomalous behaviour since it is not stabilized. As seen in Fig.(1), energy stabilizes after a certain time value and its behaviour is to increase with temperature. In the other hand, magnetization behaves differently depending on the initial temperature. For temperatures lower than the critical temperature ($T_c \approx 2.3$), the system is in its ferromagnetic state with magnetization 1 (all spins pointing upwards). It could definitely be -1, since it depends on the initial seed. For this reason, the absolute value of the magnetization is a reliable indicator to check if the system is ferromagnetic.. After reaching T_c, the magnetization oscillates around zero because it is transitioning into the paramagnetic phase, i.e, all spins are randomly oriented.

III. TEMPERATURE DEPENDENCE

As previously seen, temperature is a relevant factor when studying energy, magnetization, calorific capacity and susceptibility of the system. To understand their dependence we compute the values of each variable after 40000 MC steps and 200 initial seeds for L=30, and then we compute the average value for each variable.

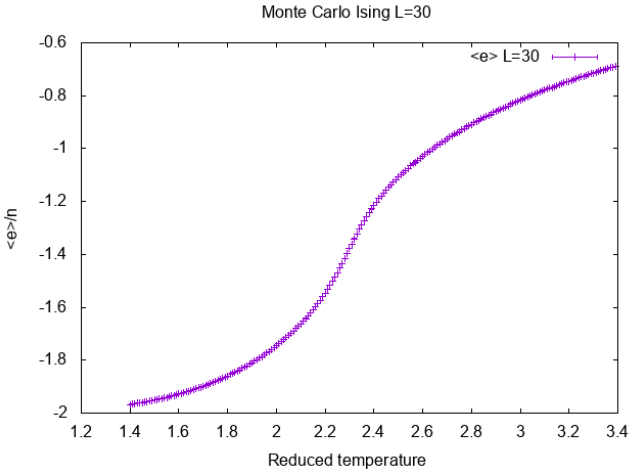

FIG. 3: Energy behaviour as a function of temperature.

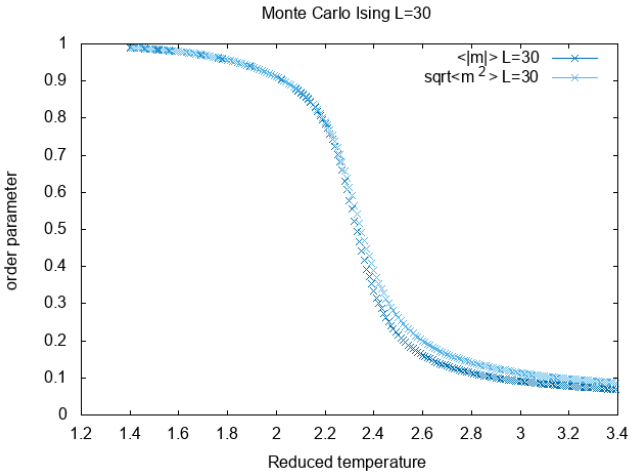

FIG. 4: Absolute value of magnetization and the square root of the square of the magnetization behaviour as a function of temperature.

As we see in Fig.(3), the average energy shows a minimum energy state at low temperatures, where all the spins have the same orientation. Increasing the temperature leads to an average energy growth until T_c is reached. It is an inflection point. Afterwards, energy continues increasing. It would eventually reach the zero value for high temepratures, meaning that all spins are randomly distributed. Error bars have been plotted, but they are indistinguishable because the error is much smaller than the energy value.

To study magnetization we have introduced the order parameter, which shows its absolute average value $|m|$ and $\sqrt{m^2}$ both normalized. As seen in the temporal evolutioon discution, the magnetization tends to -1 at low temperatures due to the same orientation of the spins showing a ferromagnetic behaviour, while at higher temperatures it leans towards 0 because the spins are randomly distributed, showing a paramagnetic behaviour. Between the this two kinds of behaviour, as showed in Fig.(3) there is an inflection point at T_c where the system changes its phase. After this point the two functions of magnetization detach from each other due to statistical errors.

The calorific capacity C_v and the susceptibility χ can be obtained from the thermodynamic variables computed before.

The calorific capacity describes how well the system is able to change its temperature when heat is introduced to the system. The susceptibility is the quantification for the change of the magnetization under magnetic field variations:

$$C_v^* = N\frac{< e^2 > - < e >^2}{T^2} \quad C_v^* = \frac{d < e >}{dT}. \tag{2}$$

$$\chi = N\frac{< m^2 > - < m >^2}{T} \tag{3}$$

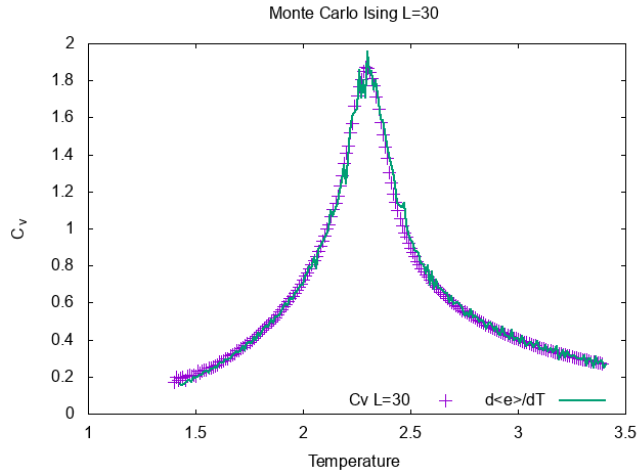

FIG. 5: Calorific capacity as a temperature function. It constitutes a graphical proof that $\frac{d<e>}{dT}$ is effectively equivalent.

As we can see, the dependence in temperature for the fluctuation method is similar in both plots. The susceptibility and calorific capacity tends to zero at low and high temperatures and in between there is a peak where the values reach their maxima. This temperature, is,

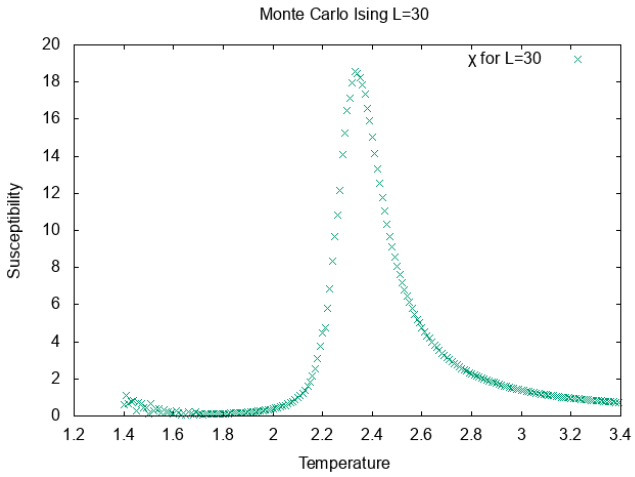

FIG. 6: Susceptibility as a temperature function.

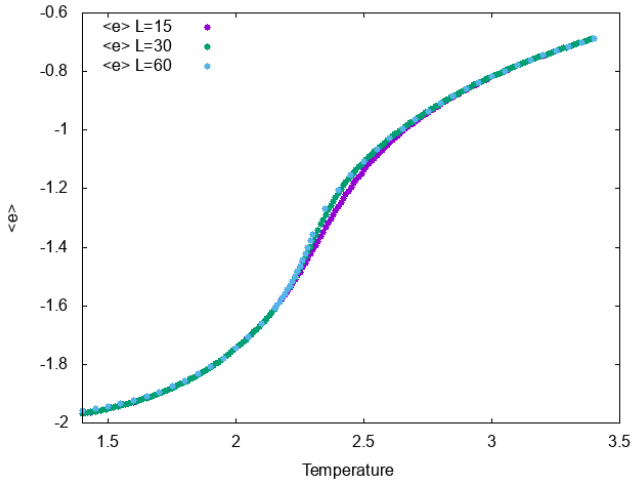

FIG. 7: Average energy as a function of temperature for L=15,30,60.

indeed, the critical temperature T_c where systems are going under a phase transition. Comparing Fig.(5) and Fig.(6), we observe that the critical temperature differs. For the calorific capacity plot, $Tc = 2.29$ whereas for the susceptibility plot $T_c = 2.33$. In Fig.(5) there is a second function that shows that we can obtain similar results using the energy derivative with respect to temperature. Obtaining matching results using two methods constitutes evidence for the success and reliability of the Monte Carlo one.

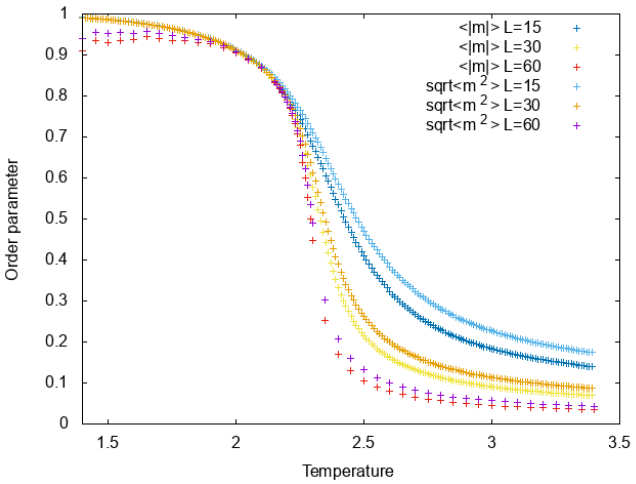

FIG. 8: Order parameter as a function of temperature for L=15,30,60.

IV. SYSTEM SIZE DEPENDENCE

We are now going to study how size variations of the system affects relevant computed quantities.

Average energy, order parameter, calorific capacity and susceptibility have been computed and plotted for 3 different systems sizes: L=15,30,60. It was suggested to do it for L=120 as well but computer limitations were suffered.

As shown by Fig.(7), energy values do not change with system size variations. However, an increase in the slope can be perceived at T_c when size grows. As far as the order parameter concerns, Fig.(8) becomes steeper as well and they detach from each other, as a consequence of the dimension of the system.

When plotting the calorific capacity and the susceptibility the dependence with the system size is, as seen in Fig.(9) and Fig.(10), significant. The peak at T_c gets higher for large values of L and it moves to low temperatures for both plots. As it can be appreciated, at low temperatures, the method is not very precise for large sized systems.

V. EXTRAPOLATION OF T_c

As seen before, critical temperature T_c presents different values for calorific capacity and susceptibility, as well as also decreasing when system size grows. For this reason we need to extrapolate the obtained values to the thermodynamic limit $N \to \infty$, where the function of calorific capacity and susceptibility diverges at the same T_c.

Plotting the critical temperature as a function of the inverse of the system's size and extrapolating the obtained values when $1/L \to 0$, we can adjust the points to a linear regression and obtain a non-size depending critical temperature T_C, as did in Fig.(11). Results yield $T_c = 2.267 \pm 0.003$ for the susceptibility and $T_c = 2.274 \pm 0.009$ for the calorific capacity. Both are near the exact value $T_{c_{exact}} = 2.269$ and within the cal-

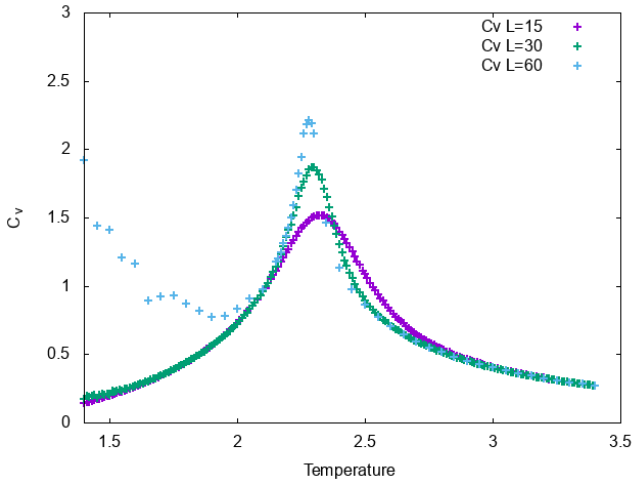

FIG. 9: Calorific capacity as a function of temperature for L=15,30,60.

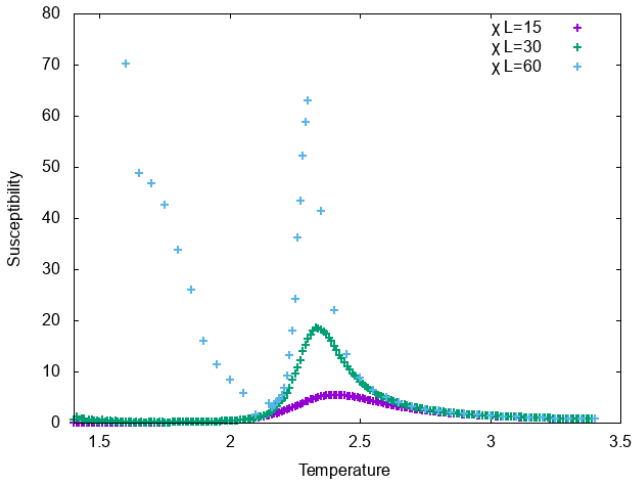

FIG. 10: Susceptibility as a function of temperature for L=15,30,60.

culated uncertainty.

VI. CRITICAL EXPONENTS

Critical exponents ν and γ are going to be determined in this section. Since the exponent ν goes as $T_{cL} - T_c = AL^{-\frac{1}{\nu}}$, the needed function to plot is $ln(T_{cL} - T_c)$ as a function of $ln(L)$, where the used exact value of T_c is $T_c = 2.269$.

Using a linear regression to find the slope of each independent variable we can compute the critical exponent ν, since $ln(T_{cL} - T_c) = ln(A) - \frac{1}{\nu} ln(L)$. We have obtained $-\frac{1}{\nu} = -1.67 \pm 0.12$ for the calorific capacity and $-\frac{1}{\nu} = -1.14 \pm 0.09$. This leads to $\nu = 0.6 \pm 0.3$ for C_v and $\nu = 0.9 \pm 0.1$ for χ. Knowing that the exact value of this exponent is $\nu = 1$, we have gotten a reasonable

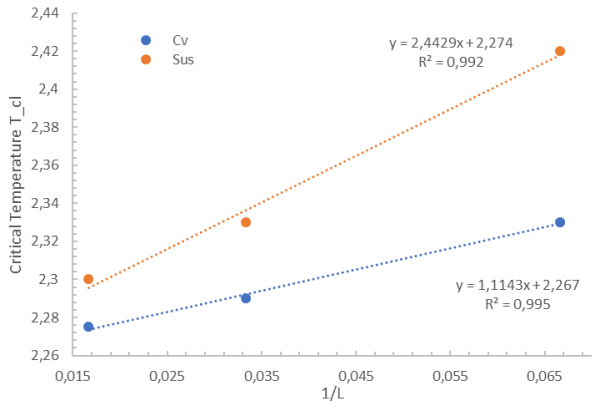

FIG. 11: Critical temperature as a function of the inverse of the system size $1/L$. Linear regressions are done for the C_v and χ cases.

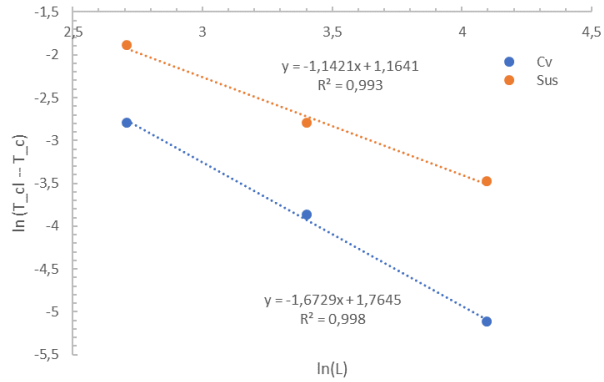

FIG. 12: Logarithm of the difference between the critical temperature depending on L and the exact critical temperature as a function of the logarithm of L.

result for the susceptibility and a less adequate result for the calorific capacity (it is not within the error interval). This fact could definitely be because there is a lack of points (there are 3). It is probable that with one extra point (computing L=120) the result for C_v would have been a better one.

In order to find the γ exponent, the following equation is used:

$$\chi = B|T - T_c|^{-\gamma} = B\left(AL^{-\frac{1}{\nu}}\right) = CL^{\frac{\gamma}{\nu}} \qquad (4)$$

Plotting the logarithm of susceptibility at T_c as function of the logarithm of L, Fig.(13) is obtained. From this plot we can find the slope of the linear regression which is, in fact, $\frac{\gamma}{\nu}$. The result is, then, $\frac{\gamma}{\nu} = 1.77 \pm 0.02$, which is a good enough result considering that $\nu_{exact} = 1$ and $\gamma_{exact} = 1.75$.

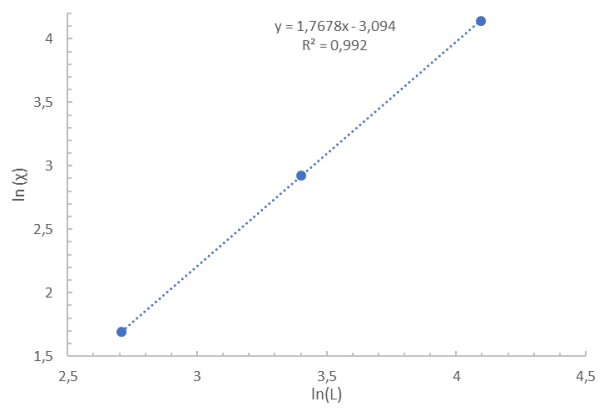

FIG. 13: Logarithm of the susceptibility at the critical point as function of the logarithm of L.

VII. FINITE SIZE SCALING

Using the recently found critical exponents, it is possible to plot the susceptibility and the order parameter with a special axis that rescales all the values in such a manner that the susceptibility peak appears at the same T_c and same height for every lattice size L, as it can be seen in Fig.(14).

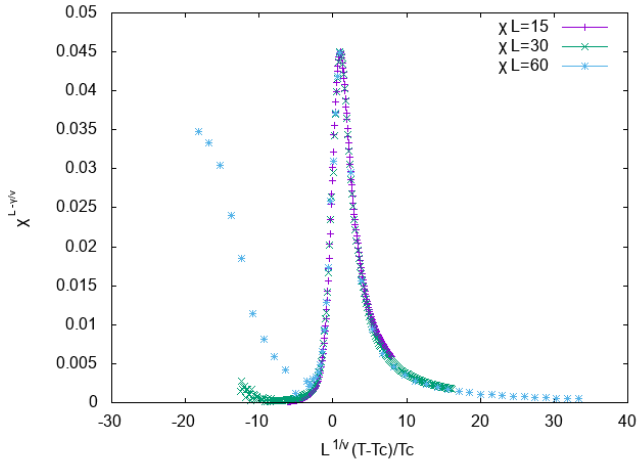

FIG. 14: Logarithm of the susceptibility at the critical point as function of the logarithm of L.

Similarly proceeding for the order parameter, we choose an axis so the slope for different sized systems is the same. The results can be seen in Fig.(15).

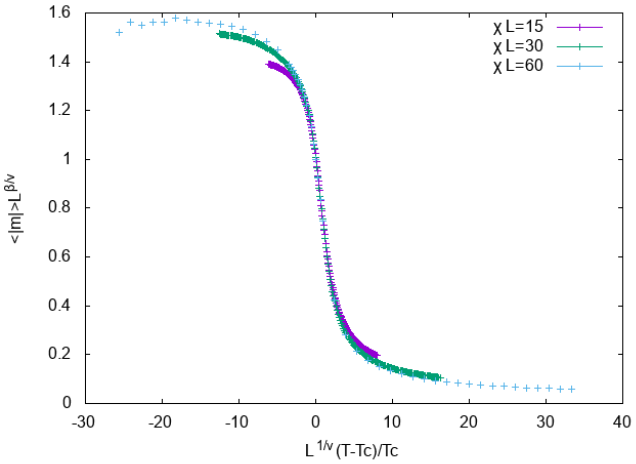

FIG. 15: Logarithm of the susceptibility at the critical point as function of the logarithm of L.

VIII. CONCLUSIONS

- Using the 2-dimensional Ising model, a thorough study of the relevant thermodynamic variables of a magnetic system has been done. In the first section we observed that the system behaves like a ferromagnet until it reaches the critical temperature where it experiences a phase transition. Above this point the system becomes paramagnetic.

- We noticed that the critical temperature T_c differs for the susceptibility and the calorific capacity and it decreases with the lattice size as well. Consequently, we analysed these dependencies and extrapolated to the thermodynamic limit, obtaining a main value of $T_c \approx 2.269$, in concordance with the exact value.

- Using the critical temperature value, we could compute the critical exponents for this two dimensional system. For the first exponent a main value of $\nu = 0.9 \pm 0.1$ has been obtained for the susceptibility, which agrees with the exact value $\nu = 1$. For the critical temperature associated with the calorific capacity, we determined that more data is definitely needed in order to calculate ν (probably computing for size L=120). A value of $\frac{\gamma}{\nu} = 1.77 \pm 0.02$ has been found which, again, agrees with the exact value for the second exponent.

- Finally, it has also been verified the finite size scaling for the susceptibility and the order parameter.

[1] *Phase transitions and collective phenomena* and *Computational physics* notes.