M.Sc. Physics of Complex Systems

Cooperative and critical phenomena

2D Ising Model

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Introduction

A numerical study of the 2D Ising Model is presented in this work. The Ising model is a physical model proposed by Ernst Ising to study the behaviour of ferromagnetic materials. The model consists in a lattice of length L with L^2 sites each of which represent an atomic spin of $s = 1/2$. The spin values are determined by the interactions with first neighbour spins and due random fluctuations given by temperature, these values (or directions) could flip. It is well-known that this system exhibits a second-order phase transition at a given critical temperature. Some properties of the system, such as susceptibility and specific heat, diverge at this critical temperature following a power-law, so that this divergence is characterised by some exponents named *critical exponents*. In this work, besides studying the thermal dependence of the system properties, the critical temperature of the system will be found and the critical exponents will be computed via the finite size scaling approach. The results will be compared with the available theoretical ones.

From a numerical point of view, a Monte Carlo method has been implemented using the Metropolis-Hastings algorithm with the sequential update method to generate representative equilibrium configurations of the system. Then, the thermal dependence of the system properties in the equilibrium stage (i.e. magnetisation, internal energy, susceptibility and specific heat) has been studied. Moreover, the critical temperature and critical exponents have been computed following the finite size scaling approach [1].

Technical details

Two set of results have been considered in this work and will be presented for each subsection. The first set of results have been obtained considering lattice lengths of $L = 4, 8, 16, 32, 64$ and temperature points in the range $T \in [0.1, 5.1]$ with a temperature increase of $\mathrm{d}T = 0.1$. In order to improve the quantitative results for the critical exponents and also the qualitative ones for the finite size scaling collapse of the data, a larger set of lattice lengths has been considered in a range of temperatures closer to the critical temperature with the same temperature increase: $L = 10, 14, 16, 20, 24, 28, 32, 36, 40, 50, 64, 70, 80, 90, 100, 110$ with $T \in [2, 3]$. We'll refere to the first set of L's as $\{L\}_1$ and to the second one as $\{L\}_2$.

In order to increase in efficiency and avoid the Metropolis-Hastings algorithm to fall in local minima an initialisation trick has been considered. As we know from the theoretical approach of the problem, for temperatures below the critical one, $T < T_c$ the absolute intensive magnetisation is nearly 1, so all spins have the same value. Thus, for "low temperatures" ($T < 2$) the lattice is initialised with all the spins with the same values. For higher temperatures it is initialised randomly. After that, a thermalisation time of $M_0 = 10^4$ MCS (Monte Carlo Steps)[1] is set along with a long run of $M = 10^6$ MCS to take measures. Moreover, in order to increase the statistical significance of the measures and decrease the statistical errors due the correlations, a spacing of $K = 5$ MCS is considered between measures. For a discussion of these values of thermalisation, run an spacing see Appendix B

[1] A Monte Carlo Step is defined as the steps needed to run over all the spins, this is, a whole lattice update. As the sequential update method is being considered, a MCS are L^2 iterations

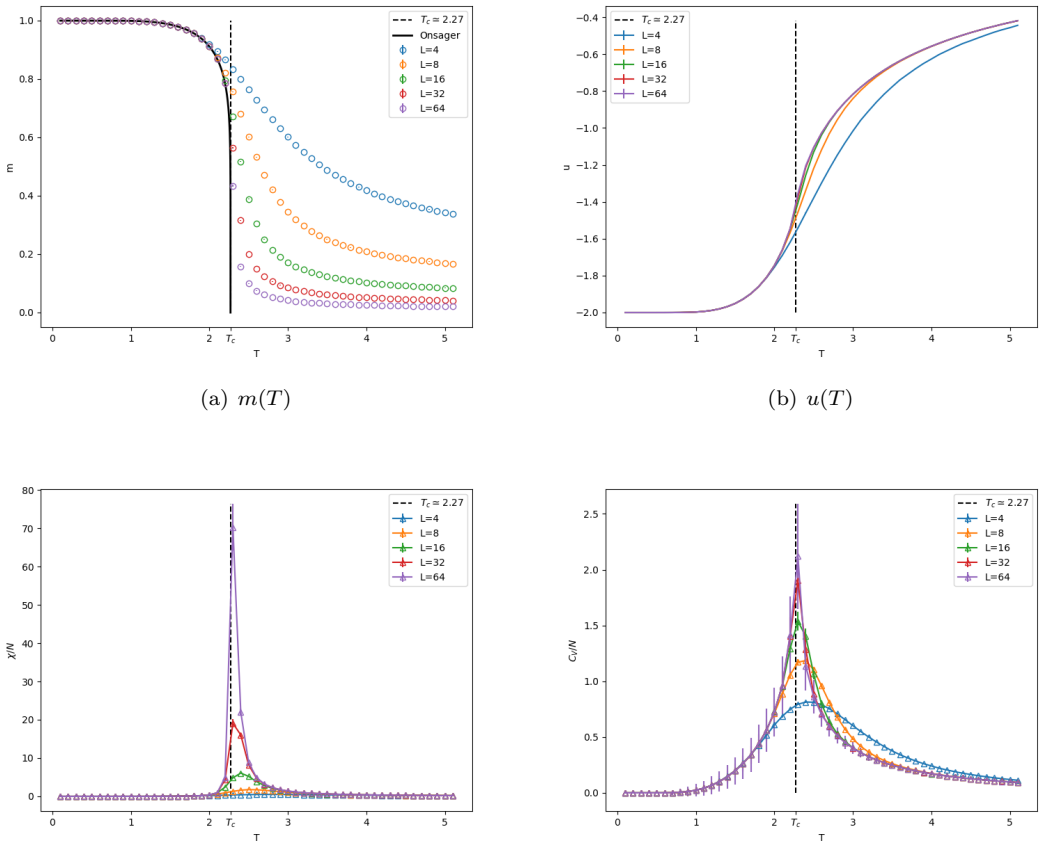
Results

Thermal dependence of system properties

In this first section the thermal dependence of the intensive quantities of magnetisation, energy, susceptibility and specific heat will be studied qualitatively for the set of results $\{L\}_1$. This quantities plotted below have been obtained from the following formulas

$$m = \frac{\langle M \rangle}{N} \qquad u = \frac{\langle U \rangle}{N} \qquad \chi = \frac{\beta}{N}\sigma^2(M) = \beta\frac{\langle M^2 \rangle - \langle M \rangle^2}{N} \qquad C_V = \frac{\beta^2}{N}\sigma^2(U) = \beta^2\frac{\langle U^2 \rangle - \langle U \rangle^2}{N}$$

where $N = L^2$ is the number of spins of the system.



(a) $m(T)$ (b) $u(T)$

(c) $\chi(T)$ (d) $C_V(T)$

Figure 1: Thermal dependence of system properties for $\{L\}_1 = 4, 8, 16, 32, 64$

Fig. 1 shows the thermal dependence of the intensive magnitudes enumerated above for the temperature range $T \in [0.1, 5.1]$. In Fig. 1(a) it can be seen how the magnetisation curve approaches the theoretical Onsager's solution as $L \to \infty$, showing an inflection point at the critical temperature $T_c \simeq 2.27$. We can see the same behaviour in Fig. 1(b), which shows the energy per spin. Fig. 1(c) and Fig. 1(d) show the fluctuations of the just described magnitudes, which are equivalent to the susceptibility and the specific heat of the system, respectively. It can be observed that there is a maximum that approaches the critical temperature as L increases. Basically this is showing the divergence of these magnitudes near the critical temperature as the system approaches the infinite system. Obviously as this is a computer simulation we'll never real get a divergence, instead we obtain these huge values of the maximums as we keep increasing the length of the system.

Finite Size Scaling: critical exponents and data collapse

It is known that the correlation length diverges near the critical temperature as $\xi \sim |t|^{-\nu}$, so that at exactly the critical temperature the correlation length should be infinite[2]. In a numerical simulation the value of the correlation length is constrained by the system size, which is finite. Thus, the correlation length in a numerical simulation will be given by $\xi \sim L$ when $T \to T_c$. Then, the divergence of all the other quantities can be expressed in terms of the system size.

$$\begin{cases} \xi \sim |t|^{-\nu} \\ \xi \sim L \end{cases} \implies |t| \sim L^{-1/\nu} \implies \begin{cases} \chi \sim |t|^{-\gamma} \sim L^{\gamma/\nu} \\ C_V \sim |t|^{-\alpha} \sim L^{\alpha/\nu} \\ m \sim |t|^{\beta} \sim L^{-\beta/\nu} \end{cases} \tag{1}$$

Then we can find the critical exponents of the system following the next procedure:

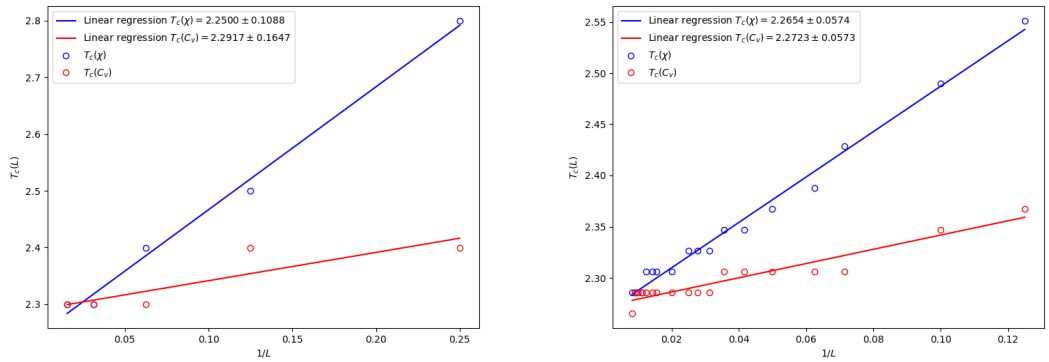
- Find the critical temperature T_c
- Fit the $|t|$, ξ, C_V and m data as function of L so that the slope is the desired critical exponent.

Determination of T_c

To find the critical temperature different methods can be applied (e.g Binder or fourth order cumulants). The one used in this work consists in finding the maximums of susceptibility and specific heat for different systems sizes, which are known to be at the critical temperature, and consider the following relation

$$T_c(L) = T_c + CL^{-1/\nu} \tag{2}$$

So that the intersection with the origin of the fitted line will be the critical temperature. The idea is that, as seen in Fig. 1, the maximums of these magnitudes approach the critical temperature when $L \to \infty$.



(a) $T_c = 2.2708 \pm 0.0987$ (b) $T_c = 2.2688 \pm 0.0405$

Figure 2: Determination of the critical temperature with (a) $\{L\}_1$ and (b) $\{L\}_2$.

Fig. 2 shows the fit of Eq. (2) where the data points are the maximums of χ and C_V for the different system sizes in $\{L\}_1$ (Fig. 2(a)) and $\{L\}_2$ (Fig. 2(b)). Then, we can consider the numerically determined critical temperature to be the average of the interceptions obtained. The final values for the critical temperature, with the proper propagation of errors considered, are summarised in Table 1

[2] $t \equiv \dfrac{T - T_c}{T_c}$

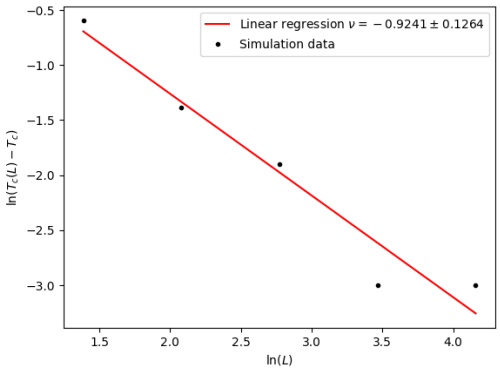
Table 1: Final values for the critical temperature with $\{L\}_1$ and $\{L\}_2$.

	T_c	Relative error (%)
$\{L\}_1$	2.2708 ± 0.0987	0.071
$\{L\}_2$	2.2688 ± 0.0405	0.017

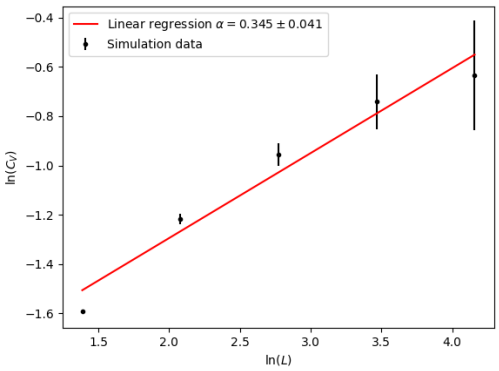
The relative error is obtained comparing with the theoretical Onsager's critical temperature $T_c = 2/(\ln\left(1+\sqrt{(2)}\right)) \approx 2.269185314213022....$ As can be observed, both values obtained for the critical temperature match with the theoretical one within errors. However, an improvement can be seen in the relative error with the second set of measures $\{L_2\}$, which also has a smaller error because more points were considered.

Determination of the critical exponents

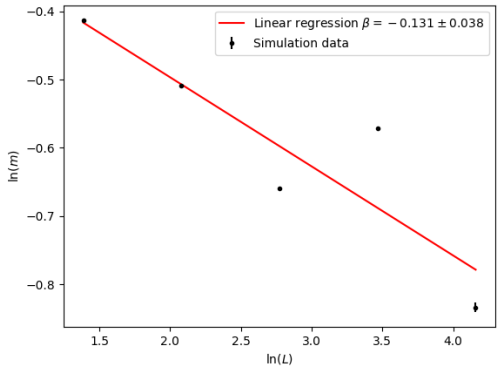
Once we have determined the critical temperature of the system the calculation of the critical exponents is straight forward. First of all the ν exponent must be computed using a linear regression in the first relation of Eq. (2). After that, the other three exponents can be determined. The figures below show the linear regressions considered to determine the critical exponents with the set of results $\{L\}_1$ and $\{L\}_2$.



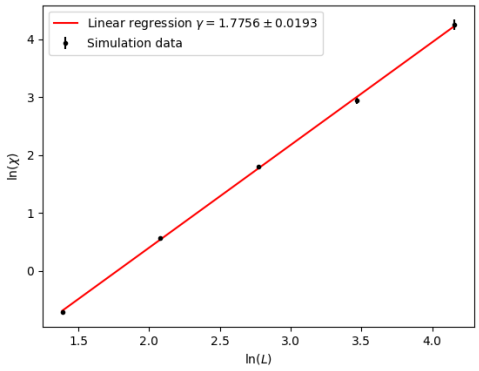
(a) $1/\nu = 0.9241 \pm 0.1264$



(b) $\alpha = 0.345 \pm 0.041$

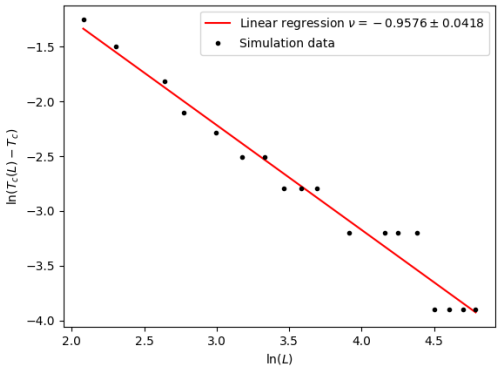


(c) $\beta = -0.131 \pm 0.038$

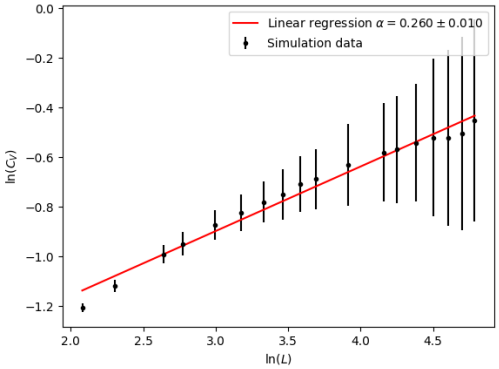


(d) $\gamma = 1.7756 \pm 0.0193$

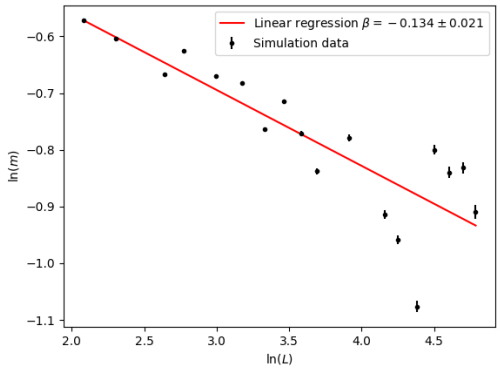
Figure 3: Determination of the critical exponents with $\{L\}_1$



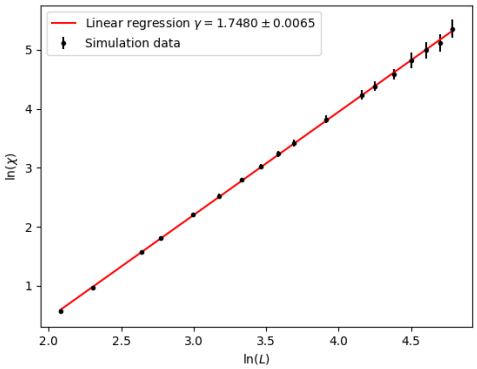
(a) $1/\nu = 0.9576 \pm 0.0418$



(b) $\alpha = 0.260 \pm 0.010$



(c) $\beta = -0.134 \pm 0.021$



(d) $\gamma = 1.7480 \pm 0.0065$

Figure 4: Determination of the critical exponents with $\{L\}_2$

Comparing Fig. 3 and Fig. 4 it is clear that the set of results $\{L\}_2$ provides a better approximation to the theoretical critical exponents. To quantify this improvement Table 2 has been written below summarising the results obtained for the critical exponents with both sets of results including the relative error to the theoretical critical exponents.

Table 2: Comparison of the results for the critical exponents obtained with both sets $\{L\}_1$ and L_2.

	α	β	γ	ν
$\{L\}_1$	0.345 ± 0.041	-0.131 ± 0.038	1.7756 ± 0.0193	1.082 ± 0.148
$\{L\}_2$	0.260 ± 0.010	-0.134 ± 0.021	1.7480 ± 0.0065	1.044 ± 0.046
Rel. Err $\{L\}_1$ (%)	$\emptyset$	4.8	1.46	8.2
Rel. Err $\{L\}_2$ (%)	$\emptyset$	7.2	0.11	4.4

Note that the relative error for α can not be computed due that the theoretical value for this critical exponent is $\alpha = 0$. However, the obtained value for α with the set of results $\{L\}_2$ is nearer to its theoretical value than the obtained with $\{L\}_1$. Furthermore, Table 2 shows that, in general, the $\{L\}_2$ set of results provide more exact and precise values for the critical exponents.

Data collapse as a finite size scaling test

As has been said at the beginning of this section, the correlation length diverges in the theoretical Ising model, but this property can not be achieved in a numerical simulation, where the correlation length will behave as $\xi \sim L$ when $T \to T_c$. Mathematically this can be expressed as follows: If we continue to denote by ξ the value which the correlation length would have in an infinite system at temperature t, then the cut-off takes place when $\xi > L$. As long as $\xi \gg L$ the value of ξ should be the same as that for the infinite system. We can express this by writing [1]

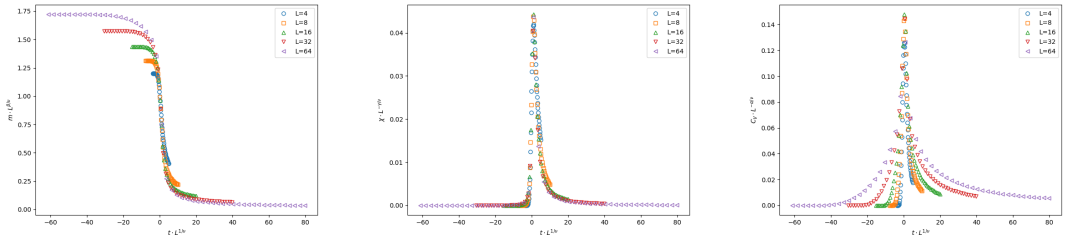
$$\chi = \xi^{\gamma/\nu} \chi_0 \left(L/\xi\right), \quad \text{where} \quad \chi_0 \left(L/\xi\right) = \begin{cases} \text{const} & \frac{L}{\xi} \gg 1 \\ \left(\frac{L}{\xi}\right)^{\gamma/\nu} & \frac{L}{\xi} \to 0 \end{cases}$$

so that for $L \gg \xi \Longrightarrow \xi \sim \xi^{\gamma/\nu}$ as in the infinite system and for $L = \xi \Longrightarrow \xi \sim L$. After that, this equation can be rearranged in a more useful form from the point of view of the numerical simulations [1], which leads to

$$\chi(L) = L^{\gamma/\nu} \chi_0 \left(L^{1/\nu} t\right) \Longrightarrow \chi_0 \left(L^{1/\nu} t\right) = L^{-\gamma/\nu} \chi(t)$$

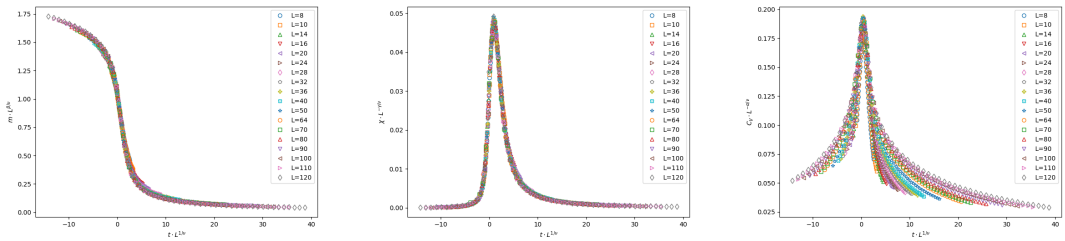
where χ_0 is the so called scaling function for the susceptibility and should be the same regardless of the system size. This procedure can be extended to the other thermodynamic quantities of the system so that their scaling functions are given by

$$m_0 \left(L^{1/\nu} t\right) = L^{\beta/\nu} m(t) \qquad C_{V0} \left(L^{1/\nu} t\right) = L^{-\alpha/\nu} C_V(t)$$



(a) $m(T)$ (b) $\chi(T)$ (c) $C_V(T)$

Figure 5: Data collapse for $\{L\}_1$



(a) $m(T)$ (b) $\chi(T)$ (c) $C_V(T)$

Figure 6: Data collapse for $\{L\}_2$

Fig. 5 and Fig. 6 show that the data actually collapses in a unique curve for the critical exponents experimentally found with $\{L\}_1$ and $\{L\}_2$. Once again, the set $\{L\}_2$ gives better results than $\{L\}_1$. Moreover, we can see that the finite size scaling fails for temperature values far enough from the critical temperature, as it is expected.

A Error calculation

In order to compute the errors for the susceptibility and the heat capacity some error propagation has been considered. The computation of the mentioned magnitudes is done from the fluctuations of the magnetisation and the energy of the system

$$\chi_T = \beta\sigma^2(M) = \beta\left[\langle M^2\rangle - \langle M\rangle^2\right]$$
$$C_V = \beta^2\sigma^2(E) = \beta\left[\langle E^2\rangle - \langle E\rangle^2\right]$$

We know the error of the averages, even considering the correlations, so we need to propagate this error to find the error of $\langle M\rangle^2$ and $\langle E\rangle^2$. The formula for error propagation is the following

$$u^2(f(\boldsymbol{x})) = \sum_i \left(\frac{\partial f}{\partial x_i}\right)^2 u^2(x_i)$$

so considering $f(x) = x^2$ we have

$$u^2(x^2) = 4x^2u^2(x) \Longrightarrow \begin{array}{l} u^2(\langle M\rangle^2) = 4\cdot\langle M\rangle^2 u^2(\langle M\rangle) \\ u^2(\langle E\rangle^2) = 4\cdot\langle E\rangle^2 u^2(\langle E\rangle) \end{array}$$

Finally, to compute the errors of the fluctuations we need to propagate the error of a difference multiplied by a constant, $f(x,y) = C(x-y)$

$$u^2(x-y) = C^2\left[u^2(x) + u^2(y)\right] \Longrightarrow u(x-y) = C\sqrt{u^2(x)+u^2(y)}$$

Thus, the errors of the susceptibility and specific heat are given by

$$\begin{array}{l} u(\chi_T) = \beta\sqrt{u^2(\langle M^2\rangle) + u^2(\langle M\rangle^2)} = \beta\sqrt{u^2(\langle M^2\rangle) + 4\langle M\rangle^2 u^2(\langle M\rangle)} \\ u(C_V) = \beta^2\sqrt{u^2(\langle E^2\rangle) + u^2(\langle E\rangle^2)} = \beta^2\sqrt{u^2(\langle E^2\rangle) + 4\langle E\rangle^2 u^2(\langle E\rangle)} \end{array} \tag{A.1}$$

Moreover, to obtain the statistical errors considered in the error propagation above correlations within measures must be considered. Measures taken at different times may be correlated, so that this correlation has an effect on the statistical error, which no longer is given by just the standard deviation. Thus, the statistical errors of the measures taking into account the correlations are given by the following expression

$$u(\hat{G}) = \sqrt{\frac{\sigma^2(\hat{G})}{N}(2\tau_G + 1)} \tag{A.2}$$

with N being the number of measurements and

$$\tau_G = \sum_{k=1}^{M-1}\left(1 - \frac{k}{M}\right)\rho_G(k) \approx \sum_{k=1}^{M-1}\rho_G(k) \qquad (\approx \text{for large } M)$$

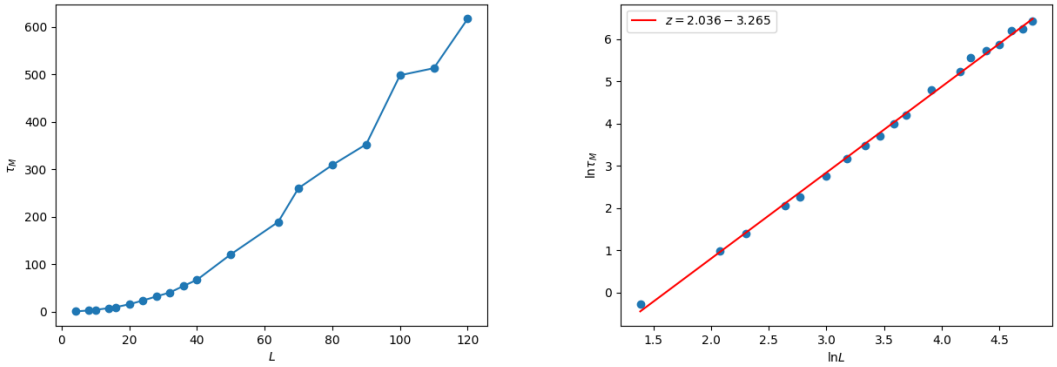
where $\rho_G(k)$ is the normalised correlation function $\rho_G(k) = \dfrac{\left\langle \hat{\mathbf{G}}_i\hat{\mathbf{G}}_{i+k}\right\rangle - \left\langle \hat{\mathbf{G}}_i\right\rangle\left\langle \hat{\mathbf{G}}_{i+k}\right\rangle}{\sigma^2[\hat{\mathbf{G}}]}$

In order to save computational time an approximation is done to compute the correlation time τ_G. An exponential decay is assumed and τ_G is computed as follows

$$\tau_G \approx \frac{\rho_G(1)}{1-\rho_G(1)} \tag{A.3}$$

B Correlation time analysis

It is already known that in the 2D-Ising Model with the metropolis algorithm the correlation time increases with the system size as $\tau \sim L_c^z$ with $z_c \approx 2.1665$. [2][3][4]. In order to determine the effect of the errors given by the correlations, the correlation time for the magnetisation has been computed for the L's in $\{L\}_2$ at the critical temperature. Then, the critical exponent z_c has been computed in an approximate way.



(a) Correlation time (τ_M) for $L \in \{L\}_2$ and $T = T_c$

(b) Linear regression $\ln \tau_M \propto \ln(L)$

Figure 7: Correlation time analysis for $\{L\}_2$

Fig. 7(b) shows how the correlation time of the magnetisation increases exponentially with the system size. With the linear regression in Fig. 7(b) a critical exponent of $z_c = 2.036 \pm 0.022$ is obtained. The result don't match with the ones in [3] and [4], although it is close to it, because of the simple method used here, which consists in just summing up the correlation function of the magnetisation until it reaches zero. Anyway, we can continue the analysis considering $z_c \approx 2.1665$ to justify the thermalisation time used.

To ensure that the system will reach the equilibrium before starting to take measures a thermalisation stage must be considered. Thus, $M_0 \gg \tau_M$ MCS must be simulated without taking any measure. Using the linear regression in Fig. 7(b) we can express $\tau_M \approx e^{-3.265} \cdot L^{2.1665} \approx 0.038 \cdot L^{2.1665}$. Thus, for the maximum L used in this work the correlation time will be $\tau_M \approx 0.038 \cdot 120^{2.1665} \approx 1221$, so that the thermalisation time used of 10^4 MCS accomplishes $M_0 \gg \tau_M$.

In order to decrease the errors two strategies can be adopted. Taking into account A.2 we can either sample a bigger number of measures or decrease the correlation time τ_G. For instance, to decrease the correlation time one can space the measures a given number of MCS. This way, the measures taken will be less correlated and have more statistical significance, so that the errors given by the correlations will decrease. To show this effect Table 3 shows the correlation time values for some system sizes using or not the spacing between measures.

Table 3: Reduction effect on the correlation time due the spacing of the measures.

	$L = 20$	$L = 24$	28	$L = 32$
Measure every 1 MCS	15.85	23.71	32.32	40.67
Measure every 5 MCS	2.75	4.32	6.35	8.36

However, we have to take into account that increasing the spacing between measures means increasing iterations, so that the simulation time will increase. It can be shown that the spacing MCS between measures can be optimised using the following relation

$$K = \sqrt{\frac{2\tau_M t_1}{t_2}}$$

For the simulations done in the present work, that value turned to be around $K = 5$ for the range of system sizes L considered.

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