

2-d Ising Model

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The 2-dimensional Ising Model is one of the simplest model exhibiting a phase transition. The model consists of classical spins σ , which can take the values ± 1 . The Hamiltonian is given by

$$H = -J \sum_{\langle \vec{i}, \vec{j} \rangle} \sigma_{\vec{i}} \sigma_{\vec{j}} = -\frac{J}{2} \sum_{i_1} \sum_{i_2} \sigma_{i_1, i_2} (\sigma_{i_1+1, i_2} + \sigma_{i_1-1, i_2} + \sigma_{i_1, i_2+1} + \sigma_{i_1, i_2-1}), \quad (1)$$

where $\langle \vec{i}, \vec{j} \rangle$ denotes the nearest neighbors, and $\sigma_{\vec{i}}$ is the spin at position \vec{i} , and we have taken the external magnetic field to zero $h = 0$. Below a critical temperature T_c , the discrete symmetry \mathbb{Z}_2 is spontaneously broken, and the system is in a ferromagnetic phase (for $J > 0$). For simplicity, we can work in units where the Boltzmann constant is $k_B = 1$ and we take $J = 1$. An alternate expression to the previous, defined on a finite lattice with periodic boundary conditions, is

$$H = - \sum_{i_1=1}^L \sum_{i_2=1}^L \sigma_{i_1, i_2} (\sigma_{i_1+1, i_2} + \sigma_{i_1, i_2+1}), \quad (2)$$

which halves the computing time compared to eq. (1). Or the alternative replacing $i+1 \rightarrow i-1$. The periodic boundary conditions are $i = L+1 \rightarrow 1$, and $i = 0 \rightarrow L$.

To simulate the Ising model on a finite lattice, we start from an initial configuration. It can be a cold-start, where all the spins are aligned, or a hot-start, where the spins are randomly distributed, for example, in a $L \times L$ square lattice with $L = 8$, we can have the initial configurations

$$\begin{pmatrix} -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 \\ -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 \\ -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 \\ -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 \\ -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 \\ -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 \\ -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 \\ -1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 \end{pmatrix}, \quad \begin{pmatrix} +1 & -1 & -1 & +1 & -1 & +1 & -1 & +1 \\ -1 & +1 & +1 & -1 & -1 & -1 & +1 & -1 \\ +1 & -1 & -1 & +1 & +1 & +1 & +1 & -1 \\ +1 & -1 & +1 & -1 & +1 & -1 & -1 & +1 \\ -1 & -1 & +1 & -1 & +1 & -1 & +1 & +1 \\ -1 & +1 & -1 & +1 & -1 & +1 & -1 & -1 \\ +1 & -1 & -1 & +1 & +1 & -1 & -1 & +1 \\ -1 & +1 & +1 & +1 & -1 & +1 & +1 & -1 \end{pmatrix},$$

for cold-start and hot-start, respectively. From eqs. (1) or (2) we can see that the energy of the cold-start is the lowest energy since all the spins are aligned, while the energy of the hot-start is higher than it.

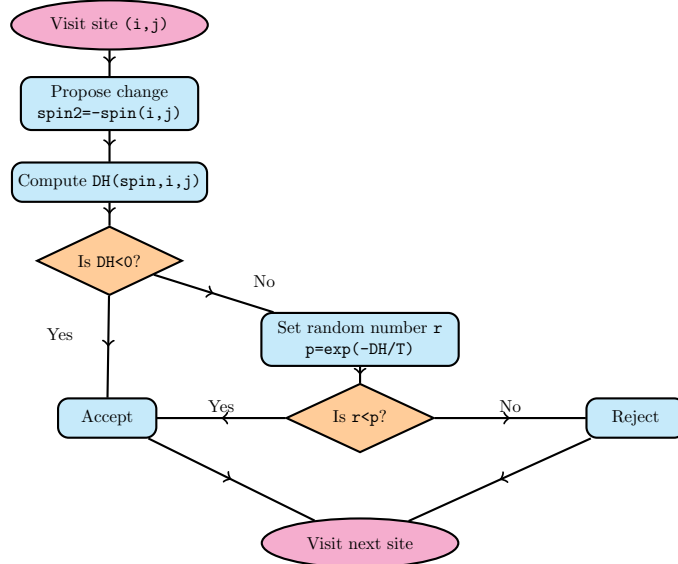
Then, we apply the Metropolis algorithm. We visit each site $\vec{i} = (i_1, i_2)$ and flip the sign of the spin if it decreases the energy, that is, if $\Delta H < 0$ then we take $\sigma'_i = -\sigma_i$. But if the change does not decrease the energy, $\Delta H > 0$, then we flip the sign with probability $p = e^{-\Delta H/T}$. A sweep is defined when we have visited all the spins on the lattice. The energy change for flipping the sign of a spin on the site \vec{i} , is

$$\Delta H = 2\sigma_{i_1, i_2}(\sigma_{i_1+1, i_2} + \sigma_{i_1-1, i_2} + \sigma_{i_1, i_2+1} + \sigma_{i_1, i_2-1}), \quad (3)$$

where σ_{i_1, i_2} is the spin before flipping its sign.

The next flowchart shows the architecture of the algorithm, where we visit all spins in lexicographic order, from 1 to L . The periodic boundary conditions are implemented inside the function $DH(\text{spin}, i, j)$, which takes the form of eq. (3) and considers the neighboring spins of the site (i, j) . To implement the boundary conditions, we define a function of the indexes $iv(i)$, that takes the form

$$iv(i) = \begin{cases} i & \text{if } i \in [1, L] \\ 1 & \text{if } i = L + 1 \\ L & \text{if } i = 0 \end{cases} \quad (4)$$



The first step is to visualize the thermalization, as shown in Fig. 1, for different temperatures. Thermalization can be studied, for example, with a plot of the energy density v.s. sweeps. In order to take measurements, we want to avoid the first sweeps that lead to thermalization, that is, when the system reaches equilibrium. Measurements should also be separated by a specific number of sweeps since they can be autocorrelated. We can also see in Fig. 1 that for $T = 1$, the system has a preference for the spins to align, so the energy fluctuates rarely. When the temperature is increased, this behavior is lost and the energy of the system varies around a determined value.

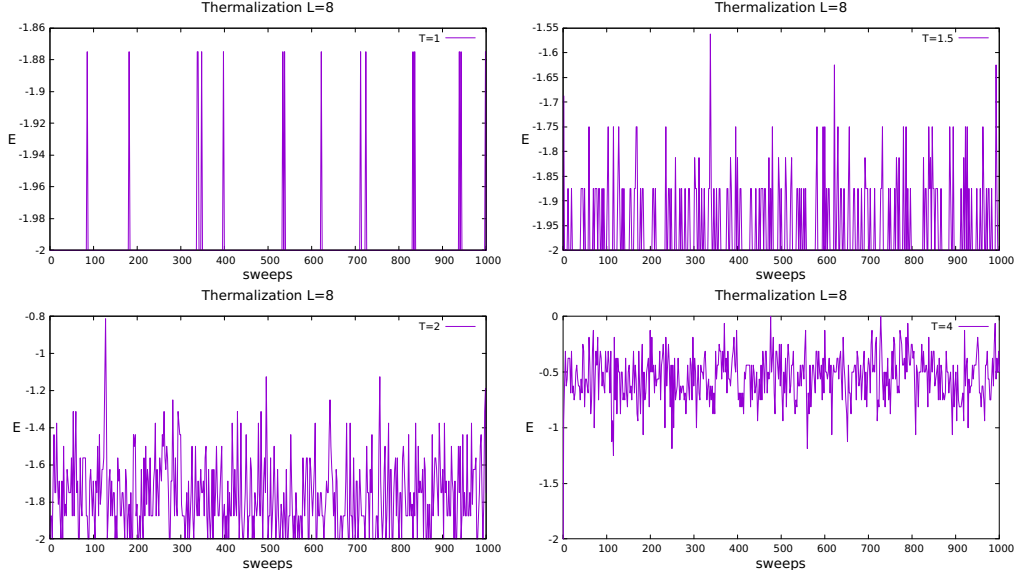


Figure 1: Thermalization for different temperatures on a square lattice of size $L = 8$.

To determine the value of an observable, we make a large number of measurements N_m . Several sweeps, N_{sweeps} , must be taken to separate these measurements, so that the statistic turns out to be independent. Otherwise, it might be the case that the measurements are autocorrelated and do not provide a reliable result. The autocorrelation time τ_{exp} is a good indicator, so we can take $N_{\text{sweeps}} \geq 2\tau_{\text{exp}}$. To determine this time, we use the connected autocorrelation function $C(t)$, for example, for the hamiltonian H ,

$$C_H(t) = \langle H_{t_0} H_{t_0+t} \rangle - \langle H \rangle^2, \quad (5)$$

which has an exponential behavior of the form

$$C_H(t) = ce^{-t/\tau_{\text{exp}}}. \quad (6)$$

We measure this function on the lattice and determine the autocorrelation time by means of a fit. This procedure is shown in Fig. 2 for different lattice sizes and distinct values of T , around the expected critical value T_c . We can see the autocorrelation time τ_{exp} increases with the lattice size. After thermalization, we take measurements of the action every one sweep and measure eq. (5), taking t_0 as each sweep in the history.

In order to fit the exponential function to the data, we select a region $t \in [t_i, t_f]$ for each curve. In logarithmic scale, the region of interest is where the curve looks like a straight line asymptotically. Before t_i , the autocorrelation might look curved or like a straight line with a different slope. After t_f there might be fluctuations, so for each curve we have to determine t_i and t_f , taking into account the reduced χ^2/dof as an indicator. We can see in Fig. 2 that $t_i \gtrsim 3$ but a good t_f depends on the temperature. For example, for $T = 2.8$ and $T = 2.3$, after $t = 12$ the points are statistically compatible with zero, as the uncertainties indicate. As a matter of fact, there are missing points since they take negative values, which are not defined in logarithmic scale.

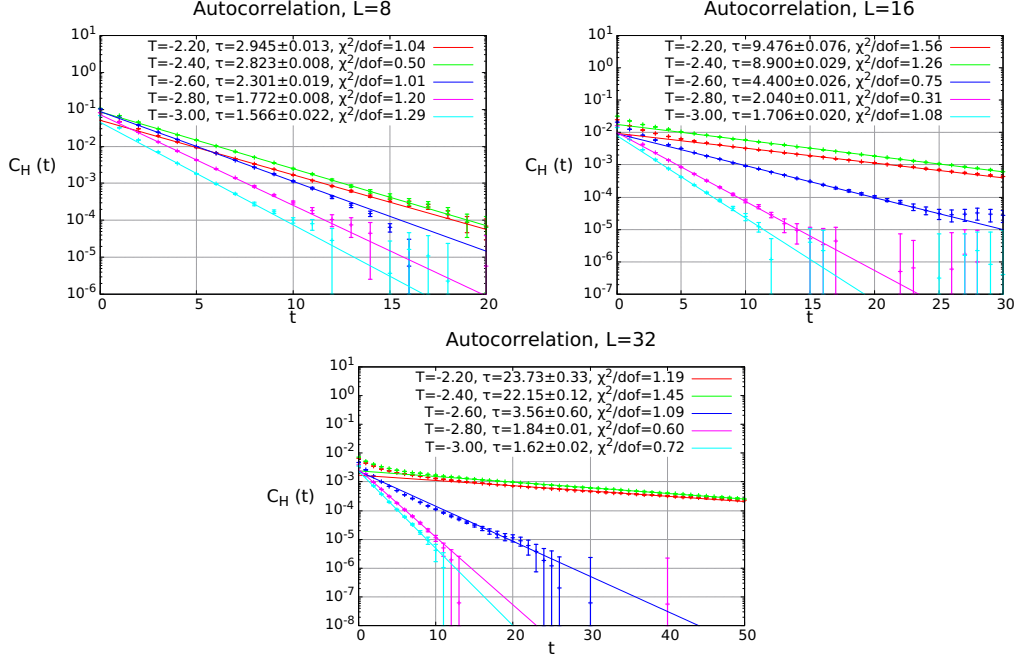


Figure 2: Autocorrelation function fits for τ_{exp} in logarithmic scale, for different temperatures at different lattice sizes.

In the remaining section of this report, we set the thermalization as 1,000 sweeps and take $N = 10,000$ measurements every 10 sweeps. A number of measurements N between 1,000 and 10,000 is enough, but with this large value, the errors are small for all the lattice sizes explored. For the special case of a lattice size of $L = 64$, we take measurements every 100 sweeps, since the errors become larger, particularly for the susceptibility. According to the autocorrelation results, we should had taken measurements every 10 sweeps for $L = 8$, but every 20 sweeps for $L = 16$, 50 sweeps for $L = 32$. But the autocorrelation was computed after the subsequent results.

The first quantity that can be measured is the energy density E , shown in Fig. 3 and given by the expression

$$E = \frac{1}{L^2} \langle H \rangle = \frac{1}{L^2} \frac{1}{N} \sum_{k=1}^N H_k, \quad (7)$$

where again, N is the number of measurements and the index k labels the lattice configuration every 10 sweeps (100 for $L = 64$) as mentioned above. We divide by L^2 so that we can compare between different lattice sizes. Another quantity we can measure is the magnetization, shown in Fig. 4, and given by the expression

$$M = \frac{1}{L^2} \left\langle \left| \sum_{i_1=1}^L \sum_{i_2=1}^L \sigma_{i_1, i_2} \right| \right\rangle = \frac{1}{L^2} \frac{1}{N} \sum_{k=1}^N \left| \sum_{i_1=1}^L \sum_{i_2=1}^L (\sigma_{i_1, i_2})_k \right|. \quad (8)$$

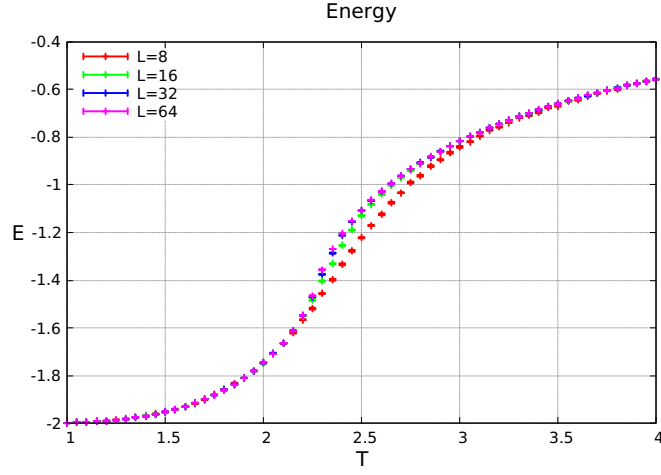


Figure 3: Energy dependence on the temperature for different lattice sizes, 8, 16, 32 and 64.

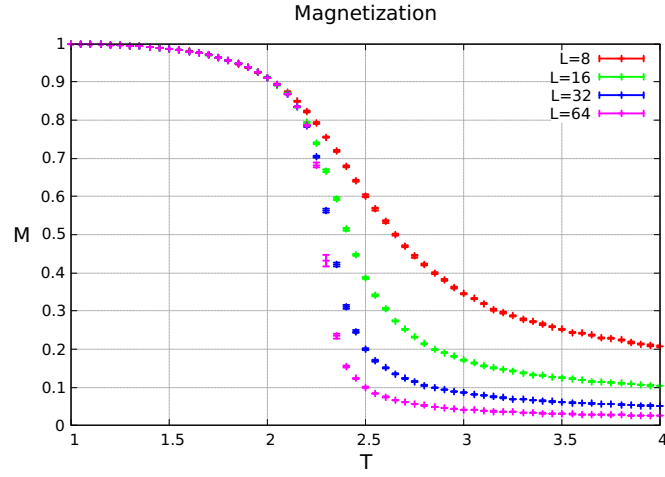


Figure 4: Magnetization dependence on the temperature for different lattice sizes, 8, 16, 32 and 64.

Each point in these figures is calculated at a fixed temperature and fixed lattice size. We vary the temperature from $T = 1$ to $T = 4$ for aesthetic reasons, but the relevant information from the model might be around the critical temperature. From the last two equations, we can see that these points are averages,

$$\langle x \rangle = \frac{1}{N} \sum_{k=1}^N x_k \quad (9)$$

with $N = 10,000$ samples. A simple way to define their associated error is using the standard error, given by

$$\delta x = \sqrt{\frac{\text{Var}}{N}} = \sqrt{\frac{1}{N(N-1)} \sum_{k=1}^N (x_k - \langle x \rangle)^2}, \quad (10)$$

where Var is the variance. The standard error for these two quantities is easy to implement. There is an alternative known as the Jackknife error, which is more convenient for other quantities such as susceptibility, specific heat, and the correlation function. Because of the structure of these quantities, using the propagation of the standard error is inaccurate and leads to errors larger than what they really are. The Jackknife error consists in dividing the samples in M bins; for example, the $N = 10,000$ samples can be divided in $M = 10$ bins, giving 10 sets of samples with 1,000 measurements each. Then, the error is computed with

$$\delta x_{\text{Jackk}} = \sqrt{\frac{M-1}{M} \sum_{m=1}^M (\langle x \rangle_m - \langle x \rangle)^2}, \quad (11)$$

where $\langle x \rangle$ is the average of x , and $\langle x \rangle_m$ is the average of x of all measurements that exclude the m -th set of samples.

A third quantity we can measure is the magnetic susceptibility, given by

$$\chi_M = \frac{1}{L^2 T} (\langle M^2 \rangle - \langle M \rangle^2), \quad (12)$$

and shown in Fig. 5 in logarithmic scale, for different lattice sizes and with jackknife errors. Notice that from eq. (12) there is a unique value for χ_M and the statistic is done on M^2 and M . This is why we use jackknife and generate a set of different χ_M 's that allow us to perform the error statistics.

As mentioned above, the 2-dimensional Ising model has an analytic solution. In the thermodynamic limit, the susceptibility is a divergent quantity at the critical temperature. But on a finite lattice, the susceptibility is a finite function with a peak, that increases its size and reduces its width with the lattice size. There is no formal phase transition in a finite volume, the maximum susceptibility depends on the lattice size, and we expect that taking the continuum limit $L \rightarrow \infty$ leads to the analytical result. That is why we fit the susceptibility peak using a Gaussian distribution

$$f(T) = A e^{-b(T-T_{\max})^2} \quad (13)$$

to find the values of $T_{\max}(L)$. These fits are shown in Fig. 6, which consider a small set of points in a region around the maxima since the full susceptibility is not a Gaussian function, but a neighborhood around the maximum can be approximated by one. These fits lead to the results presented in Table 1, along with the χ^2/dof of the fits, which we verified to be of almost order one.

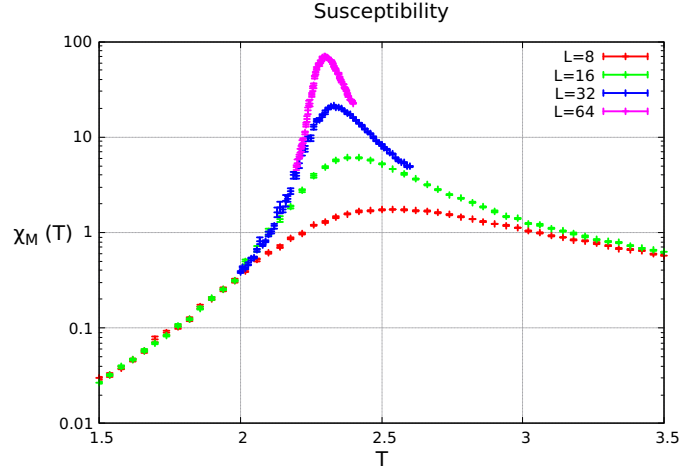


Figure 5: Susceptibility in logarithmic scale for different lattice sizes. The temperature range varies depending on the lattice size.

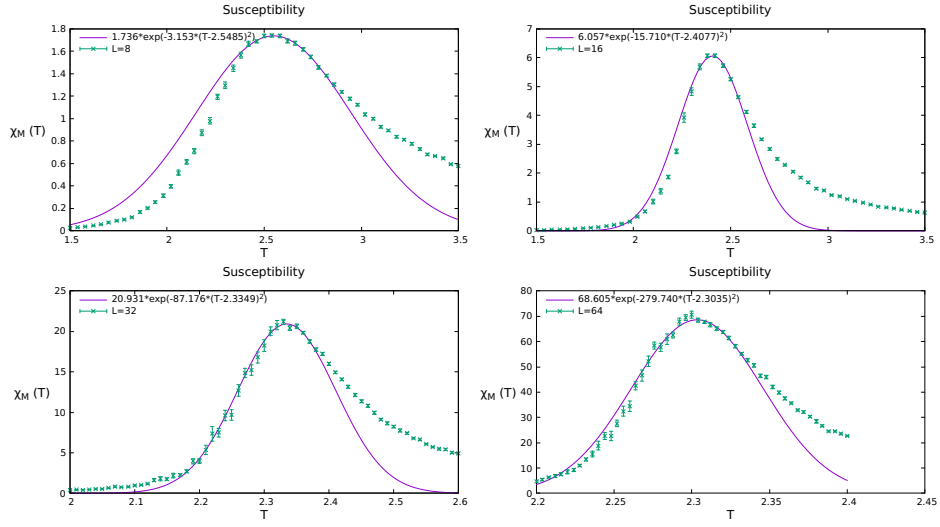


Figure 6: Gaussian fits for the susceptibility at different lattice sizes.

	$L = 8$	$L = 16$	$L = 32$	$L = 64$
A	1.736(4)	6.06(6)	20.9(2)	68.6(4)
b	3.2(1)	16(1)	87(15)	280(24)
T_{\max}	2.548(4)	2.408(4)	2.335(2)	2.3035(7)
$\chi^2/\text{d.o.f.}$	0.91	2.27	0.96	1.17

Table 1: Gaussian fit parameters for susceptibility on different lattice sizes.

With these values of $T_{\max}(L)$, we want to interpolate the final result at $L \rightarrow \infty$. To do so, we take another fit assuming $|T_{\max}(L) - T_c|^{-\nu} \sim L$. So the function to fit becomes

$$T_{\max}(L) = T_c + \frac{C}{L^{1/\nu}}, \quad (14)$$

where T_c is the critical temperature, ν is a critical exponent and C is a proportionality constant. The results are shown in Fig. 7. We get a critical temperature of $T_c = 2.274(4)$, while its theoretical value is $T_c \approx 2.269$. We also get a critical exponent $\nu = 0.93(4)$, whose theoretical value is $\nu = 1$.

T_c	2.274(4)
ν	0.93(4)
C	2.6(3)
$\chi^2/\text{d.o.f.}$	0.88

Table 2: Fit values for critical temperature T_c , critical exponent ν and proportionality constant C .

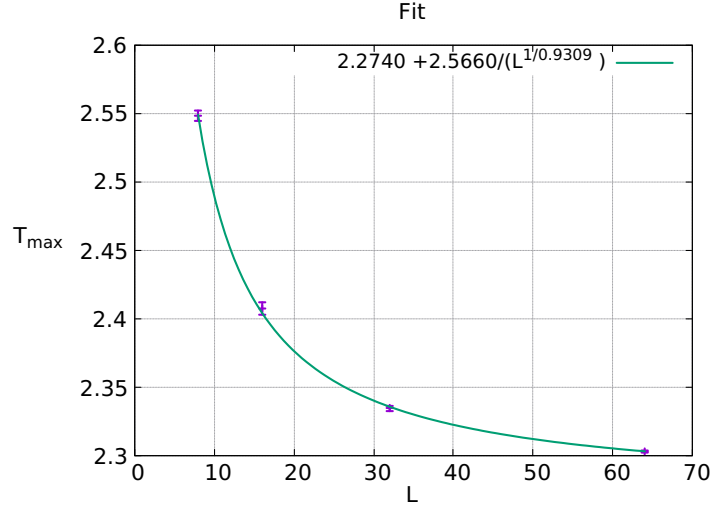


Figure 7: Fit for $T_{\max}(L)$ for different lattice sizes, 8, 16, 32, and 64.

The correlation function is an exponentially decaying function with the distance, but on a finite lattice, because of the boundary conditions, we can fit it to a hyperbolic cosine of the form

$$C(x - y) = A \cosh \left(\frac{|x - y| - L/2}{\xi} \right), \quad (15)$$

where A is an amplitude and ξ is the correlation length. To measure this function in practice, we can define a spin vector S_{i_1} , as

$$S_{i_1} = \sum_{i_2=1}^L \sigma_{i_1, i_2}, \quad (16)$$

and then, the correlation function will be

$$C(i-j) = \langle S_i S_j \rangle - \langle S_i \rangle \langle S_j \rangle. \quad (17)$$

Figure 8 shows the correlation function's behavior for different temperatures, on a lattice with size $L = 64$. To obtain their respective correlation lengths, we fit the hyperbolic cosine from eq. (15). Applying this procedure to different temperatures gives a temperature-dependent correlation length $\xi(T)$, shown in Fig. 9 for lattice sizes $L = 8$ and $L = 64$.

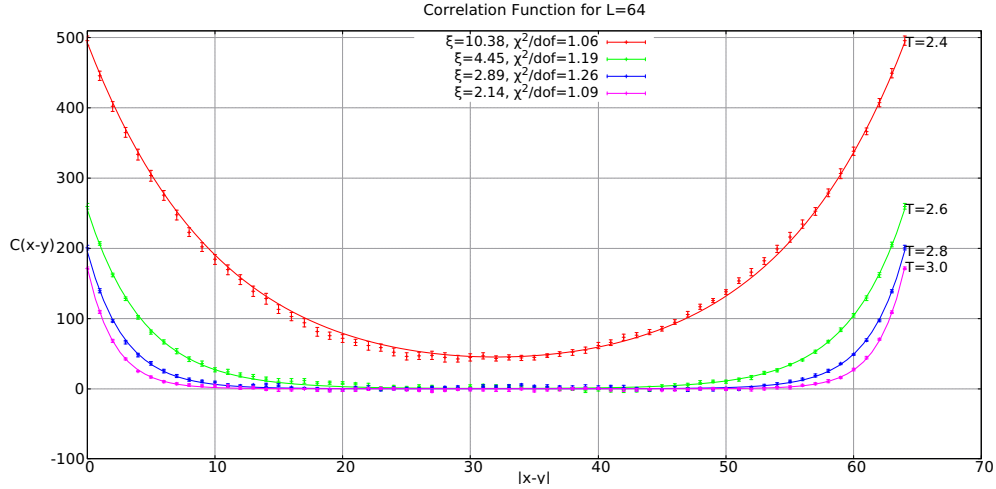


Figure 8: Correlation function fit on a lattice size $L = 64$ for different temperatures.

Again, in the thermodynamic limit, the correlation length is a divergent quantity at the critical temperature. In Fig. 9 we can see that the correlation length also depends on the lattice size. We identify that the correlation length increases towards the critical temperature, but the increment is more notorious as the lattice size is bigger. We plot for two different lattice sizes to determine the region without volume dependence. Around $T = 3$, the results seem to be independent of the lattice size, but after this temperature, the correlation length decreases slower than expected theoretically. So we select the region $T \in [2.50, 2.82]$.

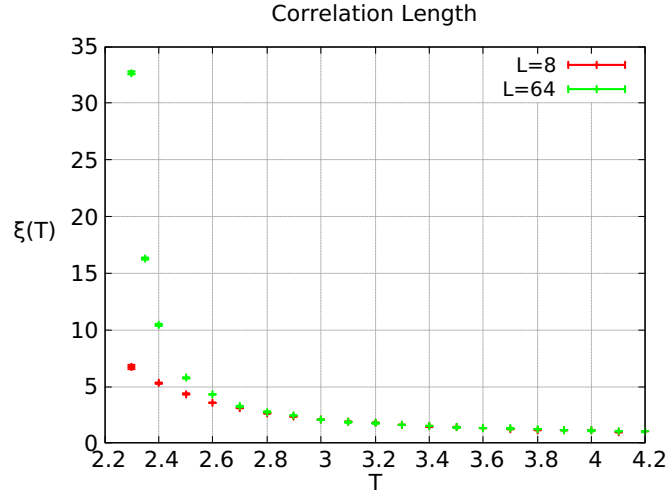


Figure 9: Temperature dependence of the correlation length for two different lattice sizes.

Figure 10 shows the temperature region chosen for the correlation length in a lattice size of $L = 64$. We fit the function

$$\xi(T) = \frac{D}{(T - T_c)^\nu}, \quad (18)$$

where D is a constant, T_c is the critical temperature and ν is the critical exponent. We also fit the same function, but introducing the theoretical value of $T_c \approx 2.269$, so that the precision can be increased only by having two fitting parameters D and ν . For the first fit, we get $T_c = 2.25(8)$ and $\nu = 1.0(2)$, while for the second we get $\nu = 0.96(2)$.

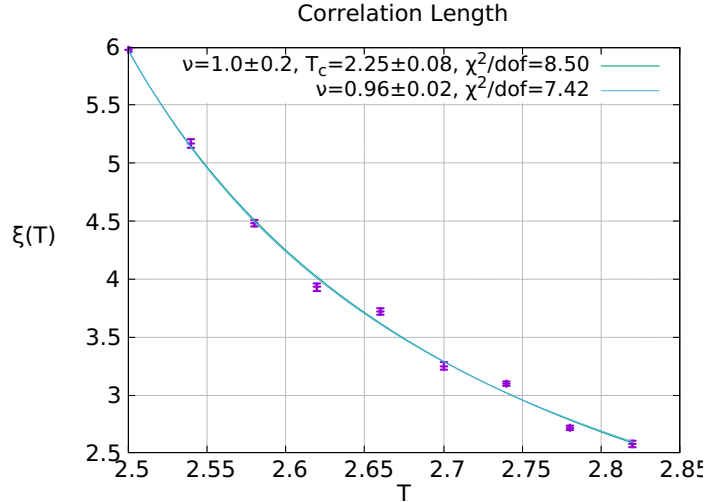


Figure 10: Correlation length fit.

Figure 10 also shows that χ^2/dof is of higher order than one. This might be because the error for the correlation length is underestimated by the fitting method. To avoid this issue, we repeat the procedure by generating a set of 5 to 10 correlation lengths for each temperature. We run our program 5 to 10 times, to generate sets of correlation functions to be fitted, one set is shown in Fig. 11 as an example. Then we can obtain a better mean correlation length with its associated standard error. As a first attempt, we can simply fit the correlation lengths of each set of correlation functions. Figure 12 shows this procedure, which provides us with a set of critical exponents and temperatures, which can be averaged with the results shown in Table 3.

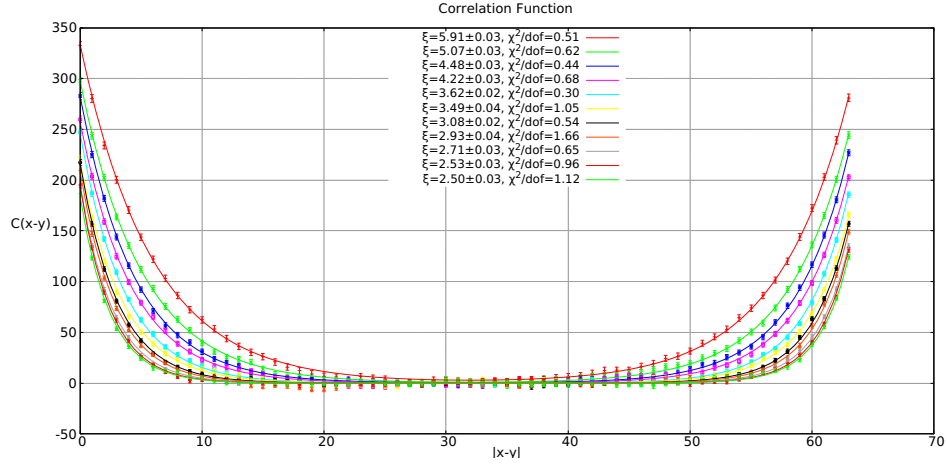


Figure 11: One set of fits for the correlation functions displaying their correlation lengths, on a lattice size of $L = 64$. Each correlation function corresponds to a temperature $T \in [2.50, 2.82]$, in steps of $\Delta T = 0.04$

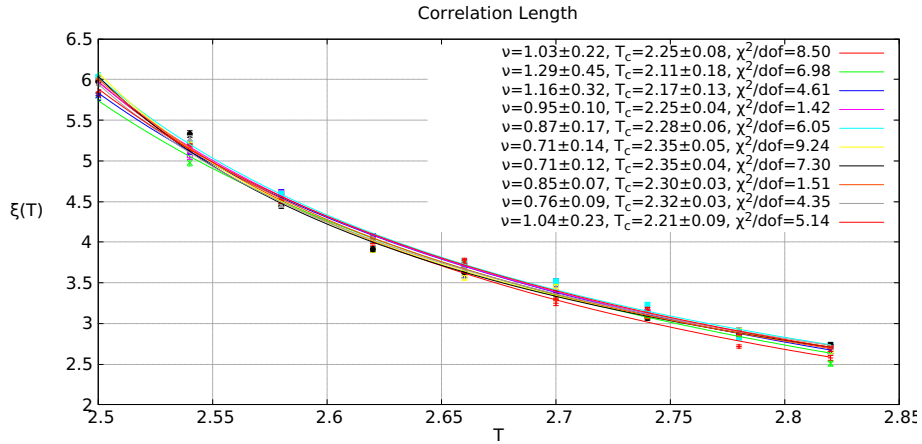


Figure 12: Correlation length fit for each one of the 10 sets of correlation functions.

T_c	2.26(2)
ν	0.94(6)

Table 3: Average values for critical temperature T_c and critical exponent ν , using fits from Fig. 12.

As an alternative, we can take the sets of correlation functions and fit them to their respective correlation length. Then we obtain a set of correlation lengths and we average them, instead of simply fit them. The results of this procedure are shown in Figs. 13 and 14, where we can see that the averaged correlation length is better behaved and with plausible errors.

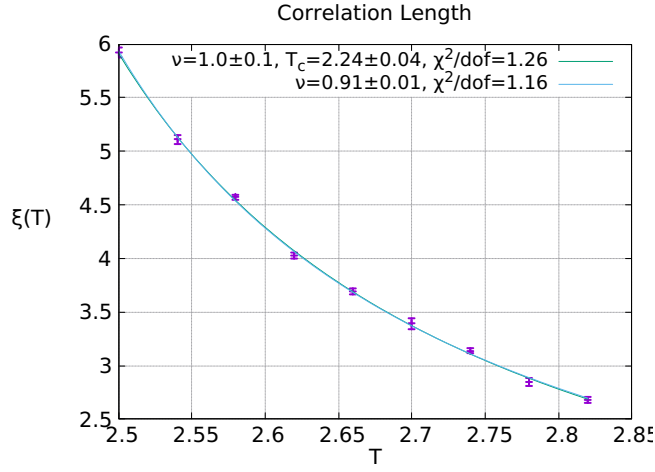


Figure 13: Correlation length fit using 5 sets of correlation functions.

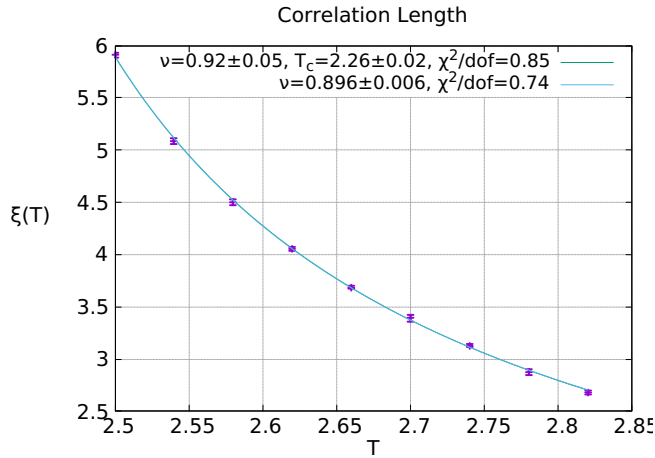


Figure 14: Correlation length fit using 10 sets of correlation functions.