

# Computational Project. Equilibrium Monte Carlo simulation of the 2D Ising model

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## **Abstract**

This project implements an equilibrium Markov-chain Monte Carlo simulation of the two-dimensional Ising model in the canonical ensemble, using the Metropolis single-spin-flip algorithm, with periodic boundary conditions. Time series of two observables (energy and magnetization) are generated for different lattice sizes and temperatures, with their corresponding statistical uncertainties, computed using a binning (block) analysis to account for autocorrelations. [2] The correctness of the implementation is validated by reproducing the Ferdinand-Fischer finite-size reference value for  $L = 20$  at  $T = 2.0$ , after discarding an initial equilibration transient. [1]

# 1 Estimates, interpretations and comments

In this section, we include all the relevant information relative to the simulations, such as direct estimates and complementary material to the figures in Sec. 2.

## 1.1 Testing our code. Estimating $\langle E \rangle / L^2$ . Comparison with Ferdinand-Fisher.

In order to test the correctness of our MC code, a simulation with  $L = 20$ ,  $T = 2$  and a sampling frequency of  $n_{\text{meas}} = 10$  was performed, starting with random initial conditions, for a total of  $n_{\text{MCS}} = 10^8$  MC steps, [1] leaving the first  $10^3$  steps, in order to compute the sample average  $\bar{E}$  directly, yielding a value of  $\bar{E} = -698.2353484\dots$ . The binning code was used to extract a statistical error of  $\sigma_E(m = 128) = 3 \times 10^{-5}$ , since from Fig. 1 we see that the errors do not depend on the choice of the binning sample size for  $m = 128$ . Therefore we obtained  $\langle E \rangle / L^2 = -1.74558 \pm 3 \times 10^{-5}$  as the final estimate. Comparing this result with the *exact* value given by Ferdinand and Fisher  $\langle E \rangle / L^2|_{\text{FF}} = -1.7455571250\dots$  we see that the exact value lies within the obtained margin of error and thus is in agreement (up to the fifth decimal place), with a relative discrepancy of  $\delta(\langle E \rangle / L^2) \approx 0.002\%$ .

## 1.2 Evolution of $E$ and $M$ for different $T$ . Comparison between $L = 20$ and $L = 100$ .

Once the code had passed the Ferdinand-Fisher test, different production runs were done for  $L = 100$  and temperatures  $2 \leq T \leq 3$  every  $\Delta T = 0.1$ , with a particular emphasis on the  $T = 2.0$ ,  $T = 2.27$ ,  $T = 2.6$  cases. A sampling frequency of  $n_{\text{meas}} = 10$  was used and a total of  $n_{\text{MCS}} = 10^8$  MC steps as well. Figures 2 and 3 show the time series for  $E$  and  $M$ , respectively, for  $T = 2.0$ ,  $T = 2.27$ ,  $T = 2.6$ .

From Fig. 2 we can see how, after the first  $10^3$  MC steps, the *energy* reaches stationary values, fluctuating around a well-defined average. As  $T$  increases, the system settles at decreasing (negative) values of the energy. It is worth mentioning that the time series for  $T = 2.27$  the energy fluctuations become more relevant, compared with the other cases.

Fig. 3 depicts the respective time series for the *magnetization*  $M$ . At a low temperature of  $T = 2$  (relative to some critical temperature  $T_c$ ) the system's spins tend to align between them, producing an ordered configuration, which is reflected on the value  $\langle M \rangle / N \sim -1$ . For a high temperature of  $T = 2.6$ , we see that the stationary configuration involves random orientations of the spins, thus  $\langle M \rangle / N \sim 0$ . Finally, and most interestingly, at  $T = 2.27$  the magnetization keeps fluctuating around all its possible values, without settling, suggesting that the system is at a critical point, i.e., a ferromagnetic-paramagnetic phase transition is taking place, with order parameter  $M$ , and thus that  $T = 2.27 \equiv T_c$ .

In order to compare any potential effect of changing the *scale* of the system  $L$ , Fig. 4 shows the time series for  $L = 20$  and  $L = 100$  at  $T = 2$ . From them, we can see that for  $L = 20$  the magnetization stabilizes much faster. Also, in both cases the system reaches an ordered stationary state, but  $\langle M \rangle / N \sim 1$  for  $L = 20$ , whereas  $\langle M \rangle / N \sim -1$  for  $L = 100$ . This difference is simply due to the fact that below the critical temperature there is a spontaneous symmetry breaking and the spins align either up or down.

## 1.3 Extracting $\langle E \rangle$ and $\langle |M| \rangle$ with its statistical errors.

With the previous MC data, a binning code was implemented to extract expected values and statistical errors. Fig. 5 and Fig. 6 show the dependence of  $\sigma$  on the block size  $m$ . Finally, we can estimate the autocorrelation time for  $m \gg \tau_{\text{int},A}$  since for a generic observable  $A$

$$\frac{s_{\bar{A}m}^2}{s_{\bar{A}1}^2} \simeq \tau_{\text{int},A}, \quad (1)$$

where  $s^2$  is the binning sample variance. [2]

### 1.3.1 Dependence of the autocorrelation time on temperature.

In order to obtain good enough estimates of the autocorrelation times  $\tau_{\text{int},A}$ , for  $T = 2$ ,  $T = 2.6$ , Eq. 1 was applied and averaged over a range of values for which we know (from binning) that the statistical

errors do not depend on  $m$ . Conversely, for  $T = 2.27$ , since the system exhibits critical behavior, we expect from theory that  $\tau_{int,A} \rightarrow \infty$  and no particular block size will remove the time correlations; as a numerical check of this fact, the value of  $\tau_{int,A}$  was computed by averaging the data points with  $m \gtrsim 128$ . Table 1 shows these results. The shortest autocorrelation time occurs for  $T = 2.6$ , for which the thermal noise is significant enough to produce faster decorrelations between successive configurations. The opposite is observed for  $T = 2$ , as expected. Note that, in terms of  $\tau$ ,  $\langle|M|\rangle$  is much more sensitive than  $\langle E \rangle$  to changes in the temperature.

Table 1: Autocorrelation times of  $\langle E \rangle$  and  $\langle|M|\rangle$ , with its statistical errors, for different temperatures.

	$\tau_{\langle E \rangle}$	$\tau_{\langle M \rangle}$
T=2.0	$1.46 \pm 0.08$	$11.4 \pm 0.2$
T=2.27	$66 \pm 32$	$148 \pm 73$
T=2.6	$1.35 \pm 0.07$	$3.0 \pm 0.1$

#### 1.4 Dependence of $\langle E \rangle/L^2$ and $\langle|M|\rangle/L^2$ on $T$ .

In figures 3 and 8, we can see the dependence on  $T$  of  $\langle E \rangle/N$  and  $\langle|M|\rangle/N$ . For the magnetization, the behavior is as expected and commented in Fig. 3: it decreases from the unity to zero, with an abrupt fluctuation at  $T_c = 2.27$ , being the point with the biggest error. For the case of the energy, the concavity changes at  $T_c$  from concave to convex, though it is expected to saturate for sufficiently high temperatures (since the system is finite and has a configuration that maximizes  $E$ ).

#### 1.5 Estimating $\chi$ and $c$ from Jackknife resampling. Dependence with $T$ .

To estimate the per spin magnetic susceptibility  $\chi = \beta(\langle M^2 \rangle - \langle|M|\rangle^2)/N$  and heat capacity  $c = \beta^2(\langle E^2 \rangle - \langle E \rangle^2)/N$ , for each temperature  $T$ , Jackknife resampling is required since the different observables are correlated, specially near the critical point. In Fig. 9 the Jackknife errors of  $\chi$  and  $c$  are represented as a function of the block size  $m$ , as well as the same error for  $\chi$  estimated from error propagating its definition given before, yielding

$$\sigma_\chi \approx \frac{1}{NT} \sqrt{\sigma_{\langle M^2 \rangle}^2 + 4\langle|M|\rangle^2 \sigma_{\langle|M|\rangle}^2}, \quad (2)$$

which naively assumes that  $\text{Cov}(\langle M^2 \rangle, \langle|M|\rangle) = 0$ , far from being true, specially at  $T_c \approx 2.27$  and thus overestimating the error.

Finally, Fig. 10 depicts the dependence of  $\chi$  and  $c$  on the temperature, by extracting the central value and its error from Jackknife resampling with block sizes optimally chosen at each point (which grew as we approached  $T_c$  and decreased beyond  $T_c$ ). We can see how, whereas  $c$  does not present a discontinuity (consistent with the  $\alpha = 0$  critical exponent for a  $2D$  Ising model), near  $T_c$ ,  $\chi$  diverges as  $\sim |T - T_c|^\gamma$ , consistent with theory.

## 2 Figures

In this section, we list the different figures obtained from the simulation data. For further comments and interpretations, see Sec. 1.

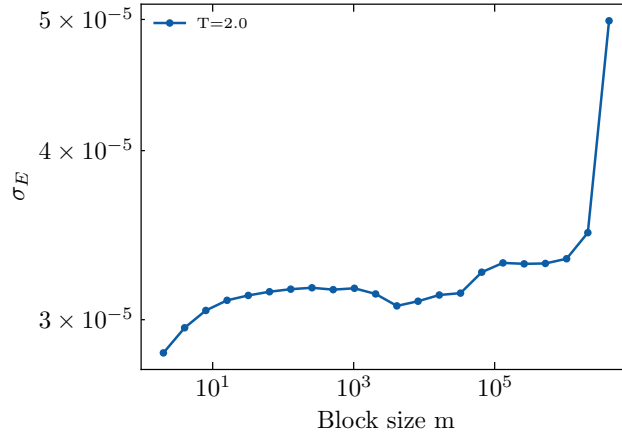


Figure 1: Statistical error (standard deviation) of the energy as a function of the block size for  $L = 20$  and  $T = 2.0$  in log-log scale.

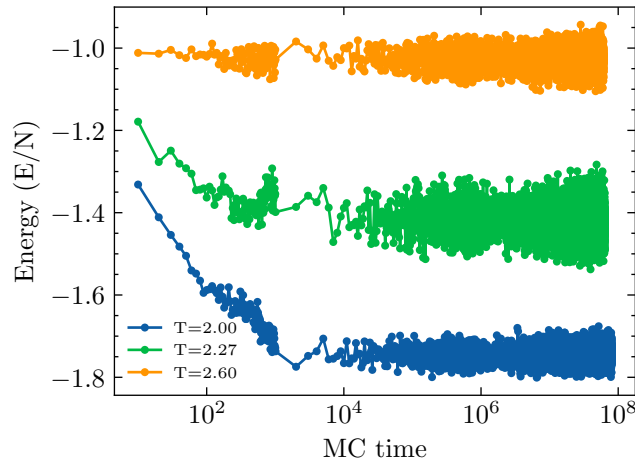


Figure 2: Energy per spin, as a function of MC time, for three temperatures, including the critical temperature, for  $L = 100$ .

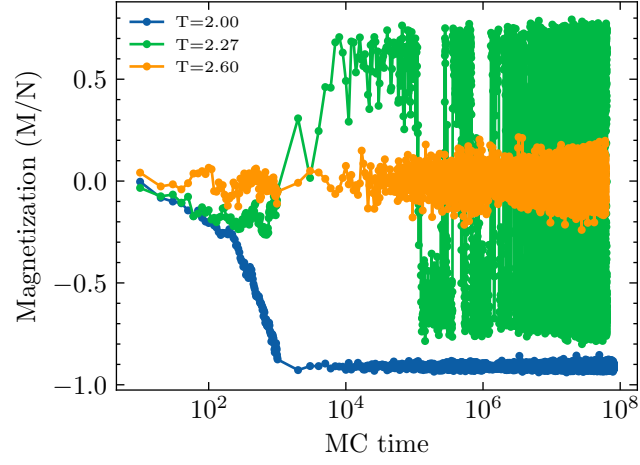


Figure 3: Magnetization per spin, as a function of MC time, for three temperatures, including the critical temperature, for  $L = 100$ .

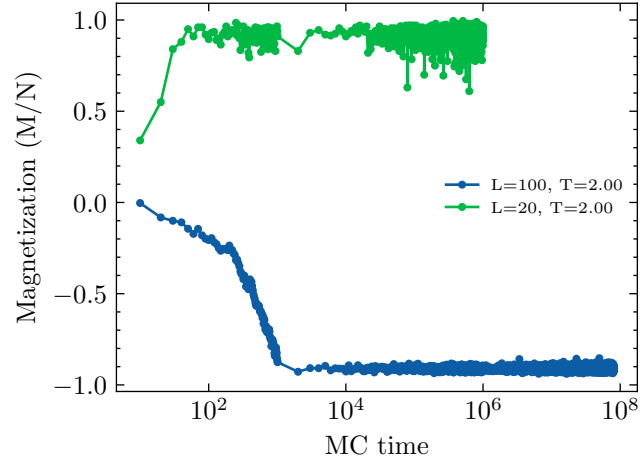


Figure 4:  $T = 2$  magnetization per spin time series for  $L = 20$  and  $L = 100$ .

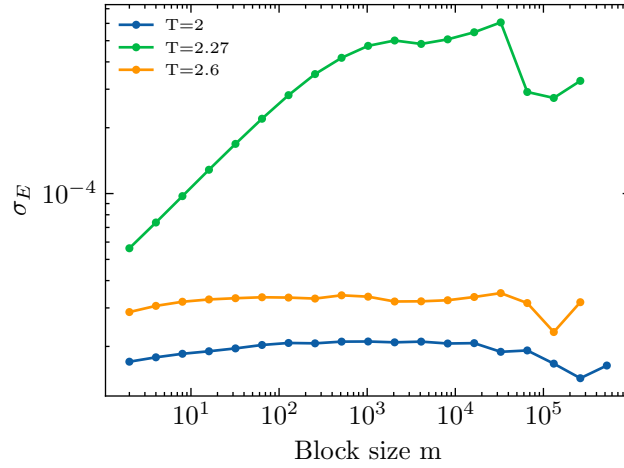


Figure 5: Statistical error (standard deviation) of the energy as a function of the block size for different temperatures, for  $L = 100$  in log-log scale.

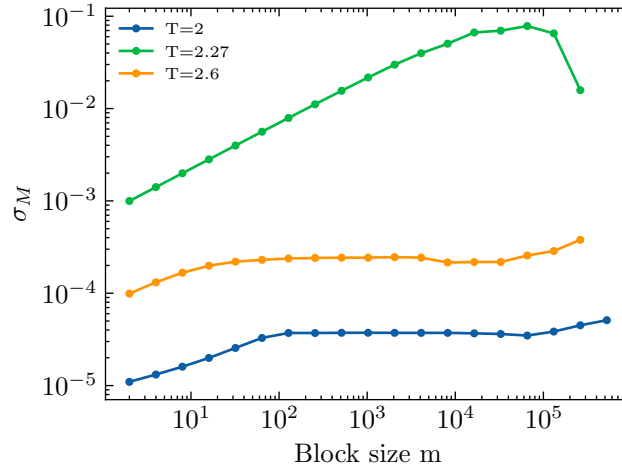


Figure 6: Statistical error (standard deviation) of the absolute value of the magnetization as a function of the block size for different temperatures for,  $L = 100$  in log-log scale.

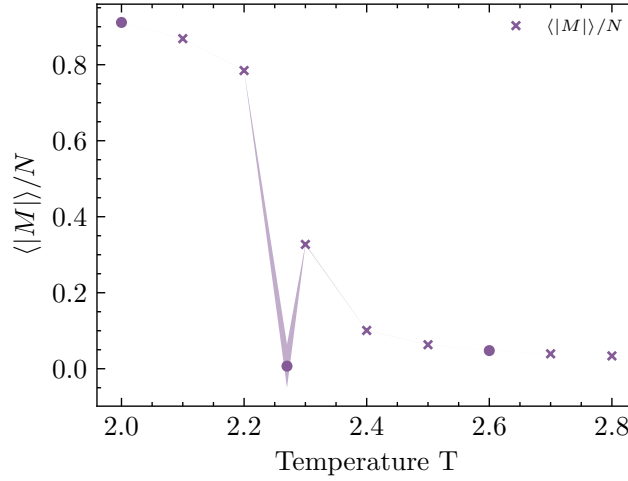


Figure 7: Average value of the absolute value of the magnetization as a function of the temperature. As dots, the requested temperatures,  $T = 2.0, 2.27, 2.6$ . Note that only at  $T_c = 2.27$  the statistical error is greater than the data markers.

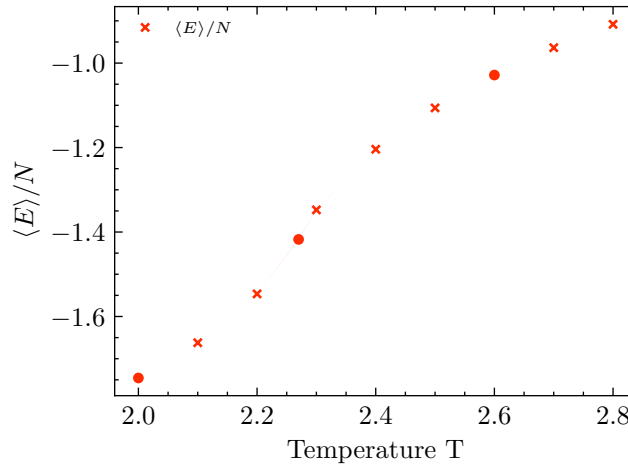


Figure 8: Average value of the energy, extracted from the binning program, as a function of the temperature. As dots, the requested temperatures,  $T = 2.0, 2.27, 2.6$ . The statistical errors are smaller than the data markers.

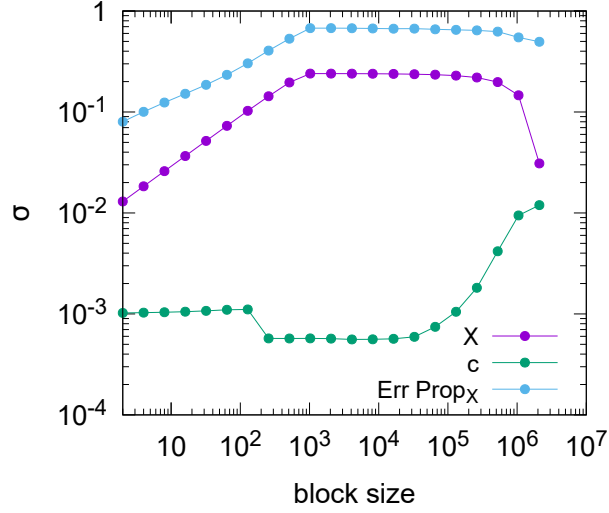


Figure 9: Log-log dependence of statistical errors on the binning block size for  $L = 100$  and  $T_c \approx 2.27$ . The Jackknife errors for the (per spin) magnetic susceptibility  $\chi$  and heat capacity  $c$  are represented in purple and green respectively. In blue is represented the error propagation for  $\chi$  as well.

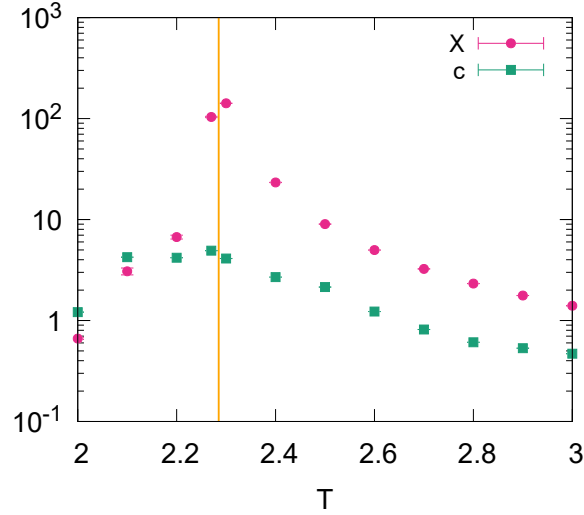


Figure 10: Semi-log per spin magnetic susceptibility  $\chi$  and heat capacity  $c$  with its corresponding statistical errors for  $L = 100$  and different  $T$ . In orange the critical temperature  $T_c \approx 2.27$  is emphasized.

## A References

### References

- [1] Molecular Modeling (MoMo), “Computational Project: Equilibrium Monte Carlo simulation of the 2D Ising model”, academic year 2025–2026 (project statement provided on Campus Virtual; file `comp_project_2025-26.pdf`).
- [2] M. Palassini, “Introduction to the Monte Carlo method”, Molecular Modeling (MoMo), Fall 2025 (lecture slides provided on Campus Virtual; file `1.MASM.slides_2025-26.pdf`).

## B Code: GitHub repository

<https://github.com/itxasoma/momo-McMC-2DIsing>