

Monte Carlo Simulation of the 2D Ising Model

Diego Ontiveros Cruz

Molecular Modelling, January 2023

In the present work, a Monte Carlo code was developed in Fortran90 to study the 2D Ising model using a square lattice. Later analysis of the data was carried out using Python scripts. All the files can be found attached to the task or online in [this GitHub repository](#).

First, to test the accuracy and correctness of the MC code, a simulation using $L = 20$ and $T = 2.0$ was performed. 10^8 MCS were employed, measuring the observables (E and M) each 10 MCS. After using the developed binning code to estimate the statistical error, see Figure 1, the average energy per spin computed was $\langle E \rangle/N = -1.74563 \pm 0.00005$ and the magnetization $\langle |M| \rangle/N = 0.91137 \pm 0.00004$. These values for the energy strongly agree with the exact value given by Ferdinand and Fisher for this system: $\langle E \rangle/N = -1.7455571250 \dots$

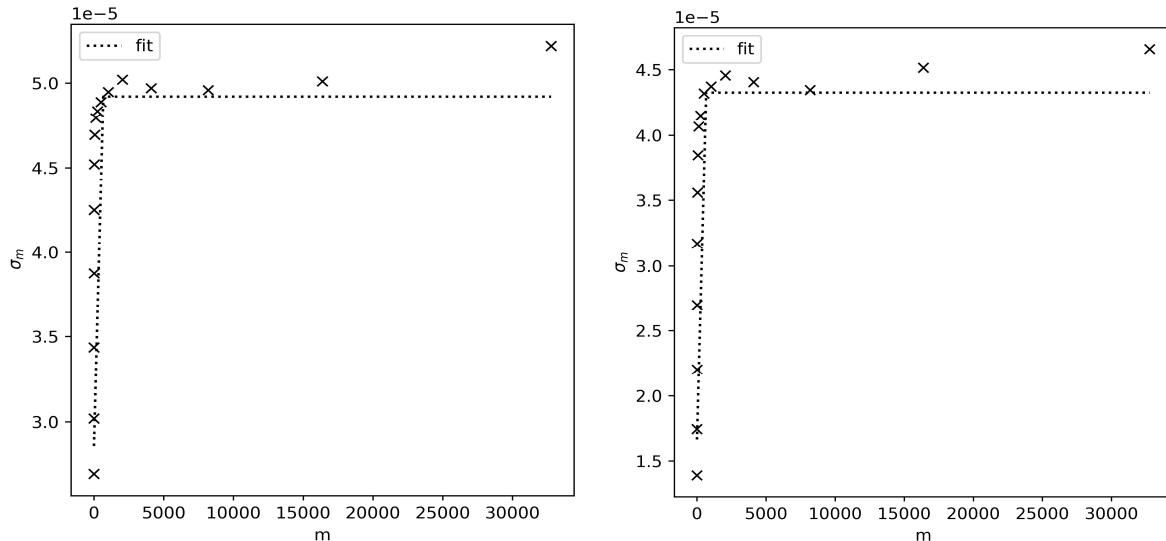


Figure 1. Statistical error σ_m for the energy (left) and magnetization (right) as a function of bin size m .

A set of production runs using $L = 100$ and 10^6 MCS were performed at different temperatures between 2.0 and 3.0 ($T = 2.0, 2.1, 2.27, 2.4, 2.5, 2.6, 2.7, 2.8, 2.9, 3.0$). The timeseries for 2.0, 2.27 and 2.6 is present in Figure 2, for the first 10^3 and 10^5 MCS. In this figure is also included the timeseries for the previous run with $L = 20$ and $T = 2.0$. In all cases, the same random seed was used (`setr1279(333)`).

In all cases, the first 10^3 MCS present a higher fluctuations than the others. In this time period, the system is still equilibrating. Comparing the simulations at $T = 2.0$, there are clear differences in the values between using $L = 20$ and $L = 100$ for the first 10^3 MCS steps, but then they quickly evolve to a very similar equilibrium value. In every case, they tend to an equilibrated value, with higher energies and lower magnetization when increasing the temperature, with the exception of the magnetization at $T = 2.27$ using $L = 100$. Given the fact that 2.27 is close to the critical point, where the system transitions between paramagnet and ferromagnet, higher fluctuations are expected, since the system may interchange between both phases.

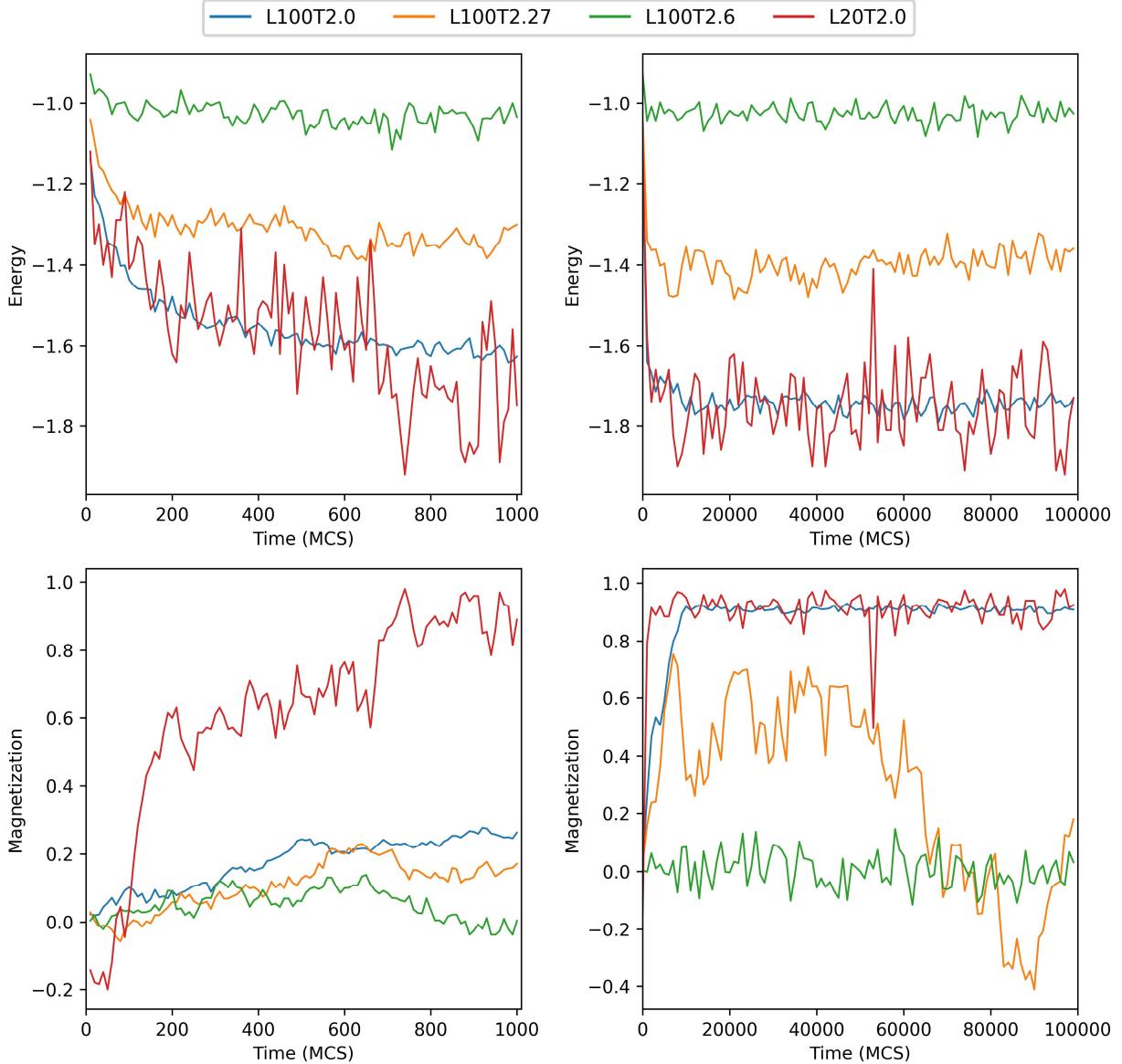


Figure 2. Time series of the energy (top) and magnetization (bottom) per spin for $L = 100$ with $T = 2.0, 2.27$, and 2.6 , and $L = 20$ with $T = 2.0$. Left are the first 10^3 MCS and right the first 10^5 .

From the production runs performed, the statistical average and error for each temperature were computed using the binning code, see Figure 3. In here we can see how as increasing the temperature, increases the energy and decreases the absolute value of the magnetization. At higher temperatures, the thermal energy is higher than the interaction between spins, and the spins evolve to a more disordered configuration, with roughly the same spins positive than negative, leading to a close to zero magnetization. On the other hand, at lower temperatures, the spins are more aligned, leading to a magnetization per spin close to 1. On Table 1 are found the values for the statistical mean, error and autocorrelation time for the studied cases.

Notice that the statistical error is higher the closer to the critical temperature. As mentioned before, in the critical temperature, phase transitions are expected, leading to higher fluctuations in the observables and thus higher statistical error. This can be supported also by the fact that the autocorrelation time is larger when approaching the critical temperature.

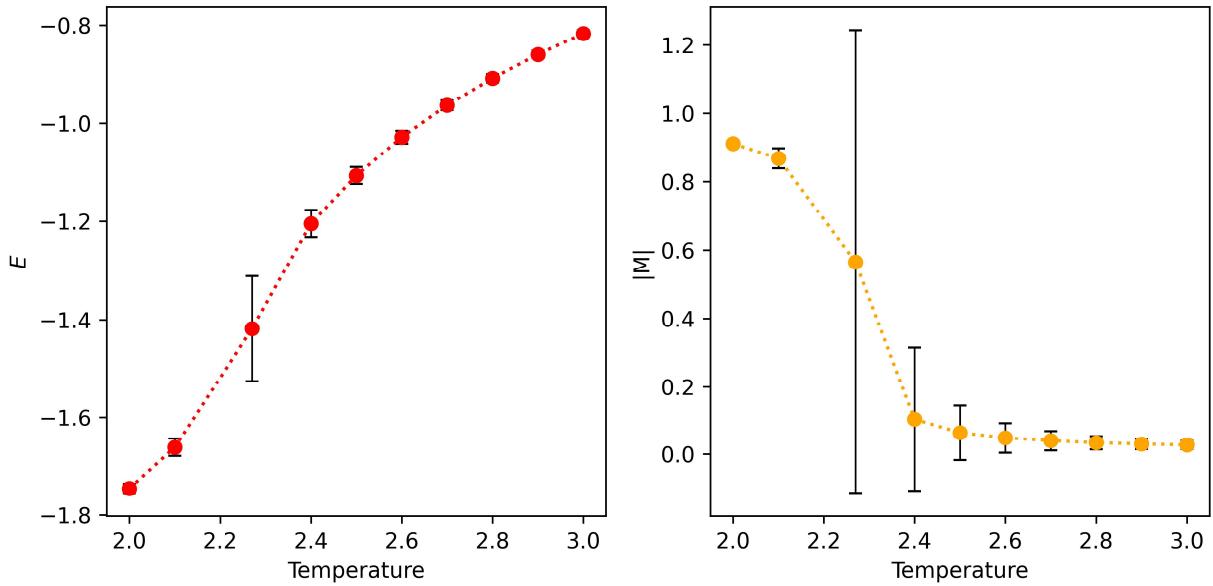


Figure 3. Mean value per spin of the computed energy (left) and magnetization (right) at the different studied temperatures. The error bars have been exaggerated by a factor of 100 in order to appreciate them.

| L | T | $\langle E \rangle$ | σ_E | τ | $\langle M \rangle$ | σ_M | τ |
|-----|------|---------------------|------------|----------|-----------------------|------------|-----------|
| 100 | 2.0 | -1.7455537 | 0.0000031 | 8.63864 | 0.9113362 | 0.0000045 | 10.28776 |
| | 2.1 | -1.6619339 | 0.0001778 | 22.20855 | 0.8682192 | 0.0002922 | 45.54713 |
| | 2.27 | -1.4181119 | 0.0010694 | 88.09364 | 0.5649028 | 0.0067822 | 108.97433 |
| | 2.4 | -1.2043724 | 0.0002795 | 22.72675 | 0.1034899 | 0.0021084 | 45.34688 |
| | 2.5 | -1.1064037 | 0.0001712 | 11.72228 | 0.0636026 | 0.0008069 | 20.37981 |
| | 2.6 | -1.0283158 | 0.0001291 | 9.98836 | 0.0480242 | 0.0004366 | 11.94336 |
| | 2.7 | -0.9635128 | 0.0000085 | 5.32919 | 0.0396256 | 0.0002839 | 8.60791 |
| | 2.8 | -0.9082234 | 0.0000055 | 3.75971 | 0.0335092 | 0.0001944 | 5.96093 |
| | 2.9 | -0.8598792 | 0.0000094 | 5.95978 | 0.0299346 | 0.0001509 | 4.74601 |
| | 3.0 | -0.8173172 | 0.0000094 | 2.87125 | 0.0269960 | 0.0001214 | 4.24625 |
| 20 | 2.0 | -1.7456252 | 0.0000092 | 12.52960 | 0.9113655 | 0.0000033 | 20.06303 |

Table 1. Statistical mean, error, and autocorrelation time obtained for the energy and magnetization per spin at the studied temperatures and lattice size.

The statistical error and autocorrelation time is computed by fitting the binned standard deviations to a function of the form $fit(m) = a - be^{-m/\tau}$, where m is the bin size and τ the autocorrelation time. The few last values were the fitting starts to be constant from the statistical error is gathered. In Figure 4 are available the plots of the statistical error as a function of bin size and the fitted function, for the temperatures of 2.0, 2.27 and 2.6. Again, the binning with the data of the critical point reveals that the fluctuations are high, and the autocorrelation is lower than in the other cases.

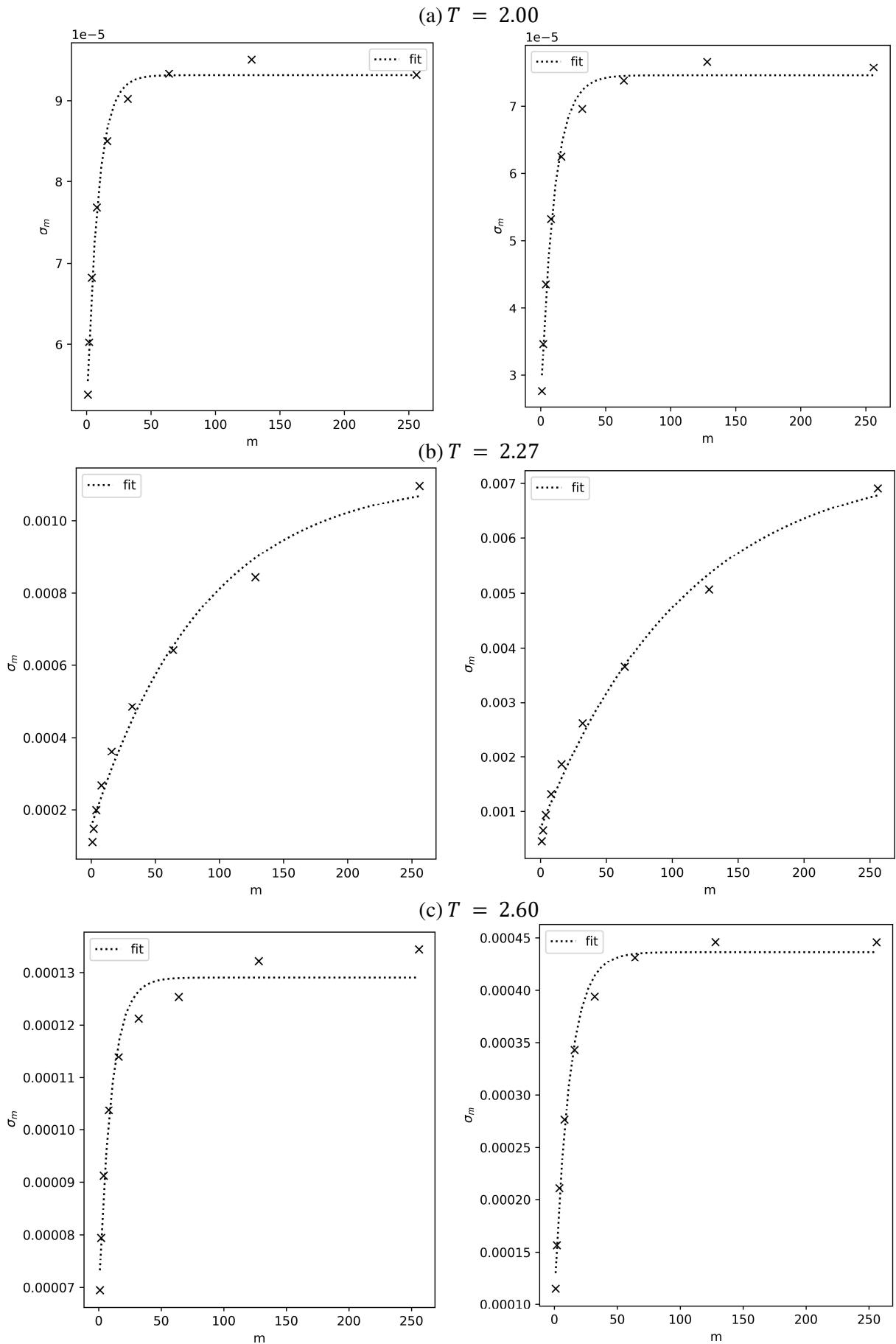


Figure 4. Statistical error σ_m for the energy (left) and magnetization (right) as a function of bin size, m , for the temperatures (a) 2.0, (b) 2.27 and (c) 2.6.