Ising model

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March 12, 2025

Part 1

Given the Hamiltonian, which is the total energy of the system in a given configuration

$$E = \mathcal{H}(\{\sigma\}) = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j \tag{1}$$

the goal is to compute $\Delta E = E(Y) - E(X)$ where the difference between the configurations X and Y is that one spin changed sign. J is the coupling constant and each spin is coupled to four of its neighbors (up, down, left, right).

The total Energy for the configuration X can be written as

$$E(X) = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j \tag{2}$$

If we assume that spin σ_i is flipped to $(-\sigma_i)$ in configuration Y, the total energy is then given by

$$E(Y) = -J \sum_{\langle i,j \rangle} (-\sigma_i)\sigma_j = J \sum_{\langle i,j \rangle} \sigma_i \sigma_j \tag{3}$$

The difference between the system can therefore be written as

$$\Delta E = E(Y) - E(X) = J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - (-J \sum_{\langle i,j \rangle} \sigma_i \sigma_j) = 2J \sum_{\langle i,j \rangle} \sigma_i \sigma_j \tag{4}$$

we can now define the neighbor field as $h_i = \sum_{\langle i,j \rangle} \sigma_j$ by factoring out σ_i since it's constant with respect to the summation resulting in the following equation

$$\Delta E = 2J \sigma_i h_i. \tag{5}$$

Part 2

I implemented this project in C++, further information on how to compile and run the code can be found in the `README.md` file located in the root folder of the project.

Part 3

Figure 1 illustrates the relationship between temperature and two key properties magnetization and energy for different sizes of square lattices in the 2D Ising model.

The left column presents the average absolute magnetization as a function of temperature. In each plot, we observe that the steepest change in magnetization, indicating the phase transition, occurs near the critical temperature, $T_c \approx 2.269$

Furthere observations on Magnetization are:

- All three lattice sizes exhibit a similar pattern: for low temperatures $T < 1$, the system remains in an ordered state with high and stable magnetization, as most spins align in the same direction.
- The most significant drop in magnetization occurs in the critical region between $T = 2.0$and $T = 2.5$ for all lattice sizes, aligning with the expected phase transition at T_c. The transition becomes steeper for larger lattices, indicating a sharper phase transition as the system size increases.

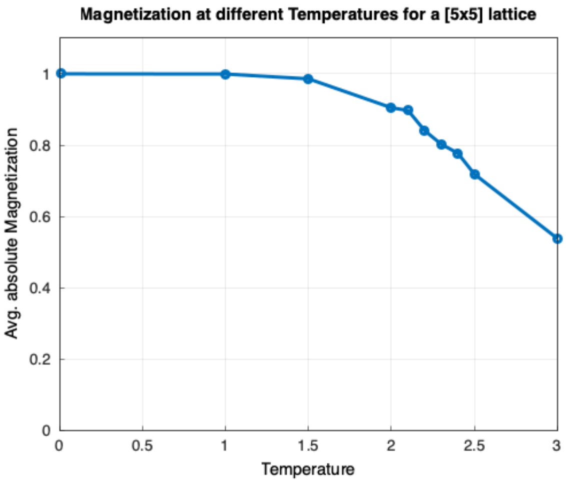
- For temperatures $T > 2.5$, magnetization continues to decrease but at a much slower rate. As T increases beyond 3.0, the system approaches complete randomness, leading to near-zero magnetization.

The right column displays the average energy as a function of temperature. We can make the following observations on Energy:

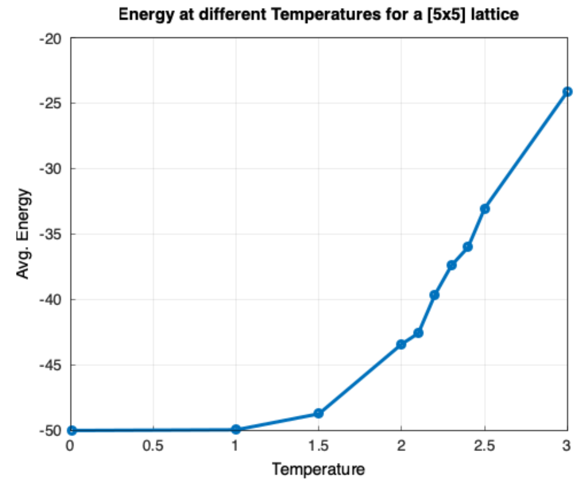
- For $T < 1$, all systems remain at their minimum energy state, corresponding to a highly ordered configuration.
- As temperature increases $T > 1.5$, the spins start to misalign with their neighbors due to increased thermal fluctuations. This occurs as thermal energy begins to overcome the exchange coupling J, leading to the disruption of ordered spin states.
- At even higher temperatures, the system gradually approaches maximum disorder, with energy increasing toward zero.

The data clearly demonstrates a phase transition near the critical temperature, showcasing the classical behavior of the 2D Ising model. As the system transitions from a low-temperature ordered state to a high-temperature disordered state, we observe a sharp drop in magnetization and a corresponding increase in energy, particularly for larger lattice sizes. The plots in Figure 2 depict the evolution of magnetization over time for an 5×5 Ising model lattice at different temperatures. Each system was initialized randomly, meaning the overall sign of magnetization may vary between subfigures (e.g., Subfigure 2c compared to 2a or 2b). The following key observation can be made on Magnetization and Sign Flipping:

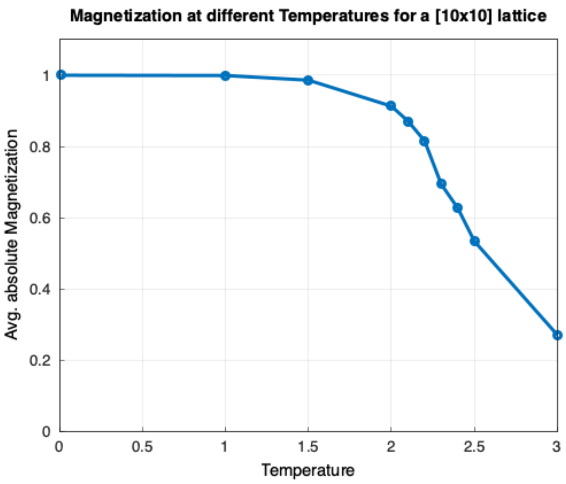
- Subfigure 2a ($T = 0.01$): At temperatures very close to zero, the system is fully ordered, with magnetization staying at -1 (or 1) throughout the entire simulation. No sign flips occur, as thermal energy is insufficient to disrupt spin alignment.
- Subfigure 2b ($T = 1.0$): The system remains predominantly magnetized in one direction, but small fluctuations appear. However, no full sign flips are observed.
- Subfigure 2c ($T = 1.5$): Larger deviations in magnetization occur, yet the system still retains a dominant direction. No complete sign flips are observed, though fluctuations increase.
- Subfigures 2d, 2e, and 2f ($T = 2.0, 2.1, 2.2$): As temperature increases and approaches the critical temperature T_c, magnetization fluctuates more violently. Frequent sign flips occur, indicating the system oscillates between states with positive and negative magnetization due to increasing thermal energy. These fluctuations become more pronounced closer to T_c, as thermal agitation competes with spin alignment.



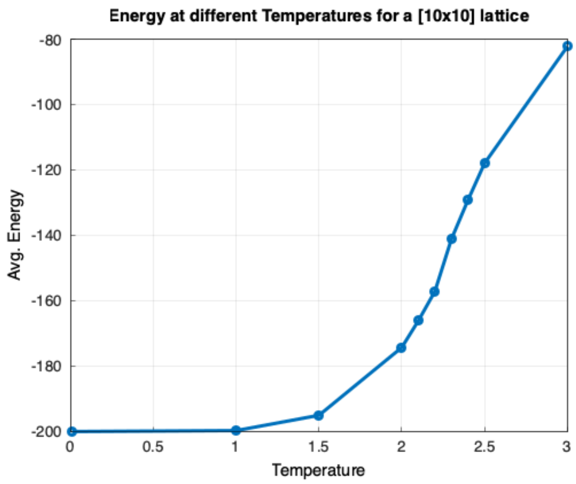
(a) $L = [5 \times 5]$



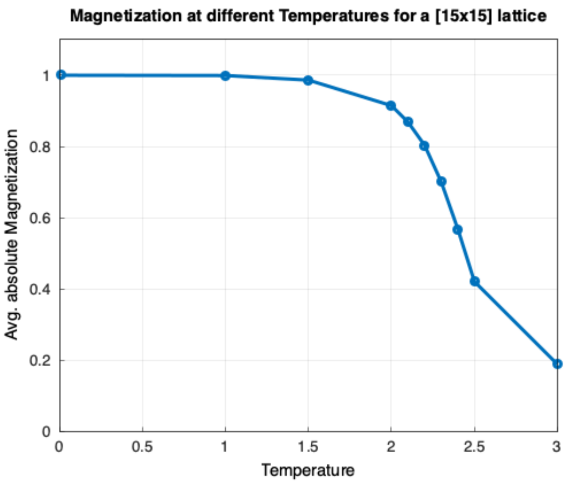
(b) $L = [5 \times 5]$



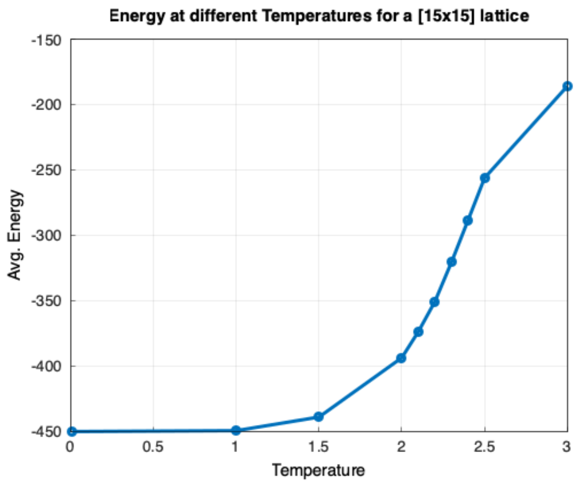
(c) $L = [10 \times 10]$



(d) $L = [10 \times 10]$

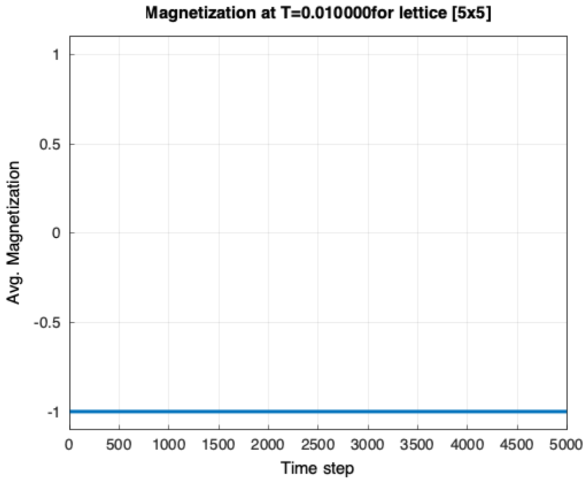


(e) $L = [15 \times 15]$

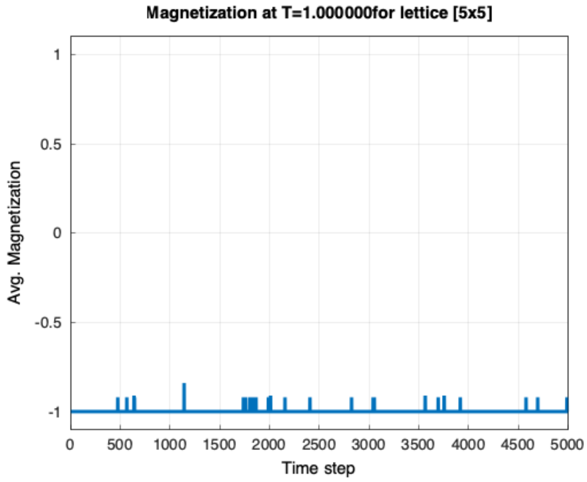


(f) $L = [15 \times 15]$

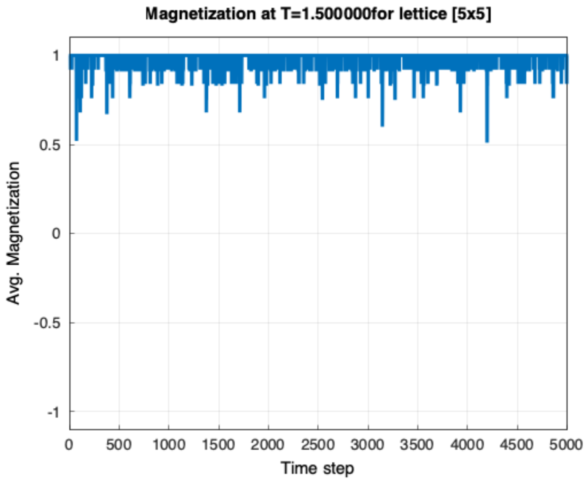
Figure 1: **Markov Chains** Average absolute magnetization at different temperature is plotted on the left, while on the right the average Energy is plotted versus the temperature.



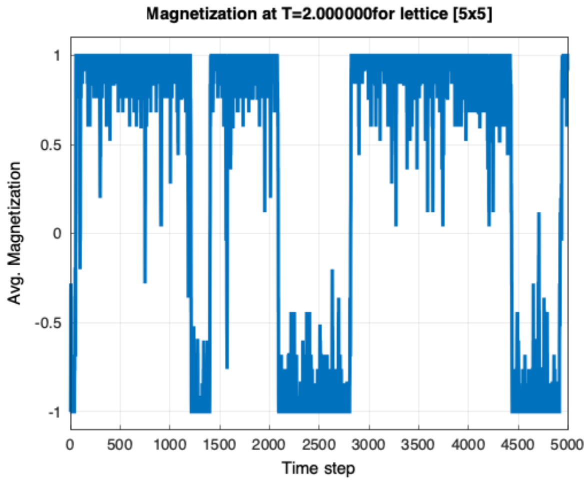
(a) $T = 0.01$



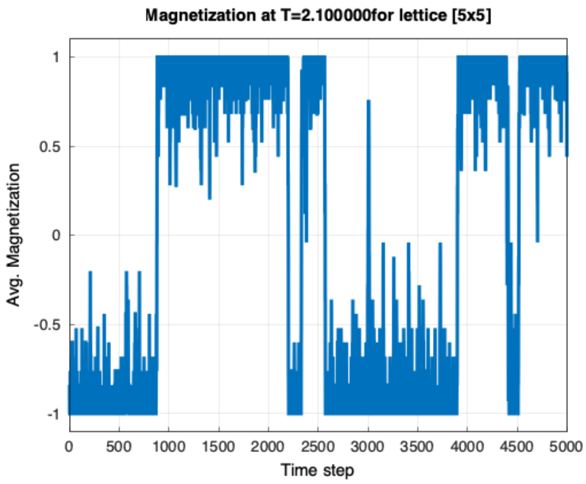
(b) $T = 1.0$



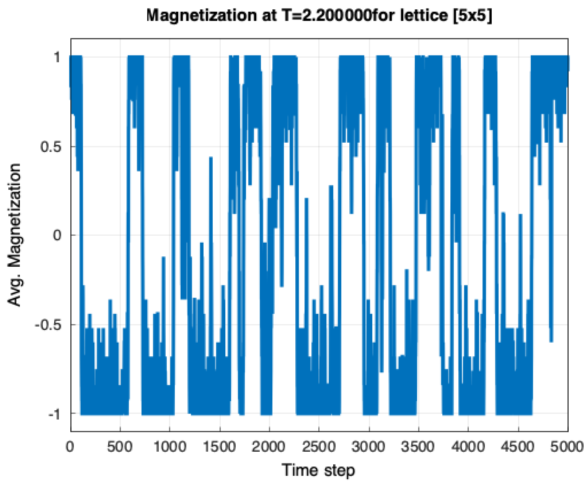
(c) $T = 1.5$



(d) $T = 2.0$



(e) $T = 2.1$



(f) $T = 2.2$

Figure 2: **Dependence of M on the simulation time at temperature $T < T_C$**