Metropolis Monte Carlo Simulation for the 2D Ising Model

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Section 1
Theory and Methods

The Ising Model

Definition: The Ising model describes a system of spins $s_i = \pm 1$ arranged on a lattice, interacting with their nearest neighbours.
Hamiltonian:

$$H = -J \sum_{\langle i,j \rangle} s_i s_j \tag{1}$$

where J is the interaction strength, and $\langle i, j \rangle$ denotes nearest neighbours.

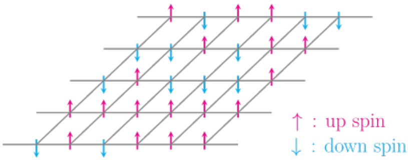

Figure 1: 2D lattice illustration of the Ising Model.

Monte Carlo Algorithm

Initialization:

- Initialize a $N \times N$ lattice with spins having a $+1$ or -1 orientation.

Calculations:

- Compute total energy using nearest-neighbour summation with periodic boundary conditions (PBCs) as well as total magnetization.

Metropolis Step:

- Choose a random spin and compute the change in energy ΔE.
- Acceptance probability given by:

$$P_{acc} = \min(1, e^{-\Delta E/T}) \tag{2}$$

- Apply Metropolis acceptance criterion:
  - If $\Delta E < 0$ or if rand $< e^{-\Delta E/T}$:
    flip the spin
    add ΔE to the total energy
    add ΔM to the total magnetization
- Repeat process for a sufficient number of steps.

Phase Transition

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Ordered phase:

- Below T_c, system exhibits spontaneous magnetization (ferromagnetic phase).
- $M \neq 0$.

Disordered phase:

- Above T_c, same amount, on average, of "up" and "down" spins(paramagnetic phase).
- $M = 0$.

Significance: At T_c, the system undergoes a second-order phase transition characterized by divergent magnetic susceptibility.

Section 2
Results and Discussion

Spin Configuration Evolution

100×100 spin system at $T = 1$:

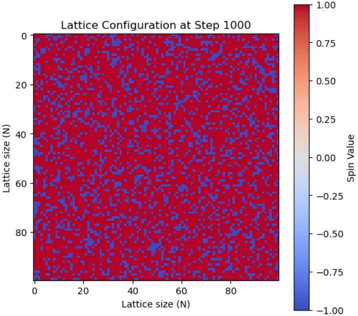

Figure 2: Initial random configuration

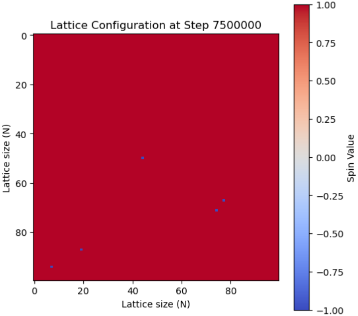

Figure 3: Configuration at equilibrium

Spin Configuration Evolution

50×50 **spin system at** $T = 1$**:**

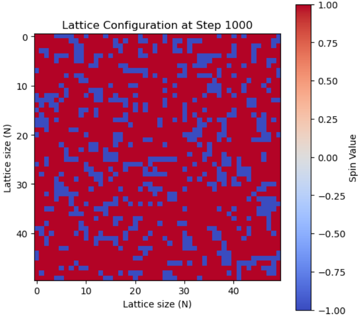

Figure 4: Initial random configuration

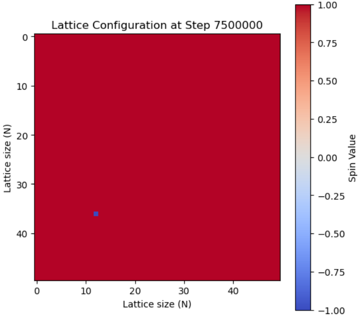

Figure 5: Configuration at equilibrium

Spin Configuration Evolution

10×10 spin system at $T = 1$:

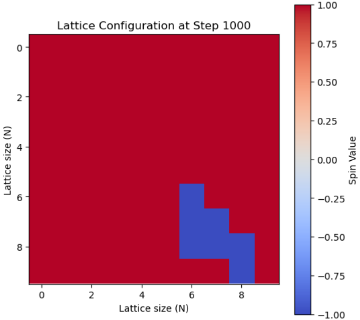

Figure 6: Initial random configuration

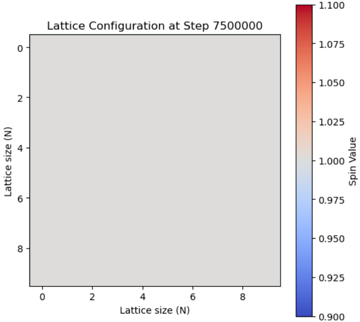

Figure 7: Configuration at equilibrium

Average Energy Per Spin

Equation for Energy:

$$\langle E \rangle = \frac{1}{K} \sum_{i=1}^{K} E_i, \qquad \frac{\langle E \rangle}{N^2} \tag{3}$$

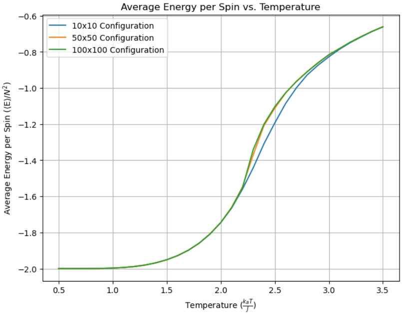

Figure 8: Comparison of the observable between the three systems.

Average Magnetization Per Spin

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Equation for Average Absolute Magnetization:

$$\langle |M| \rangle = \frac{1}{K} \sum_{i=1}^{K} M_i, \quad \frac{\langle |M| \rangle}{N^2} \tag{4}$$

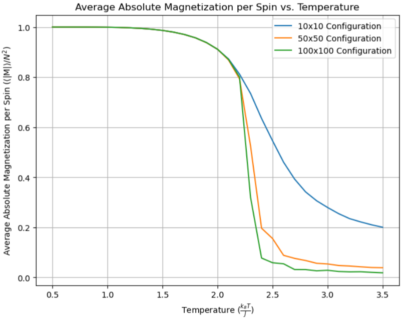

Figure 9: Comparison of the observable between the three systems.

Magnetic Susceptibility Per Spin

Equation for Magnetic Susceptibility:

$$\chi = \frac{\langle M^2 \rangle - \langle |M| \rangle^2}{T} \tag{5}$$

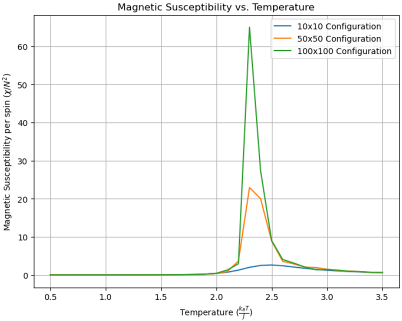

Figure 10: Comparison of the observable between the three systems.

Conclusion

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- The results given by the measured observables align with theory.
- The configuration of the systems after equilibrium at a given temperature aligns with theory.

Thank you for your attention!