Ferromagnetism in the Ising model using the Metropolis algorithm

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1. Description of the problem—2D Ising model

The Ising model is the simplest model describing phase transitions in magnetic systems. However, the interaction between spins in the model can lead to emergent phenomena that are not obvious from the properties of individual spins, granting it remarkable properties, with the most intriguing being spontaneous symmetry breaking. This model can be extended to study quantum phase transitions, dynamic critical behavior, and even complex social and economic phenomena such as wildfires, traffic congestion, and opinion dynamics.

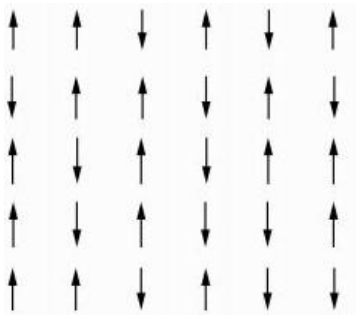

Fig.1. The lattice of Ising model.

The 2D Ising model consists of a lattice of spins, where each spin s_i takes values of either $+1$ (up) or -1 (down). These spins interact with their nearest neighbors and are also influenced by an external magnetic field. The Hamiltonian governing the system is given by

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

where $\langle i,j\rangle$ represents nearest-neighbor spin pairs and J is the coupling constant describing the strength of interaction between nearest-neighboring spins. If $J > 0$, the system favors ferromagnetic alignment (spins tend to be parallel). If $J < 0$, it favors antiferromagnetic alignment (spins tend to be antiparallel). h is the strength of the external magnetic field, which biases the spins toward alignment in its direction.

In this topic "ferromagnetism in the Ising model using the Metropolis algorithm", we consider $h = 0$ and $J > 0$. In the absence of an external field, Ising model exhibits a phase transition at a critical temperature T_c. For $T > T_c$, the system is in a disordered phase where spins fluctuate randomly. For $T < T_c$, the system has a net magnetization, which is either a predominantly up or down orientation.

When T becomes small and cross T_c, the system experiences a spontaneous Z_2 symmetry breaking, which corresponds to the emergence of ferromagnetic order (described by magnetization) in the Landau paradigm. This classical criticality (characterized by Z_2 symmetry breaking) belongs to the Ising universality class.

The order parameter, the magnetization per spin, is defined as

$$m \equiv \frac{1}{N}\sum_i s_i \,.$$

2. Simulation procedure—Markov chain Monte Carlo with Metropolis algorithm

Step 1: Define a 20×20 lattice of spins $s_i = \pm 1$, start with all spins aligned, i.e., all $s_i = +1$, and define the $J = k = 1$ (setting units so that T is dimensionless).

Step 2: The energy change ΔE when flipping a single spin s_i is

$$\Delta E = 2Js_i \sum_{nn} s_j ,$$

where nn means the sum runs over the four nearest neighbors.

Step 3: For a given temperature T, employ the Metropolis algorithm:

a. Sequentially pick a lattice site (i, j) (local updates);
b. Calculate the energy change ΔE if the spin is flipped;
c. Accept or reject the flip based on the Metropolis criterion: If $\Delta E \leq 0$, accept the flip. Otherwise, accept the flip with probability $P = e^{-\Delta E/T}$. Generate a random number $r \in [0,1]$. If $r < P$, accept the flip; otherwise, reject it;
d. Repeat for $N = 20 \times 20$ times to complete one Monte Carlo step (MCS);
e. Iterate for a total of 10^4 MCS to reach equilibrium (a Markov chain).

Step 4: After equilibrium is reached, perform 5×10^4 sampling steps. Calculate average magnetization per spin $m = \frac{1}{N}|\sum_i s_i|$, average energy per spin $\bar{E} = \frac{1}{N}\langle H \rangle$, and heat capacity $C = \frac{\langle E^2 \rangle - \langle E \rangle^2}{T^2}$.

Step 5: Repeat for different temperatures.

The detailed comments for the code are written directly in the code file.

3. Numerical Results

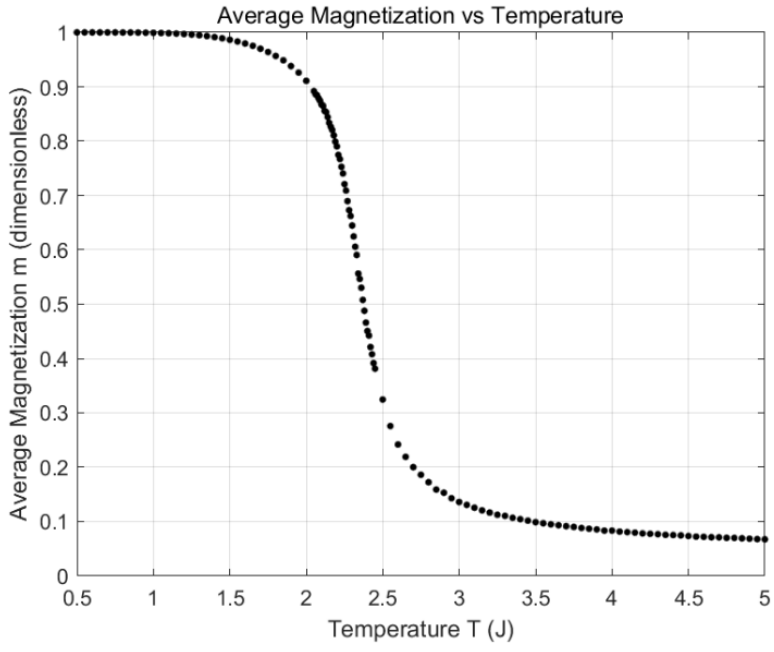

Fig.2. Average magnetization m versus T.

Critical exponent α defined by $m \sim (T_c - T)^{\alpha}$ can be obtained by fitting $\ln m \sim \alpha \ln(T_c - T)$.
It can be seen that ferromagnetic order emerges when $T < T_c \approx 2.3J$.

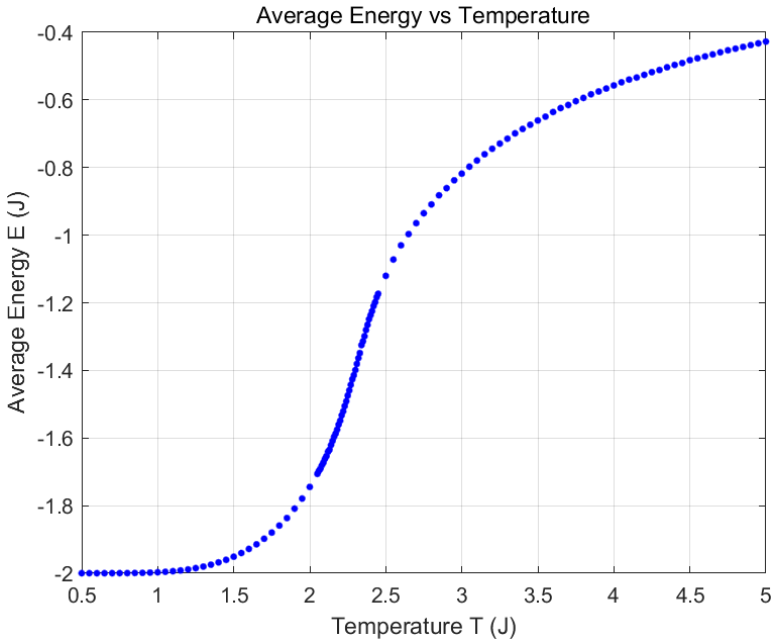

Fig.3. Average energy $\bar{E}$ versus T.

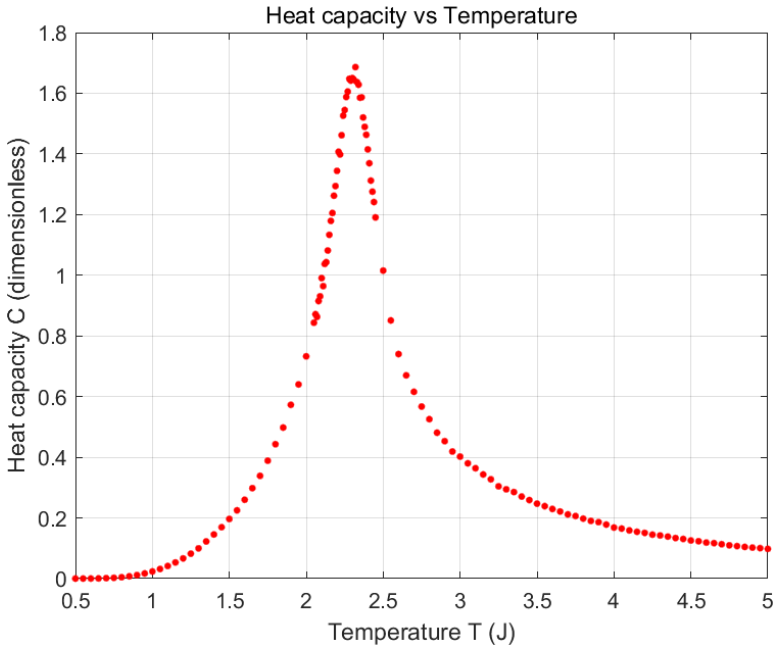

Fig.4. Heat capacity C versus T.

The more precise value of the critical point can be determined using Fig.4. Here $T_c \approx 2.27J$.

References

[1] Binder, Kurt, and Dieter W. Heermann. *Monte Carlo Simulation in Statistical Physics: An Introduction*. Graduate Texts in Physics. Cham: Springer International Publishing, 2019. https://doi.org/10.1007/978-3-030-10758-1.