Monte Carlo simulation of Two-dimensional Ising model

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Abstract

To be filled.

1 Introduction

Ising model is a simple but important model for the explanation of magnetization. It assumes that atomic spins are located on a N-dimensional lattice grid, and these spins only have two discrete states, up ($\sigma = 1$) or down ($\sigma = -1$). Only neighboring spins can interact with each other, and thus its Hamiltonian can be written as

$$H = -J \sum_{<kl>}^{N} \sigma_k \sigma_l \,, \tag{1}$$

where $J > 0$ and $< kl >$ indicates that we only sum over nearest neighbors.

In statistical physics, the equilibrium of a system described by Eq. 1 should be solved using canonical ensemble, which involves a summation over all possible microscopic states to obtain the partition function. For N-dimensional Ising model with size L in each dimension, the total number of all microscopic states is 2^{L^N}, which cannot be simply summed over. The one- and two-dimensional cases has been solved analytically and they show several interesting properties of phase transition. But the exact solution of higher-dimensional Ising model is still unavailable, and thus numerical methods which avoid the summation over all possible states are required for the simulation of Ising model.

In this report, we discuss the Monte Carlo method for the simulation of two-dimensional (2D) Ising model and compare our results with the analytical solution. In Sec. 2 several properties shown in the analytical solution are discussed, for the comparison in Sec. 4. Sec. 3 gives the outline of Monte Carlo algorithm we utilize for 2D Ising model, and then Sec. 4 discusses the results of our simulation. Conclusions are given in Sec. 5.

2 Properties of 2D Ising model from its analytical solution

In this section we discuss the properties of $L \times L$ Ising model with periodic boundary condition, which indicates that a spin on one boundary will interact with another spin on the opposite boundary. In other words, the summation over $< kl >$ in Eq. 1 includes the following cases:

$$k = (1, x), \ l = (L, x); \ k = (x, 1), \ l = (x, L) \tag{2}$$

where (x, y) gives the coordinate of a spin in the $L \times L$ lattice.

Table 1: All possible microscopic states of 2×2 Ising model. The energy is in the unit of J.

Number of spins up	Degeneracy	Energy	Magnetization
4	1	-8	4
3	4	0	2
2	4	0	0
2	2	8	0
1	4	0	-2
0	1	-8	-4

2.1 The solution of 2×2 Ising model

For simplicity, we begin our discussion of the analytical solution from the 2×2 case. Table 1 shows all the possible microscopic states of 2×2 Ising model. The corresponding partition function can be obtained by summing over all these microscopic states α

$$Z = \sum_{\alpha} e^{-\beta E_\alpha} = 2e^{8\beta} + 2e^{-8\beta} + 12 = 4\cosh(8\beta) + 12, \tag{3}$$

where $\beta = 1/T$ and T is temperature in the unit of J (Boltzmann constant k_B is absorbed into T).

Thus, the mean energy of the system (in the unit of J) is

$$\langle E \rangle = -\frac{\partial \ln Z}{\partial \beta} = -\frac{8\sinh(8\beta)}{\cosh(8\beta) + 3}. \tag{4}$$

The mean magnetization of the system is

$$\langle |M| \rangle = \frac{1}{Z} \sum_{\alpha} |M_\alpha| e^{-\beta E_\alpha} = \frac{1}{Z} \left(8e^{8\beta} + 4\right) = \frac{2e^{8\beta} + 1}{\cosh(8]\beta) + 3}. \tag{5}$$

The heat capacity is

$$C_V = \frac{\partial \langle E \rangle}{\partial T} = -\beta^2 \frac{\partial \langle E \rangle}{\partial \beta} = \beta^2 \frac{64 \left[1 + \cosh(8\beta)\right]}{\left[6 + \cosh(8\beta)\right]^2} = \beta^2 \left(\langle E^2 \rangle - \langle E \rangle^2\right), \tag{6}$$

where

$$\langle E^2 \rangle = \frac{1}{Z} \sum_{\alpha} E_\alpha^2 e^{-\beta E_\alpha} = \frac{64\cosh(8\beta)}{\cosh(8\beta) + 3}. \tag{7}$$

Similarly, we have

$$\langle M^2 \rangle = \frac{1}{Z} \sum_{\alpha} M_\alpha^2 e^{-\beta E_\alpha} = \frac{8\left(e^{8\beta} + 1\right)}{\cosh(8\beta) + 3}, \tag{8}$$

and define susceptibility as

$$\chi = \beta \left(\langle M^2 \rangle - \langle |M| \rangle^2\right). \tag{9}$$

Above results can be used to benchmark the Monte Carlo algorithm developed for 2D Ising model.

2.2 Properties of phase transition in 2D Ising model

One important aspect of the analytical solution of 2D Ising model is the second-order phase transition at a nonzero critical temperature T_C. There is a sharp transition from nonzero $\langle |M| \rangle$ to $\langle |M| \rangle = 0$

when temperature T increases from $T < T_C$ to $T > T_C$. In this section we do not discuss the details of the analytical solution of 2D Ising model. Instead, we will show several important properties of phase transition in 2D Ising model, which are used to benchmark our simulation.

Near T_C we can characterize the behavior of many physical quantities by a power law. For 2D Ising model, the mean magnetization is given by

$$\langle M(T) \rangle \sim (T - T_C)^\beta \,, \tag{10}$$

where $\beta = 1/8$ is a critical exponent. A similar relation applies to heat capacity

$$C_V(T) \sim |T_C - T|^\alpha \,, \tag{11}$$

and the susceptibility

$$\chi(T) \sim |T_C - T|^\gamma \,, \tag{12}$$

with $\alpha = 0$ and $\gamma = 7/4$. It should be noted that $\alpha = 0$ does not mean that C_V is continuous around T_C. The analytical solution shows that C_V will logarithmically diverge at T_C. Another important quantity is called correlation length, which is expected to be of the order of the lattice spacing for $T >> T_C$. Because the spins become more and more correlated as T approaches T_C, the correlation length increases as we get closer to the critical temperature. The divergent behavior of ξ near T_C is

$$\xi(T) \sim |T_C - T|^{-\nu} \,, \tag{13}$$

with $\nu = 1$. A second-order phase transition is characterized by a correlation length which spans the whole system. Since we are always limited to a finite lattice, ξ will be proportional with the size of the lattice. Through so-called finite size scaling relations it is possible to relate the behavior at finite lattices with the results for an infinitely large lattice. The critical temperature scales then as

$$T_C(L) - T_C(L = \infty) = aL^{-1/\nu} \,, \tag{14}$$

where a is a constant and ν is defined in Eq. 13. We set $T = T_C$ and obtain a mean magnetization

$$\langle M(T) \rangle \sim (T - T_C)^\beta \to L^{-\beta/\nu} \,, \tag{15}$$

heat capacity

$$C_V(T) \sim |T_C - T|^{-\gamma} \to L^{\alpha/\nu}, \tag{16}$$

and susceptibility

$$\chi(T) \sim |T_C - T|^{-\alpha} \to L^{\gamma/\nu} \,. \tag{17}$$

The exact solution gives $\nu = 1$ and $T_C = \frac{2}{\ln(1+\sqrt{2})} \approx 2.269$ (in the unit of J) when $L \to \infty$. With the help of Eq. 14, we can use our simulation results of different L to extract T_C for $L \to \infty$, which will be done in Sec. 4.

3   Monte Carlo methods for Ising model

In our work the Metropolis algorithm is adopted for the simulation of Ising model. This algorithm is based on the theory of Markov chain and detailed balance. In the example of Ising model, the transition rate between two microscopic states i and j should satisfy

$$\frac{W(j \to i)}{W(i \to j)} = \frac{w_i}{w_j} = e^{-\beta(E_i - E_j)} \,, \tag{18}$$

Input: Size of the system L, temperature T, number of Monte Carlo cycles MC.
Output: $\langle E \rangle$, $\langle E^2 \rangle$, $\langle |M| \rangle$, $\langle M^2 \rangle$, C_V and χ.

1 Initialize spin lattice a (in an ordered or random way);
2 Calculate E, E^2, $|M|$, M^2 of the initial lattice;
3 $E_{tot} = 0$, $E_{tot}^2 = 0$, $|M|_{tot} = 0$, $M_{tot}^2 = 0$;
4 for $i = 1; i <= MC; i + +$ **do**
5   **for** $j = 1; j <= L; j + +$ **do**
6   **for** $k = 1; k <= L; k + +$ **do**
7 $r =$ a uniformly distributed random number in $[0, 1]$;
8   Flip spin at position (j, k);
9   Calculate the change of energy ΔE;
10   **if** $\Delta E < 0$ or $r < \exp(-\Delta E/T)$ **then**
11   Accept this spin flip;
12   Update E, E^2, $|M|$, M^2;
13   **end**
14   **else**
15   Reverse this spin flip;
16   **end**
17   Add E, E^2, $|M|$, M^2 to their corresponding "tot" variables;
18   **end**
19   **end**
20 end
21 Calculate the average $\langle E \rangle$, $\langle E^2 \rangle$, $\langle |M| \rangle$, $\langle M^2 \rangle$ by dividing $L^2 MC$;
22 Calculate C_V and χ by Eq. 6 and 9;

Algorithm 1: Metropolis algorithm for the simulation of Ising model.

with $w_i = \frac{1}{Z} e^{-\beta E_i}$ to obtain an equilibrated (and detailed-balanced) probability distribution given by canonical ensemble. We can model $W(j \to i)$ as a product of the probability $T(j \to i)$ to make a transition from j to i and the probability $A(j \to i)$ to accept this transition, namely

$$W(j \to i) = T(j \to i)A(j \to i).$$ (19)

In the simulation of Ising model, we have no physical insight of $T(j \to i)$, so we can simply assume that all $T(j \to i)$ are the same. Then Eq. 18 can be rewritten as

$$\frac{A(j \to i)}{A(i \to j)} = e^{-\beta(E_i - E_j)},$$ (20)

which describes the probability of accepting a transition from j to i in our simulation.

Based on Eq. 20 we can develop a simulation algorithm shown in Algorithm 1. The main idea is that we flip one spin every time and use a random number r, which distributes uniformly in $[0, 1]$, to determine whether to accept this flip based on Eq. 20. If this flip reduces the energy or $r < \exp(-\Delta E/T)$ (ΔE is the energy change in the transition) we will accept. In one Monte Carlo cycle we iterate through the full lattice and try to flip each spin. Physical quantities $\langle E \rangle$, $\langle E^2 \rangle$, $\langle |M| \rangle$, $\langle M^2 \rangle$ are obtained by averaging them in the Monte Carlo process.

4 Results and discussion

In this section we will discuss the results given by our Monte Carlo simulation of 2D Ising model. Sec. 4.1 gives the results of 2×2 case for benchmark. In Sec. 4.2 we discuss the change of energy and

Table 2: Results for 2×2 case with temperature $T = 1.0$. Analytical results are provided for benchmark. Energy is in the unit of J.

Number of Monte Carlo cycles MC	10	100	1000	10000	Analytical
Mean energy $\langle E \rangle$	-7.2	-7.92	-7.986	-7.988	-7.98393
Mean magnetization $\langle |M| \rangle$	3.75	3.975	3.9955	3.99625	3.99263
Mean square of energy $\langle E^2 \rangle$	57.6	63.36	63.888	63.904	63.8714
Mean square of magnetization $\langle M^2 \rangle$	14.7	15.87	15.977	15.9805	15.9732
Heat capacity C_V	5.76	0.6336	0.111804	0.095856	0.128329
Susceptibility χ	0.6375	0.069375	0.0129798	0.0104859	0.0320873

magnetization in the Monte Carlo process for 20×20 lattice and show their probability distributions. In Sec. 4.3 the phenomenon of phase transition in 2D Ising model is discussed for different lattice size.

4.1 Benchmark: 2×2 case

Table 2 gives the quantities we obtain from our Monte Carlo simulation of 2×2 lattice with temperature $T = 1.0$. As the number of Monte Carlo cycles MC increases, our results get closer to the analytical values. For $MC = 1000$ our results are close enough to the analytical values for benchmark purpose. However, we can notice that both heat capacity C_V and susceptibility χ do not agree well with the analytical results, and they have some fluctuations as MC increases. The reason is that both $\langle E^2 \rangle$ and $\langle E \rangle^2$ are large but close to each other, so their difference, which determines C_V, will have a large numerical error. This is unavoidable when C_V and χ are small.

4.2 Details in the Monte Carlo process

For our simulation, it is important to know when the properties of our system become equilibrated, which determines how many Monte Carlo cycles are necessary. Fig. 1 shows the change of energy and magnetization as a function of the number of Monte Carlo cycles MC for 20×20 lattice with temperature $T = 1.0$ and $T = 2.4$. Blue lines are the results of ordered initialization (starting from all spins pointing up) and orange lines are the results of random initialization (starting from random spin orientation). From Fig. 1, we can see that the energy of the system converges quite fast, and different initializations give the same results after some Monte Carlo cycles. For $T = 1.0$, the system soon goes to an ordered phase with very small fluctuations. For $T = 2.4$, higher temperature will raise the probability of the system being at excitation states. Thus, the energy has a larger fluctuation around its mean value, and the magnetization also oscillates dramatically because states with different magnetization can have the same energy (degeneracy).

Fig. 2 gives the distributions of energy and magnetization per spin in the Monte Carlo process with random initialization. For $T = 1.0$, the system is almost always stays at an ordered phases, and thus we have a high peak of magnetization per spin at $M/L^2 = 1$, and a high peak of energy per spin at $E/L^2 = -2$. For $T = 2.4$, the distribution of energy centers at the most probable value, which is approximately the mean value; the distribution of magnetization is broader because of states with different magnetization but the same energy.

4.3 Phase transition

To investigate the phase transition in Ising model, we perform calculations with different lattice size $L = 20, 40, 60, 80, 100, 140$ in the temperature range $T \in [2.1, 2.4]$. The temperature step is 0.02. Fig. 3 gives the energy, magnetization, heat capacity and susceptibility per spin as a function of temperature. It
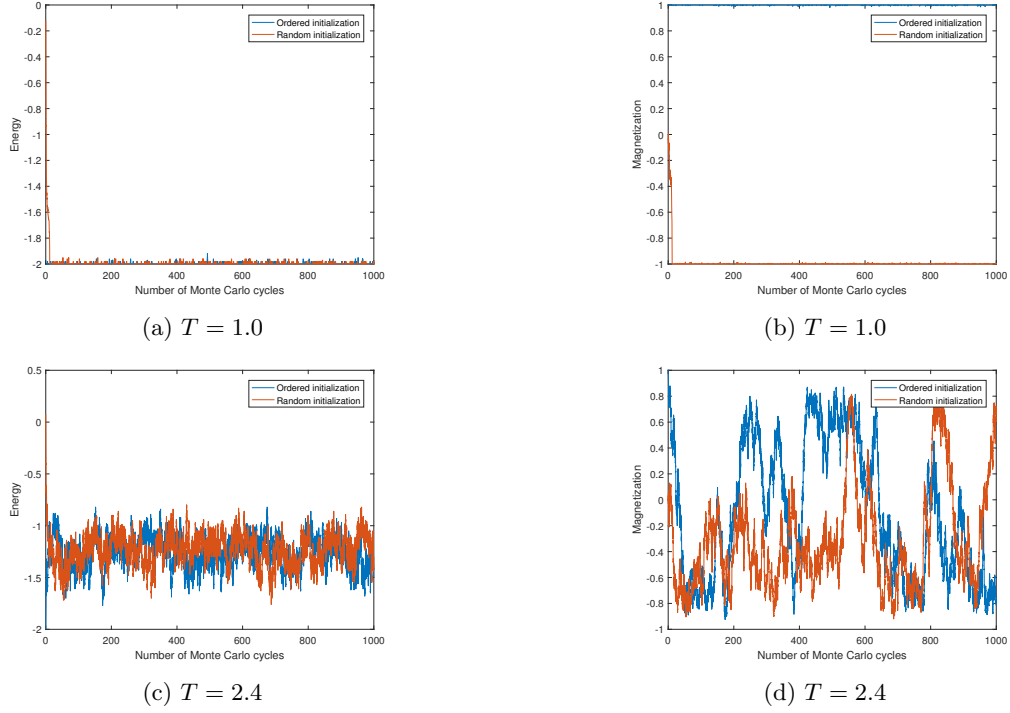
(a) $T = 1.0$

(b) $T = 1.0$

(c) $T = 2.4$

(d) $T = 2.4$

Figure 1: Energy and magnetization as a function of the number of Monte Carlo cycles. Energy is in the unit of J. Temperature $T = 1.0$ or 2.4.

can be seen that around $T = 2.28$ the magnetization drops fast as T increases, indicating that the system undergoes a transition from an ordered phase to a disordered phase. This transition is not dramatic when L is small (e.g. $L = 20$ and 40), which results from the finite size of the system. The energy of the system, however, changes smoothly when the phase transition occurs, which is a characteristic of a second-order transition. Both heat capacity and susceptibility have a high peak around the transition temperature, which agrees with the divergence of these two quantities shown in the analytical solution.

By Eq. 14 we can estimate T_C for an infinitely large system from the results with finite L. It is quite difficult to determine the critical temperature from Fig. 3 because our resolution is not small enough and the peaks of C_V and χ do not coincide. From the peaks of χ (Fig. 3d) we estimate that $T_C(L = 60) = 2.3$ and $T_C(L = 140) = 2.28$. By Eq. 14 and $\nu = 1$ we obtain

$$\begin{cases} a = 2.1\,, \\ T_C(L = \infty) = 2.265\,. \end{cases} \tag{21}$$

Our estimation is not far from the analytical result 2.269.

5   Conclusion

To be filled.

(a) $T = 1.0$ (b) $T = 1.0$

(c) $T = 2.4$ (d) $T = 2.4$
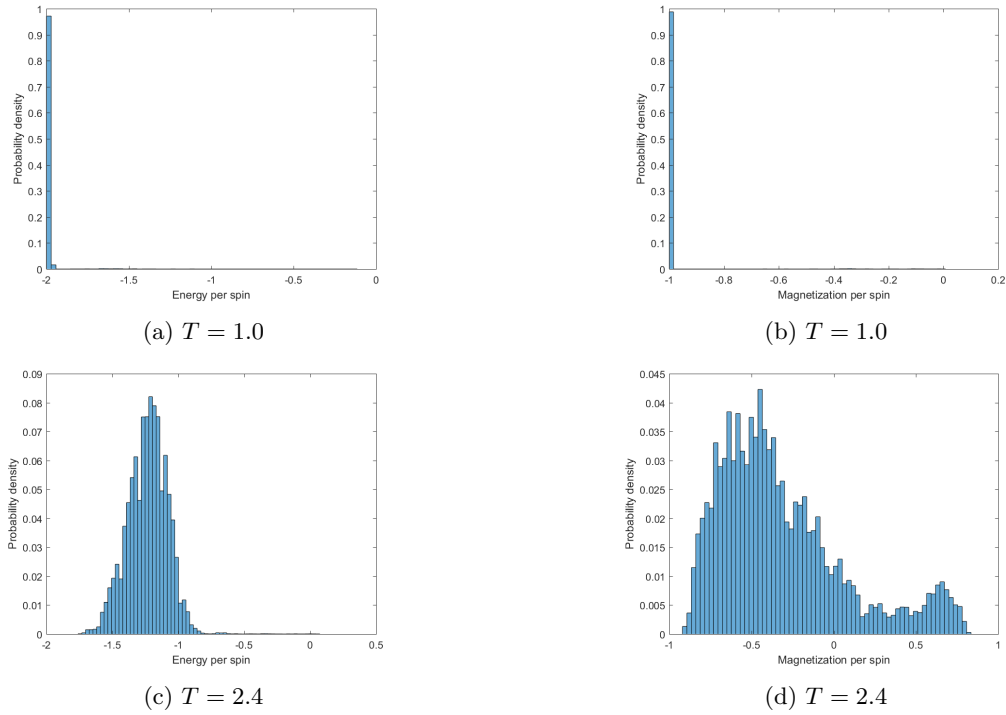
Figure 2: Probability distribution of energy and magnetization per spin. Energy is in the unit of J. Temperature $T = 1.0$ or 2.4.

Acknowledgments

We are grateful for the sincere guidance from Prof. Morten Hjorth-Jensen.

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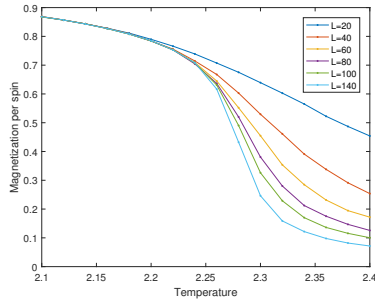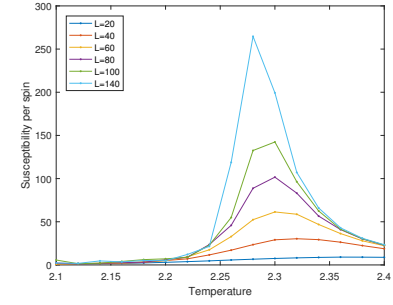
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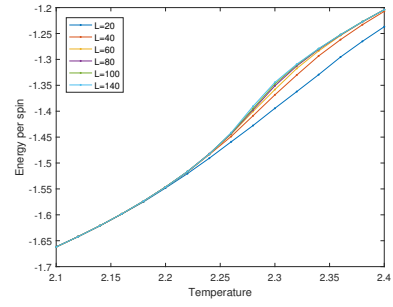
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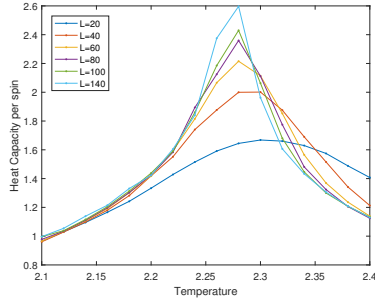
(c)

(d)

Figure 3: Energy, magnetization, heat capacity and susceptibility per spin as a function of temperature with different lattice size $L = 20, 40, 60, 80, 100, 140$ in the temperature range $T \in [2.1, 2.4]$. Temperature step is 0.02.