Monte Carlo Simulation of Phase Transition in Classical Ising Model

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Abstract. Phase transitions are widespread physical phenomena in nature and the phase transition of ferromagnetic substances which can be described by Ising model is an important part of physics. This paper discusses the phase transition of the low-dimensional Ising model. For one-dimensional Ising model, the exact solution is given and no phase transition is found when there is no external magnetic field. For two-dimensional Ising model, Monte Carlo method along with importance sampling, careful balance conditions and the Metropolis algorithm is introduced to numerically simulate it. The trends of order parameters like magnetization, specific heat and magnetic susceptibility are analyzed and the mutation of some order parameters is found around critical temperature. The influences of external magnetic field and the scale of system are discussed and critical temperature of phase transition is explored by several methods, which is eventually found around 2.269 ($k_B T/J$). Lastly, compared with theoretical values, the disadvantages are pointed out and optimization suggestions are raised for improvement.

Keywords: Ising model; Phase transition; Monte Carlo simulation; Order parameter.

1. Introduction

When the system undergoes a phase transition, the thermodynamic function will undergo a sudden change or an infinite peak caused by divergence. Though thermodynamic function derived by the partition function of the system is a good way to study the phase transition, the combination of Ising model and Monte Carlo simulation realized by computer seems to be more efficient, intuitive and simple on this topic, especially when it comes to Ising model of 2D or more [1]. Since the beginning of the last century, a large number of studies on statistical models in statistical physics have formed a specialized field, and many models have been born. In explaining ferromagnetism, the Ising model reflects its advantages. Although the Ising model is very mature and classic, it still needs to be constantly verified. As for the Monte Carlo method, it is a valuable mathematical and statistical method to solve questions about probability and statistics which are related to some phenomena in quantum mechanics and statistical mechanics [2]. Therefore, it's effective and meaningful to utilize Monte Carlo method to simulate Ising model and study the phase transition process of ferromagnetic substances.

This paper is going to talk about the exact theoretical solution of one-dimensional Ising model first and introduce some details of Monte Carlo method like important sampling, Markov process and single-spin-flip dynamics algorithm. Then this paper will present the results of simulation of two-dimensional Ising model and compare them with theoretical situation for mutual verification. Though the simulation of two-dimensional Ising model in this paper may not be so precise due to computing power and the exact solution of two-dimensional Ising model has been worked out by Onsager in 1940s, it's worth emphasizing that Ising model of 3D or more has no exact theoretical solution and can only described by numerical solution worked out by computer.

2. Ising Model: The One-dimensional Case as an Example

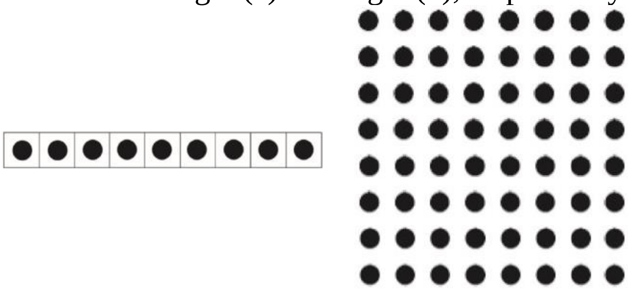
In a ferromagnetic system, the Hamiltonian is given by [3]

$$H = -\sum_{i \neq j} J_{ij} \vec{S_i} \cdot \vec{S_j} - g\mu_B \vec{B} \cdot \sum_i \vec{S_i} \tag{1}$$

Assuming that $J_{ij} = \mathrm{J}$, the Hamiltonian of Ising model is

$$H = -\frac{J}{2}\sum_{\langle ij\rangle}\sigma_i\sigma_j - \frac{1}{2}g\mu_B B\sum_i \sigma_i \tag{2}$$

In Eq. (2), σ_i represents the spin at lattice point i and the spins only have two states, up ($\sigma_i = 1$) and down ($\sigma_i = -1$). $\langle ij\rangle$ indicates that only the nearest neighbor lattice points are summed. The 1D and 2D Ising models are shown in Fig. 1(a) and Fig. 1(b), respectively.



(a) (b)

Fig. 1 (a) Schematic diagram of 1D Ising model; (b) Schematic diagram of 2D Ising model

Suppose that one-dimensional Ising model is an one-dimensional magnetic system composed of N spins which satisfy the periodic boundary condition ($\sigma_{(N+1)} = \sigma_1$), the partition function of one-dimensional Ising model can be expressed as

$$\mathrm{Z} = \sum e^{-\frac{1}{k_B T}\left(-\frac{J}{2}\sum_i \sigma_i\sigma_{i+1} - \frac{1}{2}g\mu_B B\sum_i \sigma_i\right)}. \tag{3}$$

For the convenience of calculation, define that $K = \frac{J}{2k_BT}$ and $w = \frac{g\mu_B B}{2k_BT}$. Thus, the partition function can be transformed to:

$$\begin{aligned}\mathrm{Z} &= \sum_{\sigma_1,\sigma_2,\cdots,\sigma_N} e^{K(\sigma_1\sigma_2+\sigma_2\sigma_3+\cdots+\sigma_{N-1}\sigma_N+\sigma_N\sigma_1)+w(\sigma_1+\sigma_2+\cdots+\sigma_N)} \\ &= \sum_{\sigma_1,\sigma_2,\cdots,\sigma_N}\left[e^{\frac{w}{2}(\sigma_1+\sigma_2)+K\sigma_1\sigma_2}\right]\left[e^{\frac{w}{2}(\sigma_2+\sigma_3)+K\sigma_2\sigma_3}\right]\cdots\left[e^{\frac{w}{2}(\sigma_N+\sigma_1)+K\sigma_N\sigma_1}\right].\end{aligned} \tag{4}$$

Here, the transition matrix V can be introduced [4]

$$\mathrm{V} = \begin{bmatrix} V_{1,1} & V_{1,-1} \\ V_{-1,1} & V_{-1,-1}\end{bmatrix} = \begin{bmatrix} e^{w+K} & e^{-K} \\ e^{-K} & e^{-w+K}\end{bmatrix} \tag{5}$$

Where$V_{\sigma_i\sigma_j} = e^{\frac{w}{2}(\sigma_i+\sigma_j)+K\sigma_i\sigma_j}$. Thus, the partition function can be rewritten as

$$Z = \sum_{\sigma_1,\sigma_2,\cdots,\sigma_N} V_{\sigma_1\sigma_2}V_{\sigma_2\sigma_3}\cdots V_{\sigma_N\sigma_1} = tr(V^N). \tag{6}$$

The eigenvalues can be obtained via the eigenfunction $\det(V - \lambda I) = 0$, and the eigenvalues of transition matrix V are given by $\lambda_\pm = e^K\cosh w \pm \sqrt{e^{2K}\sinh^2 w + e^{-2K}}$. The partition function can be further solved

$$Z = tr(V^N) = \lambda_+^N + \lambda_-^N = \lambda_+^N\left[1 + \left(\frac{\lambda_-}{\lambda_+}^N\right)\right] \tag{7}$$

Which turns out to be λ_+^N as $N \to \infty$. Thus, the partition function is

$$Z=\left(e^{\frac{J}{2k_BT}}\cosh\frac{\mathrm{g}\mu_\mathrm{B}\mathrm{B}}{2\mathrm{k_B T}}+\sqrt{e^{\frac{J}{k_BT}}\sinh^2\frac{g\mu_B B}{2kT}+e^{-\frac{J}{k_BT}}}\right)^N. \tag{8}$$

From Eq. (8), it can be calculated that the average magnetization is

$$M=\frac{KT}{N}\frac{\partial F}{\partial B}=\frac{g\mu_B}{2}\frac{e^{\frac{J}{2kT}}\sinh\frac{\mathrm{g}\mu_\mathrm{B}B}{2\mathrm{kT}}}{\sqrt{e^{\frac{J}{kT}}\sinh\frac{g\mu_B B}{2kT}+e^{-\frac{J}{kT}}}}. \tag{9}$$

For any temperature $T>0$, when $B=0$, $M=0$, which indicates that there is no spontaneous magnetization at finite temperature. Thus, there is no phase transition in the one-dimensional Ising model when there is no external magnetic field.

3. Monte Carlo Simulation

Monte Carlo method is a numerical simulation method which takes probability phenomena as research objects. It can estimate the unknown by obtaining statistical values through sampling surveys. In computational simulation, it can simulate the random characteristics of the system by constructing a probability model similar to the system performance and conducting random experiments on a computer. Though the improvement of accuracy consumed several times the computing power, compared with other methods, the efficiency of the Monte Carlo method increases with the increase of system complexity and can better solve statistical problems.

3.1. Importance Sampling

In the canonical ensemble, the probability of occurrence of quantum state μ_i can be written as

$$\rho_i=\frac{e^{-\beta E_i}}{\sum_i e^{-\beta E_i}}. \tag{10}$$

Here, β represents $1/k_BT$. When randomly selecting M samples, if uniform sampling is utilized, the expectation of any observable physical quantity $\langle Q\rangle$ can be expressed as

$$\langle Q\rangle=\frac{\sum_{i=1}^{M}Q_i\,e^{-\beta E_i}}{\sum_{i=1}^{M}e^{-\beta E_i}}. \tag{11}$$

However, in a Boltzmann system, ρ_i is proportional to $e^{-\beta E_i}$. Therefore, the probability of occurrence of particles in different quantum states varies greatly and uniform sampling obviously leads to errors. To solve this, importance sampling is needed. The method of determining the sampling density according to the importance of different samples is called importance sampling. Here if particles in quantum states μ_i are sampled with probability $P_i\propto e^{-\beta E_i}$, the expectation of any observable physical quantity can be modified to

$$\langle Q\rangle=\frac{\sum_{i=1}^{M}Q_i\,/e^{-\beta E_i}\cdot e^{-\beta E_i}}{\sum_{i=1}^{M}e^{-\beta E_i}/e^{-\beta E_i}}=\frac{\sum_{i=1}^{M}Q_i}{M}. \tag{12}$$

3.2. Markov Process

Knowing the sampling method, in an actual operation, how to design a mechanism to meet such sampling requirements needs to be considered. To accomplish this, Markov process can be introduced. In this process, every state μ_i is transformed from the previous state μ_j according to a certain prbability P_{ij}. What is needed is finding such P_{ij} which can made final state distribution function tend to the desired equilibrium distribution [5]

$$\rho_{eq(i)} = \frac{e^{-\beta E_i}}{\sum_i e^{-\beta E_i}} = P_i. \tag{13}$$

If Markov process is "good", which means that P_{ij} is constant and as long as there are enough steps, probability of the system transitioning to each state is determined, it needs to obey detailed balance

$$P_j P_{ji} = P_i P_{ij}. \tag{14}$$

According to Eq. (13), it can be rewritten as

$$\frac{P_{ij}}{P_{ji}} = \frac{P_j}{P_i} = e^{-\frac{\delta E}{k_B T}} \tag{15}$$

Where $\delta E = E_j - E_i$. Assume that the energy E_i of state μ_i is lower than E_j of state μ_j, naturally $P_{ji} = 1$, because it would lower the energy of the system and make the system more stable. According to, $P_{ij} = e^{-\frac{\delta E}{k_B T}}$. At this point, Metropolis criterion is introduced [6]

$$A(\delta E) = \begin{cases} 1 & \delta E \leq 0 \\ e^{-\beta \delta E} & \delta E \geq 0 \end{cases}. \tag{16}$$

3.3. Single-spin-flip Dynamics Algorithm

Single-spin-flip dynamics is a simple Markov process. A single step iteration of the process is as follows [7]:

Randomly pick a spin from the system.

Assuming the spin is flipped, calculate the increment of the energy δE of the system.

Use the Metropolis criterion $A(\delta E)$ to decide whether to actually perform this flip.

4. Tow-dimensional Ising Model

Two-dimensional Ising model is relatively more cumbersome to be solved analytically compared to one-dimensional Ising model. Thus, this paper uses Monte Carlo method mentioned above to simulate two-dimensional Ising model and study the phase transition.

4.1. Influence of finite scales

Fig. 2 show the results of Monte Carlo simulation of two-dimensional Ising model with different lattices and the coupling strength J is set to be the energy unit. The critical temperature can be calculated analytically to be [8]

$$T_C = \frac{2J}{ln1 + \sqrt{2}} \approx 2.269J = 2.269, \tag{17}$$

Where $J = 1$ is assumed. As is shown in the larger the lattice is, the closer the critical temperature get to 2.269 and the steeper the curve is around critical temperature, which means the simulation is more accurate. This is completely explainable because the simulation system gets closer to the real system with unmeasurable spins as the lattice gets larger.

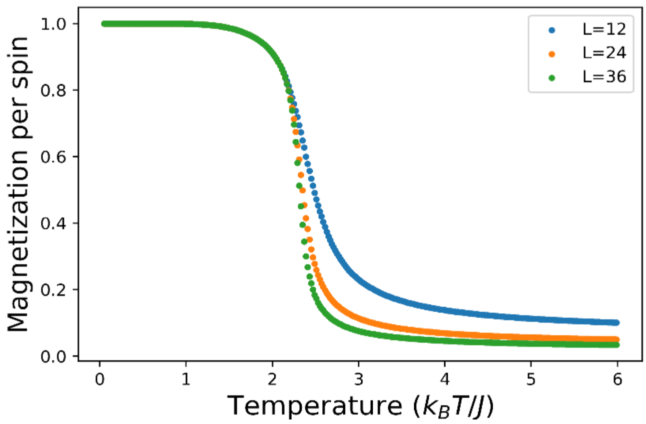


Fig. 2 Magnetization per spin of two-dimensional Ising model with different lattices

4.2. Influence of Different Magnetic Fields

Fig. 3 shows the results of Monte Carlo simulation of two-dimensional Ising model under different magnetic fields with 32×32 lattice points and coupling strength J set to 1. It is based on the simulation with 200000 steps of relaxation process and 800000 steps of steady state for each magnetic field.

As is shown in Fig. 3, the magnetic field has an obvious effect on the Ising model, which delays the phase transition temperature of the system. Because the external magnetic field makes the spins tend to be arranged in an orderly manner and the thermal motion makes the spins tend to be disordered, the larger the absolute value of the magnetic field, the higher the critical temperature of phase transition.

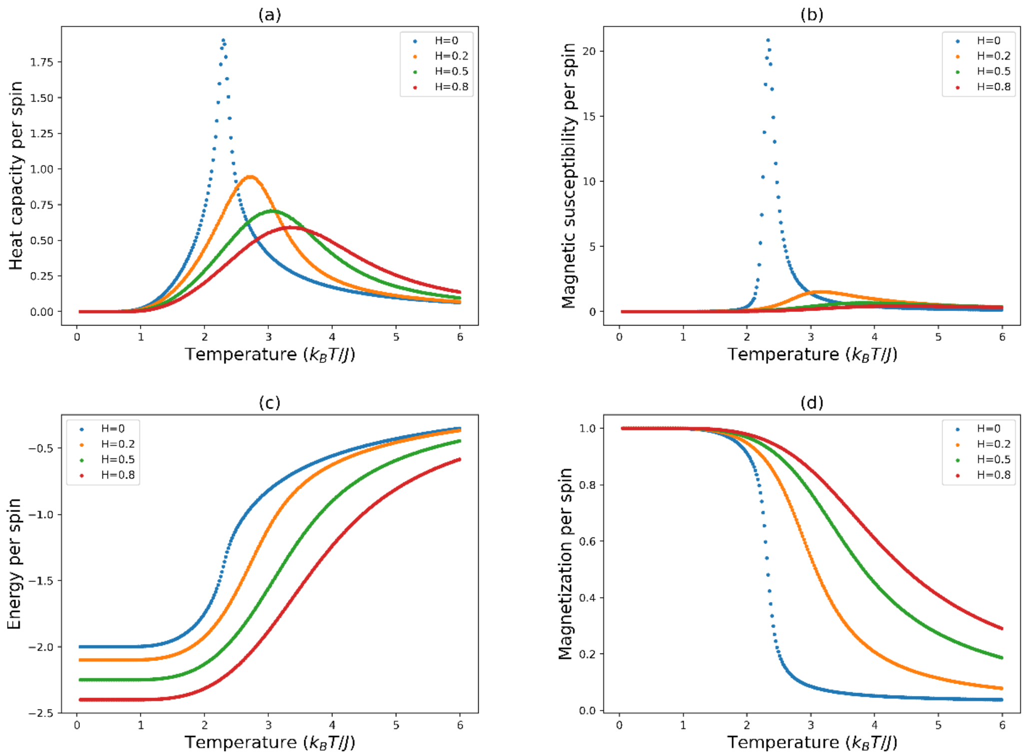


Fig. 3 Behaviours of thermodynamic quantities with temperature under different magnetic fields H. (a) Specific heat, (b) magnetic susceptibility, (c) Energy, and (d) Magnetization

4.3. Variations in Order Parameters

The calculation formulas of some order parameters are presented in Table 1 [9]. Here, the symbol $\langle \dots \rangle$ means the average value of the variables after multiple Monte Carlo iterations.

Table 1 Formulas to calculate several thermodynamic quantities.

Magnetization per spin	$m = \frac{M}{N} = \frac{1}{N}\sum_i \sigma_i$
Energy per spin	$E = -\sum_{\langle ij \rangle} \sigma_i \sigma_j - H \sum_i \sigma_i$
Heat capacity per spin	$C = \frac{1}{N k_B T^2}(\langle E^2 \rangle - \langle E \rangle^2)$
Magnetic susceptibility per spin	$\chi = \frac{1}{N k_B T}(\langle M^2 \rangle - \langle M \rangle^2)$

It can be seen in the Fig. 3 that, when the magnetic field is 0, all the system features listed change abruptly between temperature 2 and 3 ($k_B T/J$). As is known to all, these mutations and peaks imply that phase transition occurs around this temperature. Actually, there are some theoretical laws about order parameters around critical temperature under this situation

$$\mathrm{M} \sim (T_C - T)^{\beta}, \mathrm{C} \sim (T - T_C)^{-\alpha}, \chi \sim (T - T_C)^{-\gamma}, \tag{18}$$

Where α, β, γ are different critical exponents [10]. According to these formulas, the peak of heat capacity and magnetic susceptibility and the sharply decline of magnetization around critical temperature can be definitely explained.

4.4. The Critial Temperature

Because the exact critical temperature can hardly be obtained only by observing the simulation graph, so this paper just tries some methods to approximately read it out. The first method is directly extrapolating critical temperature from Fig. 2. By visually estimating when the magnetization per spin starts to decrease quickly, the critical temperature can be worked out and it's between 2.1-2.5.

The second method is that, in order to obtain relatively accurate critical temperature, (a) and (b) in Fig. 3 are chosen to estimate it by extracting the corresponding temperatures when the order parameters reach the maximum and viewing it approximately as critical temperature. The results are about 2.29 and 2.33.

The third one is more accurate. To obtain relatively precise critical temperature of infinite ferromagnetic system, results from Ising models of different sizes are needed for extrapolation. First, correlation length is introduced $\xi \sim |T - T_c|^{-\upsilon}$, where υ is the correlation length exponent. Then from (18) and (19), more derivation can be done: $\mathrm{M} \sim |T_c - T|^{\beta} \sim \xi^{-\frac{\beta}{\upsilon}}$. For actual infinite ferromagnetic system, $\xi \to \infty$ at critical temperature. But for finite Ising model, the largest length possible is the system size L. Therefore, the magnetization can be transformed to $\mathrm{M} \sim L^{-\frac{\beta}{\upsilon}}$, which can be transformed further $ML^{-\frac{\beta}{\upsilon}} = \mathrm{const}$. Thus, it can be derived that

$$\frac{\ln M(L_1)/M(L_2)}{\ln L_1/L_2} = -\frac{\beta}{\upsilon}. \tag{19}$$

From Eq. (19), relative exact critical temperature can be obtained because Ising models of different sizes need to obey this rule and intersect with each other at critical temperature. Hence, different combinations of L_1 and L_2 are plotted in Fig. 4 which is based on the simulation with 200000 steps of relaxation process and 800000 steps of steady state and critical temperature extrapolated from it is around 2.2695.

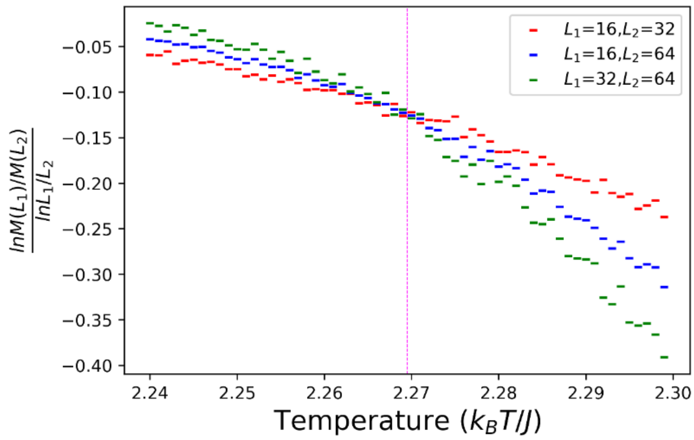


Fig. 4 Determination of critical temperature

The fourth one is to utilize Eq. (19) to perform curve fitting to data points. Fig. 5, which is based on the simulation with 100000 steps of relaxation process and 400000 steps of steady state, is the result of curve-fitting. Considering of the balance between computer arithmetic power and simulation of infinite scale system, this paper chooses 160×160 system. The critical temperature is around 2.273±0.001 and the critical index β is around 0.1377±0.0078, which are relatively close to the theoretical value 2.269 and 0.125.

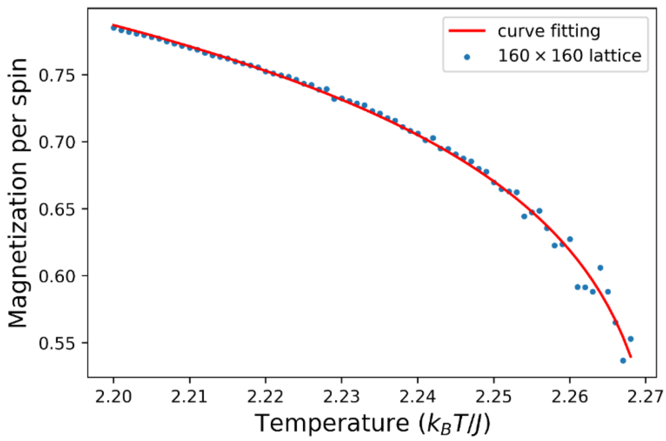


Fig. 5 Curve-fitting to determine parameters of phase transitions

5. Conclusion

This paper discusses Monte Carlo simulation and phase transition of two-dimensional Ising model after presenting the exact solution to one-dimensional Ising model and finding no phase transition when there is not external magnetic field. The influence of different scales of simulation systems on the simulation accuracy is involved and the magnetization, energy, heat capacity and magnetic susceptibility per spin are specifically studied under different magnetic fields, which successfully achieves the combination of Ising model and Monte Carlo method. This paper also explores different ways to obtain relatively accurate phase transition temperature (2.269 k_BT/J) based on simulation results, and verifies the practicality of Ising model and Monte Carlo method in solving problems about ferromagnetic phase transition. There are also some places for improvement. With more Monte Carlo steps, more accurate results can be worked out and many valuable problems are not discussed in this paper such as the coupling strength and 3D or higher dimensional Ising model. Some other methods like cluster-flip dynamics and Wolff algorithm may be more useful when simulating Ising model, which can optimize the low-efficiency of Metropolis algorithm near critical temperature.

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