The Monte Carlo Simulation of Ising Model

Abstract

Ising model is one of the most important models in the field of statistical mechanics. Despite its simplicity, it shows plenty of rich physics such as critical phenomena, and its relation to $\mathbb{Z}_2$ gauge theory. In this project, we use numerical Monte Carlo method, including the classical Metropolis and the so-called Worm algorithm to simulate the transverse field Ising model (TFI) in different spatial dimensions to reveal its critical behavior, such as its phase transition temperature, some critical exponents, as well as its critical dimension necessary to make the spontaeneous symmetry breaking possible.

1   Introduction

Ising model is one of the most fundamental model in statistical mechanics. The ferromagnetic transverse field Ising model hamiltonian is:

$$H = -J \sum_{\langle ij \rangle} \sigma_i^z \sigma_j^z - h \sum_i \sigma_i^x \tag{1}$$

where σ_i^α are the Pauli matrices representing the αth component of the spin-1/2 on site i, and $J > 0$. When $h = 0$, correspongding to the classical Ising model, the eigenstates of this hamiltonian are simply the direct product of the σ^z basis of all sites, and we can simply replace the Pauli matrices σ_i^z by their eigenvalues, which are either 1 or -1. When we turn on the transverse field h, quantum effects come in the story, since there will be fluctuations around the σ^z basis of the classical Ising model and basically the true eigenstates of the quantum Ising model with finite h will be an entangled state.

One of the main aspects that make Ising model so important in statistical mechanics is its thermodynamic fluctuation, especially its behavior near criticality. For simplicity, we let $h = 0$ and add a longitudinal field h_z in the discussion of thermodynaminc behavior, so the Hamiltonian becomes

$$H = -J \sum_{\langle ij \rangle} \sigma_i^z \sigma_j^z - h_z \sum_i \sigma_i^z \tag{2}$$

From statistical mechanics, we can easily write down its partition function, and use different methods to solve the problem (transfer matrix for dimension $d = 1$, mean field for $d > 1$, as well as various numerical methods). We take $d = 2$ as an example to see its critical behavior. At first it has a finite critical temperature between paramagnetic phase at higher temperature and ferromagnetic phase at lower temperature:

$$\sinh\left(\frac{2J}{T_c}\right) = 1 \tag{3}$$

$$T_c = \frac{2J}{\log(1 + \sqrt{2})} \tag{4}$$

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The phase transition corresponds to a $\mathbb{Z}_2$ symmetry breaking. Next we can get different physical quautities with respect to temperature: Magnetization:

$$M = \langle \sigma_i^z \rangle \sim (T_c - T)^{\frac{1}{8}} \tag{5}$$

Susceptibility:

$$\chi = \frac{\partial M}{\partial h_z} \sim (T - T_c)^{-\frac{7}{4}} \tag{6}$$

and so on.

In particular, the two-point correlation function $\Gamma(i-j) = \langle \sigma_i^z \sigma_j^z \rangle - \langle \sigma_i^z \rangle \langle \sigma_j^z \rangle$ behave differently at different temperature. When T is away from T_c, the correlation function decay exponentially:

$$\Gamma(i-j) \sim e^{\frac{|i-j|}{\xi(T)}} \tag{7}$$

with correlation length $\xi(T) \sim \frac{1}{|T-T_c|}$. As $T \to T_c$, the correlation length diverges, and the correlation function behaves like

$$\Gamma(i-j) \sim \frac{1}{|i-j|^{d-2+\eta}} \tag{8}$$

and the power-law decay remind us that the critical point of Ising model can be related to some conformal field theory. The critical exponents are listed as Fig. 1.

Exponent		Definition	Ising Value
α	C	$\propto (T - T_c)^{-\alpha}$	0
β	M	$\propto (T_c - T)^{\beta}$	1/8
γ	χ	$\propto (T - T_c)^{-\gamma}$	7/4
δ	M	$\propto h^{1/\delta}$	15
ν	ξ	$\propto (T - T_c)^{-\nu}$	1
η	$\Gamma(n)$	$\propto |n|^{2-d-\eta}$	1/4

Figure 1: Critical exponents of the Ising model.

2 Worm Algorithm

The Hamiltonian of quantum transverse-field Ising model can be written as

$$\mathcal{H} = -t \sum_{\langle ij \rangle} \sigma_i^x \sigma_j^x - h \sum_i \sigma_i^z = K + U. \tag{9}$$

And the interaction term K can be further expressed in terms of the raising and lowering operators as

$$K = K_1 + K_2 = -t \sum_{\langle ij \rangle} (\sigma_i^+ \sigma_j^- + \text{h.c.}) - t \sum_{\langle ij \rangle} (\sigma_i^+ \sigma_j^+ + \text{h.c.}). \tag{10}$$

Then with the Holstein-Primakoff transformation $b_i(b_i^\dagger) = \sigma_i^+(\sigma_i^-)$ and $n_i = b_i^\dagger b_i = (\sigma_i^z + 1)/2$, the QTFI model can be mapped onto a Bose-Hubbard (BH) model whose Hamiltonian is

$$\mathcal{H} = -t \sum_{\langle ij \rangle} (b_i^\dagger b_j + \text{h.c.}) - t \sum_{\langle ij \rangle} (b_i^\dagger b_j^\dagger + \text{h.c.}) - \mu \sum_i n_i, \tag{11}$$

where the chemical potential $\mu = 2h$. For this BH model, K_1 accounts for the hopping of a particle, and K_2 simultaneously creates or deletes a pair of nearest neighbouring (NN) particles.

We can use the imaginary-time path integral to represent the partion function:

$$\mathcal{Z} = \text{Tr}\left(e^{-\beta \mathcal{H}}\right) = \sum_{a_0} \langle \alpha_0 | e^{-\beta \mathcal{H}} | \alpha_0 \rangle \tag{12}$$

$$= \lim_{d\tau = \frac{\beta}{n}, n \to \infty} \sum_{\{\alpha_i\}} \langle \alpha_0 | e^{-\mathcal{H}d\tau} | \alpha_{n-1} \rangle \cdots \langle \alpha_i | e^{-\mathcal{H}d\tau} | \alpha_0 \rangle \tag{13}$$

$$= \sum_{\alpha_0} \sum_{\mathcal{N}}^{\infty} \int_0^\beta \int_{\tau_1}^\beta \cdots \int_{\tau_{\mathcal{N}-1}}^\beta \prod_{k=1}^{\mathcal{N}} d\tau_k \, F(t, h), \tag{14}$$

with the integrand function

$$F(t, h) = t^{\mathcal{N}_h + \mathcal{N}_p} e^{-\int_0^\beta U(\tau)\,d\tau}, \tag{15}$$

where $\mathcal{N}_h$ and $\mathcal{N}_p$ are the number of hopping and pairing kinks. So the partition function $\mathcal{Z}$ can be regarded as the summation of different configuration in the $(d+1)$D space-time, of which the statistical probability is

$$W_\mathcal{Z}(t, h) = \prod_{k=1}^{\mathcal{N}} d\tau \, F(t, h). \tag{16}$$

In this representation, each configuration can be viewed in the following way. For each lattice site i, the spin σ_i^z may be flipped by the hopping or pairing at some imaginary time τ_k. Since either hopping or pairing term simultaneously flips spins at two NN sites, so one can construct a loop by following the spin-up segments along the imaginary time, and kinks which labels the spin flips of two NN sites. Hence, a configuration can be indentified with several loops of spin-up in the $(d+1)$D space-time.

Then, we can extend the configuration space $\mathcal{Z}$ to $\mathcal{G}$ by including two defects, which corresponds to the spin-spin correlation function:

$$\mathcal{G}(\boldsymbol{x}_I, \tau_I; \boldsymbol{x}_M, \tau_M) = \text{Tr}\left[T_\tau \left(\sigma_I^x(\tau_I)\sigma_M^x(\tau_M)e^{-\beta \mathcal{H}}\right)\right], \tag{17}$$

where T_τ is the τ-ordering operator. In the configuration space $\mathcal{G}$, each configuration can be viewed as several loops and an open path with two ending points "Ira" (I) and "Masha" (M), which correspond to the two spins in the correlation function. Similarly, the statistical weight of the $\mathcal{G}$ configuration can be written as

$$W_\mathcal{G} = \frac{d\tau_I d\tau_M}{\omega_\mathcal{G}} \prod_{k=1}^{\mathcal{N}} d\tau_k \, F(th), \tag{18}$$

here $\omega_\mathcal{G}$ is an arbitary positive number. And when I coincides with M, the open path forms a loop, the configuration in the $\mathcal{G}$ space turns into one in the $\mathcal{Z}$ space.

The key idea of the worm algorithm is to move the defects I and M of the open path (like a worm wriggling) to produce different $\mathcal{G}$ and $\mathcal{Z}$ configurations for sampling. For ergodicity, the simulation should be able to change the number of kinks, the space-time location of kinks, and that of the defects I and M. So we perform the following three kinds of updates:

1. *Create/annihilate defects I and M.* If the current configuration is in the $\mathcal{Z}$ space, then "creating defects" is the only possible update. We randomly picks up a point (x_I, τ_I) in the whole space-time, draws a uniformly distributed time displacement $\delta \in [-\tau_a/2, \tau/2]$ and $\delta \neq 0$, assigns $x_M = x_I$ and $\tau_M = \text{mod}(\tau_I + \delta, \beta)$, and flips the spin state between I and M.

   The reverse operation of "creating defects" is "annihilating defects", which is chosen with an *a priori* probability $\mathcal{A}_a$ in the $\mathcal{G}$ space. By annihilating defects I and M and flipping the spin state inbetween, a $\mathcal{G}$ configuration are changed into a $\mathcal{Z}$ configuration. The annihilation is possible only if I and M are on the same world line $x_I = x_M$ and their imaginary-time displacement $\min\{|\tau_I - \tau_M|, \beta - |\tau_I - \tau_M|\} \leq \tau_a/2$.

   The detailed-balance condition of creating and annihilating defects reads as

   $$\frac{\mathrm{d}\tau_I}{\beta N} \frac{\mathrm{d}\tau_M}{\tau_a} \cdot W_{\mathcal{Z}} \cdot \mathcal{P}_{\text{crea}} = \mathcal{A}_a \cdot W_{\mathcal{G}} \cdot \mathcal{P}_{\text{anni}}, \tag{19}$$

   which leads to the acceptance probabilities

   $$P_{\text{crea}} = \min\left[1, \mathcal{A}_a \tau_a \frac{\beta N}{\omega_G} \frac{F_{\text{new}}}{F_{\text{old}}}\right], \tag{20}$$

   $$P_{\text{anni}} = \min\left[1, \frac{1}{\mathcal{A}_a \tau_a} \frac{\omega_G}{\beta N} \frac{F_{\text{new}}}{F_{\text{old}}}\right], \tag{21}$$

   where F_{old} and F_{new} are given by Eq. 15. And here we choose $\omega = \beta N$ to make the calculation simpler.

2. *Move imaginary time of defect M.* This kind of update is chosen with a probability $\mathcal{A}_b$ in the $\mathcal{G}$ space. We randomly select a imaginary-time displacement $\delta \in [-\tau_b/2, \tau_b/2]$ and $\delta \neq 0$, assigns $\tau_M' = \text{mod}(\tau_M + \delta, \beta)$ for the new temporal location of defect M, and flips the spin states inbetween. The acceptance probability is

   $$P_{\text{move}} = \min\left\{1, \frac{F_{\text{new}}}{F_{\text{old}}}\right\}. \tag{22}$$

3. *Insert/delete a kink.* Each operation is chosen with a probability $\mathcal{A}_c$ in the $\mathcal{G}$ space. When "inserting a knik", we randomly choose one of the $z_d = 2d$ neighbouring world lines of x_M, denote it as x_M', and updates the location of M from (x_M, τ_M) to (x_M', τ_M). Meanwhile, we insert a kink k between world lines x_M and x_M' at imaginary time $\tau_k = \text{mod}(\tau_M + \delta, \beta)$, with a random displacement $\delta \in [-\tau_c/2, \tau_c/2]$ and $\delta \neq 0$. Further, the spin states between τ_M and τ_k, on both x_M and x_M', are flipped.

   In the reverse operation, "deleting a kink", we also pick up a random neighbouring world line x_M' of x_M and moves M from (x_M, τ_M) to (x_M', τ_M). If there is no kink that connects world lines x_M and x_M' in the imaginary-time domain $[\tau_M - \tau_c/2, \tau_M + \tau_c/2]$, the operation is rejected. Otherwise, we randomly

pick up one of those n_k in this region and delete it, and meanwhile flip the spin states on both world lines between τ_M and the imaginary time of the deleted kink. The detailed balance conditon of this pair of operations is

$$\mathcal{A}_c \cdot \frac{1}{z_d} \cdot \frac{d\tau}{\tau_c} \cdot W \cdot \mathcal{P}_{\text{inse}} = \mathcal{A}_c \cdot \frac{1}{z_d} \cdot \frac{1}{n_k} \cdot W_+ \cdot \mathcal{P}_{\text{dele}}, \qquad (23)$$

which leads to the acceptance probabilities

$$P_{\text{inse}} = \min\left[1, \frac{\tau_c}{n_k + 1} \frac{F_{\text{new}}}{F_{\text{old}}}\right], \qquad (24)$$

$$P_{\text{dele}} = \min\left[1, \frac{n_k}{\tau_c} \frac{F_{\text{new}}}{F_{\text{old}}}\right]. \qquad (25)$$

The worm algorithm can be concluded as Algorithm. 1, in which *a priori* probabilities satisfy $\mathcal{A}_a + \mathcal{A}_b + 2\mathcal{A}_c = 1$.

Algorithm 1 Worm algorithm

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initialization;
thermalization;
loop
    if it is a $\mathcal{Z}$ configuration **then**
        compute statistical quantities of this configuration;
        choose the "creating defects (I, M)" operation;
    else
        choose an operation with its *a priori* probability; except "creating defects (I, M)";
    end if
    calculate the acceptance probability P and carry out the operation with the probability P;
end loop

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3 Numerical Results