Contents

Notes On Ising Model

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1 Abstract

The Ising Model, developed by Dr. Ernst Ising, is a mathematical model of ferromagnetism in statistical physics. Dr. Ernst Ising gave the analytical solution in one dimension. The result shows the phase trasition point is at $T = 0$. While people believed that here is no phase transition point in two dimensions, the result given by Dr. Onsager showed phase transition point exists indeedly. After that, other methods were developed like mean-field theory, renormalization group and so on. They all indicate two-dimension Ising Model has phase transition. In this article, I will introduce these thoeries and perform some numerical methods such as Metropolis algorithm and cluster algorithm.

2 Ising Model

In Ising Model, each atom can adopt two states, corresponding to $S = \{-1, 1\}$ where S represents the spin. The spin interaction are dependent of the coupling parameter J_{ij} between the adjacent atoms. For the sake of simplification, I set $J_{ij} = J$, which indicate the system is isotropic. As a result, the Hamiltonian of ferromagnetic Ising Model is:

$$H = -J \sum_{<ij>} S_i S_j, \tag{1}$$

where $J > 0$ and $S_i \in \{1, -1\}$.

The partition function is given by:

$$\mathcal{Z} = \sum_i \exp\{-\beta E_i\} = \sum_{S_0} \sum_{S_1} \dots \sum_{S_N} \exp\{-\beta H\}, \tag{2}$$

in the canonical ensemble, free energy can be written as:

$$\mathcal{F} = -kTln(\mathcal{Z}). \tag{3}$$

At the same time, energy has the form:

$$U = \frac{Tr(exp\{-\beta H\})}{\mathcal{Z}}, \tag{4}$$

As a result, heat capacity is:

$$C_v = \frac{\partial U}{\partial T} = \frac{\overline{E^2} - \overline{E}^2}{kT^2}, \tag{5}$$

Similarly, magnetic susceptibility can be obtained.

$$\kappa = \frac{\partial M}{\partial B} = \frac{\overline{M^2} - \overline{M}^2}{kT}. \tag{6}$$

As above, Ising Model is described briefly. Next, I will introduce some analytical methods.

3 Mean Field Theory

3.1 Bragg-Williams Approximation

The main idea of this approximation is to ignore the correlation between the different spins. As a result, the hamiltonian could be simplified:

$$\mathcal{H} = -J \sum_i S_i * (\sum_j{}' S_j) = -Jq\overline{S} \sum_i S_i, \tag{7}$$

where the $\sum_i'$ represents sum over the spins near the ith spin. Then, a self-consistent equation could be obtained.

$$\overline{S} = \frac{\sum_{\{S_i\}} S_1 exp\{\beta Jq\overline{S} \sum_i S_i\}}{\sum_{\{S_i\}} exp\{\beta Jq\overline{S} \sum_i S_i\}} = tanh(\beta Jq\overline{S}). \tag{8}$$

It's convenient to get the solution by using iterative method.

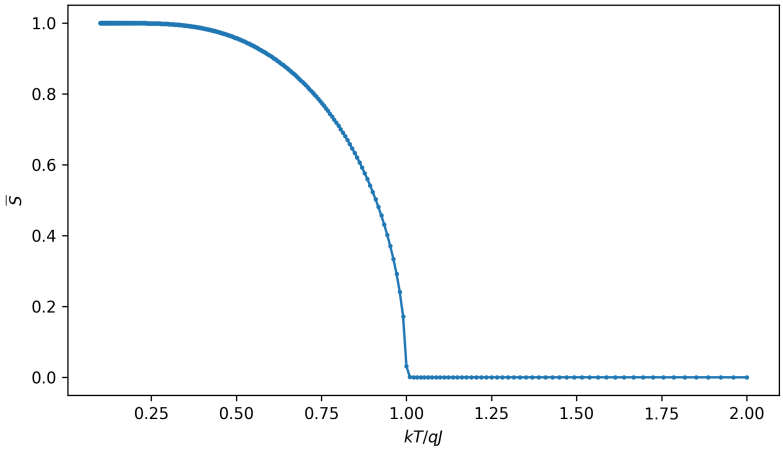


Figure 1: solutions for different T

It's easy to make a conclusion that the phase transition point is $\frac{kT}{qJ} = 1$, that is, when $q = 4, J = 1$, $kT_c = 4$. The stric solution is about $kT_c = 2.269J$, so Bragg-Williams method is a rough approximation.

3.2 Bethe-Peierls Approximation

The main idea of this method is to ignore the correlations between three different spins or more. As a result, the hamitonian could be simplified as:

$$\mathcal{H}_0 = -J\sum_{j=1}^{q} S_0 S_j - \mu B \sum_{j=1}^{q} S_j, \tag{9}$$

where B is the parameter which represents the mean field. Let $\alpha = \frac{\mu B}{kT}, \gamma = \frac{J}{kT}$. It's not hard to get the self-consistent equation:

$$\alpha = \frac{q-1}{2} ln(\frac{cosh(\alpha+\gamma)}{cosh(\alpha-\gamma)}). \tag{10}$$

With the same method mentioned in Sec3.1, the average of S is as follows.

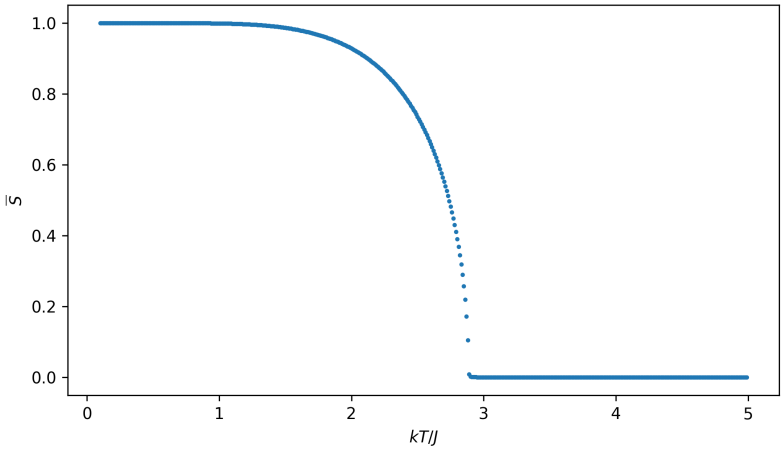


Figure 2: solutions for different T

It's also easy to confirm that the phase transition point is about $\frac{kT}{J} = 2.88$ for $q = 4$. That is, when $J = 1$, $kT_c = 2.88$, which performs better than Bragg-Williams approximation.

4 Metropolis Algorithm

4.1 Algorithm Details

1.Locally trail move the current conformation.
2.Calculate the energy change caused by the trial move, dE.
3.If dE is negative, the trial move is allowed; Else allowed the trial move but with a probability $exp(-dE/kT)$. Whether the trial move is allowed or not, a new conformation is thought to be generate.
4.Repeat 1,2,3 enough steps.

4.2 Results

4.2.1 Random Engine

The first thing of implementing this algorithm is to choose a suitable random engine. With trying a lot of times, I find the random function in random.h which is a library of Cpp is not as good as I imagine. The main reason is that the biggest random number generated is about 60000. Because the random float number is generated by n(integer numer generated by random function)$/N$(the biggest number generated by random function), the precision is $1/N$ which is not enough. As a result, I choose a more powerful random engine, which is, mt19937.

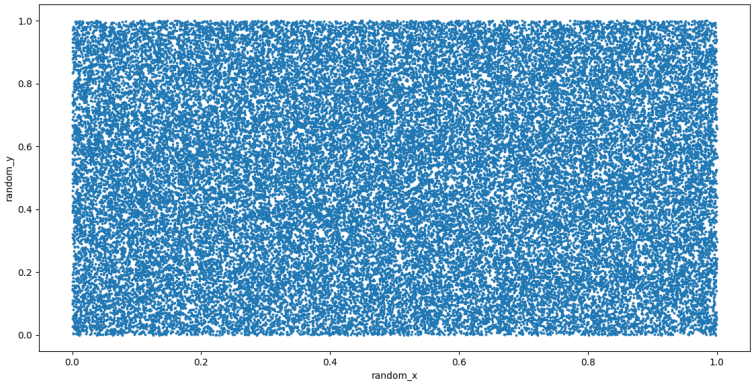
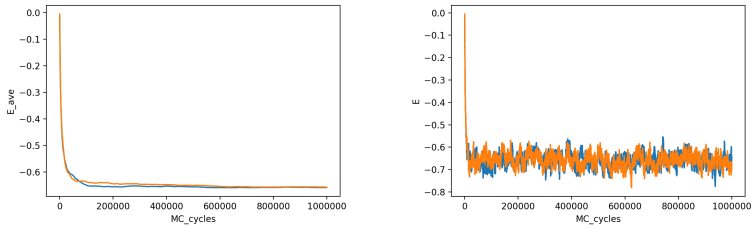


Figure 3: random numbers generated by mt19937

From the Fig.3, mt19937 performs well.

4.2.2 Mente Carlo Cycles

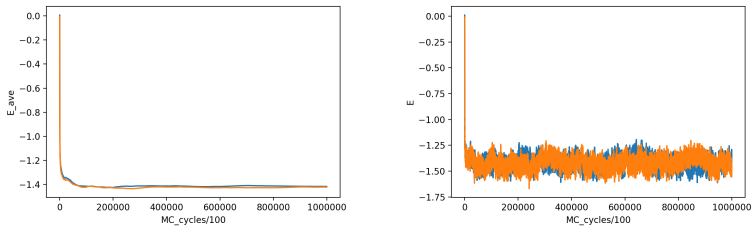
It would be interesting to investigate how the algorithm behaves with the number of Mente Carlo cycles inceasing.



(a) pic1.energy average (b) pic2.energy

Figure 4: Energy's dynamic change for two different configurations at $kT = 3.5$

From the figures above, at $kT = 3.5$, two different configurations performs well. They both converges quickly, so the chain number could be reduced appropriatly. But things will be different when near the phase transition point, that is, $kT_c = 2.269$.



(a) pic1.energy average (b) pic2.energy

Figure 5: Energy's dynamic change for two different configurations at $kT = 2.27$

As a result, it needs a longer Mente cycles to achieve an equilibrium at T_c. So I set 10^6 cycles when far from T_c and 10^8 cycles when near T_c.

Moreover, the accept rate increases with temperature incresing, which indicates that higher temperature means more states the sysytem can have.

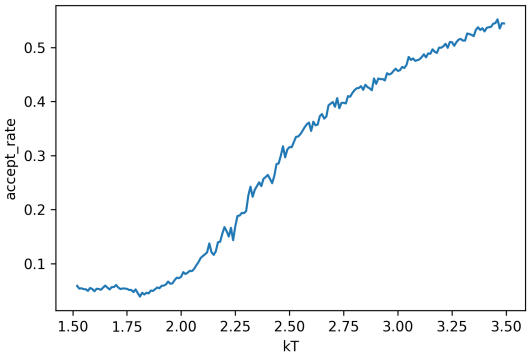
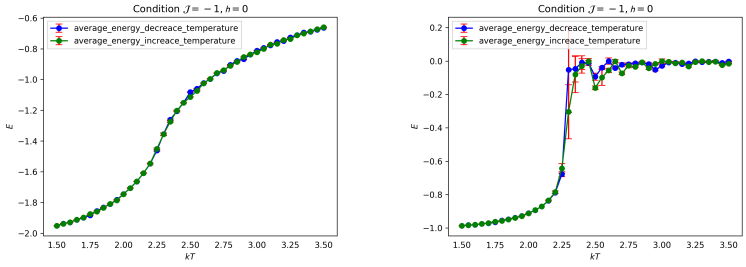


Figure 6: accept rate versus T

4.2.3 Numerical Results



(a) pic1.Average Energy at different T (b) pic2.Average Magnet at different T

Figure 7: Energy and magnet versus kT