Determining the critical temperature of Ferromagnetism by using Monte Carlo Algorithm

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Abstract——**Ferromagnetic phase transition occurs from disorder phase state(no net magnetisation) to order state(non-zero magnetisation) at critical temperature (Curie temperature). However, it is extremely difficult to determine the critical temperature theoretically, and even impossible for real materials. Approximations such as mean field theory provide reasonable answers, but they are not accurate enough. Thus, it is proper to use stochastic process like Monte Carlo simulation to tackle the problem. In this project, Marcov chain is used to generate samples representative of the system, and physical quantities of the system are extracted from samples. Robbins-Monro algorithm is applied to find the critical temperate automatically. This paper checks the consistency between Monte Carlo simulation and theoretical result for two-dimensional Ising model, determines the critical temperature of system with more complex structure and coupling strength automatically, and further explores the relation between critical temperature of ferromagnetism and the structure of the materials.**

I. Introduction

One of the most important property of ferromagnetism is that it only has magnetization without external magnetic field below critical temperature. Above the critical temperature, spins are randomized, and the collective behavior of system presents no magnetization. At critical temperature, the balance between minimizing energy and maximizing entropy is achieved, and the system shows critical behavior such as divergent susceptibility and infinite correlation length. This condition can be stricter for some applications of ferromagnetism than others, so it is important to find the critical temperature of different materials.
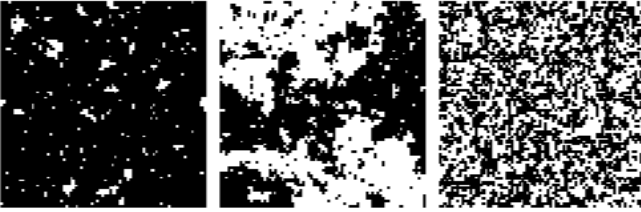

Figure 1: Configurations of system below Curie temperature, at Curie temperature and above Curie temperature (from left to right)

Analytically, the critical temperature of 2D Ising model is solved by Lars Onsager in1944. However, real materials have far more complicated structures and are difficult to solve theoretically. Even though other analytic method like mean field theory provides a sensible solution ignoring the fluctuation of the spins, Monte Carlo simulation achieves more accurate result.

In this project, simulation of 2D Ising model by Monte Carlo method is performed. Robbins-Monro algorithm is utilized to locate the critical temperature accurately and accuracy of the simulation is examined by comparison to the theoretical result. Then the same algorithm is applied for Heisenberg model with other structures and various coupling coefficient. Further improvements of the simulation are also discussed.

II. Theory

The Hamiltonian of the ferromagnetism without external magnetic field is given by

$$H = -\sum_{<i,j>} J_{ij}\sigma_i\sigma_j \, , \qquad eq(1)$$

where J is the coupling coefficient for each bond, σ is the value of spin, and the sum is over all neighbors in the system. For ferromagnetism, J is always positive. The partition function of the system, in this way, cam be shown as

$$Z = \sum_{\{\sigma\}} e^{-\frac{H_{\{\sigma\}}}{k_bT}} \, , \qquad eq(2)$$

where the sum is over all possible configurations. As the system size increases, the number of possible configurations increases exponentially. Simple traversal fails to calculate partition function efficiently even for the most modern computer. Therefore, stochastic process is a proper approach to the problem.

A. Monte Carlo Method

The idea of Monte Carlo algorithm is to repeat random sampling representative of the behavior of the system and then extract physical quantities from the samples. In this way, the expectation value of magnetization can be expressed as

$$< \text{m} > = \frac{1}{Z}\sum_i m_i e^{-\frac{H_i}{k_bT}} \, , \qquad eq(3)$$

where the sum is over samples and m_i is the magnetization of sample i. Nonetheless, the weight of each sample is different. Configurations with large Hamiltonian almost don't contribute to the result, which reduces computing efficiency. To maximize computational efficiency, the desirable distribution of samples is also Boltzmann distribution, which cancels the weight factor, making each sample equally important. In this way, the expectation value of magnetization is simply the arithmetic mean of the samples.

$$< \text{m} > = \frac{1}{N}\sum_{i=1}^N m_i \, . \qquad eq(4)$$

B. Marcov Chain

It can be proved mathematically that if the transition matrix (the probability from previous sample to next sample) satisfies ergodicity, normalization and detailed balance equation shown below,

$$w^{(c_l)(c_k)}e^{-\frac{E_{c_k}}{k_bT}} = w^{(c_k)(c_l)}e^{-\frac{E_{c_l}}{k_bT}} \quad , \qquad eq(5)$$

the distribution of generated samples will obey Boltzmann distribution. In equation 5, $w^{(c_l)(c_k)}$ is the transition matrix from configuration c_k to configuration c_l. One of the simplest choices of transition matrix in statistical mechanics is Metropolis method, where

$$w^{(c_l)(c_k)} = e^{\frac{E_{c_l}-E_{c_k}}{k_bT}}$$
$$w^{(c_k)(c_l)} = 1$$

for $E_{c_l} > E_{c_k}$.

C. Robbins-Monro Algorithm

Due to the finite size effect, order parameter itself (magnetization) cannot locate the critical temperature accurately. Instead, binder cumulant, which is universal at critical temperature independent of system size, can be used to determine the critical temperature with much greater accuracy. Therefore, Robbins-Monro algorithm is applied to find the intersection of binder cumulant of different system sizes.
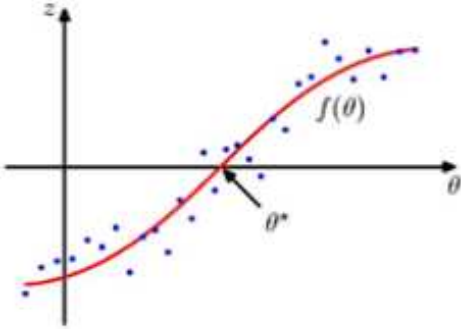

Figure 2: Using Robbins-Monro algorithm to find zero of the function with statistical noises

The updating equation to find zero of the function is shown below,

$$\theta^{(n+1)} = \theta^{(n)} - \frac{\alpha}{n}f(\theta^{(n)}) \qquad , \qquad eq(6)$$

where α is the feedback parameter that determines how quickly the result updates itself. The denominator n guarantees that θ will converge to the zero of the function. The prerequisite condition is that the function is monotonically increasing.

III. METHODS

The main algorithm of this project is MCMC(Monte Carlo Marcov Chain). After we use it to generate series of samples according to Boltzmann distribution, we can extract physical quantities such as magnetization, energy, structure factor and correlation length. Binder cumulant is used specifically to locate the critical temperature.

The first model implemented is two dimensional Ising model, which is compared with theoretical value to validate the simulation. Then we extend it to three-dimensional Heisenberg model and implement it on real material like Fe with body-centered structure, which is obtained by defining the structure of unit cell and then spanning it to the desired system size. As there are many types of bonds in Fe, we increase the threshold for coupling coefficient from 300K to 20K step by step to approach the real material.

IV. RESULTS AND ANALYSIS

In this section, the critical temperature of two-dimensional Ising model calculated by simulation is presented. Face-centered cubic(fcc) and Body-centered cubic(bcc) are also examined with comparison to simple cubic structure. Then different types of bond in the system are incorporated in the model and applied to real material Fe. The disadvantage of Robbins-Monro algorithm and further possible improvements of the simulation are also mentioned.

Based on the theoretical result given by Lars Onsager, the critical temperature for 2D Ising model is 2.269. After 50 Robbins-Monro steps (50000 Monte Carlo steps in each Robbins-Monro step), the critical temperature converges closely to 2.269 as shown below.
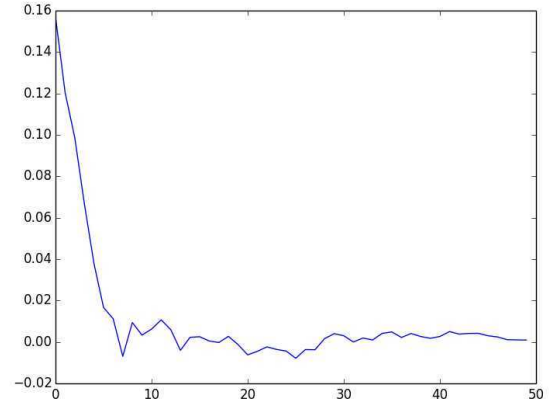

Figure 3: Difference with theoretical value vs. Robbins-Monro steps for 2D Ising Model

As the initial condition for Robbins-Monro algorithm changes arbitrarily, the error is within 0.003. However, the accuracy can be hardly improved by further increasing the Robbins-Monro steps.
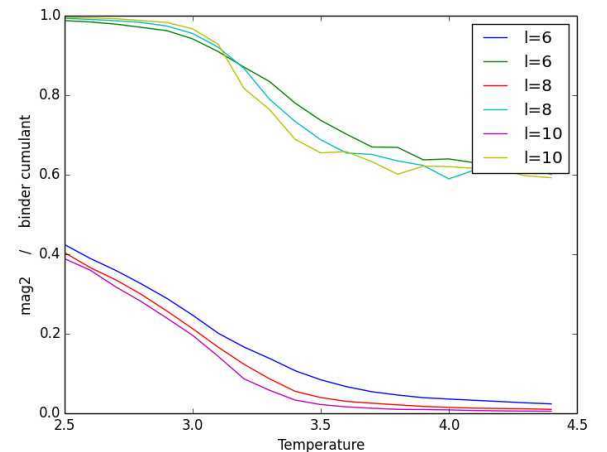

Figure 4: FCC Heisenberg model for different system sizes

Then the same algorithm is applied on fcc Heisenberg model. Magnetization squared and binder cumulant are presented in figure 4 to provide qualitative information. In Heisenberg model, spin can take value on the unit sphere instead of ±1. Now the limit of binder cumulant is 0.6 instead of 1/3 at high temperature, as shown in the figure above. It can be observed that the system size has substantial effect on the order parameter, but binder cumulant has a universal value about 0.88 at critical temperature, which even can be used for other structures like BCC as well.

Using unbiased binder cumulant estimator (detail in reference) can help reduce the Monte Carlo steps in each Robbins-Monro step but make it more difficult to find the proper feedback parameter for Robbins-Monro method to converge. The problem arises when we hope to find the zero of the function $0.88*< m^2 >^2 -< m^4 >$. Apart from the solution at critical temperature, the function is also almost zero, as shown in figure 5, above critical temperature as a trivial solution (both $< m^2 >^2$ and $< m^4 >$ are close to zero). The asymmetry of the function on left and right side of the zero makes it particularly difficult to choose initial value and feedback parameter. A too small feedback parameter will make result stuck at the trivial solution at high temperature while a too large feedback parameter can make result skip over the ideal solution.

As a result, we first use mean field theory to obtain an approximate value for critical temperature, and then plot the estimator to find the correct order of feedback parameter for Robbins-Monro method to converge to the desirable result.
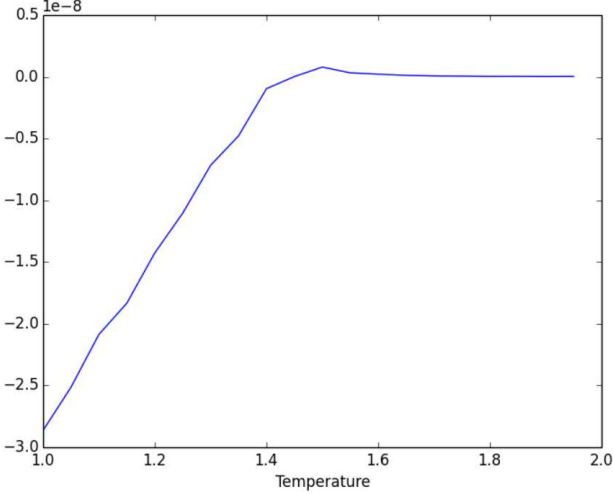
Figure 5: estimator $0.88*< m^2 >^2 -< m^4 >$ vs temperature for three-dimensional simple cubic lattice Heisenberg model

Furthermore, derived from first principle calculation, 40 different types of bond for Fe are incorporated in the model to determine its critical temperature. Considering 40 nearest neighbors (coupling coefficient ranging from 324 to -0.15) for each site in the system will dramatically increase the complexity of the computation, so thresholds of 300, 100, 40, 20 are set to ignore the trivial coupling effect first. Also, Monte Carlo steps are reduced to 1/10 of the original steps. The statistical error does not affect much as the scale of the temperature also increases compared to the model without real coupling constant.
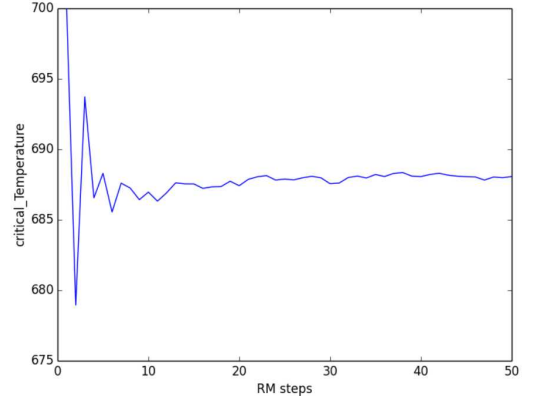
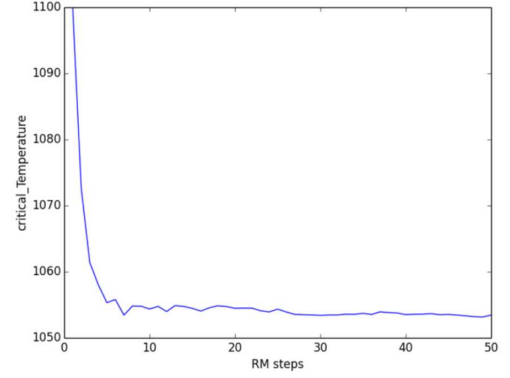Figure 6: BCC Fe with threshold 300
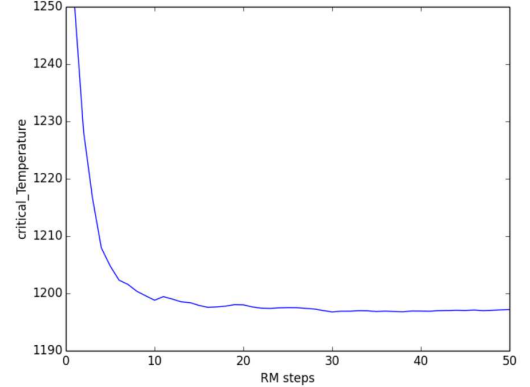
Figure 7: BCC Fe with threshold 100
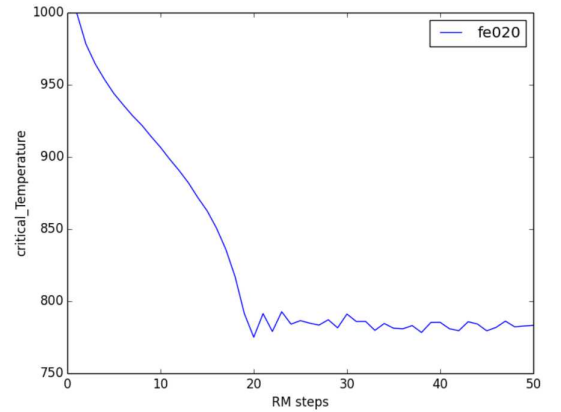
Figure 8: BCC Fe with threshold 40

Figure 9 : BCC Fe with threshold 20

As shown above, as more coupling intereactions in Fe are counted, the crticial temperature increases genereally. However, for coupling constant below 40, there are also negative coupling coefficient in Fe, which represents

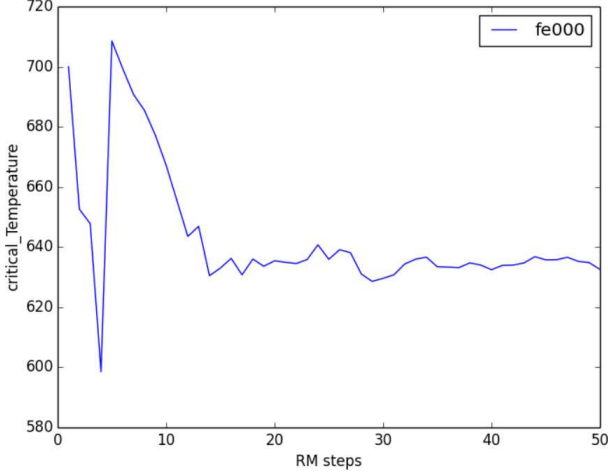antiferromagnetic behavior. The convergent behavior is thus different and the critical temperature decreases.

Figure 10: BCC Fe including all coupling interaction

Figure above considers the full description of atom strucute in Fe. It is still possible to further converge the result by increasing Robbins-Monro steps, but the complexity of the algorithm becomes too demanding.

	MFT	MCMC
Fe 300	893	688
Fe 100	1308	1053
Fe 040	1420	1197
Fe 020	1088	782
Fe 000	1060	632

Table 1: Cirtical temperature calculated by mean field theory(MFT) and Monte Carlo Markov Chain(MCMC)

By comparison with MCMC simulation, mean field theory generally overestimates the value of critical temperature by extra 30%. This error is even enlarged when negative(antiferromagnetic) coupling interactions are taken into account. This may also be caused by the statistical error of MCMC simulation as the Monte Carlo steps are reduced due to the complexity of the problem.

Further Possible Improvements

To further increase the computational efficiency, we can probably implement cluster algorithm instead of Metropolis algorithm used in this project, which can effectively reduce the critical slowing down near the critical point. In this way, Robbins-Monro steps can also be increased.

Machine learning based on artificial neural network can be applied to predict the critical temperature of ferromagnetism given the lattice Hamiltonian. Exploration of new material with different structures can be realized.

V. CONCLUSION

In this project, we use MCMC(Monte Carlo Markov chain) simulation to determine the critical temperature of ferromagnetism. Particularly, Metropolis algorithm is used to generate random sampling and Robbins-Monro algorithm is used to locate the intersection of binder cumulant of different system sizes. The result of two-dimensional Ising model is very consistent with the theoretical result. The application on

body-center cubic Fe is implemented step by step according to different threshold of coupling coefficient, and the result is compared with the estimation of mean field theory. The trend of simulation is consistent while the value of mean field theory generally is above that of simulation by 30%. It is possible to further increase the computational efficiency of simulation by implementing cluster algorithm. Machine learning can also be used to predict critical temperature of ferromagnetism given the lattice Hamiltonian.

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