2-D Ising Model with MMC Method

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Abstract: Ising model and Monte Carlo method are introduced briefly in this paper. The way of applying Metropolis Monte Carlo (MMC) method to a two dimensional Ising model is discussed in detail. The way of computing several thermodynamic quantities is compared with Wang-Landau method.

Key words: Ising model, Monte Carlo method, statistical mechanics, phase transition.

1. Introduction

The Ising model, named after the physicist Ernst Ising, is a mathematical model of ferromagnetism in statistical mechanics. The model consists of discrete variables that represent magnetic dipole moments of atomic spins that can be in one of two states (+1 or −1). The spins are arranged in a graph, usually a lattice, allowing each spin to interact with its neighbors. The model allows the identification of phase transitions, as a simplified model of reality. The two-dimensional square-lattice Ising model is one of the simplest statistical models to show a phase transition.

A key ingredient in the theory of magnetism is the electron's spin and the associated magnetic moment. Magnetism is an inherently quantum phenomena. It is interesting that Niels Bohr made a seminal contribution to the field of magnetism. Ferromagnetism arises when a collection of such spins conspire so that all of their magnetic moments point in the same direction, yielding a total moment that is macroscopic in size. A central issue in the study of ferromagnetism is to understand how the interactions between spins gives rise to this overall

alignment. Since we also know that systems generally lose their magnetism at high temperatures, we would also like to understand why and how the magnetic properties depend on temperature.

2. Theoretical consideration [1]

The model of a ferromagnet that will be considered is shown in Fig 1. It consists of a collection of magnetic moments, which we denote by arrows and which we can think of as being atoms with spin =1/2 magnetic moments.

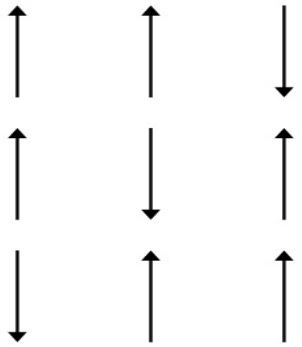


Figure 1: (3x3 Lattice)

For simplicity we assume these spins are situated on a regular lattice. Since spin is a quantum mechanical phenomena, this is in a sense a quantum model. A fully quantum mechanical treatment of the model would require that we include all of the quantum rules for dealing with spin angular momentum. Again for simplicity, a few simplifications are taken, yet, we still capture the essential physics of magnetism.

In this model, the simplest case is that each spin is able to point along either +z or –z direction. No other orientation is permitted. Hence, the *i*th spin in the system with orientation up or down can be denoted as $s_i = \pm 1$(or $\pm$½ if you like). Each of these spins interacts with other spins in the lattice; in a ferromagnet this interaction will favor parallel alignment of pairs of spins. In a real magnetic material, the interaction will be largest between spins that are nearest

neighbors and fall off rapidly with increasing separation between the spins. So the energy of this kind of system attributes to the exchanging energy between the nearest neighbors, i.e. the energy of the system is

$$E = -J \sum_{<i,j>} s_i s_j \tag{1}$$

where the sum is over all pairs of the nearest neighbor spins <*ij*>, and *J* is an exchange constant, which should be positive here in a ferromagnetic system. It is useful to imagine that the spin system is in a particular state, corresponding to a particular arrangement of the individual spins. Equation (1) is the total energy of the particular state of the entire system.

For canonical ensemble, or to say a system in equilibrium with a heat bath, the probability of finding the system in any particular state is proportional to the Boltzmann factor

$$P_\alpha = \frac{e^{-\frac{E_\alpha}{k_B T}}}{\sum_\alpha e^{-\frac{E_\alpha}{k_B T}}} \tag{2}$$

where E_α is the energy of state α as calculated from Eq.(1), k_B is the Boltzmann's constant, and P_α is the possibility of finding the system in state α. Each of these states which is called a microstate of the system is a particular configuration of spins. For example, if we have N Ising spins, there will be 2^N different possible microstates, thus a tremendously large number.

3. Thermodynamic quantities

Individual spins flip from +1 to −1 or vice versa when they gain energy from or loose energy to the heat bath the system in contact with. Once we get the probabilities P_α of finding the system in its various microstates, various macroscopic quantities readily to get. the magnetic moment of the system is

$$M = \sum_\alpha M_\alpha P_\alpha \tag{3}$$

where $M_\alpha = \sum s_j$. After getting the energy of the system as a function of temperature T using Eq. (1), we can easily calculate the heat capacity C of this system with finite differential method (i.e. FDM)

$$C = \frac{\Delta E}{\Delta T} \tag{4}$$

Also, the trick to calculate Helmholtz free energy is shown as following. From the first principle of thermodynamics, $dE = dQ + dW = dQ$. For quasi-static process, $\Delta S = S_b - S_a = \int_a^b \frac{dQ}{T}$, where S denotes the entropy of the system of a certain state. Thus,

$$S(\infty) - S(T) = \int_T^\infty \frac{dE}{T'} = \frac{E(T')}{T'}\bigg|_T^\infty + \int_T^\infty \frac{E(T')}{T'^2} dT'$$

noting that $\lim_{T\to\infty} \frac{E}{T} = 0$, so we have

$$S(T) = S(\infty) + \frac{E(T)}{T} - \int_T^\infty \frac{E(T')}{T'^2} dT' \tag{5}$$

4. Monte Carlo algorithm

According to statistical mechanics, the role of a heat bath is to exchange energy with the spin system and thereby bring it into equilibrium at some temperature T. As the system gains energy from, or loose energy to, the heat bath, spins are flipped, causing the system to move to new microscopic states. Monte Carlo method uses a stochastic approach to simulate the exchange of energy between the spin system and the heat bath. We can first choose a spin in the system, or easy to say in the lattice, then make it flip, and the energy E_{flip}, is calculated using Eq. (1). If E_{flip} is negative which means this flip lowers the total energy of the system, this spin is correctly flipped. Otherwise, we compare the Boltzmann factor $e^{-\frac{E_{flip}}{k_B T}}$ with a random number generated by computer. If this Boltzmann factor is larger than the random number, the spin flip is

correct or this spin should not be flipped. Hence, this system may or may not move to a new microstate. After completing one Monte Carlo time step the next spin is chosen and the similar procedure is carried out. This is repeated a large number of times, so that every spin is given many chances to flip. We can view each Monte Carlo time step as one interaction with the heat bath. Since T enters Boltzmann factor for flipping a spin, the effect of this interaction varies according to the temperature.

Quantitatively, a MC spin process connects two microstates such as state 1 and state 2 with energies $E_1 > E_2$. The flipping rules specify the probability for flipping the selected spin during a given step. Denote this rate $W(1 \rightarrow 2)$ and from the assumption that $E_1 > E_2$, it is clear that $W(1 \rightarrow 2) = 1$. However, if the system is in state 2, the probability is $W(2 \rightarrow 1) = \exp\left[-(E_1 - E_2)/k_B T\right]$. When the system reaches equilibrium the probability of finding it in any particular state will be independent of time and the number of transitions from state 1 to state 2 must be equal to the number of transitions in the reverse direction, i.e.

$$P_1 W(1 \rightarrow 2) = P_2 W(2 \rightarrow 1) \tag{6}$$

where P_1 and P_2 are the probabilities of the system being found in these two microstates. With $W(1 \rightarrow 2) = 1$, we get $\frac{P_1}{P_2} = \exp\left[-(E_1 - E_2)/k_B T\right]$. Compare this with Eq. (2), we see that this is exactly what is expected for a system in thermal equilibrium.

In this simulation, period boundary conditions (PBCs) are assumed. [2] For example, the top line spins' upper neighbors are those bottom line spins with the same column number in the lattice. Though this is one of the simple boundary conditions, other kinds of conditions bring different properties for the similar system.

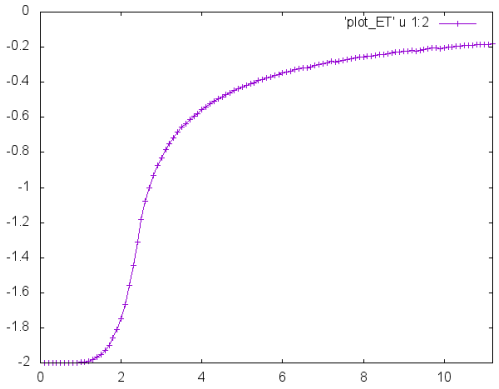


Figure 2: (E - T) 10x10 lattice

Using Eq. (1) we get the energy versus temperature graph shown as Fig 2. Y-axis denotes reduced energy average on each spin and x-axis denotes reduced temperature. Here $k_B = J = 1$ are reduced constants. Noting that under the above circumstances, we should have $\lim_{T\to 0^+} E = -2$ and $\lim_{T\to\infty} E = 0$. Some calculations lead to $T_c = \frac{2}{\ln(1+\sqrt{2})} \approx 2.27$. [1]

After the structure is established, i.e. each given temperature has a given sets of spins to correspond to it, the mean magnetization can be quickly sought out.

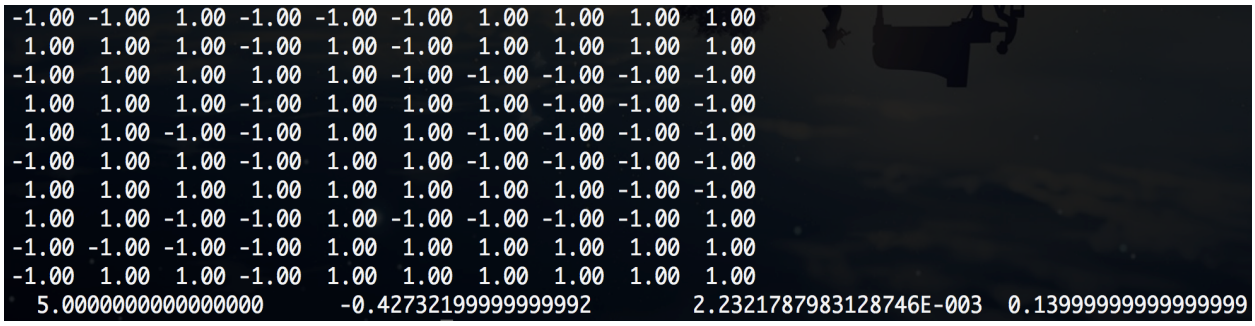


Figure 3: Magnetization at reduced temperature 5

As Fig. 3 shows, the mean magnetization at reduced temperature 5 is 0.14 with mean reduced temperature -0.427. And 2.23×10^{-3} is the error bar of the mean energy.

By the finite difference method (FDM), we can calculate the heat capacity of this system. The difference step is 0.1, which is so small that a conspicuous fluctuation is observed no matter how many times of warm up steps are taken before measure. Virtually, the heat capacity *C* peaks

at $T_c \approx 2.27$ and approaches zero when temperature are either very low or very high, shown as Fig 4.

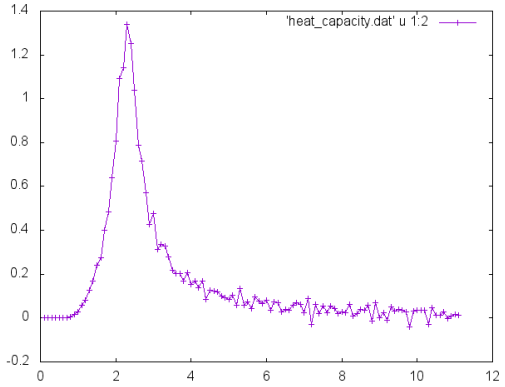


Figure 4: (C - T)

Using Eq. (5) we can get entropy-temperature relation, shown as Fig. 5. From the aspect of calculation, since $\lim_{T\to 0} E/T = -\infty$ and $\lim_{T\to 0} \int_T^{\infty} \frac{E(T')}{T'^2} dT' = +\infty$, entropy is divergent. Hopefully, however, we know clearly that when temperature approaches 0, entropy approaches 0 and that when temperature approaches infinity, entropy approaches ln2. So the *S*-*T* relation of low temperature (T<0.7) should be fixed to become a horizontal line leaving other parts the same as before. Also, if the relation between energy and temperature are gained through an in direct way such as $E(\beta)$ where $\beta = \frac{1}{k_B T}$, that is energy given as a function of the reciprocal of temperature. Then entropy can be calculated also in a thermal integral (TI) fashion and avoid the divergence at T=0 since when temperature approaches 0, β approaches infinity and there always exists a cut-off error, you can raise the upper limit of the integral as large as you need.

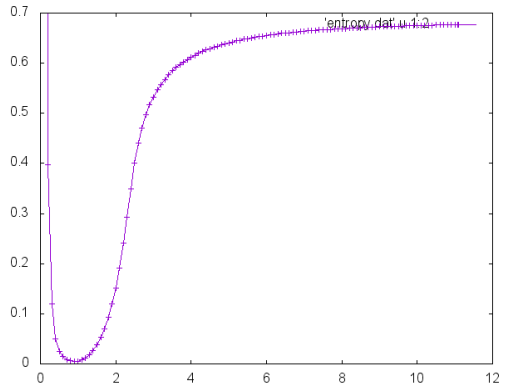


Figure 5: (S - T)

Compare the result [3] given by Wang-Landau method in Fig 6, we find the low-temperature range should be fixed.

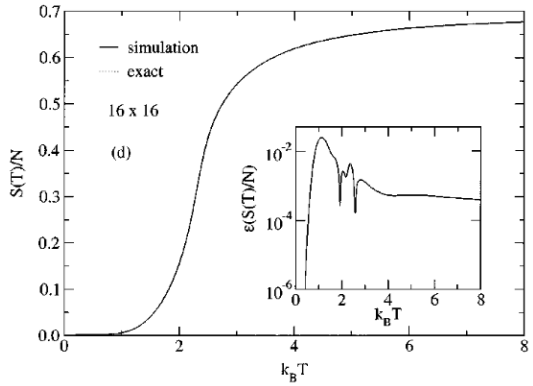
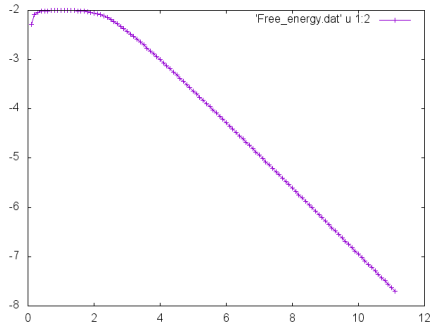


Figure 6: (S - T)by WL method

Last, the Helmholtz free energy F can be calculated directly as

$$F = E - TS \tag{7}$$

This also shows the advantages of collecting $E - T$ relation rather than $E - \beta$ relation. Fig 7 gives the $F - T$ graph.



5. Conclusion

For that a large spin system with $O(10^{23})$ spins the analytic approaches are formidable, and only a relatively few exact results are known, which makes simulations very valuable for this problem. Also, the fact that interaction will be largest between spins that are nearest neighbors and fall off rapidly with increasing separation between the spins permits even the nearest neighbor approximation still catches most spirit of physics in this case. The advantages and disadvantages of my way to calculate various thermal quantities are discussed as above. Another important thing deserves noting is that the error for MMC is reciprocal to the square root of the loop times *n*, that means if you want to raise the precision for only 1 digit you have to repeat 100 times more calculations. For this simple model MMC is viable, however this can only act as a prelusion for some other methods.

6. Reference

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[3] *A new approach to Monte Carlo simulations in statistical physics: Wang-Landau sampling*. 2004 American Association of Physics Teachers.