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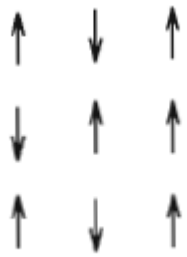
Computational Physics Final Project – Ising Model

Ising model describes a system of N sites. The model of a ferromagnet that we will consider is shown schematically following. 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. For simplicity we assume that these spins are situated on a regular lattice. We will assume that each spin is able to point along either $+z$ or $-z$; that is, either up or down. No other orientation is permitted. Hence, the ith spin in the system can have one of only two possible values, which for convenience we take to be $s_i = \pm 1$. Each of these so-called Ising 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 between the two spins. With this motivation, the simplest Ising model assumes an interaction only between nearest neighbors so that the energy of the system is

$$E = -J \sum_{(ij)} s_i s_j$$

where the sum is over all pairs of nearest neighbor spins $\langle ij \rangle$, and J is known as the exchange constant, which we will assume to be positive.

The magnetization is closely related to the average spin alignment $\langle s_i \rangle$, where the angular brackets denote a thermal average. The total magnetization at temperature T for a system of N spins will then be

$$M = \sum_i \langle s_i \rangle = N \langle s_i \rangle$$

Since the sum is over all possible various microstates, we mainly discuss two algorithms: Local Metropolis Algorithm (Local Monto-Carlo Algorithm) sampling directly in space with Markov chain. However, it is to be noticed that this method progresses very slowly at critical condition. Therefore, we use the improved Global Cluster Algorithm.

If we can sum over all possible microstates, we can calculate physical quantities such as specific heat and magnetization.

Partition function

$$Z(\beta) = \sum_i e^{-\beta E_i} = \sum_{E_i} n(E_i) e^{-\beta E_i}$$

$n(E_i)$ is density of state of energy E_i. Then we can consider the following quantities

$$\langle E \rangle = -\frac{\partial}{\partial \beta} \log(Z) = \frac{1}{Z} \sum_{E_i} n(E_i) e^{-\beta E_i}$$

$$\langle E^2 \rangle = -\frac{\partial}{\partial \beta} \log(Z) = \frac{1}{Z} \sum_{E_i} E_i^2 n(E_i) e^{-\beta E_i}$$

and the specific heat capacity is

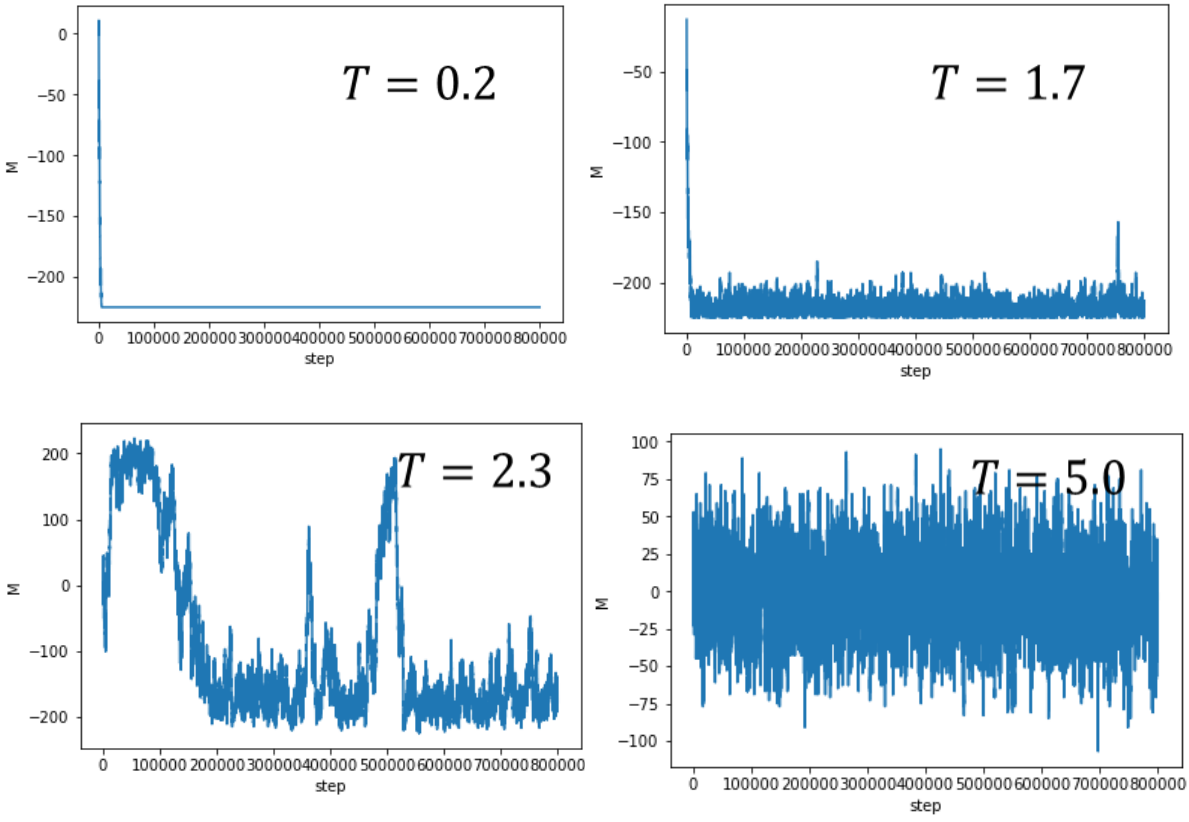
$$C_V = \frac{\partial}{\partial \mathrm{T}} \langle E \rangle = -\beta^2 \frac{\partial}{\partial \beta} \langle E \rangle = \frac{\beta^2}{N} (\langle E^2 \rangle - \langle E \rangle^2)$$

For a very large analogue scale N, it is too slow to go through all possible states. The complexity will be an over-exponential $\mathrm{T(n)} = \mathrm{O}(2^{n^2})$. Therefore, it is unrealistic to count a large system through an exhaustive method, while it is possible to take samples with Monto-Carlo Algorithm.

To be specific, we can take sample directly in space to construct a Markov chain satisfying thermal equilibrium condition through Local Monto-Carlo Algorithm, and count up properties above.

In Local Monto-Carlo Algorithm, we randomly pick up a spin, and try to make it flip and the system will move into a different microstate (a to b). In order to make the transition between two states satisfy the thermal equilibrium condition, only the transition with probability P can be accepted

$$\mathrm{P} = \min\{1, e^{-\beta(E_b - E_a)}\}$$



When different temperatures T are set, the plot of total magnetization against states of a certain Markov sampling chain is shown above; the analogue scale L is 15, a 15*15 two-dimensional lattice. It is to be noticed that as the temperature rises, the degree of order is reduced from its values at lower temperature, and when T=5.0K, the system macroscopically does not show magnetism.

One major problem of the above Local Monto-Carlo Algorithm is, at the critical temperature, the algorithm shows low convergence rate. In order to take samples quickly, we hope to modify multiple spin at a time appropriately. However, the rate of rejection increased simultaneously if we simply try to flip multiple spins.

Global Cluster Algorithm can modify a great number of spins which have the same orientation at one time to achieve a high rate of convergence at critical temperature without violating the thermal equilibrium condition.

We are now ready to apply the Global Cluster Algorithm to the study of phase transitions is the Ising model. It starts with a randomly chosen spin, through gradually increasing the number of the spin which have the same orientation by probability P, we now have a cluster. In addition, the newly added member is active as well, which means they can also make spins with same arrangement outside the collection join the cluster by probability P. After the cluster is constructed, all members of it will flip altogether, which moves the system into a new state b. Our goal is to choose P appropriately so as to make the transition legally.

Note P(a) and P(b) are the probabilities of the system being found in these two microstates, the rate of transitions from state a to state b is $\mathrm{P}(a \to b)$, and the rate of transitions from state b to state a is $\mathrm{P}(b \to a)$. On account of the thermal equilibrium condition

$$\mathrm{P}(a)\mathrm{P}(a \to b) = \mathrm{P}(b)\mathrm{P}(b \to a)$$

be aware that $\mathrm{P}(a \to b)$ is equivalent to the probability of constructing a cluster first and then accept the cluster

$$\mathrm{P}(a)P_{con}(a \to b)P_{ac}(a \to b) = \mathrm{P}(b)P_{con}(b \to a)P_{ac}(b \to a)$$

When all spins in the cluster are reversed, it is the boundary terms that actually influence the energy. To be specific, the difference between the number of spin co-direction and n_1 and spin reverse n_2 at the boundary. Therefore, the energy of state a is proportional to $n_1 - n_2$, and $n_2 - n_1$after the system is reversed.

Meanwhile, the newly added spin is probability-independence $P_{ac}(a \to b) \propto (1-P)^n$, we have

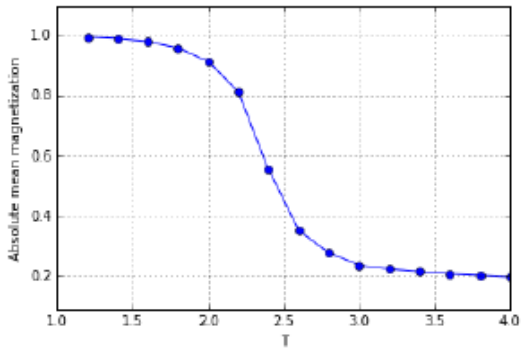
$$e^{-\beta(n_1-n_2)}(1-P)^{n_2}P_{ac}(a \to b) = e^{-\beta(n_2-n_1)}(1-P)^{n_1}P_{ac}(b \to a)$$

the probability of acceptance

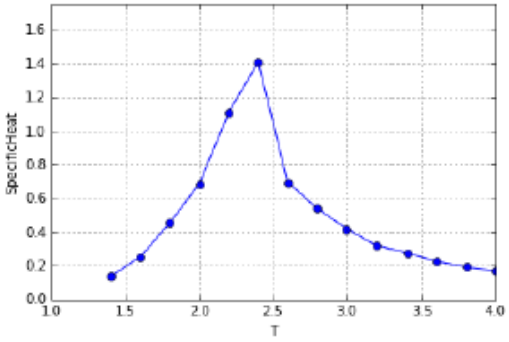
$$P_{ac}(a \to b) = min\left\{1, \frac{e^{-\beta(n_2-n_1)}(1-P)^{n_1}}{e^{-\beta(n_1-n_2)}(1-P)^{n_2}}\right\} = min\left\{1, (\frac{e^{-2\beta}}{1-P})^{n_2}(\frac{1-P}{e^{-2\beta}})^{n_1}\right\}$$

Only need to set $\mathrm{P} = 1 - e^{-2\beta}$ to make the probability of acceptance equals to unity without violating the equilibrium condition.

The algorithm constructs a cluster by constantly put in neighboring spins with the same arrangement and then flipping directly, without considering probability of acceptance. Analyzing the Markov chain generated at different temperatures respectively, obtain the thermal and magnetic properties. (analogue scale L = 15)

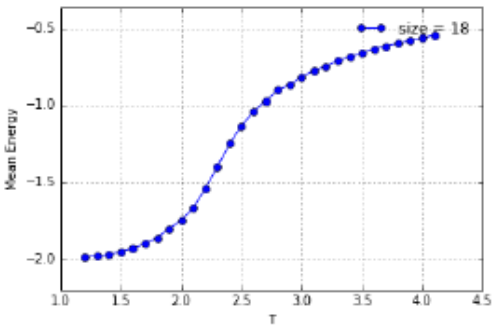


(a) Absolute mean magnetization

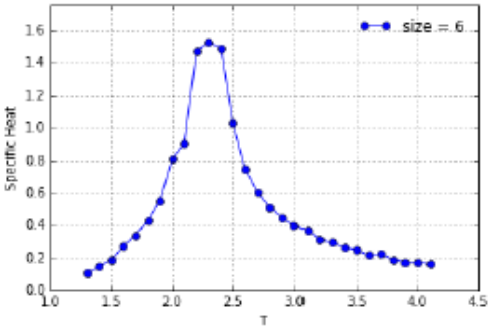


(b) Specific Heat

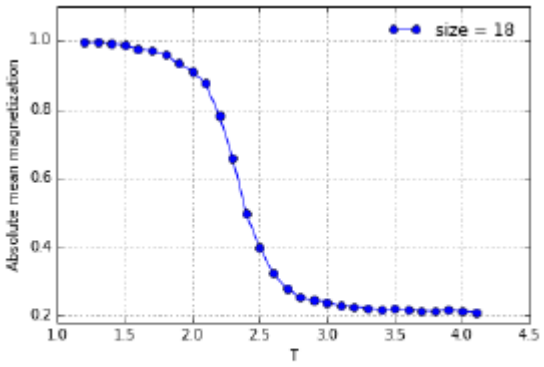
Analyzing the Markov chain generated at different temperatures respectively, obtain the thermal and magnetic properties. (analogue scale L = 18)



(a) Absolute mean magnetization



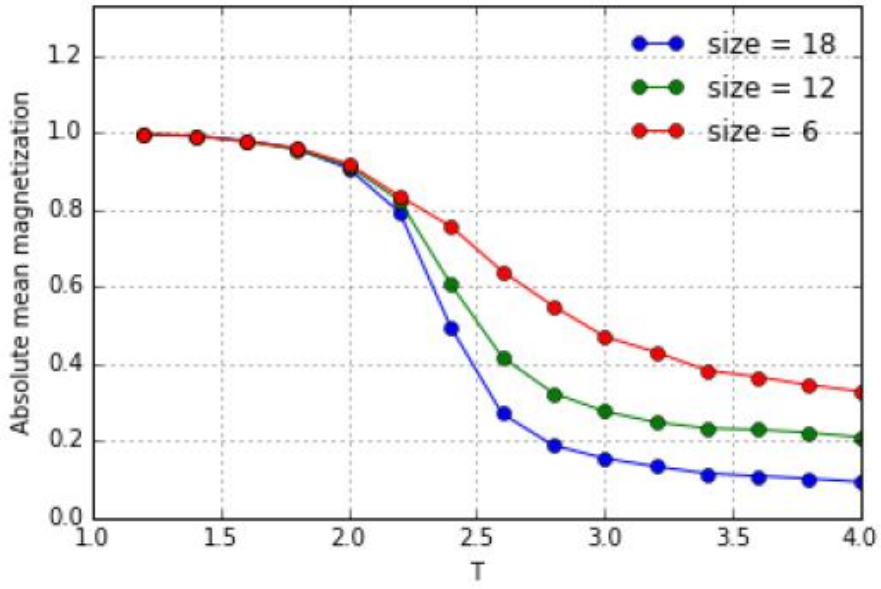
(b) Specific Heat



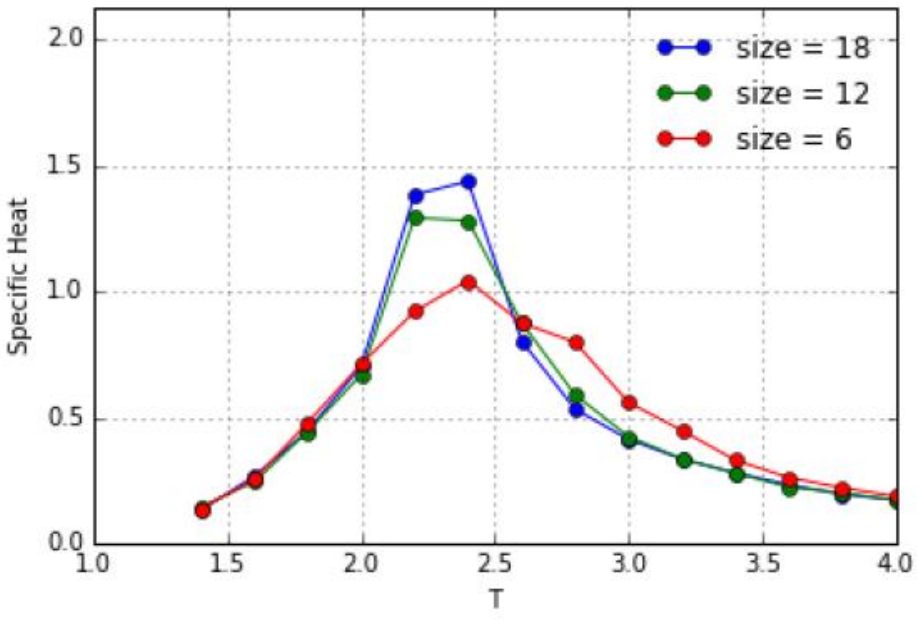
(c) Mean Energy per spin

For different analog scale, the obtained absolute value of average magnetization changes with temperature. We can observe that the phase transition becomes obvious as the analogue scale L increases, and the phase transition point approaches the theoretical value

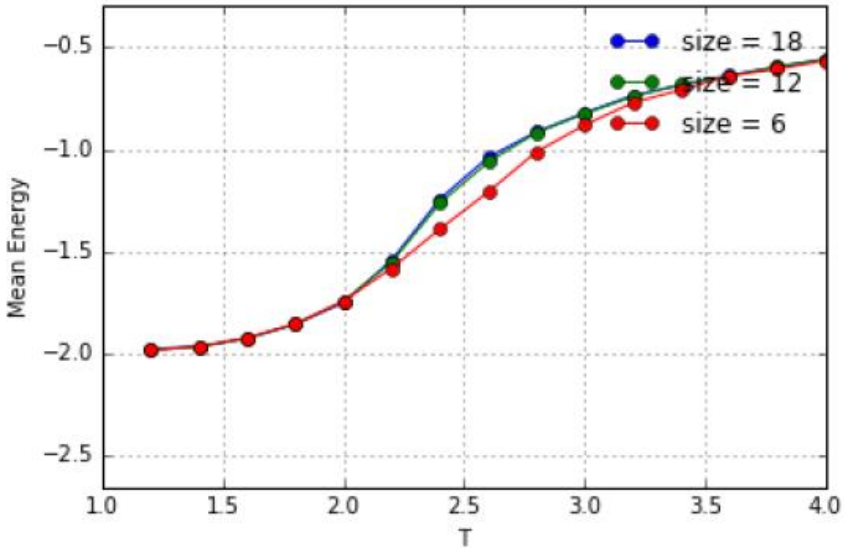
$$T_C = \frac{2}{\log(1+\sqrt{2})} = 2.27.$$



Absolute mean magnetization



Specific Heat



Mean Energy per spin

Through the gradual improvement of these two algorithms, we can analyze the system's statistical properties including magnetization and specific heat. These two sampling method is useful and effectively in a system of Ising model as well as other statistical systems which have vast state space.