Monte Carlo Simulation on 2D Ising Model

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October,2020

1. Introduction

Ising model is a simplified model to study ferromagnetic phase transition,which make it one of the simplest and best studied of statistical mechanical models.It is a periodic lattice system consisting of N lattice points with n(n=1,2,3) spatial dimensions.Each lattice has a spin $s_i(i=1,2,...N)$ on it,the direction of which can be up or down,represented by $s_i=\pm 1$,and these spins have nearest neighbor interaction.

A given set of $\{s_i\}$ is called a configuration of the system,that is,a microscopic state of the system.Give a configuration,the Hamiltonian of the system can be written by:

$$H_{\{s_i\}}=-\sum_{\langle i,j\rangle} Js_is_j-\mu B\sum_{i=1}^{N}s_i\ .$$

Here $\langle i,j\rangle$ represents the nearest neighbor pair, J denotes the coupling constant where $J>0$ describes ferromagnetic coupling and $J<0$ describes antiferromagnetic coupling. B is the external magnetic field and μ is the spin magnetic moment.

For the moment,we consider a 2D model with coupling constant $J>0$ and without a external field.Most of the interesting questions concerning physical quantities associated with phase transitions can be answered in this way.By the way,the ferromagnetic phase transition described by ising model is second order phase transition,also known as continuous phase transition.At the phase transition point,free energy and its first derivative are continuous,and its second derivative is discontinuous.The transition point of second order phase transition is also called critical point.

Next,we will introduce you the Metropolis Algorithm,some measurements and their physical significance such as magnetization,binder parameter,heat capacity,susceptibility,correlation function,etc.These are the foundations of statistical physics learning.

2.The Metropolis Algorithm

Monte Carlo method is a kind of extensive computing algorithm,which is based on probability theory and relies on random sampling to obtain numerical results.It can be used to simulate thermodynamic problems in various equilibrium or non-equilibrium states.Usually,our goal in the Monte Carlo simulation is the expectation value $\langle Q \rangle$ of an observable quantity Q,which can be written as

$$\langle Q \rangle = \frac{\sum_\mu Q_\mu e^{-\beta E_\mu}}{\sum_\mu e^{-\beta E_\mu}},$$

in which the core idea is to make a weighted average of Q_μ of all possible states,where the weight is Boltzmann factor.However,this simple sampling method is easy to cause computational problems in simulation.Taking 2-dimension ising model we discuss now as an example,if we have a 16*16 spin lattice,then the system will have 2^{256} states totally.Obviously,it is going to take a long,long time to traverse through all of these possible states.But what if we take a more clever route?

In stead of going through all the microscopic states and averaging them with Boltzmann factors as their weights,it would be much easier to sample these states with Boltzmann factors as their weights and then average them equally.This sampling method is called importance sampling,and it is the basic of metropolis algorithm.

The next question now is that how to generate points in configuration space with a relative probability proportional to the Boltzmann factor.The detailed balance condition tells us that given an initial configuration,if we accept the change based on the following probability:

$$P = e^{-\beta u_n}/e^{-\beta u_o}, \text{ if } e^{-\beta u_n} < e^{-\beta u_o},$$

$$P = 1, \qquad \text{if } e^{-\beta u_n} > e^{-\beta u_o},$$

We will achieve our goal. Here is how the Metropolis Method works specifically:

1）Select a spin at random,and calculate the contribution to the energy involving this spin.

2）Flip the value of the spin,and calculate the new contribution.

3）If the new energy is less,keep the flipped value.

4）If the new energy is more,accept the flip with probability:

$$acc(o \to n) = \exp\{-\beta[H(n) - H(o)]\}$$

5）Repeat.

3.Measurements and their physical significance

3.1 Order parameter:magnetization

One of the most important quantities used to study phase transition is order parameter, which is a measure of how ordered a system is.The order parameter of ising model is magnetization,which is defined by

$$m = \frac{1}{N}\left\langle \sum_{i=1}^{N} S_i \right\rangle$$

and $\langle\ \rangle$represents ensemble average.

To understand how magnetization varies with temperature,let us consider *Gibbs-Boltzmann distribution*

$$P(S) = \frac{e^{-\beta H}}{\sum_{s} e^{-\beta H}}$$

where numerator is Boltzmann factor and denominator is partition function Z.In the high temperature limit $\beta \to 0$,the numerator $e^{-\beta H} \to 1$,which implies that microscopic state with different energies occur with equal probability.Therefore,each spin S_i will flip frequently,implying that the macroscopic system is in disordered phase at this time,and magnetization will vanish in an infinite system.However,at low temperature $T \to 0$,*Gibbs-Boltzmann distribution* tells us that low-energy states are more likely to emerge than high-energy states.In the absence of external field, $S_i = 1$ or $S_i = -1$ at all sites will minimize energy,in which case magnetization is 1 or -1.

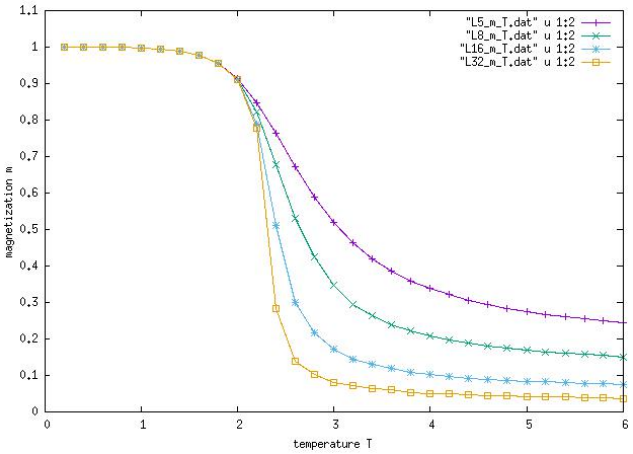

Figure 1:magnetization per site varies with temperature T for L=5,8,16,32.

The result of our simulation is shown in figure 1.It is worth noting that the magnetization measured here is taken in absolute value to avoid the problem causing by states jumping between two free energy valleys.As the system increases, the phase transition becomes more and more obvious.

If you want to figure out why doesn't magnetization goes to zero at high temperature as we expected,let us go to figure 2.It show us how the distribution of magnetization varies with temperature.At low temperature,the magnetization shows bi-modal distribution,corresponding to $S_{\mathrm{i}}=1$ or $S_{\mathrm{i}}=\text{-}1$ at almost all sites.At high temperature,the magnetization is approximately a Gaussian distribution with zero mean,corresponding to frequent spin reversals.In the thermodynamic limit,the fluctuation of magnetization is negligible compared with the magnetization,and the distribution is going to be a delta one.However,because the system size is finite,the variance of this distribution is a finite value instead of zero,so that the absolute value of magnetization that we calculated is not zero at any temperature.

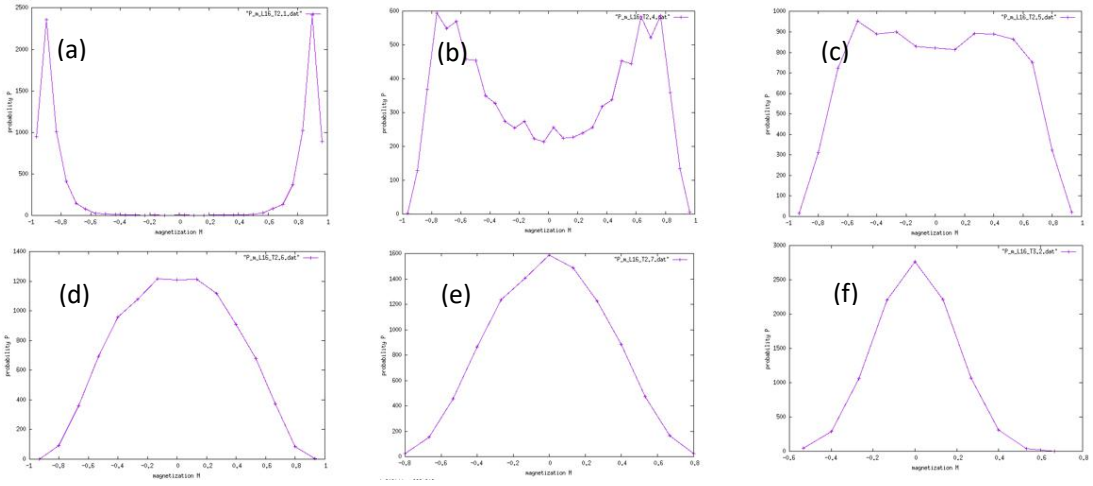

Figure 2:The distribution of magnetization varies with temperature T for L=16.Temperature increases gradually from fig.2(a) to fig.2(f).

3.2 Binder parameter

Magnetization tells us the difference between symmetric phase and broken phase,however,we still can't figure out where the critical point is located.Binder parameter is another quantity to help us,which is defined as

$$U_L = 1 - \frac{\langle S^4 \rangle_L}{3\langle S^2 \rangle_L^2}$$

and S here is just magnetization we have introduced before.In an infinite system, $U_L \to 0$ in the high temperature limit and $U_L \to \frac{2}{3}$ in the low temperature limit.At the critical point, U_L tends towards an universal value where $0 < U_L^* < \frac{2}{3}$.We show the behavior of U_L in figure 3.We can see that the intersection point of systems with different sizes is $T \approx 2.219$,which is very close to the critical point $T = \frac{2J}{k \ln(1+\sqrt{2})} \approx 2.269$ given by Onsager exact solution.

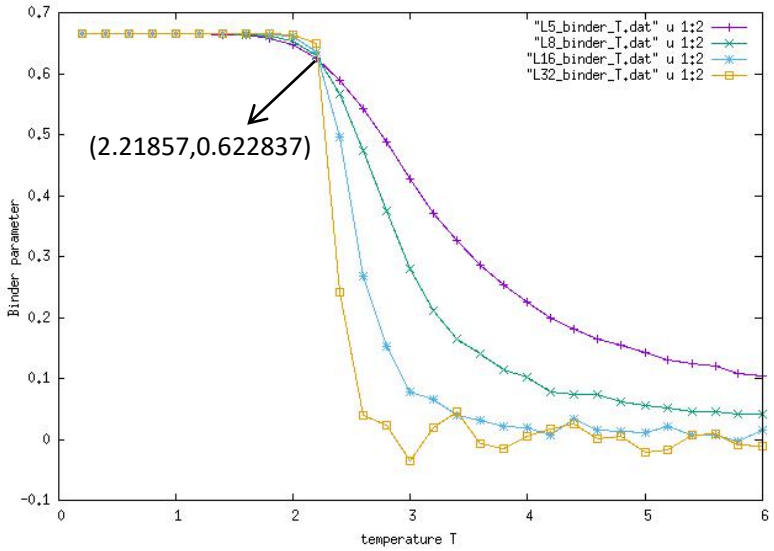

Figure 3:The behavior of binder parameter.

3.3 Fluctuation: The specific heat and Magnetic susceptibility

Fluctuations in observable quantities is another one of interesting properties that statistical mechanics can tell us.In other words,the standard deviation of those observable quantities also play an important role in understanding physical behavior of a system.The specific heat capacity and magnetization susceptibility are two examples of fluctuations in observable quantities,and we will proceed with a simple derivation below.

If we write the expectation value of the energy $\langle E \rangle$ in terms of a derivative of the partition function:

$$\langle E \rangle = \frac{1}{Z} \sum_{\mu} E_{\mu} e^{-\beta E_{\mu}} = -\frac{1}{Z} \frac{\partial Z}{\partial \beta} = -\frac{\partial \log Z}{\partial \beta} ,$$

then heat capacity,which is the derivative of the internal energy,is written by:

$$C=\frac{\partial\langle E\rangle}{\partial T}=-k\beta^2\frac{\partial\langle E\rangle}{\partial\beta}=k\beta^2\frac{\partial^2\log Z}{\partial\beta^2}=k\beta^2\left(\frac{1}{Z}\frac{\partial^2 Z}{\partial\beta^2}-\left[\frac{1}{Z}\frac{\partial Z}{\partial\beta}\right]^2\right)=k\beta^2\left(\langle E^2\rangle-\langle E\rangle^2\right),$$

that is to say,heat capacity is actually the fluctuation of energy,and this is known as the Fluctuation Dissipation Theorem.

Similarly,we can also write magnetization in terms of a derivative of the partition function:

$$\langle M\rangle=\frac{1}{Z}\sum_{\mu}M_{\mu}e^{-\beta E_{\mu}}=\frac{1}{\beta Z}\frac{\partial}{\partial B}\sum_{\mu}e^{-\beta E_{\mu}}=\frac{1}{\beta}\frac{\partial\log Z}{\partial B},$$

in which the third term is derived from the coupling term of magnetic field and magnetization in Hamiltonian.Then the magnetic susceptibility,which is the derivative of magnetization,can be written by:

$$\chi=\frac{\partial\langle M\rangle}{\partial B}=\frac{1}{\beta}\frac{\partial^2\log Z}{\partial B^2}=\frac{1}{\beta}\left(\frac{1}{Z}\frac{\partial^2 Z}{\partial B^2}-\left[\frac{1}{Z}\frac{\partial Z}{\partial B}\right]^2\right)=\beta\left(\langle M^2\rangle-\langle M\rangle^2\right)$$

implying that susceptibility is the fluctuation of magnetization.

First,let us look at the behavior of internal energy.According to the Hamiltonian expression without external field,the ordered phase at low temperature will have lower energy than the disordered phase at high temperature.Figure 4 shows that internal energy is a continuous function of temperature and increases with temperature T as we have expected.

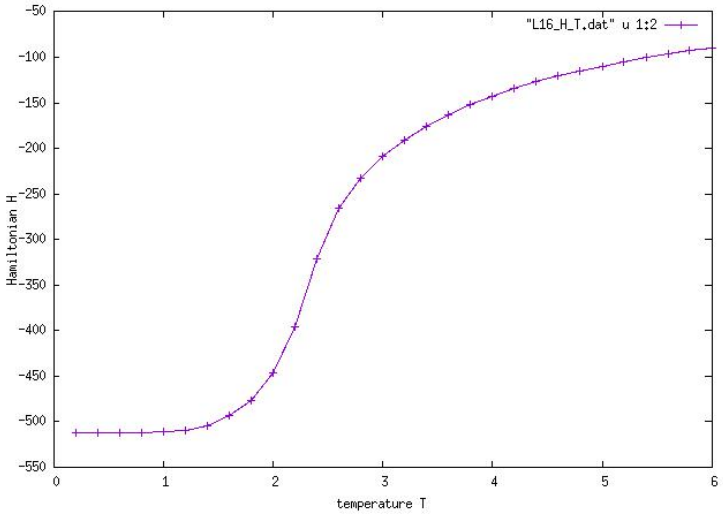

Figure 4:The internal energy varies with temperature T for L=16.

Having obtained the internal energy and magnetization,their fluctuations heat capacity and susceptibility,are easy to calculate.Results are shown in figure 5 and figure 6.These two plot have many similarities.They all have sharp peaks near the critical point and these peaks become sharper and sharper as the system becomes larger.Therefore,we can imagine that in the thermodynamic limit,both heat capacity and susceptibility will diverge at the critical point.

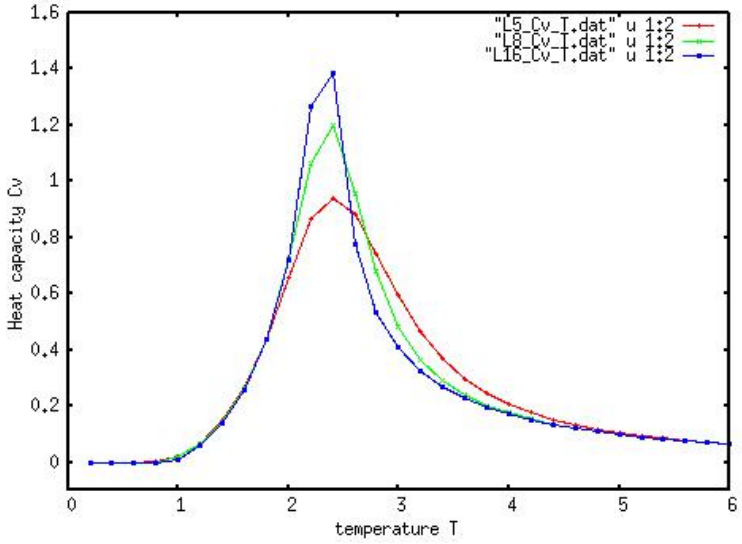

Figure 5:Heat capacity per spin varies with temperature T for L=5,8,16.

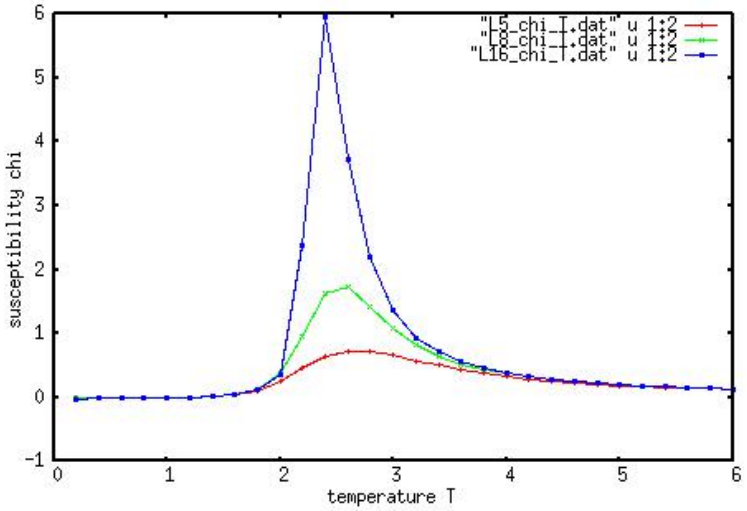

Figure 6:Magnetic susceptibility per spin varies with temperature T for L=5,8,16.

3.4 Spacial correlation function

In order to figure out why does susceptibility diverge at the critical point,we can continue to calculate another quantity,spacial correlation function $G_c^2(i,j)$,which is defined as

$$G_c^2(i,j) = \langle S_i S_j \rangle - \langle S_i \rangle \langle S_j \rangle = \langle S_i S_j \rangle - m^2$$

and you must have noticed that there is a connection between correlation function and magnetic susceptibility.If we measure the response of $\langle M_i \rangle$ to a variation of the magnetic field B_j at a different lattice site to get a generalized susceptibility χ_{ij} ,we will have

$$\chi_{ij} = \frac{\partial \langle M_i \rangle}{\partial B} = \frac{1}{\beta} \frac{\partial^2 \log Z}{\partial Y_i \partial Y_j} = \beta(\langle S_i S_j \rangle - \langle S_i \rangle \langle S_j \rangle) = \beta G_c^2(i,j)$$

that's how they relate to each other.

In fact,the transition symmetry of the ising model enables $G_c^2(i,j)$ to be a function only of the relative distance r between two spins:

$$G_c^2(r) = \frac{1}{N} \sum_{i,j(r_i - r_j = r)} \left[\langle S_i S_j \rangle - m^2 \right]$$

and N is the number of pairs whose distance is r.

More strictly speaking,the function above we defined is called connected correlation function,and we can start with the other one,disconnected correlation function,to make out them.disconnected correlation function $G_c^2(i,j)$ is defined to be

$$G_c^2(i,j) = \langle S_i S_j \rangle$$

Then,it is easy to understand that if two spins fluctuate in the same direction,the function will take a positive value.Inversely,it will take a negative value if two spins fluctuate in the opposite directions.If two spins are completely unrelated,they will fluctuate sometimes in the same direction and sometimes in the opposite direction,and the average will be close to zero.In this way,we can distinguish easily that whether spins are relevant or not.

However,system at low temperature are so ordered that almost all spins are in the same direction even if they are unrelated,leading to a non-zero value of disconnected correlation function.Therefore,connected correlation function,where the average is taken on the fluctuation about variable expectations, is introduced to avoid this problem.Figure 7 shows us the difference between these two correlation functions.

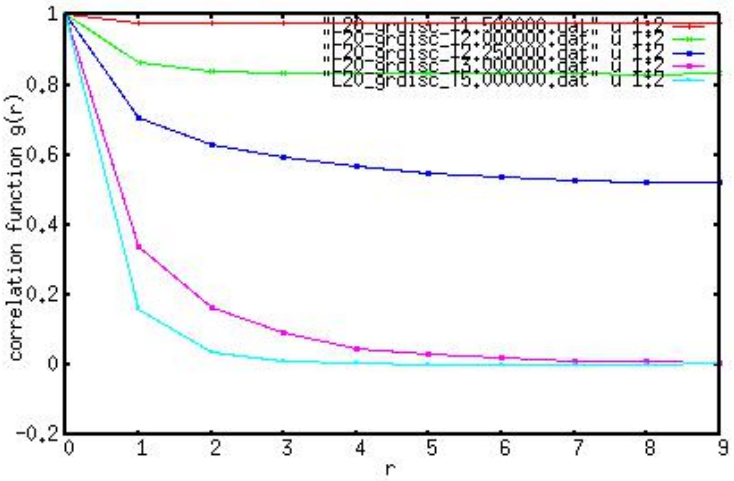

Figure 7(a):Behavior of disconnected correlation function for L=20.

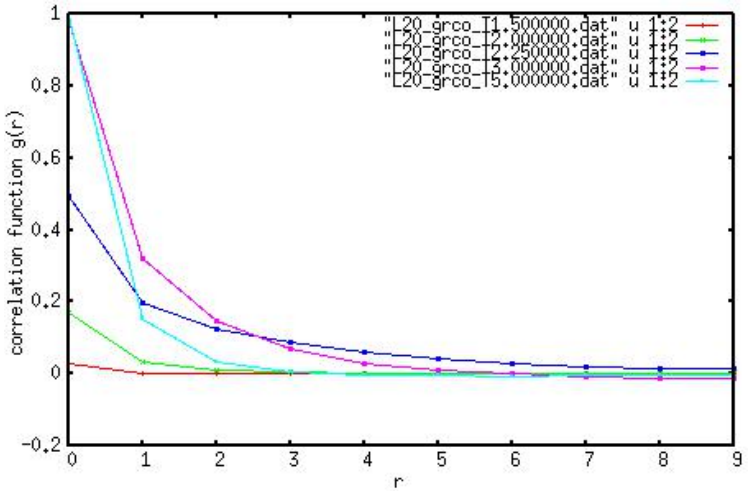

Figure 7(b):Behavior of connected correlation function for L=20.

We can also learn from figure 7(b) that the correlation function seems to decay more slowly near the critical point. In order to prove that we simulate a larger system at various temperature near the critical point.The results are plotted in figure 8.As we have expected,the distance that two spins are related to each other becomes much

longer near the critical point,and it increases as the system gets larger.That is why susceptibility diverges at the critical point in the thermodynamic limit.

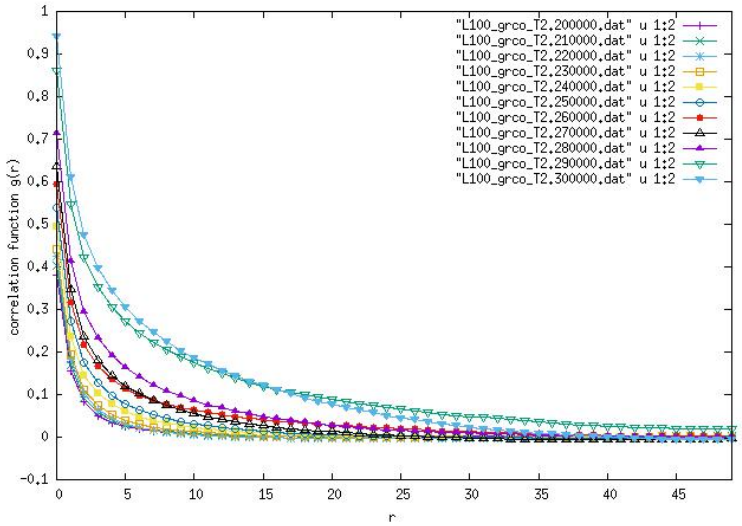

Figure 8:Behavior of connected correlation function for L=100.

3.5 Time-displaced Autocorrelation function

In the simulation,we have to take thousands of unrelated samples to ensure the ergodicity.So how long will it take for a system to drop off autocorrelation? We can define the following time-displaced autocorrelation function:

$$\chi(t)=\int dt'\left[m(t')-\langle m\rangle\right]\left[m(t'+t)-\langle m\rangle\right]=\int dt'\left[m(t')m(t'+t)-\langle m\rangle^2\right]$$

where $m(t)$ is magnetization at time t and $\langle m\rangle$ is the average value.This function gives us a measure of correlation at different times.If fluctuations of magnetization are in the same direction on average during time interval t' then $\chi(t)$ will take a non zero value,that is to say,these configurations are correlated.If they are not, $\chi(t)$ will be zero.People define a typical time-scale that $\chi(t)$ decreases to $1/e$ as the time when two configurations are drop off correlation.Figure 9 shows our results of autocorrelation function for some different temperatures.Here we use a slightly larger system L=64 to make the difference of curves from various temperature more obvious.

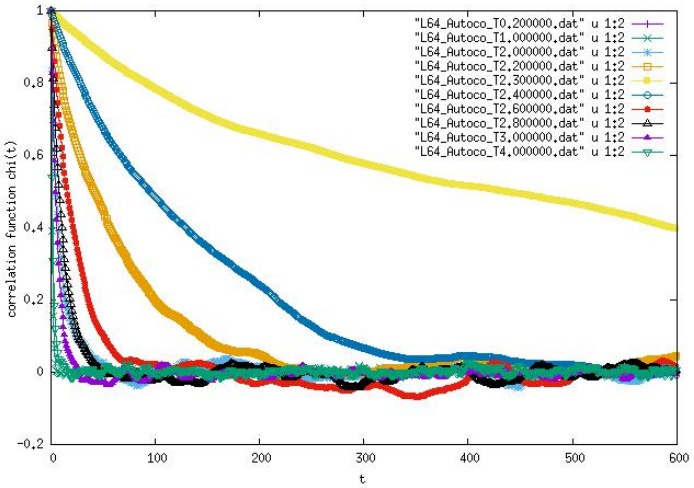

Figure 9:Autocorrelation function at various temperature for L=64.
Time is measured in Monte Carlo steps per site.

From the figure above,we can make a reasonable conclusion that for a system at given size,the correlation time gets its maximum at the critical point,and this time can be used as the interval for taking two unrelated samples at any temperature during the simulation.

Acknowledgment

I wish to thank my professor Dr.Yuliang Jin sincerely for his great help and support.

References

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