PHYS 8601 – Problem 3

Yier Wan

March 18, 2018

1 Introduction

In this work, we still study the two-dimensional square-lattice Ising model. Instead of calculating physical quantities, we are focusing on the correlation of the simulated results. It is assumed that the Metropolis algorithm we are using can generate statistically independent configurations through a series of spin flips, but we do not know exactly how many Monte Carlo steps are required between two configurations can be considered statistically independent. To answer this important question, the relaxation functions are studied.

2 Relaxation time

For a quantity A, the relaxation function can be defined which describes time correlations within equilibrium

$$\phi_{AA}(t) = \frac{\langle A(0)A(t)\rangle - \langle A\rangle^2}{\langle A^2\rangle - \langle A\rangle^2} \tag{1}$$

where the averages are over the time-index k. We consider one Monte Carlo step as one time step here. Noted that $\langle A(0)A(t)\rangle = \sum_k A(k) \times A(k+t)$ and $\langle A^2\rangle = \sum_k A(k) \times A(k)$ are different. In the simulation, we do 5100 MCS each time and burn in the first 2000 MCS results.

The asymptotic behavior of the correlation function is $\phi_{AA}(t) \to \exp(-t/\tau_{AA})$. The linear regression model is used to fit the coefficient α in $\log\phi = \alpha t$, where $\tau = -\frac{1}{\alpha}$. Propagation of uncertainty is needed to obtain the error of τ_{AA} from the error of α in this case. For fraction like $R = \frac{A}{B}$, we have

$$\sigma_\tau = R \times \sqrt{\left(\frac{\sigma_A}{A}\right)^2 + \left(\frac{\sigma_B}{B}\right)^2}. \tag{2}$$

So the error of σ_τ is calculate by σ_α/α^2.

We can also define an integrated relaxation time

$$\tau_{int} = \int_0^\infty \phi(t)dt. \tag{3}$$

However, we can not really simulate the value of relaxation function at infinity and after certain t value, the simulated values of relaxation function will contain fluctuations. So we divide the entire integral into two parts. The term 1, $\int_0^{t_0} \phi(t)dt$, is numerical integral and the term 2, $\int_{t_0}^\infty \phi(t)dt = \tau e^{-t_0/\tau}$, is estimated by the asymptotic behavior of the relaxation function.

3 Results and Discussion

Figure. 1 and Figure. 2 plots the relaxation functions for energy and magnetization on different lattice conditions. The left panel shows the raw data and right panel shows the logarithm-transformed figure, which helps us better locate the exponential region. We actually have data for $t \geq 40$ until

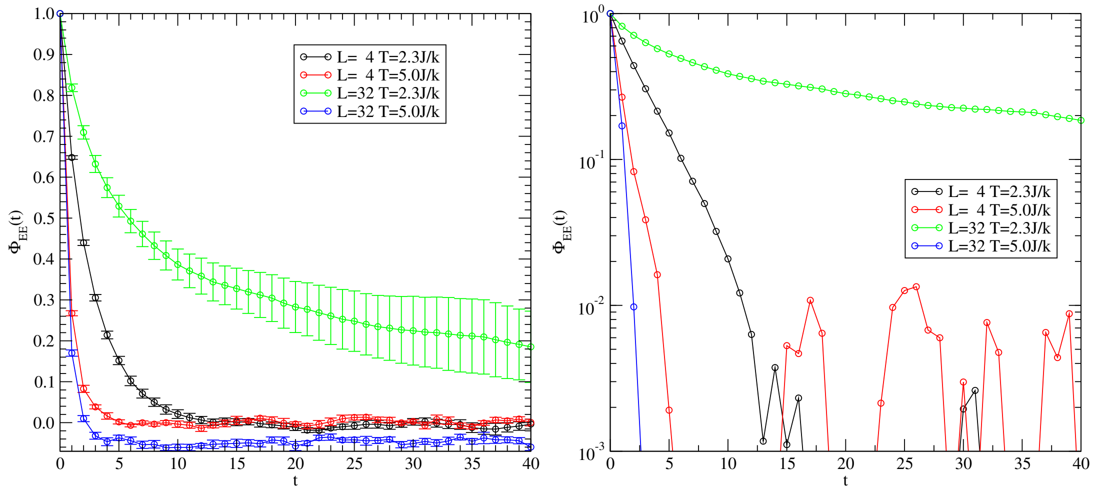

Figure 1: Relaxation function for energy on different lattice conditions.

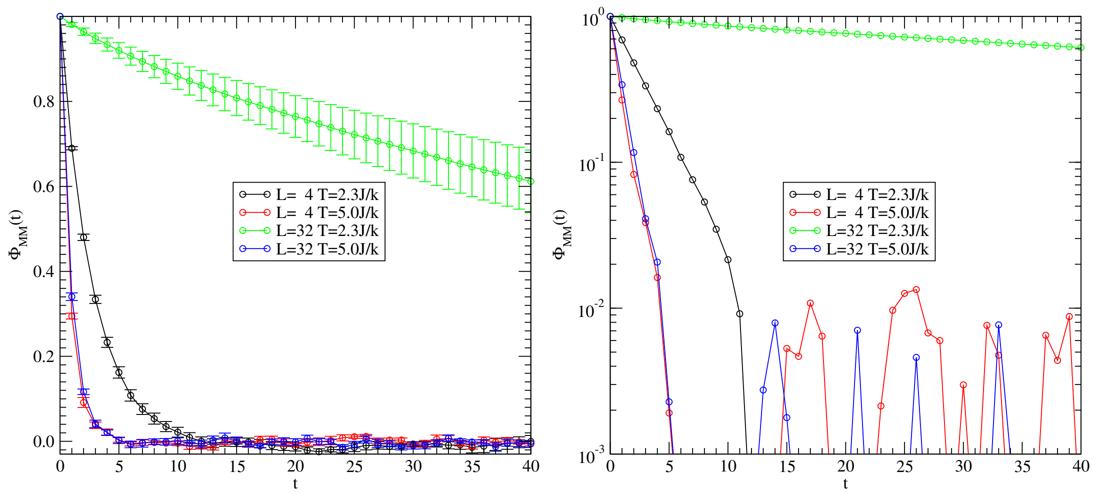

Figure 2: Relaxation function for Magnetization on different lattice conditions.

100, but there are too many fluctuations, so that part is not plotted here. For each condition (one combination of L and T), we run the code 10 times to get the averaged values and error bars.

Table 1: Simulated results

Condition	quantity	Region II	τ	Error	τ_{int}	Term1	Term2
L= 4, T=2.3J/k	Energy	[1,11]	2.5870	0.0206	2.5699	2.5331	0.0368
	Magnetization	[1, 9]	2.7115	0.0088	2.6680	2.5699	0.0981
L= 4, T=5.0J/k	Energy	[1, 3]	0.8710	0.0463	0.8176	0.7898	0.0278
	Magnetization	[1, 3]	0.8843	0.0293	0.8281	0.7984	0.0297
L= 32, T=2.3J/k	Energy	[10,35]	18.3054	0.6749	18.1535	15.4482	2.7052
	Magnetization	[10,40]	78.2414	0.6256	78.2414	31.3159	46.9255
L= 32, T=5.0J/k	Energy	[0, 2]	0.4533	0.0315	0.4897	0.4842	0.0055
	Magnetization	[0, 4]	0.9847	0.0240	0.9898	0.9729	0.0170

From those figures, we can conclude the following things:

1) For fixed lattice size, the relaxation function decays to zero slower as the temperature gets closer

to the critical temperature.
2) For fixed temperature, the relaxation function of the larger lattice decays slower then that of the smaller lattice size.

Table. 1 gives the simulated values of relaxation time and the integrated relaxation time. The problem we got is that at high temperature ($t = 5.0J/k$), the relaxation function decays so fast to almost zero and then fluctuates, so we only have few data points to fit the linear model and find the relaxation time, which makes the results questionable.

4 Attachment

Since we use the same Ising model program to generate the data, only the newly written part for relaxation function is attached. The R code for data analyzing and model fitting is also attached.