PHYS 8601 – Problem 3

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March 2, 2018

1 Introduction

The Ising model, named after the physicist Ernst Ising, is a mathematical model of ferromagnetism in statistical mechanics. This model uses discrete variables to represent the magnetic dipole moments of atomic spins that can be in one of two states (+1 or -1). This model allows the identification of phase transitions. Specially, we are going to study a two-dimensional square-lattice Ising model, which is one of the simplest statistical models to show a phase transition.

2 Physics Background

2.1 Ising model

Consider a set of $L \times L$ lattice sites. Each lattice site represents a spin. For any two adjacent spins i, j, there is a ferromagentic coupling $J > 0$. (We ignore the magnetic moment in this work). The energy of a lattice with a certain microstate (μ) is given by the Hamiltonian

$$H(\mu) = -J \sum_{(i,j)} \sigma_i \sigma_j, \tag{1}$$

where $\sigma_i = \pm 1$. The notation (i, j) indicates that spin i and j are nearest neighbors, so the sum is over pairs of adjacent spins. The energy per site $E(\mu)$ can be obtained by dividing the number of sites ($N = L \times L$) in the lattice

$$E(\mu) = -J \times \frac{1}{N} \sum_{(i,j)} \sigma_i \sigma_j. \tag{2}$$

Define

$$\epsilon(\mu) = \frac{1}{N} \sum_x \epsilon_x(\mu), \tag{3}$$

$$\epsilon_x(\mu) = -\sigma_x \sigma_a - \sigma_x \sigma_r, \tag{4}$$

where a and r stands for the spin sits above and right to spin x.
Then we have

$$E(\mu) = J \times \epsilon. \tag{5}$$

Because we consider only two nearest neighbors instead of four in Eq. 4, there will be no double counting.

The order parameter is defined differently in different kinds of physical systems. In a ferromagnet it is simply the spontaneous magnetization. Similarly, we use magnetization per site in this work.

$$M(\mu) = \frac{1}{N} \sum_i \sigma_i \tag{6}$$

2.2 Measure fluctuating quantity

Define the scaled temperature parameter $t = k_B T/J$.

Internal energy per site:

$$\bar{E}(t) = \langle E(\mu) \rangle = J \times \langle \epsilon(\mu) \rangle \,, \tag{7}$$

Scaled specific heat per site can be obtained by either numerical differentiation of the internal energy per site:

$$C_V(t) = \frac{1}{N} \times \frac{\partial H(t)}{\partial T} = k_B \times \frac{\partial \langle \epsilon(\mu) \rangle}{\partial t}, \tag{8}$$

or using the fluctuation relation

$$C_V(t) = \frac{1}{N} \times \frac{1}{k_B T^2} \left(\langle H(\mu)^2 \rangle - \langle H(\mu) \rangle^2 \right) = k_B \times \frac{N}{t^2} \left(\langle \epsilon(\mu)^2 \rangle - \langle \epsilon(\mu) \rangle^2 \right). \tag{9}$$

The magnetization per site is estimated by

$$\bar{M}(t) = \langle M(\mu) \rangle = \frac{\sum_\mu M(\mu) \times \exp(-\epsilon(\mu)/t)}{\sum_\mu \exp(-\epsilon(\mu)/t)}, \tag{10}$$

and the scaled susceptibility can be obtained from the fluctuation relation

$$\chi = \frac{N}{k_B T} \times \left(\langle M(\mu)^2 \rangle - \langle M(\mu) \rangle^2 \right) = \frac{1}{J} \times \frac{N}{t} \left(\langle M(\mu)^2 \rangle - \langle M(\mu) \rangle^2 \right), \tag{11}$$

where

$$\langle M(\mu)^2 \rangle = \frac{\sum_\mu M(\mu)^2 \times \exp(-\epsilon(\mu)/t)}{\sum_\mu \exp(-\epsilon(\mu)/t)}. \tag{12}$$

3 Sampling Algorithm

Metropolis importance sampling Monte Carlo method is used to flip the spins:

Step 1 Initialize the lattice and choose a scaled temperature parameter t.

Step 2 Randomly choose a site x and flip it.

Step 3 Compute energy change ($\Delta\epsilon$) before (ϵ^{old}) and after (ϵ^{new}) the spin at site x is flipped.

Because only nearest-neighbor interactions are considered, flipping spin x would merely influence ϵ_x, ϵ_b and ϵ_l, where b and l denote the spin sits below and left to site x, respectively. So we actually calculate and $\Delta\epsilon = (\epsilon_x^{new} + \epsilon_b^{new} + \epsilon_l^{new})/N - (\epsilon_x^{old} + \epsilon_b^{old} + \epsilon_l^{old})/N$.

Step 4 Generate a random number r such that $0 < r < 1$.

Step 5 If $r < \exp(-N \times \Delta\epsilon/t)$, accept this spin-flip and record $\epsilon^{new} = \epsilon^{old} + \Delta\epsilon$; else flip spin x back and record $\epsilon^{new} = \epsilon^{old}$.

Step 6 Go to **Step 2** until equilibrium is reached.

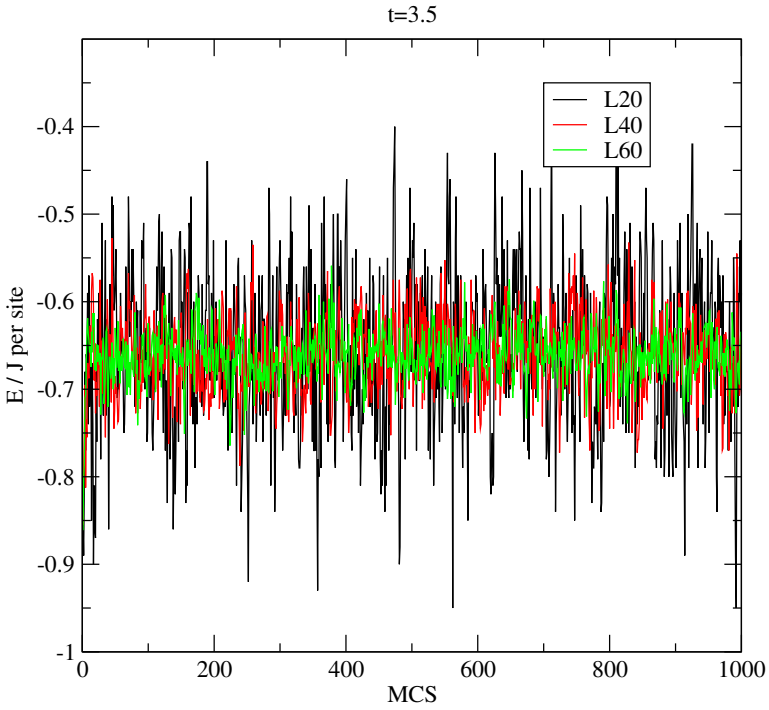

Figure 1: Dependence of the data on lattice size and on the length of runs in MCS.

4 Calculation Details

4.1 Monte Carlo step/site

The standard measure of Monte Carlo time is the Monte Carlo step/site (MCS) which corresponds to the consideration of every spin in the system once. Approximately, every site would be hit once after $N = L \times L$ draws because we randomly and equally choose a spin in the entire lattice to flip. One MCS is equivalent to N spin-flip trials. Figure 1 shows the influence of length of MCS runs on the simulated data. We can clearly see that the system gets into equilibrium very quickly. In the calculations, we run 1000 MCS in total, and throw away the first 200 MCS runs.

4.2 Numerical differentiation

We use a simple two-point formula to compute the slope of a nearby secant line through the points $(t_{i-1},\ f(t_{i-1}))$ and $(t_{i+1},\ f(t_{i+1}))$

$$f'(t_i) = \frac{f(t_{i+1}) - f(t_{i-1})}{t_{i+1} - t_{i-1}} \tag{13}$$

4.3 Coding Details

The sampling is done in code `pb3v5.c`, which contained two outputs:
`out1.dat`: scaled temperature parameter (t), lattice size (L) and number of MCS.
`lattice.dat`: spin configuration (optional).
Scaled internal energy, magnetization, specific heat and susceptibility are printed to the screen.
`void initial(int *ptl, float p)` is used to create a lattice of randomly arranged spins at a given temperature. Input `p` is the percentage of spins up.
`double fepx(int *ptl, int x)` returns the value of ϵ_x as defined in Eq. 4.
`double fep3(int *ptl, int x)` returns the value of sum $(\epsilon_x + \epsilon_b + \epsilon_l)/N$.
`double fdep(int *ptl, int x)` flips spin x and returns $\Delta\epsilon$.
`double fmag(int *ptl)` returns $M(\mu)$. This function is only called once at the beginning of the

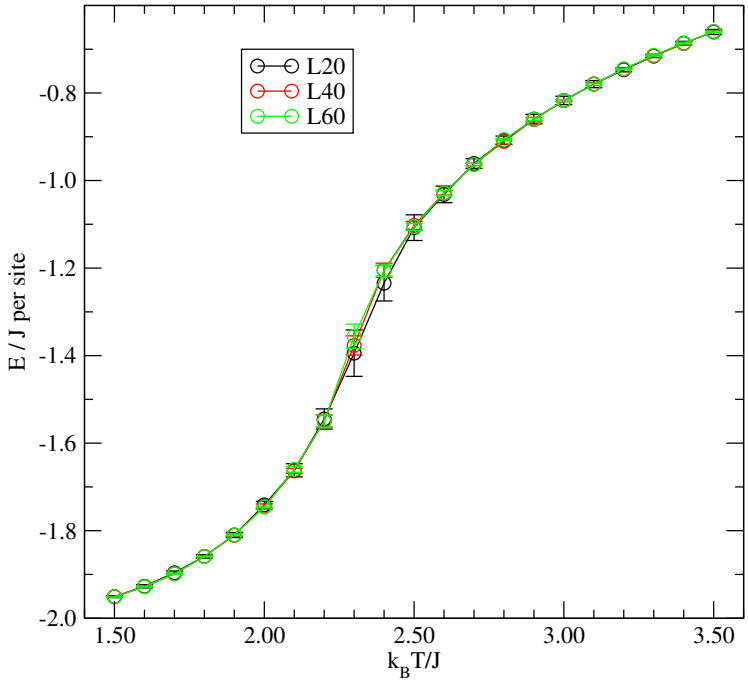

Figure 2: Temperature dependence of the internal energy for different lattice sizes.

calculations. Because the change in magnetization can only be +2 or -2, so we keep track of the spin-flip and magnetization of last step..

5 Results and Discussion

First, from Figure. 2 we can see that at low temperature, the internal energy per site is very small. When temperature increases to some certain value, the internal energy per site changes dramatically. The lattice size does not influence the internal energy per site. Figure. 3 gives similar results. The magnetization drops from nearly 1 to almost zero in region 2.1 - 2.4. By applying numerical differentiation or computing from fluctuations of internal energy, we obtain specific heat per site. The results obtained from these two methods are in good agreement. We can also see from Figure 4 that although the lattice sizes are different, the three curves reach their maximum value at the same temperature point 2.3. In Figure. 5, susceptibility takes its maximum value at around 2.4.

To find out the real critical temperature, we run more simulations with a finer temperature grid. The results are plotted in Figure. 6. Because the error bars are relatively big around the critical temperature. It's hard to say when we get the maximum value of specific heat. The critical temperature should be in region 2.29 - 2.31 from Figure. 6,which should be valid for infinite square lattice.

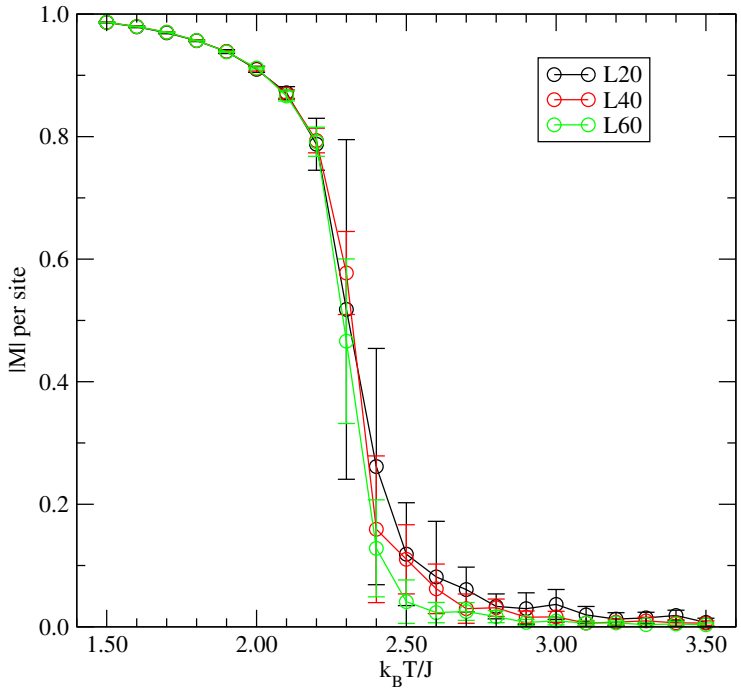

Figure 3: Temperature dependence of the magnetization for different lattice sizes.

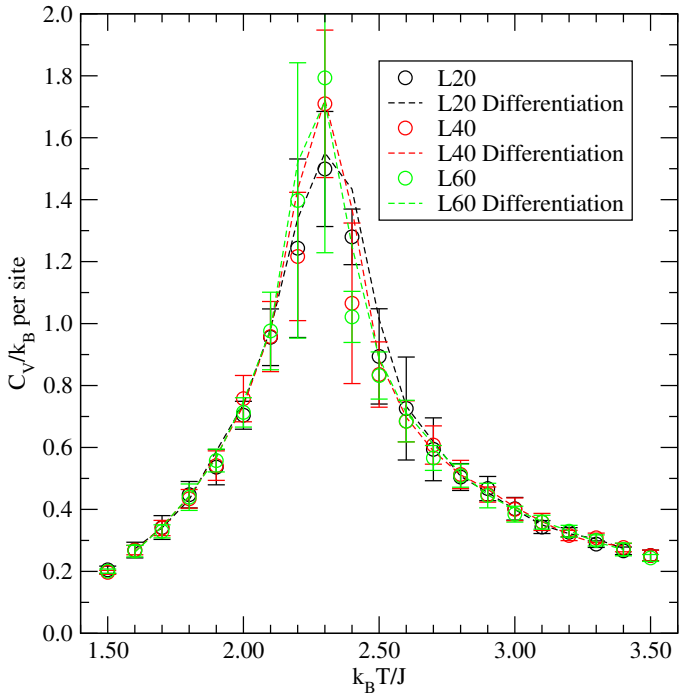

Figure 4: Temperature dependence of the specific heat for different lattice sizes. The circles present results calculated from fluctuations of the internal energy; the dash lines present results calculated by numerical differentiation.

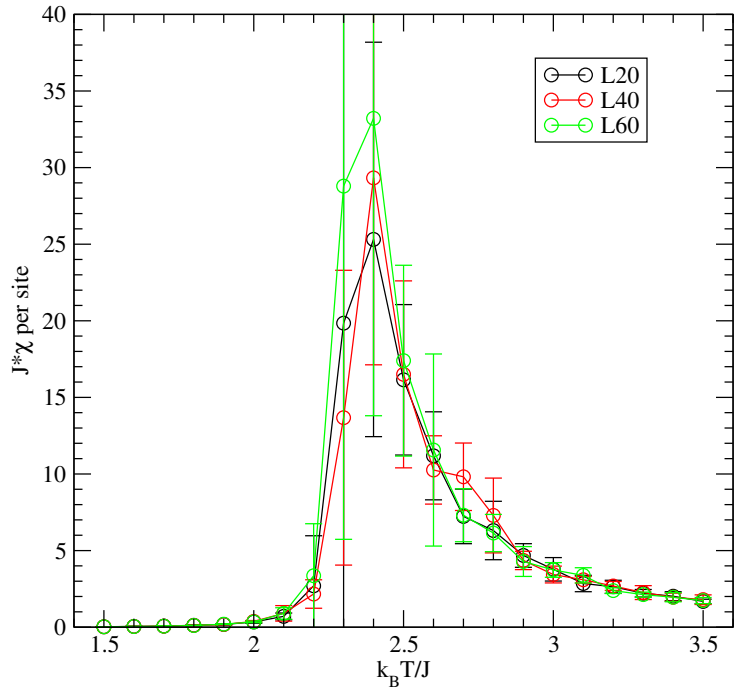

Figure 5: Temperature dependence of the susceptibility for different lattice sizes.

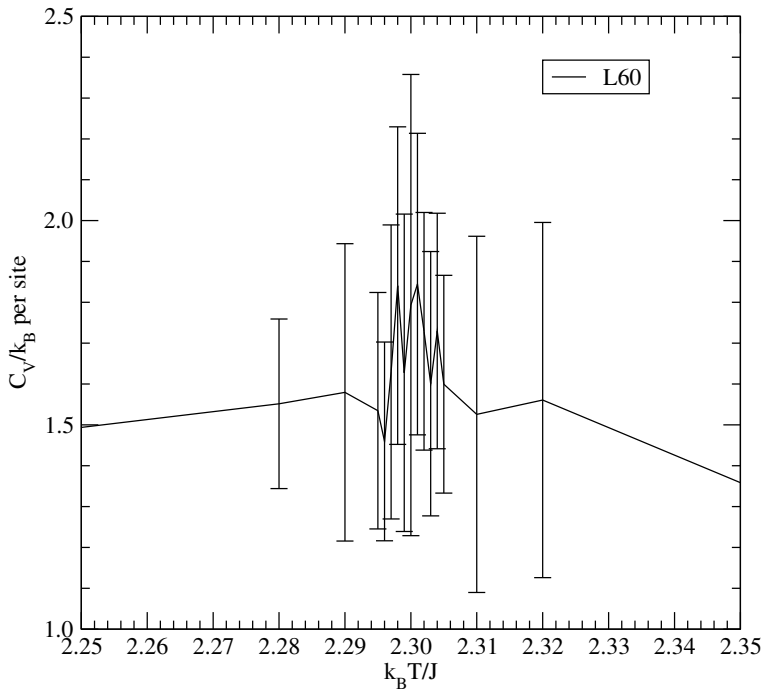

Figure 6: Specific heat near critical temperature.

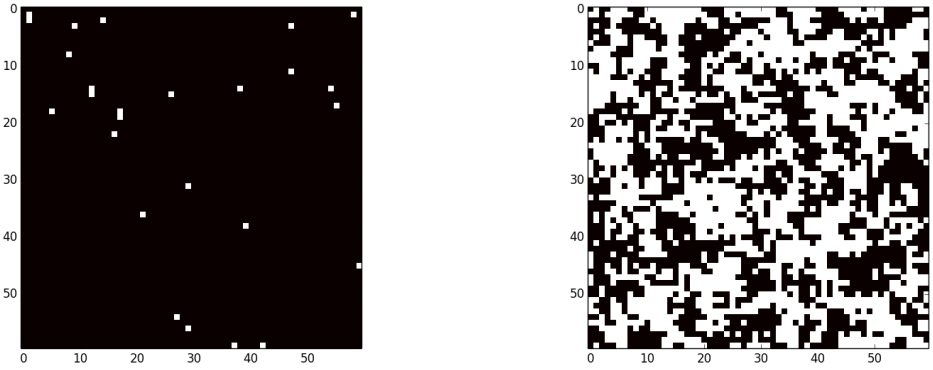

Figure 7: Left panel: configuration at t=1.5; right panel: configuration at t=3.5.

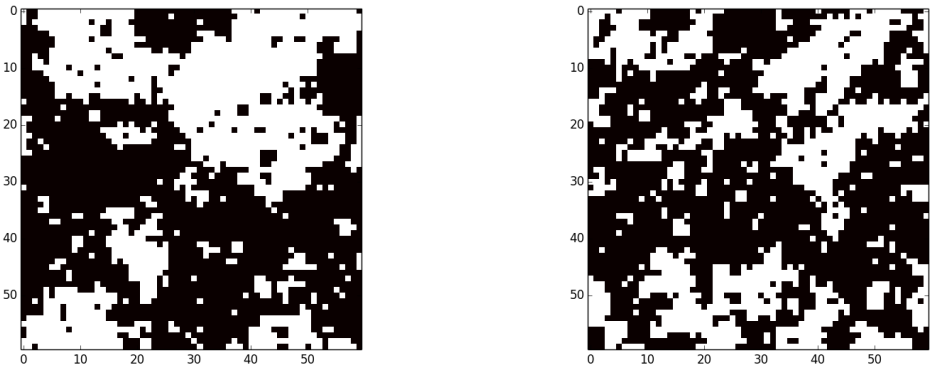

Figure 8: Left panel: configuration at t=2.3 (close to critical temperature); right panel: configuration at t=2.5 (slightly away from the critical temperature).