Research on Diluted Ising Model

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In this problem, I have studied the 2D diluted Ising model. We looked the bahaviors of site energy e, magnetization m, site density n, specific heat C, susceptibility χ, compressibility κ and Binder ratio Q versus temperature for different system sizes. Also, the critcal temperature for para-ferro magnetic phase transition Tc has been determined and finite-size scaling behaviors near Tc has been investigated. Also, I compared the obtained results with the standard 2D Ising model.

Introduction and Theory

In this report, I will study the 2D diluted Ising Model, which the spins can have three states, +1,-1 and 0. Because the spin can be zero, so the number of spin-occupied sites can be changing, thus we will apply grand-canonical ensemble statistics to do the measurements. For this Model, the Hamiltonian can be written as

$$H = -J \sum_{<i,j>} \sigma_i \sigma_j ; \sigma = -1, 0, 1$$

Here we use J=1, which is a Ferromagnetic Ising Model. Next, let's discuss about some messurements of physical properties of this model. As discussed above, N is not fixed, hence we can calculate the particle density $n = < N > /V$ and its fluctuation. Also the compressibility κ can be de

ned as the response of the particle density to a chemical potential μ and is given by the fluctuation of the particle number;

$$\kappa = \frac{1}{T}\frac{1}{V}(< N^2 > - < N >^2)$$

For susceptibility χ, and specific heat c, they are difined as:

$$\chi = \frac{1}{T}\frac{1}{V}(< M^2 > - < |M| >^2)$$

$$c = \frac{1}{T^2}\frac{1}{V}(< E^2 > - < E >^2)$$

We will also be interested in the Binder ration,

$$Q = \frac{< M^2 >}{< |M| >^2}$$

as a way to locate the phase transition through the crossing points for Q versus T for different L.

Data and Analysis

I wrote a Metropolis Monte Carlo program to do simulation on periodic L*L lattices, which L=4, 8, 16, 32, 64. I quenched temperature from 3.0 to 1.0 with a step of 0.02, also, I used 30 bins to do binaverage, and at each temperature the Monte Carlo steps I applied are 5000. In the following, I will present the analysis of the data I got.

1. Energy and Specific heat

As shown in Fig.1, the energy decreases with the temperature, and at the limit T→ ∞, the energy becomes -2, which concides with our prediction(the lowest energy happens when all the spins will point to one direction). From Fig.2, we can see the specific heat vs temperature curve has a peak, and the peak increases as the system size increases, from which we can predict that the specific heat will diverge if the system size goes to infinity.

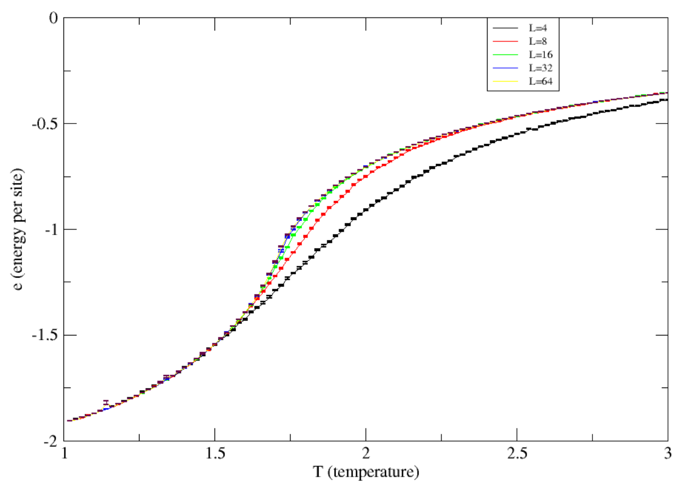

FIG. 1: Average energy per site $< e(T) >$ versus tmperature for different system sizes(with error bar).

2. Magnetization and Susceptibility

As shown in Figure 3 and 4, we plot the behavior of magnetization m and susceptibility χ versus temperature for different system sizes. Here we use logarithmic y-axis for more clearer view for behavior of χ.

As we can see, as T goes to very high, magnetization m will go to zero and as T goes to zero, m will go to 1. At T near Tc, we observed a paramagnetic to ferromagnetic phase transition behavior and as L increases, the transition edge becomes sharper. For the susceptibility, the increasing rate near critical temperature is very high and shows a behavior of divergence.

3.Density and Compressibility

Fig.5 and Fig.6 showed the behavior of site density and compressibility versus temperature. From Fig.5 we can see that as T$\rightarrow\infty$, n$\rightarrow \frac{2}{3}$, which can be predicted by equal partitional theory at high-T equilibrium state. Also, as T $\rightarrow$ 0, n$\rightarrow$1, which shows that as T approches to zero, all the sites tend to be occupied and the spins point to the same direction. Also, similiar to the behavior of specific heat and susceptibility, we can predict that as L $\rightarrow\infty$, the compressibility κ will diverge.

4.Binder ratio

At T=Tc, Binder ratio should be independent of L for large L, so that all the curves of binder ratios will cross over each other at the same point, which will help us to locate Tc. Fig.7 showed the curve of Binder ratio Q versus temperature T for different system sizes. From the crosspoint, we can get Tc/J 1.7.

5. Critical Temperature

The critical temperature for standard 2D Ising Model is Tc/J 2.27, but as now we are considering diluted Ising model, we need to consider J_{eff} instead of J. We can estimate that J_{eff} should be proportional to $n(T)^2$, if we take the middle point of site density , which is n=0.83, we can found J_{eff}=0.64*J, thus the Tc_{eff}/J is approximately 1.57. In order to locate Tc from the data I got, I can either use Binder ratio crossing or we can get it from the curve of specific heat and susceptibility. From Binder ratio crossing, I found Tc/J 1.70, while Tc/J 1.70 and Tc/J 1.72 from the behavior of specific heat and susceptibility correspondingly. From these, we can see that the approximate Tc we get from J_{eff} is close to the value I got from the data.

6. Finite size scaling

From finite-size scaling theory prediction, we know that for finite size system with size L, the peak value of susceptibility show power-law behavior χ L^{γ}. Now we can plot peak value for susceptibility for different system sizes(as shown in Figure 8). From which we can see in double ln coordinates, χ shows approximately linear behavior versus system size L. The slope of the linear fitting is 1.6346. For standard Ising model, the predicted value for finite-size scaling is γ=4/7. Our value for γ is smaller, but close to 1.75.

Fig.8 shows the behavior of C vs. ln(ln(L)), where c is the maximum value of specific heat at each L. Suprisingly, unlike the 2D normal Ising Model C vs L doesn't show a linear behavior but it's C vs.ln(ln(L)) , however this result is accordance with some results from

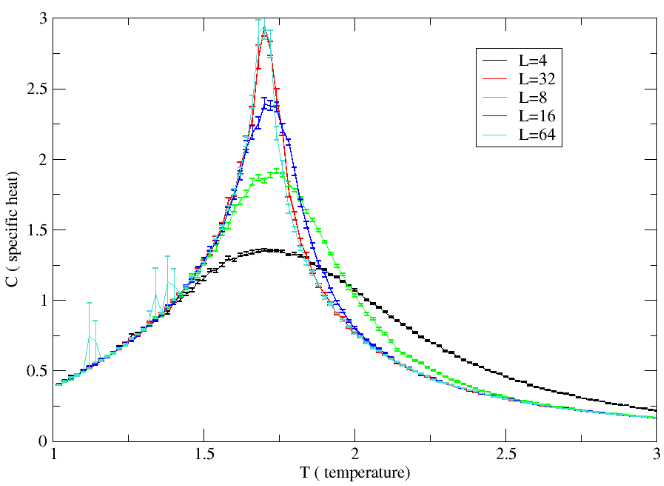

FIG. 2: Specific heat per site c versus temperature T for different system sizes(with error bar).

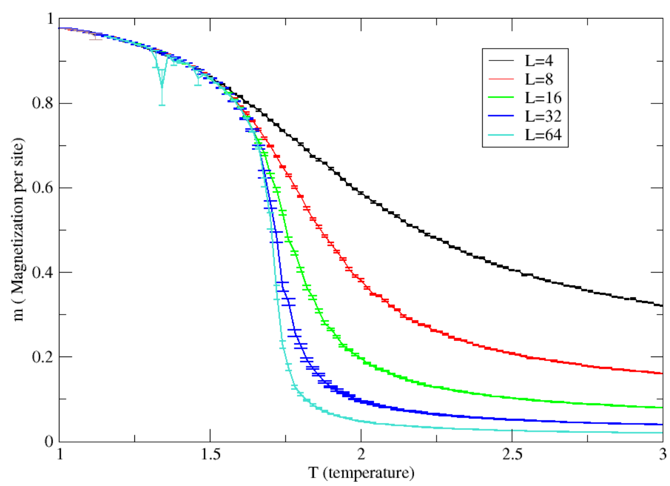

FIG. 3: Magnetization per site m versus temperature T for different system sizes(with error bar).

previous literatures(PRL 72(1994)2785).

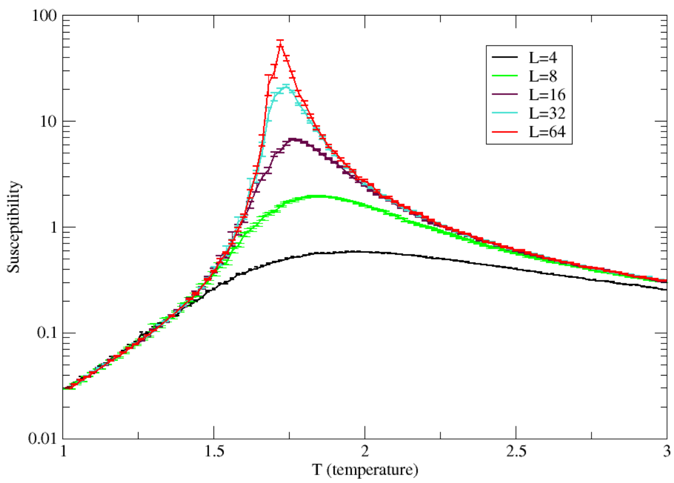

FIG. 4: Susceptibility χ per site versus temperature T for different system sizes(with error bar).

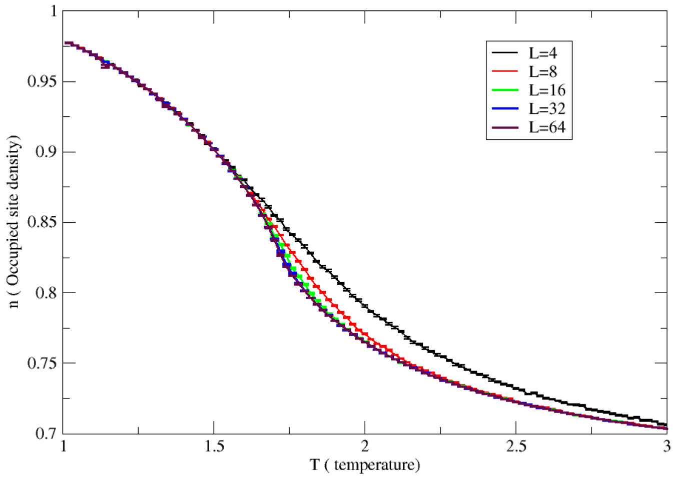

FIG. 5: Site density n versus temperature T for different system sizes(with error bar).

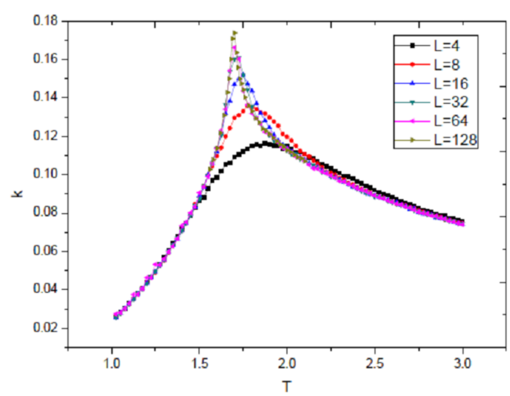

FIG. 6: Compressibility κ per site versus temperature T for different system sizes(with error bar).

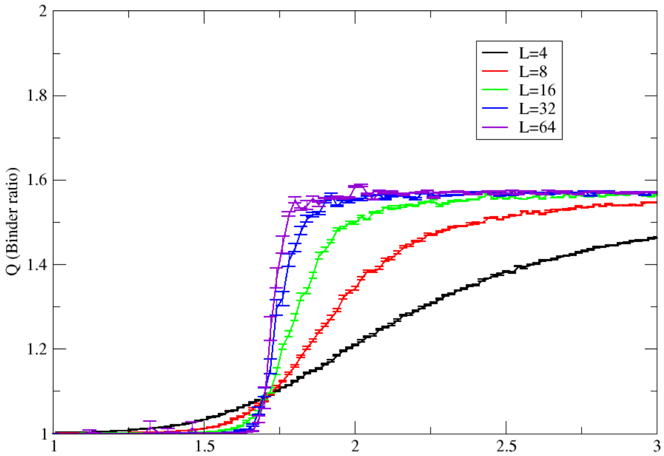

FIG. 7: Binder ratios Q versus temperature T for different system sizes(with error bar).

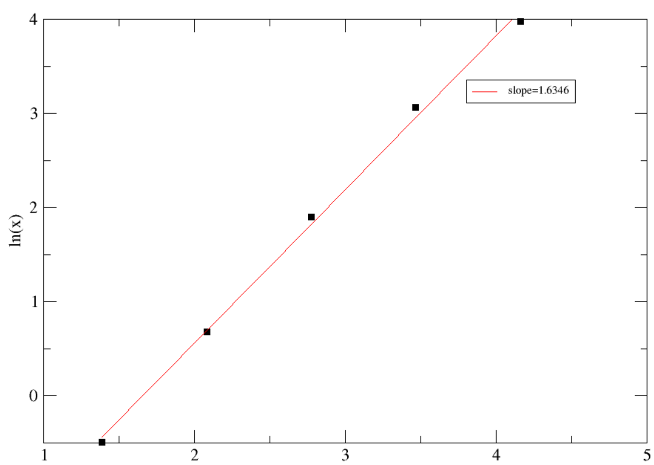

FIG. 8: ln(x)vs.ln(L).

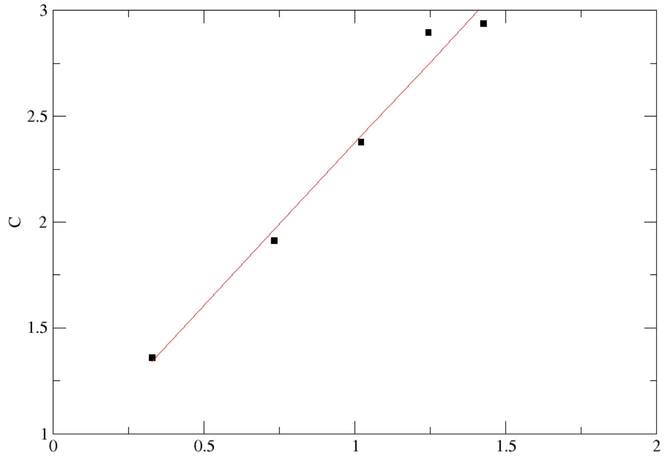

FIG. 9: c vs. ln(ln(L))