Assignment 2

Mainak Roy (20PH20020), Yash Rana (20PH20045), Govind Wanjalkar (20PH20047), Edwin Somy (20PH20012)

November 14, 2024

1 Preliminary note

For ease of implementation, we define $k_B = 2$ and J = 1. This means we get half the critical temperature value that is quoted in the literature. This is not an issue though, it is simply a choice of units.

The simulation code was written in C++. Below we have provided only the numerical results. The plots can be seen in the cpp_analysis.ipynb file.

2 Datasets used

Three datasets were created for the assignment, the basic dataset and two higher resolution datasets, $zoom_ex$ and cr3, each having data for L = 16, L = 25, and L = 40. The parameters are as follows:

2.1 Basic

Equilibriation time: 10⁴ MC timesteps Autocorrelation time: 10² MC timesteps

Number of snapshots per temperature value: 10^4 snapshots Temperature values: [0.1, 4] with 40 linearly spaced values

2.2 zoom_ex

Equilibriation time: 10^4 MC timesteps Autocorrelation time: 10^2 MC timesteps

Number of snapshots per temperature value: 10⁵ snapshots Temperature values: [0.8, 1.3] with 26 linearly spaced values

2.3 cr3

Equilibriation time: 10⁴ MC timesteps Autocorrelation time: 10² MC timesteps

Number of snapshots per temperature value: 10^4 snapshots Temperature values: [1.0, 1.2] with 32 linearly spaced values

3 Histograms

The histograms are only generated for the basic dataset. From the histograms, we can see that the variance decreases as the system size increases. This makes sense because the finite size effects are disappearing as the system size increases. The energy is lowest and magnetisation is close to 1 below T_c . The energy is highest and magnetisation is close to 0 above T_c . Again, this is to be expected because of the symmetry broken phase below T_c and the disordered phase above T_c .

4 Critical temperature and exponents from finite size scaling

The finite size scaling analysis was done by first taking guesses for T_c , ν , and η , where η is the critical exponent of the quantity. Then, the data was scaled, and a 4^{th} order polynomial was fitted through it by least squares minimisation. The final answer was taken to be the set of guesses which minimised the mean least squares (that is, the least squares value divided by the number of points). Only those guesses were considered which had at least 10 data points inside the x-axis window.

The zoom_ex dataset was used for this question.

4.1 Magnetisation

Estimated values:

$$T_c = 1.135$$

$$\nu = 0.936$$

$$\beta = 0.118$$

4.2 Susceptibility

Estimated values:

$$T_c = 1.134$$

$$\nu = 0.982$$

$$\gamma = 1.734$$

4.3 Specific heat

Estimated values:

$$T_c = 1.135$$

$$\nu = 1.088$$

$$\alpha = -0.31$$

5 Critical exponents from curve fitting

The question requires us to find the exponents on both sides of T_c . We only found it on the side of T_c where the critical exponent is typically defined however (above T_c for susceptibility and specific heat, and below T_c for magnetisation).

The cr3 dataset was used for this question, because of the need of a large number of points in the critical region.

Estimated value of β : 0.071 ± 0.0005 Estimated value of γ : 1.754 ± 0.0726 Estimated value of α : -0.373 ± 0.0336

Critical exponent	Exact value	Calculated value	MFT value
α	0	-0.373	0
β	0.125	0.071	0.5
γ	1.75	1.754	1
$\overline{\nu}$	1	1.1865	0.5
δ	15	32.42	3
η	0.25	0.52	0

6 Two point function

The L=40 data from zoom_ex dataset was used for this question. At T=1.1, we fitted the points for small r (whereas the question asked us to do it for large r). This choice was forced upon us because the system size is simply not big enough for it. In any case, we have power law behaviour at T_c , so it should be fine. We got the estimated value of η as 0.2494 ± 0.0295 .

7 Bonus: Critical temperature from Binder cumulant

The critical temperature can also be estimated from the crossing point of the Binder cumulant for different system sizes. This method gave T_c as 1.132.