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Computational Physics – Exercise 2

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1 Simulating the Ising model in $d = 2$

We simulated the Ising model in $d = 2$, the code can be found at [1].

2 Numerical cost of the calculation of the energy

We know that calculating the energy of a given spin configuration involves summing over all the sites, thus the numerical cost of calculating the energy is $\mathcal{O}(\Lambda)$ for $\Lambda = N_x \times N_y$ or $\mathcal{O}(N^2)$ for $N = N_x = N_y$.

3 Numerical cost of the calculation of the change in energy

We know that to calculate the change in energy of a spin update, we only need to consider neighbouring spins which depends on dimensionality d for $N_x = N_y$ and not on the system size Λ, thus the numerical cost of calculating the change in energy is $\mathcal{O}(\lambda)$ where λ is some constant independent of system size.

4 Significance of the critical coupling

The critical coupling is point at which the average magnetization vanishes. We observer a phase transition at that point [2].

5 Estimating the average magnetization per site

We can estimate the average magnetization per site, $\langle m \rangle$ as a function of $J \in [-1, 1]$ while we hold $J = 0.5$ and $N \in [2, 4, 6, 8, 10, 12, 14, 16, 18, 20]$

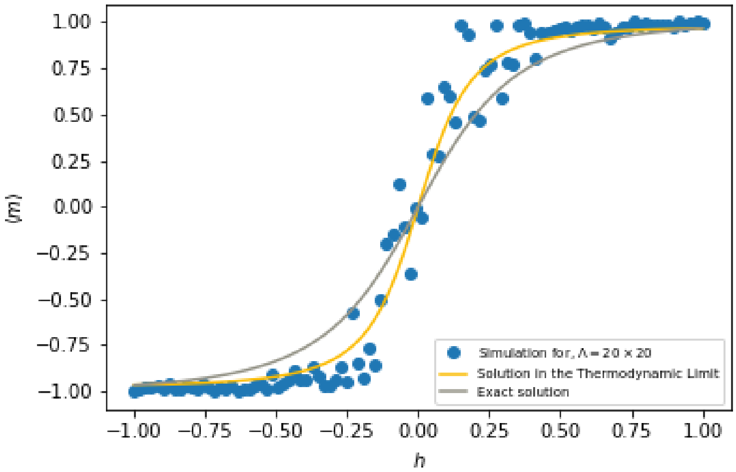

Figure 1: A plot of the average magnetization per site $\langle m \rangle$, as a function of h for $N = N_x = N_y = 20$ sites

6 Estimating the average energy per site

We can estimate the average energy per site, $\langle \epsilon \rangle$ as a function of $J^{-1}, \forall J \in [0.25, 2]$ while we hold $h = 0$ and $N \in [2, 4, 6, 8, 10, 12, 14, 16, 18, 20]$

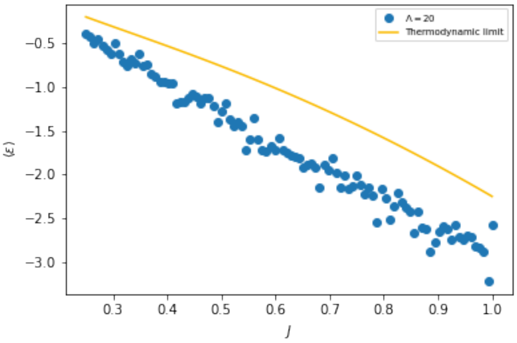

Figure 2: A plot of the average magnetization per site $\langle m \rangle$, as a function of h for $N = N_x = N_y = 20$ sites

The simulation comes close to displaying the qualitative behaviour of what we observe in the thermodynamic limit however there is a quantitative difference, we expect this to disappear as N becomes larger.

7 Estimating the absolute value of the mean magnetization

We plot for absolute value of the mean magnetization, $\langle |m| \rangle$ the versus the reciprocal of the nearest neighbour coupling, $J^{-1} \in [0.25, 1]$ in figure 3. We observe a drop in absolute magnetization as predicted at

$$J_c = \frac{1}{2} \log\left(1 + \sqrt{2}\right) \approx 0.440686793509772 \tag{1}$$

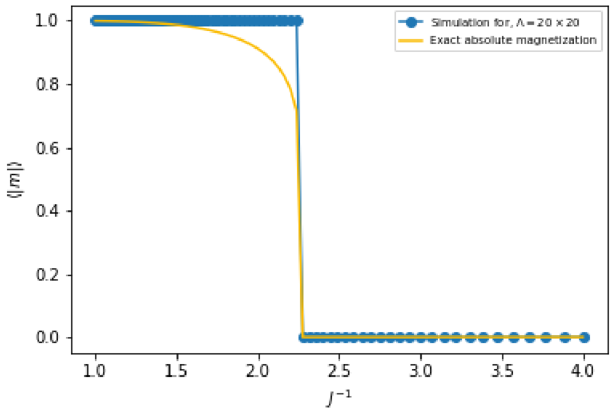

Figure 3: A plot of the average absolute magnetization per site $\langle |m| \rangle$, as a function of J^{-1} for $N = N_x = N_y = 20$ sites.

Moreover, the simulation misses this phase transition's shape and displays a sharp drop, we expected this as we know that the Hasting's algorithm is not effect near critical points. However, when we plot for mean magnetization versus the reciprocal of the nearest neighbour coupling, J^{-1} as shown in figure 4, we completely miss out on the phase transition.

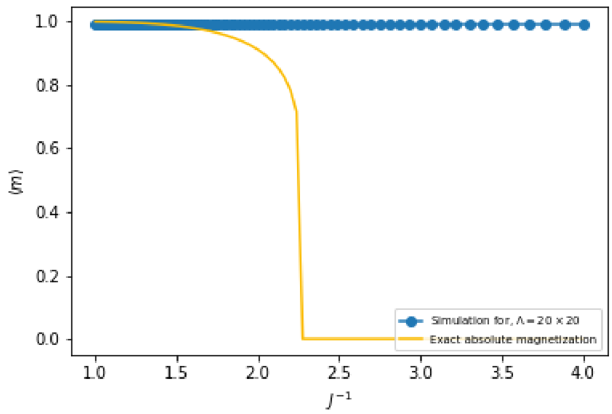

Figure 4: A plot of the average magnetization per site $\langle m \rangle$, as a function of J^{-1} for $N = N_x = N_y = 20$ sites.

8 Computing the specific heat

Specific heat is given by,

$$C = \Lambda * \left(\left\langle \epsilon^2 \right\rangle - \langle \epsilon \rangle^2\right) \tag{2}$$

and in the thermodynamic limit

$$C = \frac{4J^2}{\pi \tanh^2(2J)} \left(K\left(\kappa^2\right) - E\left(\kappa^2\right) - \left(1 - \tanh^2(2J)\right)\left[\frac{\pi}{2} + \left(2\tanh^2(2J) - 1\right) K\left(\kappa^2\right)\right]\right) \tag{3}$$

where $K(m)$ and $E(m)$ are the incomplete elliptic integral of the first and second kind, respectively, and

$$\kappa = \frac{2\sinh(2J)}{\cosh^2(2J)} \tag{4}$$

Here we plot figure 5 for C/J^2 as function J^{-1} for $J \in [0.25, 1]$ and

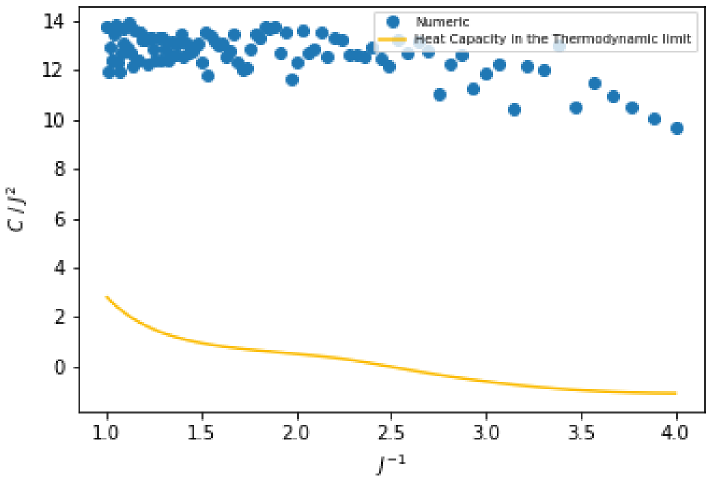

Figure 5: A plot of the scaled specific heat C/J^2, as a function of J^{-1} for $N = N_x = N_y = 20$ sites.

Although there is a quantitative difference by at least an order of of a magnitude. After some trial and error, we found that this factor is independent of N. However, if we were to subtract a constant (10 in our case) we obtained the following plot.

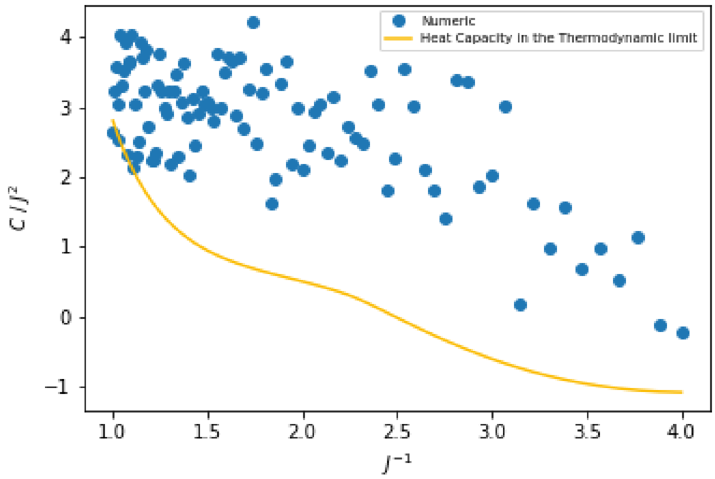

Figure 6: The plot we obtain after subtracting a constant from C/J^2 in figure 5

We think that this due to us not having a perfect Markov chain i.e. presence of correlations. In the lecture, a "autocorrelation" correction was mentioned as the cure for this. However, we were unable to find it.

References

[1] P. Anancia Devaneyan and R. K. Senthilkumar. Exercises for the Physics 760: Computational Phyics course during the WS 22/23 Term.

[2] J. Thijssen. *Computational Physics*. Cambridge University Press, 2 edition.