

# Simulation of 2-Dimensional Ising Model

Harilal Bhattarai & Marcel Schindler

November 18, 2020

## 1 Introduction

In this exercise we want to examine the Ising model in two Dimensions. We already did the Analysis in one Dimension. So we just have to expand our Analysis. After we got the Analysis part right we want to look for the magnetization per spin in dependency of the coupling  $J$ . Also we look for the average energy per site.

## 2 Theory

We can still start with the Hamiltonian:

$$H(s) = -J \sum_{\langle x,y \rangle} s_x s_y - h \sum_x s_x$$

$\langle x, y \rangle$  denotes the nearest-neighbor pair  $x$  and  $y$  on the chain,  $J$  is the coupling constant and we assume periodic boundary conditions in  $x$ - and  $y$ - axis. That means that spins couple only to the nearest neighbor and  $s_{N-1}$  couples with  $s_0$  with  $N$  the number of total spin-particles. The partition function stays the same in two dimensions:

$$Z = \sum_{s'} \exp\left(-\frac{H(s')}{k_B T}\right)$$

It is possible to examine the magnetization for  $h = 0$  analytically

$$|m| = \begin{cases} (1 - \frac{1}{\sinh(2J)^4})^{\frac{1}{8}}, & J > J_c \\ 0, & J \leq J_c \end{cases}.$$

We can also examine the energy per site analytically

$$\epsilon = -J \coth(2J) \left[ 1 + \frac{2}{\pi} (2 \tanh 2J^2 - 1) K\left(4 \frac{\tanh(2J)^2}{\cosh 2J^2}\right) \right]$$

where  $K(m)$  is the complete elliptic integral of the first kind.

For  $h \neq 0$  the analytic solution is not known yet.

### 3 Analysis

We first want to answer some important questions to write the code in a smart way. The numerical cost to calculate the energy is proportional to  $\Lambda = N_x \cdot N_y$ , Where  $N_{x/y}$  is the number of spin particles in the axis x or y. Because we look at a quadratic field of spin particles the numerical cost is  $N^2$ . On the other hand if we flip one Spin and examine the difference in energy  $\Delta S$  the numerical cost is independently of N because we have to only examine the difference to the nearest neighbours of the flipped spin. We get the formula

$$\Delta S = 2 \cdot s_{xy}(h + s_{(x+1),y} + s_{(x-1),y} + s_{x,(y+1)} + s_{x,(y-1)})$$

where x and y are the coordinates for the flipped spin. In this case we also take boundary conditions.

We saw that the magnetization depends on  $J_c = \frac{1}{2} \log(1 + \sqrt{2}) \approx 0.44069$ . If the coupling is higher than  $J_c$  then the material will start building a magnetic field without an outside source. If the coupling is smaller than  $J_c$  then the coupling is too small to start a magnetic field on its own.

In this exercise we want to use the Metropolis-Hasting algorithm. That means we do the following steps:

- 1 Choose some random spin  $s_i$
- 2 Flip the spin  $s_i = (-1) \cdot s_i$
- 3 Determine the change in energy  $\Delta S$
- 4 Metropolis-Hasting step:
  - if  $\Delta S < 0$  ACCEPT the spin flip
  - else sample  $Y \propto U(0, 1)$ 
    - \* if  $y \leq \exp\{-\Delta S\}$  ACCEPT the spin flip
    - \* otherwise REJECT the spin flip
- 5 repeat steps 1-4 for  $\Lambda$  times- This is called a "sweep" through the lattice
- 6 Make a measurement and store result  $O_1, \dots, O_{N_{meas}}$
- 7 Go back to 1

After we done these steps a few times we can estimate the observable.  $\bar{O} = \frac{1}{N_{meas}} \sum_{i=1}^{N_{meas}} O_i$ . In the following we put  $J = 0.3$ ,  $N_{x/y} = 20$  and vary h. The result of the Metropolis-Hasting algorithm is in graph 1. We see that the result looks familiar. It looks like the result from sheet 1. We also can see that with higher N we get a greater magnetization.

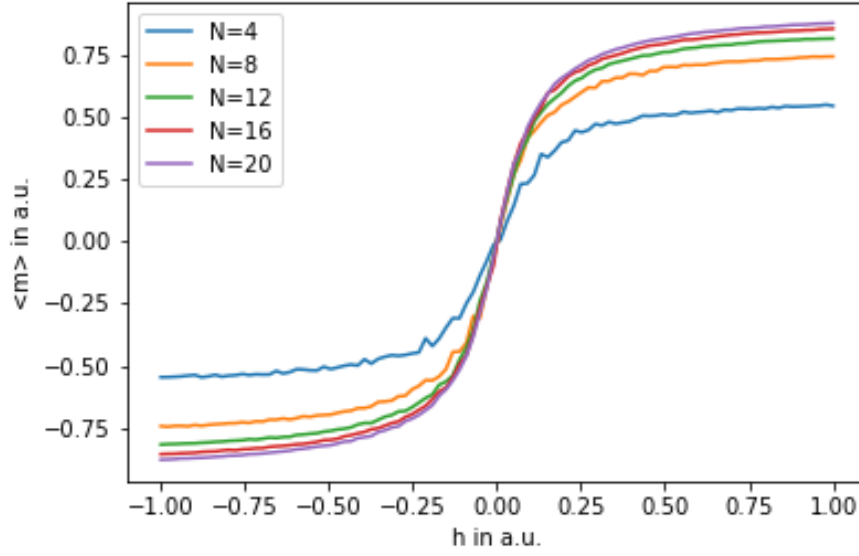


Figure 1: Magnetization dependency of  $h$ .

For the next Graph 2 we plotted the absolute value of the magnetization per particle against  $J^{-1}$ . We can see that for higher  $N$  the curve goes to the analytical one and we see for lower  $N$  the error seems to be high. In this graph the magnetization is zero until the  $J_c$  is reached. Then we see a fast rise in the magnetization. This is because with  $h=0$  an external field will only build if the coupling constant is high enough. For the graph on the right side we did not plot the absolute value. We can see that it is for higher  $J$  it is mirrored on the x-axis.

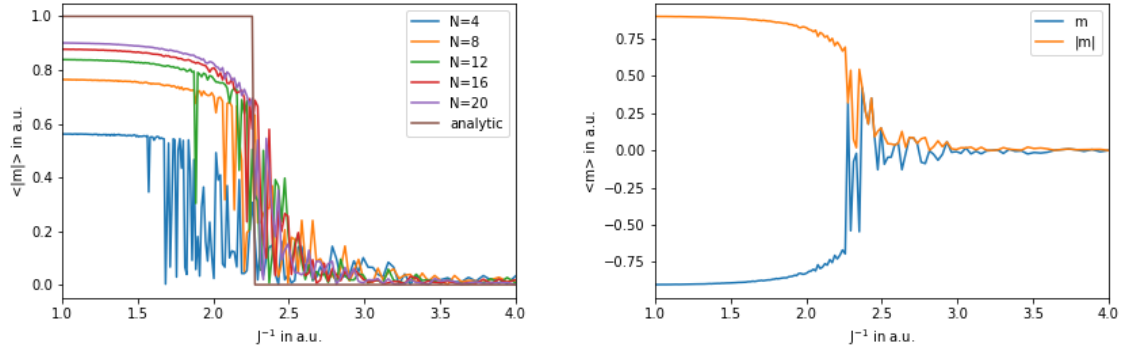


Figure 2: Magnetization dependency of  $J^{-1}$ .

For the next part we want to look at the energy per site. We plotted for different  $N$  the energy in graph 3. Again we can see with lower  $N$  the error gets higher. We can also see that until the critical coupling is reached all graphs are nearly the same. After the critical coupling we can see that the thermodynamic limit is way lower than the rest. This makes sense because the thermodynamic limit is for  $N \rightarrow \infty$  and with higher  $N$  the energy per site can get higher.

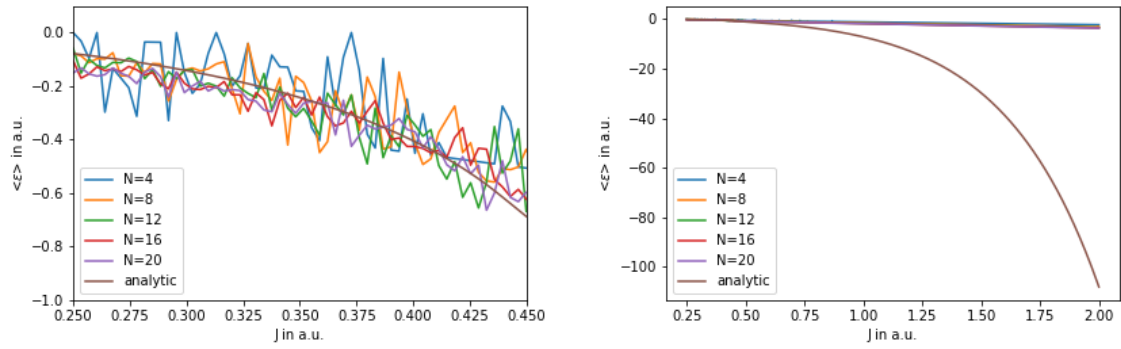


Figure 3: Energy per site compared to  $J$ .

For the extra homework we should look at the specific heat  $C = \Lambda \cdot (\langle \epsilon^2 \rangle - \langle \epsilon \rangle^2)$ . In the Graph 4 we plotted it out. We again see that we get a change in curve by  $\frac{1}{J_c} \approx 2.27$ . If  $N$  is higher we get a greater value of  $C$ .

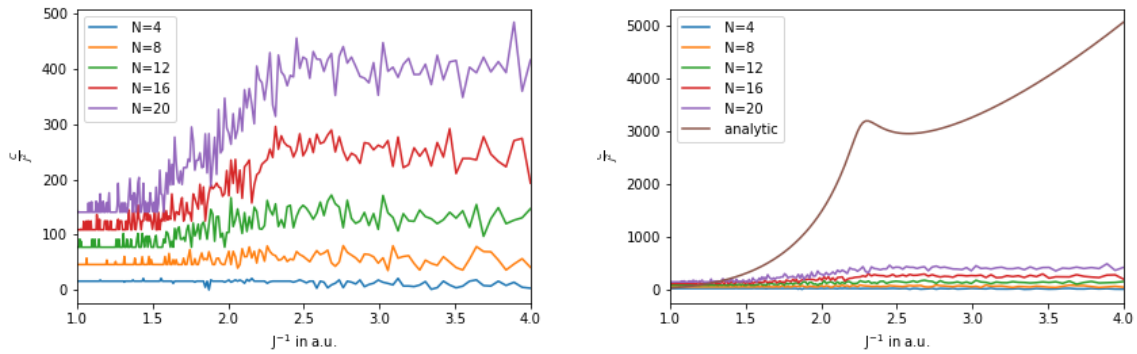


Figure 4: Specific heat

## 4 conclusion

In this exercise we saw that we get an internal magnetization if the coupling constant is high enough and we could replicate the graph from week one but now for two dimensions. Furthermore we saw that with lower  $N$  the error is a lot higher. Lastly we can see that the energy per site scales with  $\Lambda$ , so it scales with how many sites are there.

## References

- [1] Thomas Luu, Andreas Nogga, Marcus Petschlies and Andreas Wirzba, Exercise-sheet, 2020.