Exercise 02: Simulating the 2-D Ising model

Computational Physics WS20/21

Marc Vöhringer Carrera und Helen Meyer

November 18, 2020

1 Introduction

In last week's exercise we implemented the Ising model in one dimension and calculated the average magnetization per spin $\langle m \rangle$. Now we want to do the same thing for a two-dimensional lattice with $N_x \cdot N_y$ spin sites. The Hamiltonian for this system

$$\mathcal{H}(\mathbf{s}) = -J \sum_{\langle x,y \rangle} s_x s_y - h \sum_x s_x \tag{1}$$

is the same as for one dimension with the coupling constant J and the coupling to an external magnetic field h. However in two dimensions, each spin has four nearest neighbours. We again assume periodic boundary conditions. In the following, we want to calculate not only the average magnetization per spin as a function of the coupling h, but also the average of the absolute value of the magnetization and the average energy per spin as a function of the coupling constant J, using importance sampling when implementing the Ising-model.

2 Importance sampling: Metropolis-Hastings-Step

In the last exercise we have seen, that the random sampling of spin configurations yields good results only for a small number of sites N. In order to solve this problem in two dimensions, we implement something called importance sampling. First, we randomly generate a spin configuration $\mathbf{s}$. Now, randomly choose one spin $s_{i,j}$, flip it and calculate the change in energy ΔS, which is

$$\Delta S = \mathcal{H}(s_{1,1}, ... - s_{i,j}, ...s_{N_x,N_y}) - \mathcal{H}(s_{1,1}, ...s_{i,j}, ...s_{N_x,N_y}) \tag{2}$$

$$= 2s_{i,j} \cdot \Big(h + J(s_{(i-1) \pmod{N_x},j} + s_{i,(j-1) \pmod{N_y}} + s_{(i+1) \pmod{N_x},j} + s_{i,(j+1) \pmod{N_y}})\Big) . \tag{3}$$

The modulo ensures the periodic boundary condition. Then we generate a number y between 0 and 1 randomly and check, if $y < \exp(-\Delta S)$. If yes, we accept the spin flip, otherwise we reject it. Doing that $\Lambda = N_x \cdot N_y$ times is called a sweep through the lattice.

2: *The numerical cost for the calculation of the energy of a system with $\Lambda = Nx \cdot Ny$ spin sites scales proportionally with Λ. For the interaction term we have to perform 2Λ calculations (because each site has four nearest neighbours). For the term porportional to h we calculate another Λ times.*

3: *The calculation of the change in energy ΔS is independent of the system size Λ, as only the coupling to the four nearest neighbours and of course the site itself is affected by the spin flip.*

When simulating the Ising-model, we first want to thermalize the system, meaning we generate a random spin configuration and sweep through that N_{therm} times. Then we start with our first measurement and sweep once through the lattice. After that we calculate

$$m = \frac{1}{N_x N_y} \sum_k s_k \tag{4}$$

$$\epsilon = \frac{1}{N_x N_y} H(\mathbf{s}). \tag{5}$$

By measuring N_{meas} times and averaging over all measurements we get the average magnetization per spin $\langle m \rangle$, the average absolute magnetization $\langle |m| \rangle$ per spin (when summing over $|m|$) and the average energy $\langle \epsilon \rangle$ per spin.

3 Thermodynamic limit

The 2d Ising model exhibits a thermal phase transition at a critical coupling

$$J_c = \frac{1}{2} \log\left(1 + \sqrt{2}\right) \tag{6}$$

when $h = 0$.

4: *The critical coupling J_c corresponds to a critical temperature at which the spin system transitions from an unordered system ($J \leq J_c$) to an ordered one ($J > J_c$). Ordered meaning here, that all spins point in the same direction, whereas in an unordered system the spins point randomly in any direction (which is the case for high temperatures).*

There has also been determined an exact solution for absolute magnetization per site and energy per site for $h = 0$:

$$|m| = \begin{cases} \left(1 - \frac{1}{\sinh^2(2J)}\right)^{1/8} & \forall J > J_c \\ 0 & \forall J \leq J_c \end{cases} \tag{7}$$

$$\epsilon = -J \coth(2J) \left(1 + \frac{2}{\pi} \left(2 \tanh^2(2J) - 1\right) K(4 \operatorname{sech}^2(2J) \tanh^2(2J)\right), \tag{8}$$

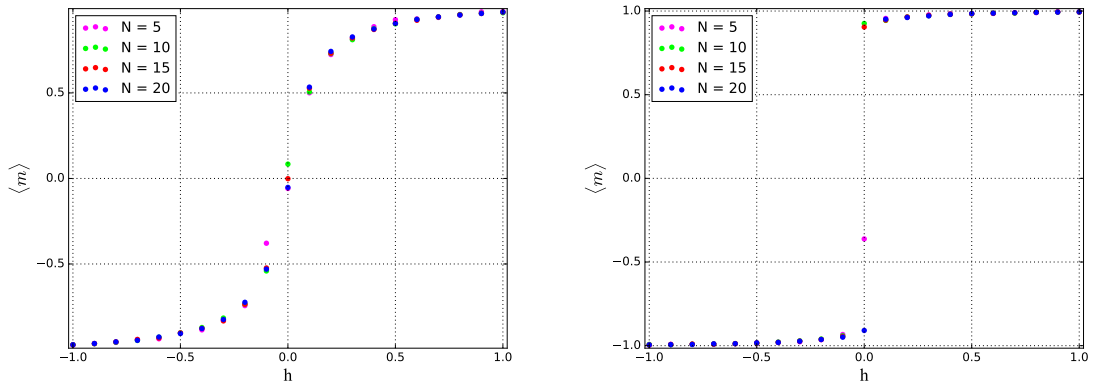

Figure 4.0.1: Average magnetization per spin $\langle m \rangle$ as a function of external coupling h. Left: $J = 0.3 < J_c$, Right: $J = 0.5 > J_c$ for different N.

with $K(x)$ the complete elliptic integral of the first kind.

4 Results

Having implemented the importance sampling and the sweep through the lattice in `ising2d.py`, we want to first calculate the average magnetization per spin $\langle m \rangle$ as a function of the external coupling $h \in [-1, 1]$ for a fixed value of J. We choose $N_{\text{therm}} = N_{\text{meas}} = 500$.

The results can be seen in Fig. (4.0.1). What is interesting to see, is the influence of the coupling J: For $J < J_c$ the system is unordered, so even for small h not all spins point in the same direction. The average magnetization is therefor not strictly either 1 or -1 as is the case for $J > J_c$.

Secondly, with the same values for N_{therm} and N_{meas}, we want to calculate the average absolute value of the magnetization per spin and the average energy per spin as a function of the coupling J for $h = 0$ and compare the results to the exact solution obtained from equation (7).

As can be seen in Fig. (4.0.2) the results obtained for $\langle \epsilon \rangle$ fit very well to the exact solution. However especially for large N and J, there are some points that do not fit in. In Fig. (4.0.2) there are two simulations shown and we can see, that the points that deviate are random. We suppose there is a problem in the algorithm, where for large N and J sometimes a random spin configuration is generated for which the Metropolis-Hastings-Step does not work well.

A similar problem can be seen in Fig. (4.0.3), where for large N random points deviate from the exact solution for large J. This problem might be solved by increasing the number of measurements or N_{therm}.

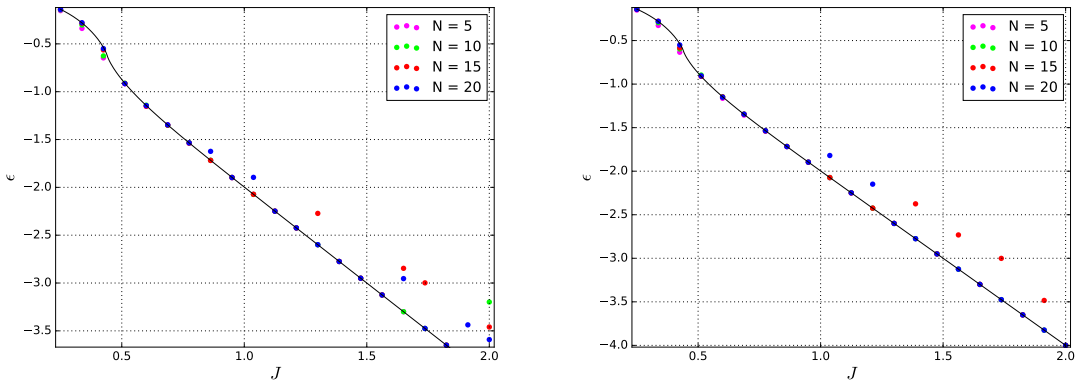

Figure 4.0.2: Average energy per spin $\langle \epsilon \rangle$ as a function of coupling J for $h = 0$. Black line is the exact solution.

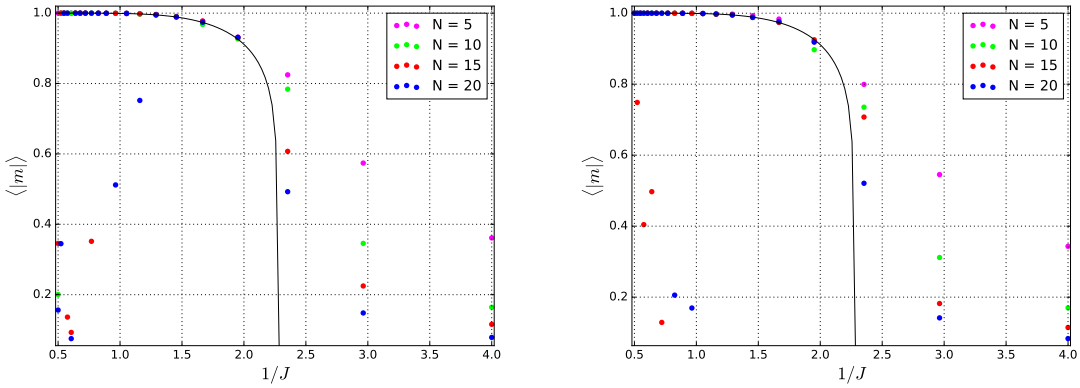

Figure 4.0.3: Average absolute magnetization per spin $\langle |m| \rangle$ as a function of coupling J for $h = 0$. Black line is the exact solution.

Otherwise the results fit very well to the exact values, at least for $J > J_c$. For $J < J_c$ the average absolute value of the magnetization does not drop immediately to zero as is the case in the exact solution. However we can see, that for larger N this deviation is smaller. This is expected as the exact solution was calculated for a system where $N \to \infty$.

If we would plot $\langle m \rangle$ instead of $\langle |m| \rangle$ against $1/J$, we would see very little as for $h = 0$ $\langle m \rangle$ is zero.