Computational Physics
Excercise 1

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1 Intro

The Ising model consists of a lattice of sites x with spins $s_x \in \{\pm 1\}$ attached. In the 1-dim Ising model, the lattice reduces to a simple chain. Each spin couples to its neighbouring spins and an external magnetic field. Thus the Ising Hamiltonian of a spin configuration $s = \{s_x : \forall x\}$ is:

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

were $\langle s_x, s_y \rangle$ denotes a pair of neighbouring spins. For more information on the Ising model, please refer to the exercise sheet or the relevant literature.

2 Task 1

In the Ising model J is a coupling strength between to neighbouring spins. A positive value means that spins aligned in the same direction are energetically favorable. A negative value makes neighbouring spins aligned in opposite direction energetically favorable. For negative values the material is diamagnetic, for positive para- or ferromagnetic.

3 Task 2

Periodic boundary conditions mean that the first spin neighbours the last.

4 Task 3

We have implemented the Ising model by writing functions that can calculate the Ising Hamiltonian and the corresponding Boltzmann factor for any given spin configuration. The exact partition function Z of the 1-dim Ising model with N spins is then calculated by summing the Bolzmann factors of all possible spin configurations.

$$Z = \sum_s \exp\left(-\frac{\mathcal{H}(s)}{k_B T}\right) \tag{2}$$

The expectation value of an observable is the sum of the observable weighted with its Boltzmann factor over all possible spin configurations, devided by the partition function.

$$\langle O \rangle = \frac{\sum_s O(s) \exp\left(-\frac{\mathcal{H}(s)}{k_B T}\right)}{Z} \tag{3}$$

The observable that we want to study is the expected magnetization per spin:

$$\langle m \rangle = \frac{T}{N} \frac{\partial \log Z}{\partial h} = \frac{\langle \sum_{s_x=s_0}^{s_N} s_x \rangle}{N} \tag{4}$$

This can be exactly calculated numerically by actually performing the sum over all possible spin configurations. In the 1-dim Ising model, the partition function Z can alternatively be calculated analytically:

$$Z = \lambda_+^N + \lambda_-^N \quad ; \quad \lambda_\pm = e^{\frac{J}{T}} \left(\cosh\left(\frac{h}{T}\right) \pm \sqrt{\sinh^2\left(\frac{h}{T}\right) + e^{-4\frac{J}{T}}} \right) \tag{5}$$

As one can see in equation 5 the relevant dimensionless ratios for this problems are $\frac{J}{T}$ and $\frac{h}{T}$.

We have plotted both exact solutions in figure 1 to show that they are indeed equivalent, except that the analytic solution has a much shorter runtime. Figure 1 also includes the analytic solution in the thermodynamic limit $N \to \infty$.

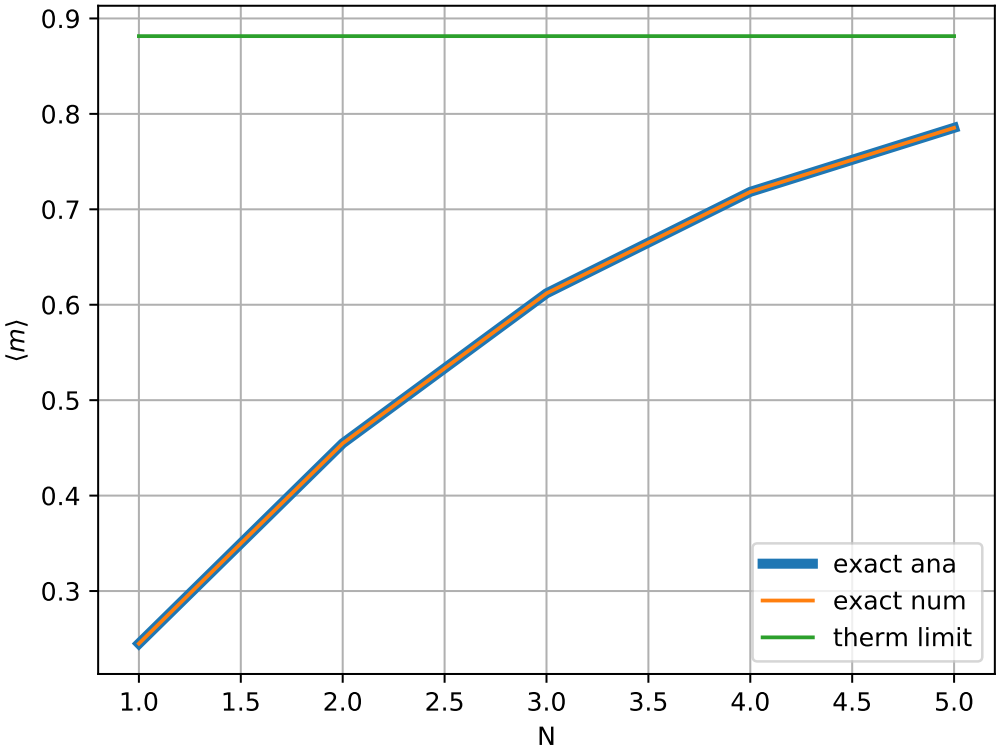

Figure 1: Comparison of the analytical and numerical exact solution.

The solution (for fixed N) can also be approximated by a Monte-Carlo simulation. In this case one does not sum over all possible spin combinations in equations 2 and 3, but over a number of randomly sampled spin configurations. For N spins we decided use 2^{N+1} samples for each Monte-Carlo simulation. For much lower amounts of samples the simulations do not give meaningful results. Since the exact (numerical) solution only includes 2^N different spin

combinations and therefore has a better runtime while also being exact, a brute force Monte-Carlo simulation is obviously a bad choice.

Performing the Monte-Carlo simulation and calculating the exact solution for various N and fixed $h = 0.25$ results in the plot of figure 2. Additionally we plot the average of 10 such Monte-Carlo simulations and use their standard deviation as an error estimate. This is shown in the plot as a shaded area. One can see that the MCs roughly follows the exact solution. It rises slowly and approaches the (constant) thermodynamic limit solution for large N.

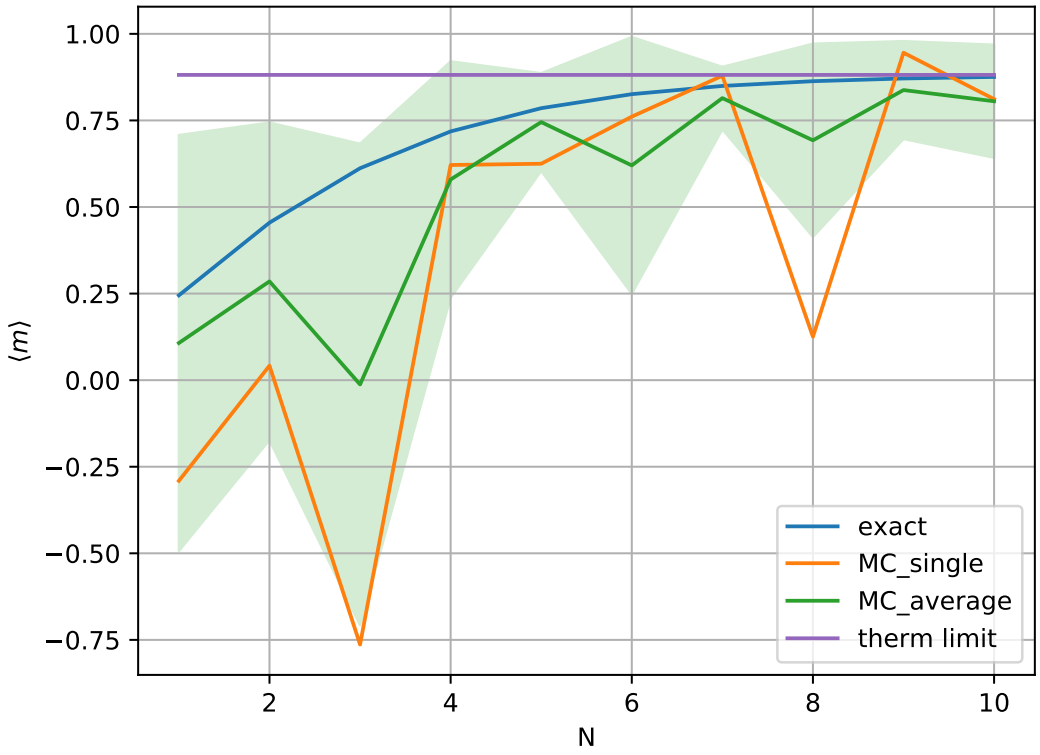

Figure 2: Dependence of the magnetization on N

In order to study the influence of h on the results, we plot both the exact and the Monte-Carlo solution for various values of h from -1 to $+1$ and fixed $N = 10$ (see figure 3). Again we plot the average of 10 Monte-Carlo simulations and use their standard deviation as an error estimate.

Since we used $N = 10$ for this plot the thermodynamic limit is already almost indistinguishable from the exact solution.

We also created a 2d-plot of the exact and Monte-Carlo simulated solution with varying values for N and h to get a better overview. These are shown in figures 4 and 5. For $h = 0$ the average magnetization is 0, which is expected, since in this case the problem is symmetric in the direction of spin quantization. For positive h the average magnetization get shifted to positive values and for negative h to negative values. This shift is stronger for larger amounts of spins J.

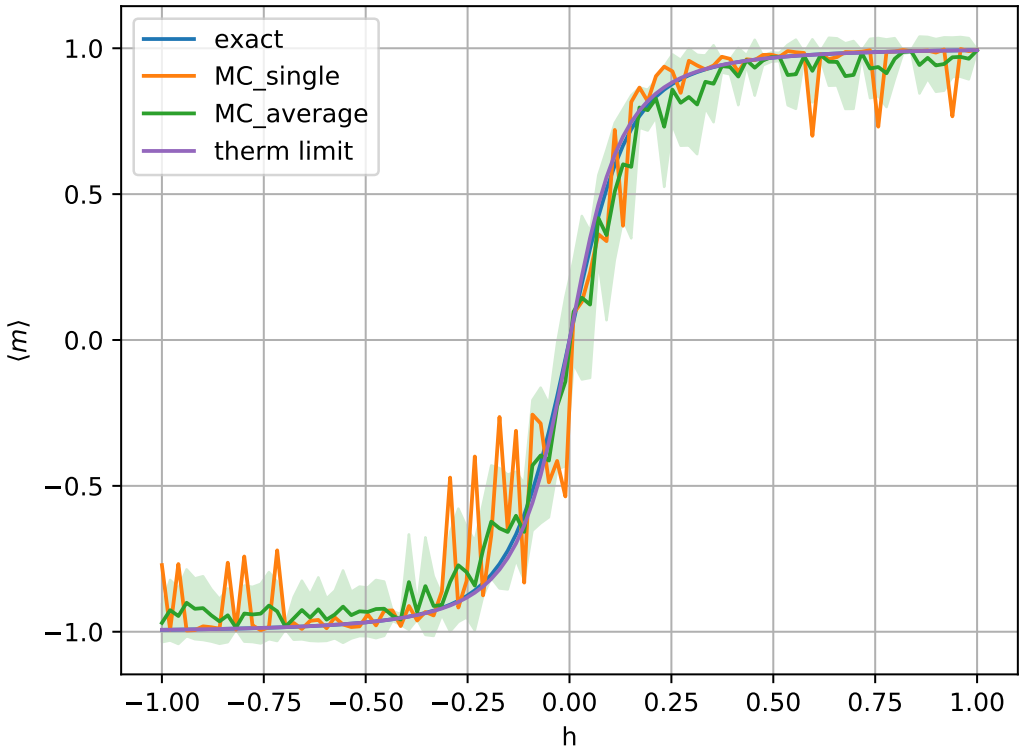

Figure 3: Dependence of the magnetization on h

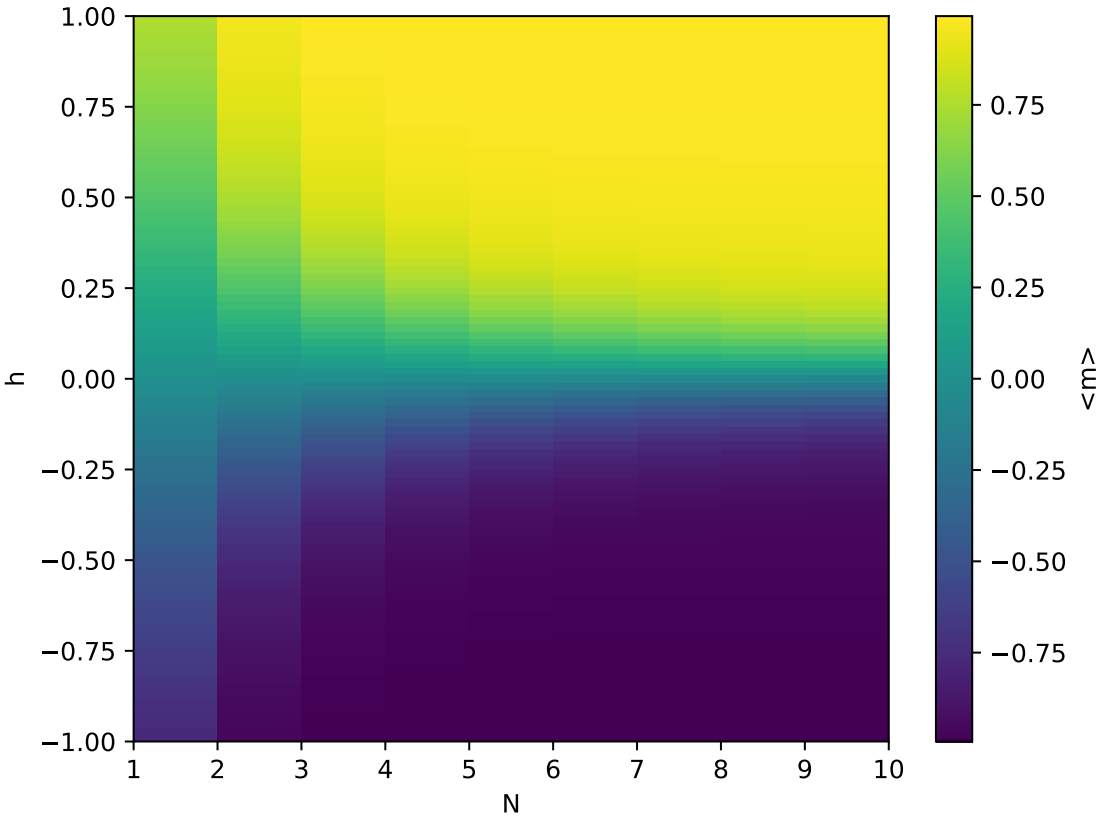

Figure 4: Exact dependence of the magnetization on N and h

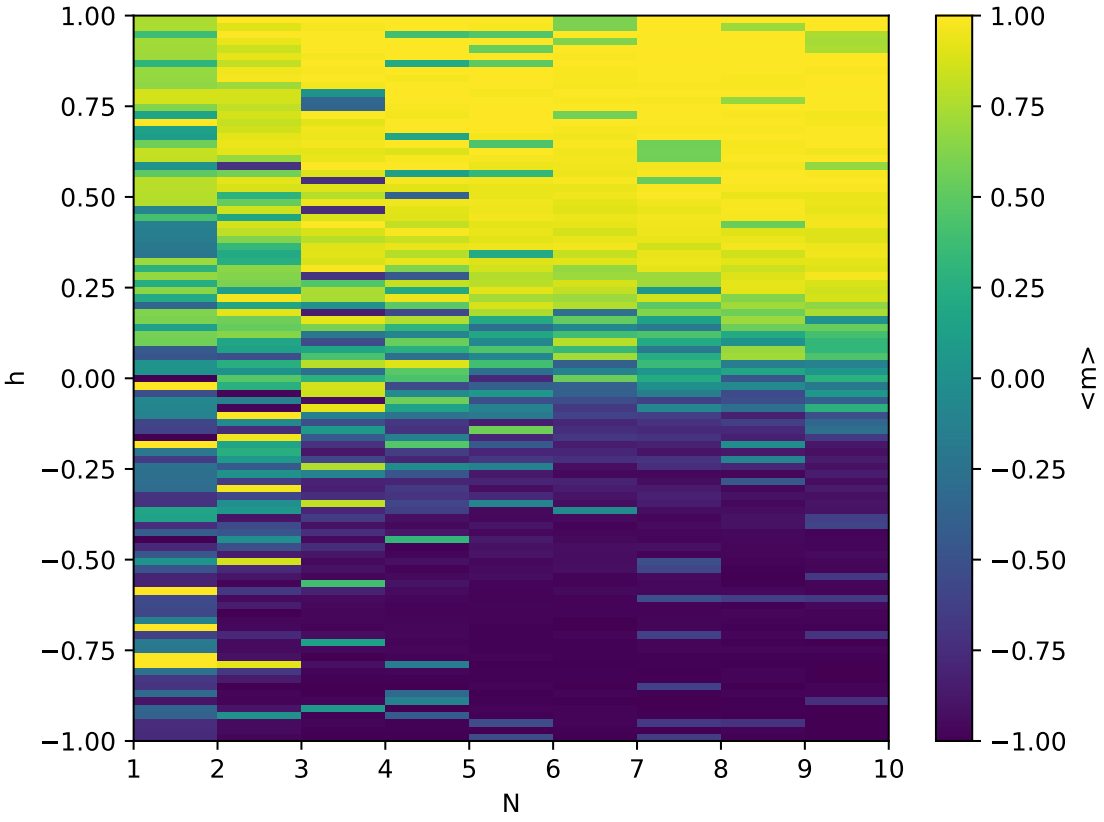

Figure 5: Monte-Carlo simulated dependence of the magnetization on N and h