UNIVERSITÄT BONN
PHYSIKALISCHES INSTITUT

Homework 1 - Computational Physics Monte-Carlo-Simulation of the 1-D Ising model

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Contents

18/20 Good job !! Keep it up!

1 Introduction

1.1 Goal

In this homework we try to verify the theoretical magnetization of the 1D-Ising-Model. We use a Monte-Carlo-Simulation to generate the ~~constellations~~ configurations which build the ensemble and calculate the magnetization of the ensemble.

1.2 Theory

The 1D-Ising-Model is a lattice-model at which on each grid-point a spin is placed. As the name states the lattice is 1-dimensional (i.e. a chain) and we label the grid-points with $x \in 0, ..., N-1$. The spins are 1-dimensional as well s.t. to each grid-point x we attach a spin $s_x \in \pm 1$. One specific state is called $s = s_1, ..., s_{N-1}$.
The grouping of similar systems in thermodynamic equilibrium is called an ensemble. Even if they are similar with regard to the defined state variables, they differ in the realization of the microstates. The constellations examined below, which are characterized by the same number of particles N, the same volume V and the same temperature T, form canonical ensembles.
For canonical ensembles the probability of occurrence for a specific state s is given by:

$$P(s) = \frac{1}{Z_c(\beta)} e^{-\beta E_s}, \tag{1.1}$$

where E_s is the energy of state s, $e^{-\beta E_s}$ is the Boltzmann-factor with $\beta = \frac{1}{k_B T}$ and Z_c is the canonical partition function with

$$Z_c = \sum_{s'} e^{-\beta E_{s'}}, \tag{1.2}$$

where the sum is over all possible configurations that fulfill the defined state variables. The energy of a configuration can be calculated with the Hamiltonian

$$E_s = H(s) = -J \sum_{\langle x,y \rangle} s_x s_y - h \sum_x s_x. \tag{1.3}$$

2 Theoretical questions

2.1 1.

J is the coupling constant of two spins. If $J > 0$ the model favors parallel spins. This would represent a ferromagnetic interaction. At low temperatures we would expect the spins to point mostly in the same direction.

If $J < 0$ we call it an antiferromagnetic interaction. For low temperatures neighboring spins will point mostly in different directions. At high temperatures we expect spins to fluctuate randomly, because the entropy dominates the system.

3

2.2 2.

Periodic boundary conditions mean that the spin at position 0 is a direct neighbor of the spin at position $N-1$. Limiting the interaction of spins to their nearest neighbours means that they only interact with those spins who are closest to them. For a 1D Model these are the direct neighbours.

not required

1/2

(here what would it imply for a chain physically... it would become a ring and how did you implement it numerically)

2.3 3.

Since the value in the exponential function has to be dimensionless, $\frac{J}{T}$ has to be dimensionless and therefor J needs to have dimension of T.

1/2

$H(s) = -J \sum_{\langle i,j \rangle} s_i s_j - h \sum_n s_n$

$P(s) = \exp(H(s)/k_B T)$

$\therefore$ h also needs to have dimension of temperature.

3 The Code

We use a Metropolis Algorithm to implement a Monte-Carlo-Simulation. Since this is asked for on the next sheet I'll provide a detailed explanation of this Algorithm there.

3.1 calc-magn

This function calculates magnetisation for a spin for you!

10/10

Code

This function calculates the magnetization of a given constellation by summing over all spins and adding up their value.

3.2 theo-mag

(try not to write the entire formula in a line very hard to read!)

Return the theoretical expected magnetization for a given N and h. We calculated the theoretical magnetization as suggested on the exercise-sheet.

3.3 main

We first define some parameters for our algorithm such as the amount of steps for the initialization, correction for autocorrelation and the number of configurations for one ensemble as well as the fineness of our final curve. Lastly with D we can change the Number of runs of the simulation which will be 1 for creating our best graphs and will be lager for error-estimation. More on that later.
Several 'for'-loops handle the parameters I mentioned above and the magnetization is

calculated for every configuration in the ensemble. For every run, the final curves is plotted together with the expected theoretical curve.

4 Results

As suggested we fix $J = 1$, $k_b = 1$ and use $h = 0.2$ and $N = 20$ for the fixed values. As N should not be much larger than 20 we use $N = 20$ as the thermodynamic limit. → see below

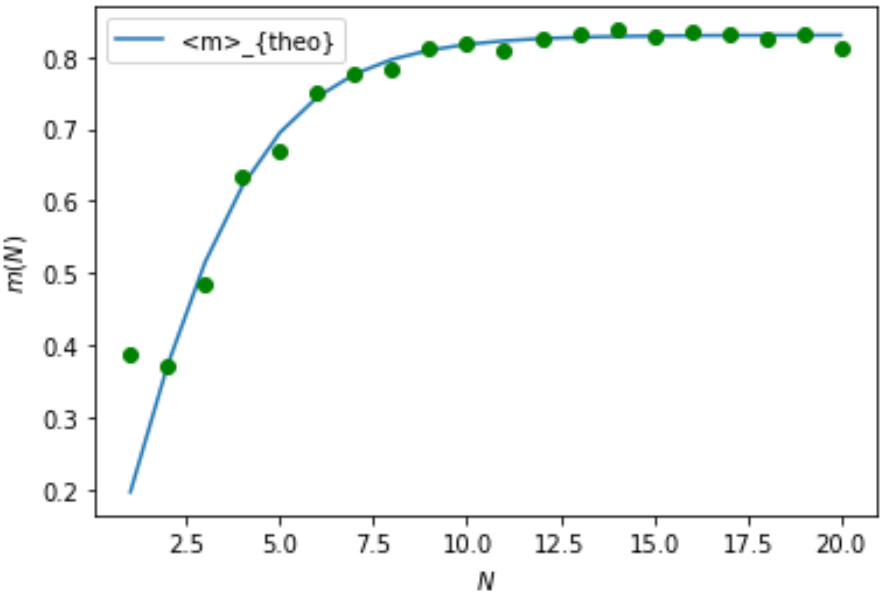


Figure 4.1: Magnetization from simulation as dots together with the theoretical expectation. We used 5000 constellations for the ensemble.

For fixed h one can see that the magnetization rises for increasing N and runs against an asymptotic value in the thermodynamic limit. This is expected because for small N fluctuations have a larger impact. For larger configurations the flip of one spin against the external magnetic field doesn't change the overall magnetization of the system too much. For fixed N the magnetization runs fast against -1 and 1 for $h = -1$ and $h = 1$ respectively.

for thermodynamic limit: take the limit of the theoretical expression in case $N \to \infty$ you should get

$$\langle m \rangle = -\frac{\sinh(h)}{\sqrt{\sinh^2(h) + e^{-4J}}}$$

where $h = \frac{h}{T}$, $J = \frac{J}{T}$

and you had to compare that!

your simulation time is very large and in general you don't need 5 for loops try to reduce the computation time for next increases

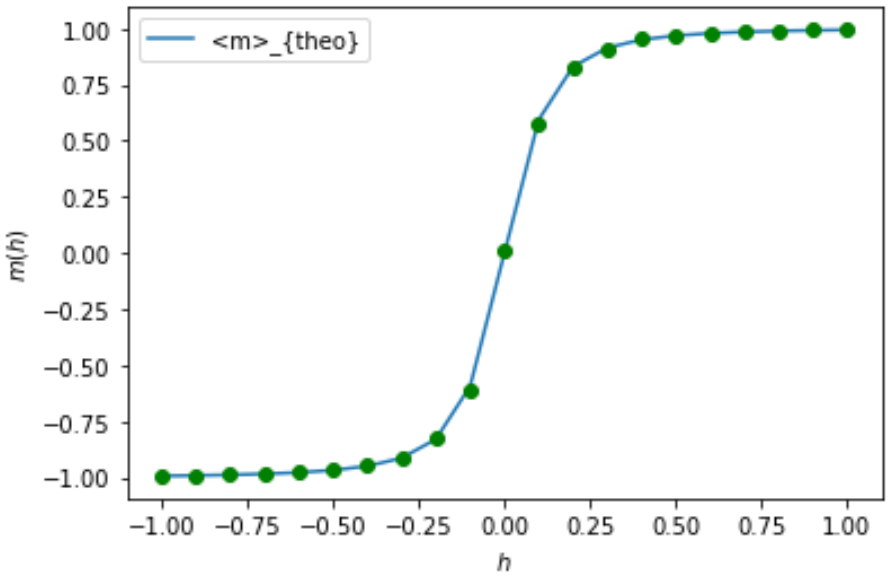


Figure 4.2: Magnetization from simulation as dots together with the theoretical expectation. We used 5000 constellations for the ensemble.

5 Error estimation

(later you will learn better method for error estimation)

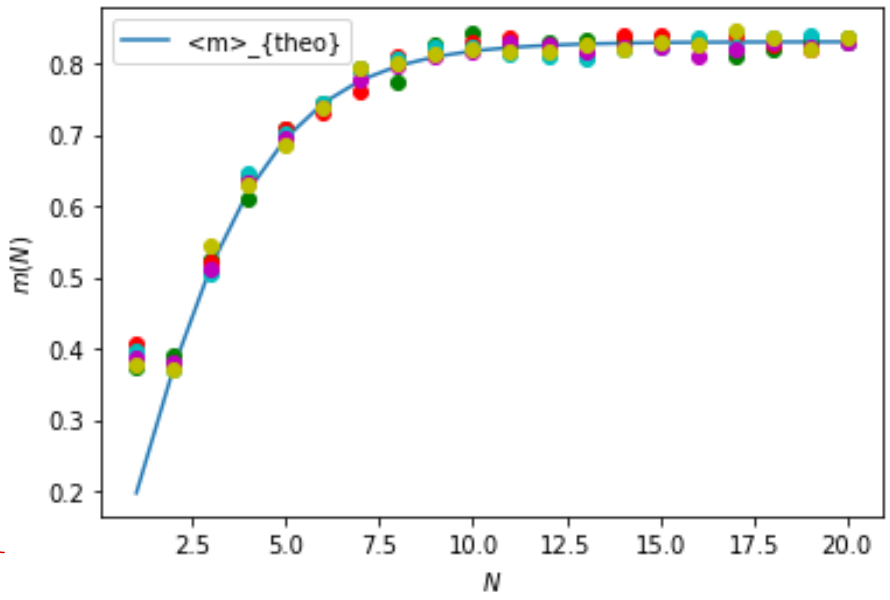
We want to estimate the error of our calculated magnetizations. We make the assumption that every calculated magnetization m_i follows a normal distribution around the theoretical expected value μ_i.

$$m_i \sim N(\mu_i, \sigma_i^2) \tag{5.1}$$

If we now subtract the theoretical magnetization μ_i for every m_i and further assume that all these magnetizations have the same variance, i.e. $\sigma_i = \sigma \forall i$, then the distribution of the errors is as follows:

$$m_i - \mu_i \sim N(0, \sigma^2). \tag{5.2}$$

The Maximum-Likelihood estimator for σ is then $\sqrt{\frac{1}{n}\sum_{i=1}^{n} m_i - \mu_i}$. We calculate these σ for varying h and N with 5 runs and each get $\sigma_h = 0.0442$ and $\sigma_N = 0.0101$. These values are quite low and match with the observation from the plotted graphs. These vary little from the theoretically expected value. What can be observed is that the variation is larger for the case of fixed h, which is also reflected in a lager σ for this case.



4/5

1 Point deducted for $N \to \infty$ lim

Figure 5.1: Magnetization from simulation as dots together with the theoretical expectation. We used 5000 constellations for the ensemble and simulated the final result 5 times, $\sigma_h = 0.0442$.

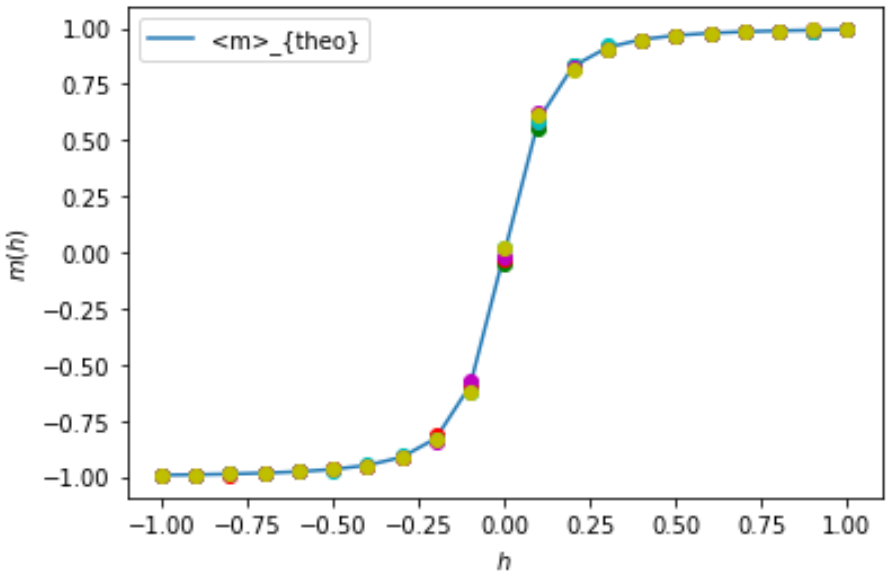


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Figure 5.2: Magnetization from simulation as dots together with the theoretical expectation. We used 5000 constellations for the ensemble and simulated the final result 5 times, $\sigma_N = 0.0101$.