Exercise 1. Ising model

Goal: We start by simulating the 3D Ising model using the Metropolis-based single-spin flip Monte Carlo method. For those who attended last semester's lecture it is (to some degree) a revision.

Write a program for a Monte Carlo simulation to solve the three-dimensional Ising model with periodic boundary conditions. Implement the single-spin flip *Metropolis algorithm for sampling. As you will have to reuse this code for upcoming exercise sheets, it might be worth to make sure that it is well-structured!*

Task 1: *Measure and plot the* energy E, *the* magnetization M, *the* magnetic susceptibility χ *and the* heat capacity C_V *at different temperatures* T.

Task 2: *Determine the critical temperature* T_c.

Hint: You should obtain $T_c \simeq 4.51$.

Task 3: *Study how your results depend on the system size.*

Hint: Start with small systems to reduce the computation time.

Task 4 (OPTIONAL): *Save computation time by avoiding unnecessary reevaluations of the exponential function. To achieve this, use an array to store the possible spin-flip acceptance probabilities.*

Task 5 (OPTIONAL): *Plot the time dependence of* M *for a temperature* $T < T_c$.

Hint: For small systems you should be able to observe sign-flips in M.

Solution. For the implementation of the 3D Ising model several ideas from the lecture were used. For example, to minimize the computation time the possible acceptance probabilities were stored in a look-up table. Furthermore, for each temperature T a number of thermalization sweeps was performed - prior to the sampling process - to let the system thermalize from the initial random configuration to a configuration that is more likely to be expected at this temperature. The computations of the susceptibility χ and the specific heat C_V were realized by using the fluctuation-dissipation theorem:

$$\chi(T) = \beta \left(\langle M(T)^2\rangle - \langle M(T)\rangle^2\right) \tag{S.1}$$

$$C_V(T) = \beta^2 \left(\langle E(T)^2\rangle - \langle E(T)\rangle^2\right). \tag{S.2}$$

The results for a system with parameters $L = 20$, $J = 1$, $N_{thermalization} = 100L^3$, $N_{sample} = 3000$ and $N_{subsweeps} = 3L^3$ are shown in Fig. 1. The critical temperature is found to be somewhere between $\beta = 0.2$ and $\beta = 0.25$. Note that the error is higher in the regime around T_c. This is related to the so-called *critical slow-down.*

Larger system sizes would cause the phase transition to be more abrupt (visible in M and E). This leads to increased peaks of χ and C_V at T_c.

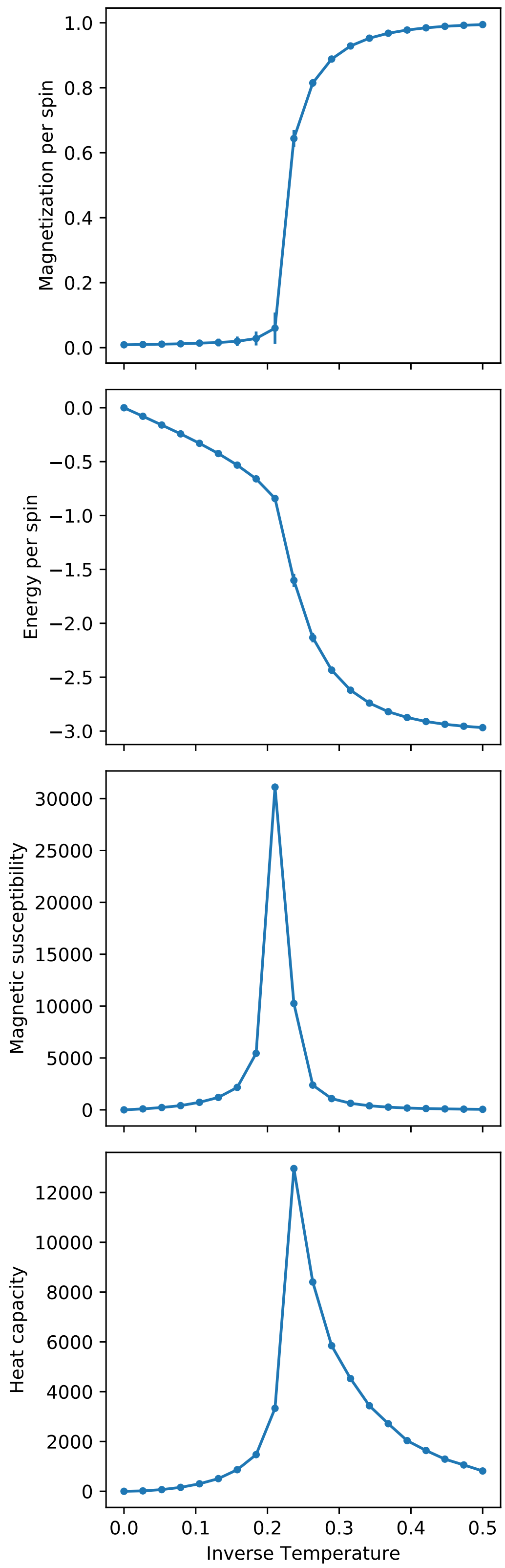

Figure 1: Magnetization, energy, magnetic susceptibility and heat capacity for different temperatures.