

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 .