Exercise 1. Monte Carlo simulation of the 2D Ising model

Goal: In this exercise we learn how to do a Monte Carlo simulation of the 2D Ising model using the single-spin flip Metropolis algorithm.

The Ising model is a simple model for simulating the magnetic properties of a material. It consists of a square lattice of (classical) spins where every site represents e.g. an atom or a molecule. Every spin can only take the values ± 1. The spins only interact with their nearest neighbors. The Hamiltonian of the system is given by

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} S_i S_j.$$

We consider the canonical ensemble that means a system at fixed temperature. Therefore, the thermal average of any quantity A of the system is given by

$$\langle A \rangle = \frac{1}{Z} \sum_i A_i e^{-\beta \mathcal{H}_i}, \quad \beta = \frac{1}{k_B T} \tag{1}$$

where

$$Z = \sum_i e^{-\beta \mathcal{H}_i}$$

is the so-called partition function and i labels the different microstates.

Task: Write a program for a Monte Carlo simulation to solve the 2D Ising model with periodic boundary conditions. Implement the single-spin flip Metropolis algorithm. Plot the average energy as well as the magnetization as a function of the temperature T. Are your results reliable? What is the statistical error?

Hint: The thermal average of a quantity A (Eq. 1) is estimated by

$$\langle A \rangle \approx \frac{1}{M} \sum_{i=1}^{M} A_i$$

where M is the number of samples.

Please consider the following points:

- As a starting configuration you may use the ground state. The system will automatically relax towards thermal equilibrium.
- For equilibration to a given temperature you may have to perform a couple of system sweeps (L^2 new configurations). Take about 100 system sweeps to be relatively safe (more details e.g. next semester). It might be useful to plot the relaxation process of e.g. the system energy for some temperatures i.e. $\mathcal{H}$ as a function of the number of system sweeps.
- For every new sample to be sufficiently uncorrelated from the previous one perform at least one system sweep. This will be enough for most temperatures (be careful about the region around the phase transition where the 'critical slow-down' happens (more details e.g. next semester)).

- For the 2D Ising model the critical temperature is known exactly: $T_c = 2/\ln\left(1+\sqrt{2}\right) \approx 2.27$ (in units of J/k_B). Use this to check if your results look reasonable.
- To speed up your code you may consider the following (OPTIONAL):
  - You can store the values of the exponential function (only a few discrete values are needed).
  - Use integer variables inside your main loop (e.g. for the values of the magnetization and energy).
  - The current values of the magnetization and energy can be easily updated after each spin flip.
  - Re-use equilibrated systems from the previous temperature (T_i) when going to the next temperature ($T_i + \Delta T$). This saves throwing away a lot of configurations to get to the equilibrium.