Exercise 1. Microcanonical Monte Carlo

Goal: So far, we treated the Ising model in the canonical ensemble (fixed temperature) where the samples were drawn according to the Boltzmann distribution. In this week's exercise we are going to perform a microcanonical Monte Carlo simulation of the 3D Ising model according to the Creutz algorithm (M. Creutz, Phys. Rev. Lett., 50, 1411, (1983)).

The Creutz algorithm is defined in the following way:

1. Start with an initial spin configuration x of a given energy E and define a container energy E_d (demon energy) such that $E_{max} \geq E_d \geq 0$.
2. Choose a spin at random and flip it to obtain the configuration y.
3. Calculate the energy diffference ΔE between the configurations x and y.
4. If $E_{max} \geq E_d - \Delta E \geq 0$ choose a new spin and repeat the process. If not revert the spin flip and choose a new spin.

Task 1: Modify your program of the first exercise to simulate a microcanonical Ising system using the Creutz algorithm.

Task 2: Determine the corresponding temperature T using

$$P(E_d) \sim e^{-\frac{E_d}{k_B T}}.$$

Task 3: Compute T for different E. Plot energy and magnetization as a function of temperature and compare your results to the results obtained with the Metropolis algorithm.

Task 4: Repeat the above tasks for different system sizes and compare your results.

Task 5 (OPTIONAL): What happens in the case $E_{max} = 0$ (Q2R algorithm)? Discuss the issue of ergodicity.