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)).*

Task 1: Modify your program of the first exercise to simulate a microcanonical Ising system on a 3-d cubic lattice using the Creutz algorithm as described in the following:

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 difference 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.

Determine the corresponding temperature T using

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

Task 2: 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 3: Repeat the above tasks for different system sizes and compare your results.

Task 4 (OPTIONAL): What happens in the case $E_{\max} = 0$ (Q2R algorithm)? Discuss the issue of ergodicity.