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.*

Solution. Starting point is a configuration where all spins are parallelly aligned. By accepting every spin flip that increases the energy we are able to eventually arrive at the desired energy E from which the microcanonical Monte Carlo simulation begins. The corresponding temperature can be obtained by fitting the energy distribution of the demon energy E_d with a semi-logarithmic scale ($P(E_d) \sim e^{-\beta E_d}$) as it is presented in Fig. . However, it is also possible to obtain the temperature from

$$\beta = \frac{1}{4} \log(1 + \frac{1}{4 < E_d >}).$$

For the simulations an average of both quantities was used. The energy and magnetization curves are found in Fig. and Fig. . (To have uncorrelated samples $3 \times L^3$ configurations were thrown away.) The graphs are similar to the ones obtained with the Metropolis algorithm. However, the magnetization appears to be steeper around the critical temperature. Moreover, the differences in system size are not as apparent as in the Metropolis algorithm. Creutz's paper says: *finite-size effects differ from those in the canonical approach [..] one cannot directly use the fluctuations in the lattice energy to measure the specific heat.*

For $E_{max} = 0$ one obtains the Q2R algorithm which is deterministic and reversible. It was found that the Q2R algorithm is non-ergodic (*Schulte et. al.: Period in the chaotic phase of Q2R automata*).

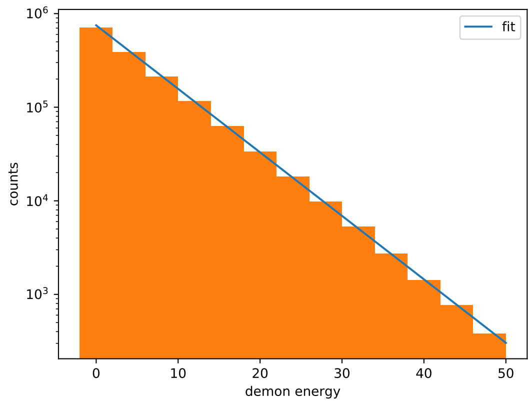

Figure 1: Obtaining the temperature T from the Boltzmann distributed demon energy on a system with $L = 12$ and $E_{max} = 50$. The fit yields $T_{fit} = 6.4$ and the averaged quantity $T_{average} = 6.5$.

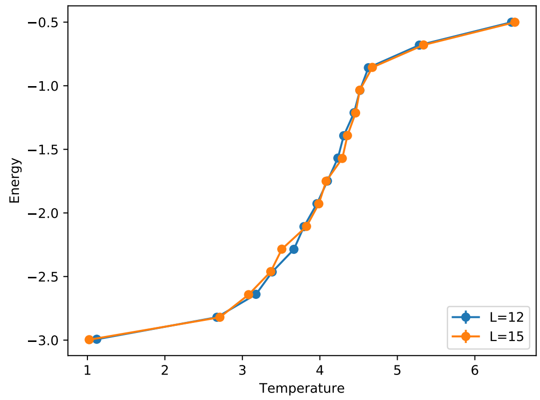

Figure 2: Energy E as a function of temperature T for $L = 12$ and $L = 15$ with $E_{max} = 50$ and 300 samples.

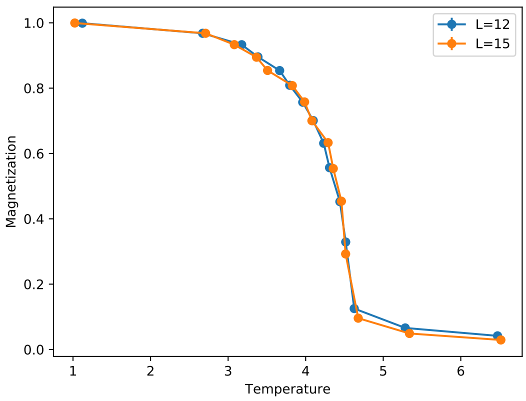

Figure 3: Magnetization M as a function of temperature T for $L = 12$ and $L = 15$ with $E_{max} = 50$ and 300 samples.