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

$$P(E_d) \sim e^{-\frac{E_d}{k_{\mathrm{B}}T}}.$$

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.*

Solution. The starting point is a uniform ground state configuration with energy $E = -3JL^3$. We also fix an initial demon energy of $E_d = 12$ and capacity $E_{\max} = 48$ (note that both need to be integer multiples of 4 for the Ising model).

First, we reach equilibrium by accepting every spin flip that increasing energy until the system reaches the fixed energy E of the microcanonical ensemble.

After reaching the equilibrium, the Creutz algorithm proceeds to construct the Markov chain by picking a random site and flipping the spin if the condition $E_{\max} \geq E_d - \Delta E \geq 0$ is satisfied and update the demon energy $E_d \to E_d - \Delta E$ in case of acceptance.

The coupling with the small demon reservoir leads to an effective temperature of the system at each fixed energy. That is, in the steady state the demon energy is exponentially distributed as $E_d \sim e^{-\beta E_d}$, where β is the effective inverse temperature. In the case of Ising spins, $s = \pm 1$, the restriction $E_d = 4k$ with $k \in \mathbb{Z}^+$ leads to closed expression for the effective temperature:

$$\beta = \frac{1}{4} \log \left(1 + \frac{4}{\langle E_d \rangle} \right). \tag{S.1}$$

An alternative approach is to directly fit the histogram for E_d with a semi-logarithmic scale, see Fig.1, which can be useful in cases where the degrees of freedom have a continuous symmetry, *e.g.*, XY spins with $O(2)$.

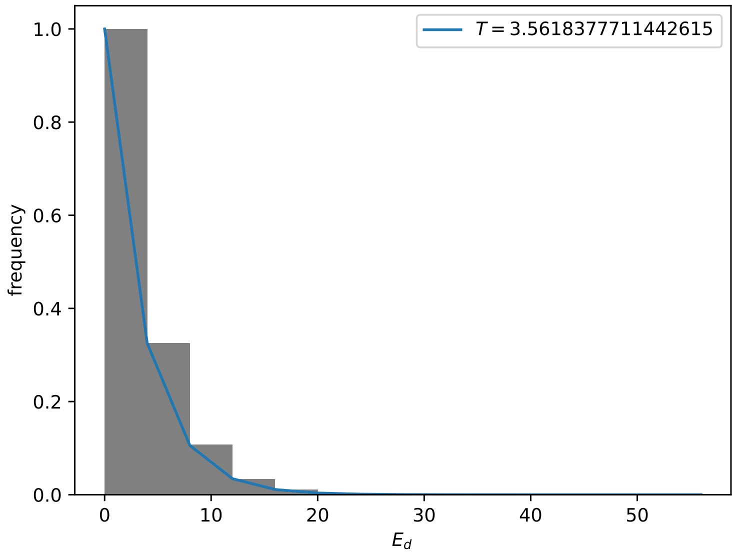

Figure 1: Effective temperature of the system is determined by the demon energy E_d.

The details of the simulation are as follows: after reaching the energy of the microcanoncial ensemble, we measure the magnetisation and energy at every $N_{\text{subsweeps}} = 3 \times L^3$-th step of the Markov chain. In total we take 10^4 measurements for each of the 16 linearly spaced energy values in the range $[-3JL^3, 0]$.

The estimates for the thermodynamic quantities are shown in Fig. 2 for linear system sizes $L \in \{2^n\}_{n=2}^4$. Firstly, we observe in Fig. 2.a that the absolute magnetisation density approaches a sharp kink at $T = T_c$ with growing system size. However note that the finite-size scaling of these curves differ from those of the canonical ensemble simulation (see *e.g*, solutions of last week's exercise with Metropolis-Hastings algorithm). In particular also note that one cannot use the fluctuation-dissipation formulas for the susceptibility and the specific heat. One way to estimate the specific heat is to use the fluctuations in the Fourier transform of the energy density and extrapolating to the $\mathbf{k} = 0$ component.

For $E_{\max} = 0$ (Q2R algorithm) the algorithm becomes non-ergodic as the possible Markov chains are largely restricted by the chosen initial state due to the fixed energy condition.

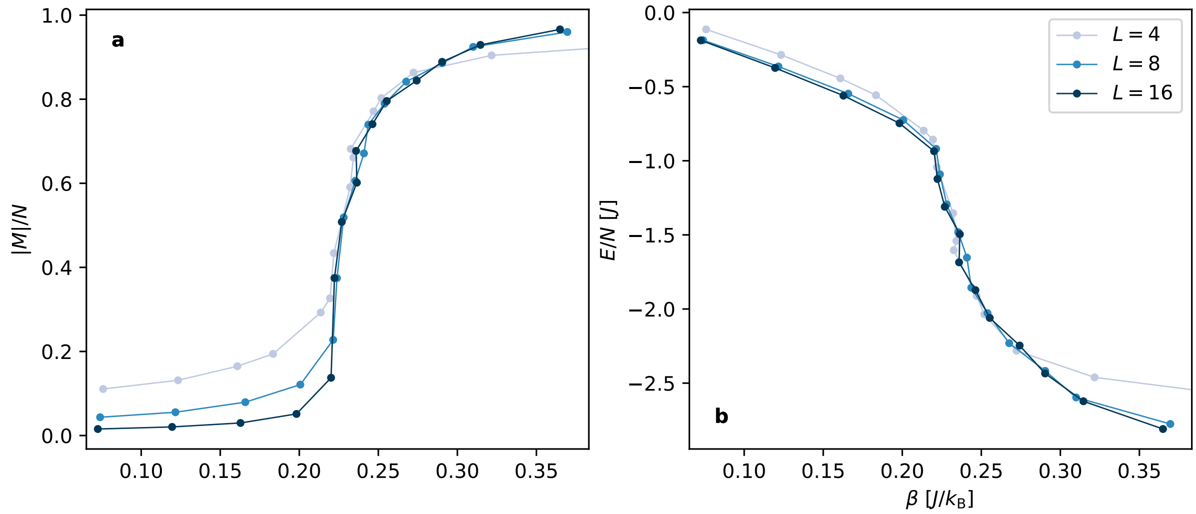

Figure 2: The Creutz algorithm reproduces the qualitative behaviour of the average quantities in 3-d Ising model. In **a** the magnetisation density and in **b** the energy density for the 3-d Ising model, which indicate a critical temperature $T_c \approx 4.51$.