Exercise 1. 2-d Ising model

Goal: We start by simulating the 2-d Ising model using the Metropolis-Hastings-based single-spin flip Monte Carlo method.

Write a program for a Monte Carlo simulation to solve the two-dimensional Ising model on the square lattice with periodic boundary conditions. Implement the single-spin flip *Metropolis-Hastings algorithm for sampling. As you will have to reuse this code for upcoming exercise sheets, it might be worth to make sure that it is well-structured!*

Hint: If you get stuck you can use the python skeleton provided.

Task 1: *Measure and plot the* energy E, *the* magnetization M, *the* magnetic susceptibility χ *and the* heat capacity C_V *at different temperatures* T.

Task 2: *Determine the critical temperature* T_c.

Hint: You should obtain $T_c \approx 2.27$.

Task 3: *Study how your results depend on the system size.*

Hint: Start with small systems to reduce the computation time.

Task 4 (OPTIONAL): *Save computation time by avoiding unnecessary re-evaluations of the exponential function. To achieve this, use an array to store the possible spin-flip acceptance probabilities.*

Task 5 (OPTIONAL): *Plot the dependence of* M *on the simulation time at a temperature* $T < T_c$.

Hint: For small systems you should be able to observe sign-flips in M.

Solution. We can make use of the fluctuation-dissipation theorem to construct an simple estimators for the magnetic susceptibility and the specific heat using total magnetisation M and the total energy E measurements on the Markov chain constructed by the Metropolis-Hastings algorithm:

$$\chi(T) = \frac{1}{NT}\left[\langle M(T)^2\rangle - \langle M(T)\rangle^2\right], \tag{S.1}$$

$$c_V(T) = \frac{k_\mathrm{B}}{NT^2}\left[\langle E(T)^2\rangle - \langle E(T)\rangle^2\right], \tag{S.2}$$

where $N = L^2$ is the system size. Note that in what follows, we measure temperature in units of k_B/J.

The details of the simulation are as follows: we throw away the first $N_\text{thermalisation} = 100 \times L^2$ samples until reaching the steady state in thermodynamic quantities, and afterwards we measure the magnetisation and energy at every $N_\text{subsweeps} = 10 \times L^2$ step of the Markov chain. In total we take 10^4 measurements.

The estimates for the thermodynamic quantities are shown in Fig. 1 for linear system sizes $L \in \{2^n\}_{n=2}^{6}$. Firstly, we observe in Fig. 1 that the absolute magnetisation density approaches a sharp kink at $T = T_c$ with growing system size. In particular we find that the Monte Carlo estimator is close to the analytical result

$$|M|/N = \left[1 - \sinh^{-4}(2/T)\right]^{1/8}, \tag{S.3}$$

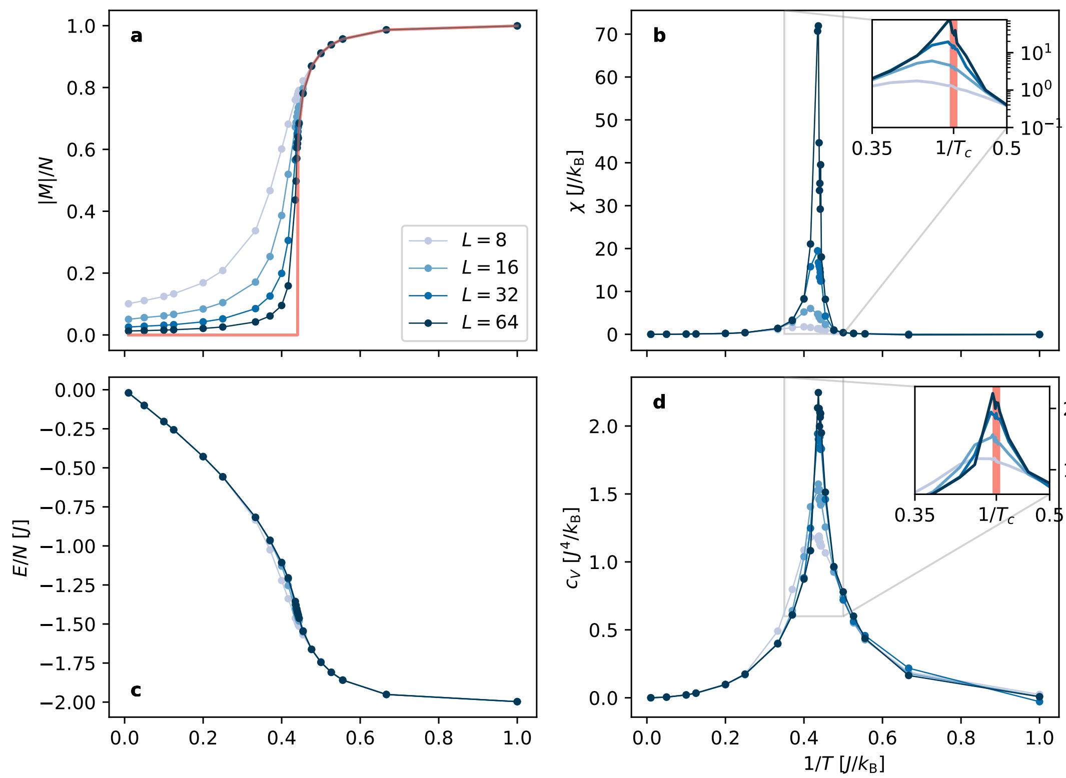

Figure 1: **a.** For large enough systems, the magnetisation density $|M|/N$ rapidly increases from 0 to 1 at around $T = T_c \approx 2.27$. **b.** The magnetic susceptibility has a peak at $T \approx T_c$ which gets sharper with growing system size. **c.** The inverse-temperature dependence of the energy density E/N. **d.** The qualitative behaviour of specific heat is analogous to the magnetic susceptibility.

also shown in red. The location of the peaks of c_V and χ give an estimate of $T_c \approx 2.28(1)$. Furthermore in both cases we find that the peak gets sharper and higher with growing L.

Finally, we look into the dynamics of the Metropolis-Hastings algorithm. In Fig. 2 we plot the time-series of signed magnetisation density (left column) and the histograms of magnetisation samples (left column). For a specific instance of the Markov chain generated by the algorithm we observe spin flips for $L \leq 16$ at temperatures $T \lesssim T_c$. In which cases the, histograms indicate that the $\mathbb{Z}_2$ symmetry of magnetisation is approximately recovered.

The average magnetisation density should vanish at all temperatures for the Ising model without an external field due to the $\mathbb{Z}_2$ symmetry of spins. This means that a faithful simulation should be able to generate random spin flips at all temperatures, including first-order phase transitions at $T < T_c$. However we find that the local Metropolis-Hastings updates can only provide this at very small systems. The reason for this is that in the ordered phase (in thermodynamic limit), the phase space is perfectly segregated into two magnetised sectors. Once the system spontaneously selects a magnetised state during the thermalisation, the ergodicity is broken thereafter and the simulation gets stuck in this sector, as it is extremely unlikely to flip all of the spins with local updates in a large uniform configuration.

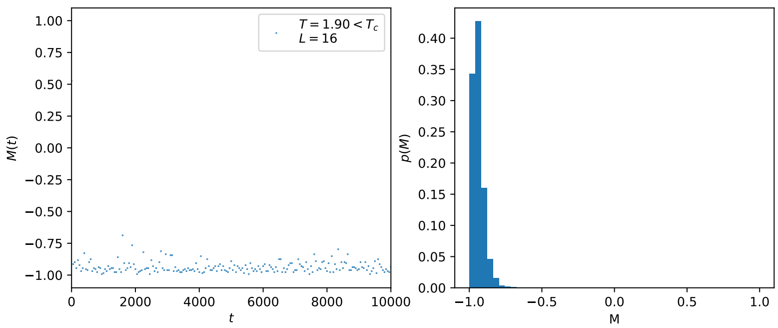

Figure 2: The spin-flips in the long-range ordered (magnetised) phase become less an less probable with local Metropolis-Hastings updates with growing system sizes. For large L and $T < T_c$, the dynamics experience an ergodicity breaking and the simulation gets stuck at one of the segregated sectors of the phase space after it spontaneously picks up one of the magnetisations.