UNIVERSITEIT VAN AMSTERDAM

Advanced Numerical Methods in Many-Body Physics - Homework 1

Spin flip Metropolis algorithm

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Exercises

We have implemented Metropolis algorithm in a 2D Ising model on a square lattice with periodic boundary conditions. The representation of the spin lattice is given by a numpy array of size $L \times L$ with spins down represented as -1 and spins up as 1.

We have set $N_{steps} = 2^{14} = 16384$ spin-flip steps together with $N_{therm} = 2^{12} = 4096$ thermalization steps and $N_{sweep} = L^2$ sweeps.

Exercise 1

Using this code and the binning analyisis function to estimate the error bars, we compute the following observables for the test scenario $L = 4$ and $T = 3$:

- The energy per site, $\langle E/N \rangle = -0.9975 \pm 0.0088$
- The magnetization per site, $\langle E/N \rangle = -0.0059 \pm 0.022$
- The order parameter, $m = \langle |M|/N \rangle = 0.5920 \pm 0.0044$
- The magnetization squared, $\langle M^2 \rangle = 112.66 \pm 1.29$

As a comparison, here are the reference values obtained from the ALPS library using 10^{10} sweeps.

```
<E/N> = -1.017786 +/- 0.000374
<M/N> = 0
<m> = 0.601592 +/- 0.0002
<M^2> = 115.554048 +/- 0.058112
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We can see how the obtained values are close to the reference values, nevertheless they do not seem compatible. This may be due to the fact that we are using a low amount of sweeps, $2^{14} \approx 1.6 * 10^4$ as opposed to the 10^{10} sweeps used for the simulation with the ALPS library.

Exercise 2

Now, we simulate some different configurations of the Ising model in order to observe finite size effects. In particular, we will plot three observables with respect to the lattice size L and the temperature T for different values of them. The chosen observables will be the order parameter $m(L, T)$, the self-correlation time for the order parameter, $\tau_m^{(int)}(T, L)$ and the magnetization per site $M(T, L)$.

We will choose L between $L \in \{4, 8, 12, 16, 24\}$ and the temperatures T will be choosen between 0 and 4 adding more density of points close to the critical temperature $T_c = 2.269$. In particular, the temperatures chosen are $T \in \{0.1, 1, 2, 2.1, 2.2, 2.269, 2.3, 2.4, 2.5, 2.6, 2.7, 2.8, 2.9, 3, 4\}$.
The error bars will again be obtained using binning analysis, as well as the self-correlation time $\tau_m^{(int)}(T, L)$.

The results are as follows:

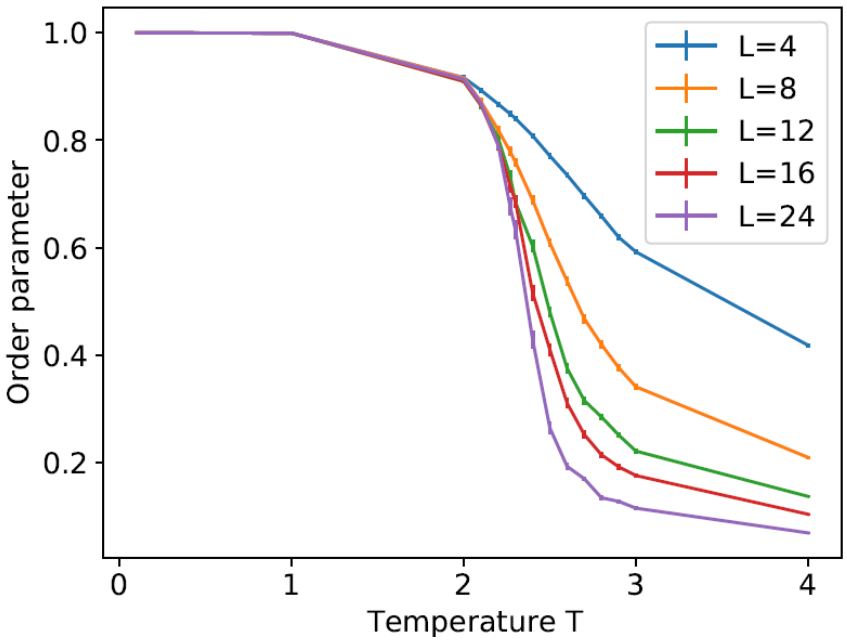

Figure 1: *Order parameter m as a function of T and L*

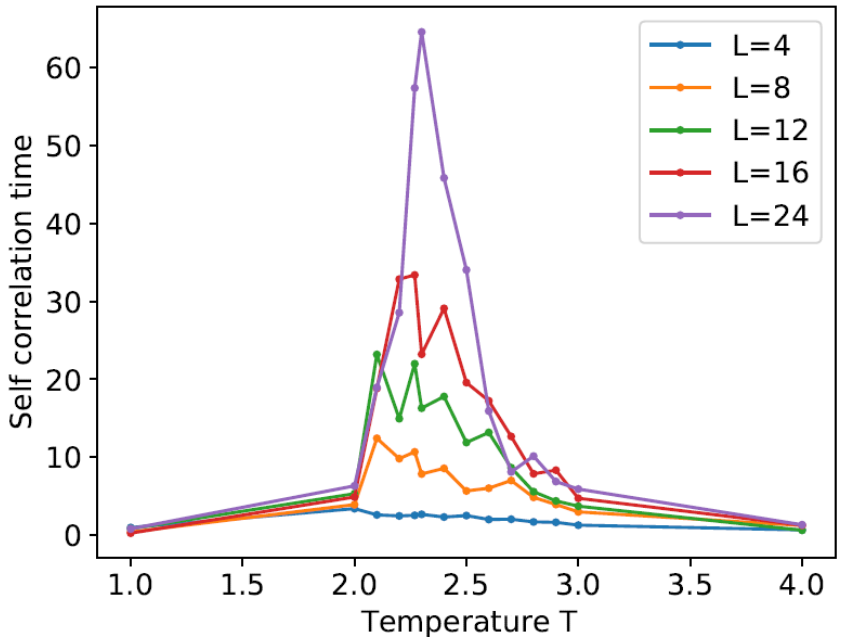

Figure 2: *Self correlation time of the order parameter, τ_m^{int}, as a function of T and L*

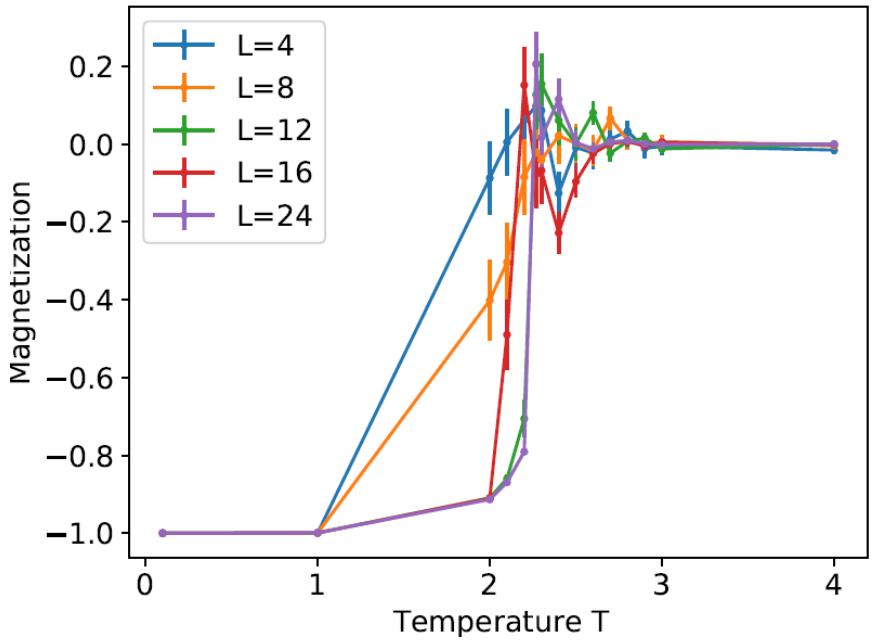

Figure 3: *Magnetization per site as a function of T and L*

We can see how the critical temperature $T_c = 2.269$ defines a phase transition because there is a sudden drop in the order parameter and a sudden spike at it's self-correlation time around that value of T. Moreover, this variations get more pronounced as we increase the lattice size L.

We can observe the finite-size effects in the sense that this changes are softened for low values of L. In the thermodinamic limit $L \to \infty$, the order parameter would drop to zero after T_c and its self-correlation time would diverge, but in finite size systems decreases continuously to zero with a rate proportional to the size of the system, reaching the value of 0 at $T \to \infty$, and the self-correlation time spikes proportionally to L but not diverges. For example, we see how for $L = 4$ the self-correlation time almost doesn't change.

This also happens for the magnetization per site, as it behaves expectedly going from the initial value of -1 (all spins pointing down) to an average magnetization of 0 after the phase transition at T_c. We can appreciate how for larger values of L this transition becames more sudden, but for lower values of L the change is smooth.

With respect to the error bars, we can see how the order parameter m has much smaller errors than the average magnetization per site. The self-correlation time for m doesn't have error bars because it is actually a result from binning analysis.

The magnetization per site has large fluctuations on its values after the phase transition, before it stabilizes at 0. This could make this results unreliable if we needed these values quantitatively. This can be seen more easily if we plot the two largest lattices $L = 16$ and $L = 24$:

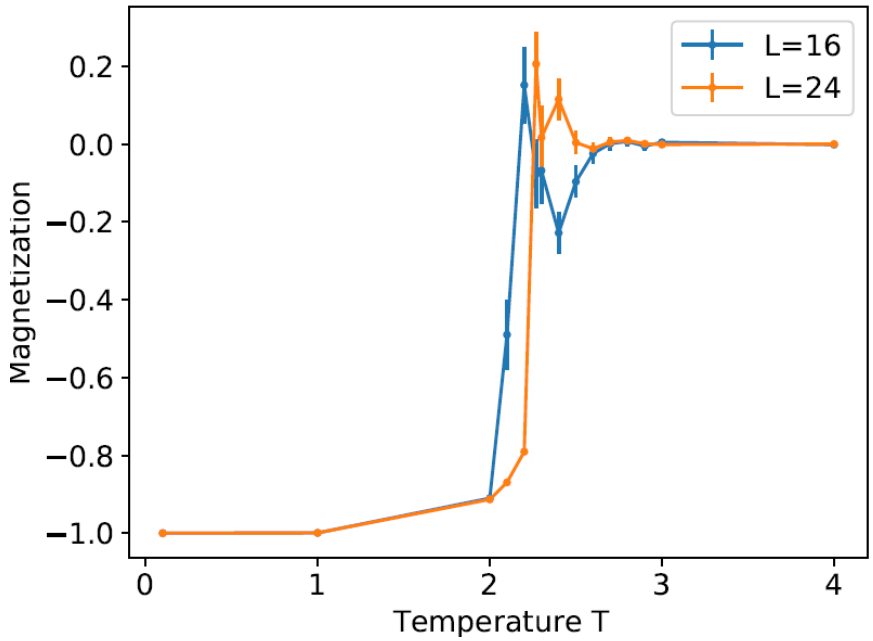

Figure 4: *Magnetization per site for the two largest lattices*

The magnetization per site varies considerably before stabilizing at 0 after the phase transition, which could make the results unreliable.

Exercise 3

Lastly we show how the heat-bath algorithm, characterized by the probability of flipping a spin

$$p_{\text{accept}} = \frac{e^{-\beta\Delta E}}{1 + e^{-\beta\Delta E}}$$

fulfills detailed balance.

Basically, this algorithm will fullfill the detailed balance condition if it satisfies

$$\frac{W_{xy}}{W_{yx}} = \frac{p_y}{p_x}$$

where

$$W_{xy} = \frac{e^{-\beta\Delta E(x,y)}}{1 + e^{-\beta\Delta E(x,y)}} \qquad W_{yx} = \frac{e^{-\beta\Delta E(y,x)}}{1 + e^{-\beta\Delta E(y,x)}} = \frac{e^{\beta\Delta E(x,y)}}{1 + e^{\beta\Delta E(x,y)}}$$

$$p_x = \frac{e^{-\beta E(x)}}{Z} \qquad p_y = \frac{e^{-\beta E(y)}}{Z}$$

substituting on the previous condition:

$$\frac{1 + e^{-\beta\Delta E}}{1 + e^{\beta\Delta E}} = \frac{e^{-\beta E(y)}}{e^{-\beta E(x)}} = e^{-\beta\Delta E}$$

using the identity

$$\frac{1+e^{-a}}{1+e^{a}} = e^{-a}$$

we see that the detailed balance condition indeed holds for this design of the amplitude matrix W_{xy}.