Statistische Physik im Gleichgewicht

WS 2023/2024 – Blatt 6

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Problem 12: Monte Carlo Simulation of the 2D Ising model (*15 Points*)

The aim of this exercise is to perform a Monte Carlo simulation of the Ising model

$$H = -J \sum_{\langle ij \rangle} S_i S_j$$

using importance sampling. Specifically, we want to find out the value of the magnetization in a heat bath at different temperatures. Without loss of generality, we can set $J = 1$.

Preliminary comment: It is possible that the simulations take some time for larger system sizes. Therefore, please save the values that we want to plot (temperature and mean square magnetization) in a file for each system size. Separating the simulation from the plotting in this way avoids costly re-runs. Please also upload these data files as part of your solution (you can use csv files or numpy files, for example).

Write a program that performs the following tasks:

(a) Sample a quadratic array of spins (size $L \times L$) according to the importance sampling method. You can choose which of the definitions for the transition probabilities you want to use. The spins take values $S_i = \pm 1$, therefore the only possible transitions are the spin flips $+1 \to -1$ and $-1 \to +1$. Accept or reject a flip for each site individually, according to the importance sampling algorithm. One sweep consists of going through all $L \times L$ sites once. One run consists of performing $5L$ sweeps for equilibration and then $30L$ sweeps, where the magnetization is measured and averaged.

(b) The Hamiltonian sums over next neighbors. Make sure that you use periodic boundary conditions at the boundaries of the system. As an initial condition at the start of each run, choose $S_i = 1$ for all i.

(c) Sample the system sizes $L = 8$, $L = 16$ and $L = 32$. In order to ensure good statistics, repeat at least 20 runs (consisting of equilibration and measurement) for each system size. Concerning the temperatures, choose 10 values for $k_\mathrm{B}T$ between 1.5 and 3.0.

(d) Measure the mean square magnetization per volume $\langle m^2 \rangle$ as a function of temperature, averaged over all runs. Plot this quantity for the three different system sizes. Draw a vertical line at the critical temperature of the system at $k_\mathrm{B}T_c = \frac{2}{\ln(\sqrt{2}+1)}$, this serves as a good verification of your simulation results.

(e) Calculate the error of m^2. For this, use the following estimation of the standard deviation of a statistical quantity A

$$\sigma_A = \frac{1}{N-1} \sqrt{|\overline{A^2} - \overline{A}^2|}$$

where N is the number of runs and $\overline{\{...\}}$ denotes the average over all runs. Use these standard deviations for errorbars in the figure.

Feedback:

Roughly how much time did you spend on this problem set?