

https:
//www2.physik.uni-muenchen.de/lehre/vorlesungen/sose_24/thermodynamik/index.html

Sheet 09

Discussion: Thursday 11.07.2024

Exercise 1 Monte Carlo simulations

The Monte Carlo method aims at solving the problem of the effective statistical sampling of suitable observables by a reversible, ergodic Markov chain.

1. Describe the (Metropolis) Monte Carlo Algorithm as introduced in the lecture notes.

2. **Estimating π :**

Write a code that computes $\pi = 3.1415\dots$ by Monte Carlo sampling.

- How does the probability for a point to be found inside the circle look like?
- Run the code multiple times for $N = 10^i$, $i = 1, 2, 3, \dots$ random numbers.
- How does the estimate for π improve with increasing N ? Compute the deviation from the exact result and plot it on a log-log scale as a function of N . Which scaling do you get?

3. **Simulating the 1D Ising model:**

The goal of this exercise is to simulate the one-dimensional Ising model

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} S_i^z S_j^z \quad (1)$$

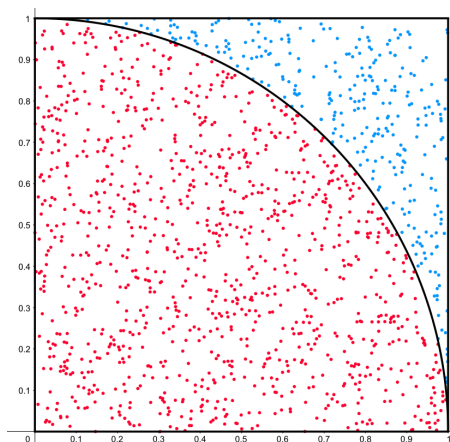


Abbildung 1: Figure from <https://de.wikipedia.org/wiki/Monte-Carlo-Simulation>

for periodic boundary conditions and temperatures $T \in [0.2, 5]$.

- How does the probability for accepting a new state look like?
- How does the acceptance rule arise from detailed balance?
- Compare your results to the analytical expression

$$E = \frac{e^{-J/T} - e^{J/T}}{e^{-J/T} + e^{J/T}}. \quad (2)$$