Numerische Methoden der Physik

WiSe 2023-2024 – Prof. Marc Wagner

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Exercise sheet 14

To be handed in on 31.01.2024 and discussed on 02.02.2024 and 05.02.2024.

Exercise 1 [*Ising model*] (2 + 10 + 8 = 20 pts.)

Consider the 1-dimensional Ising model with n spins $s_j = \pm 1$, $j = 1, \ldots, n$:

$$H = -\lambda \sum_{<j,k>} s_j s_k - B \sum_j s_j,$$

with coupling λ, external field B and where $\sum_{<j,k>}$ denotes the sum over neighboring spins. We are interested in Monte Carlo simulations of such a system using the heat bath algorithm.

(i) Provide an analytical expression for the probability for $s_j = +1$ and $s_j = -1$ for a randomly chosen spin, when connecting it to a heat bath, while keeping all other spins fixed.

(ii) Implement the heat bath algorithm for the Ising model with periodic boundary conditions. Run a simulation with the parameters $\beta\lambda = 0.1$, $n = 100$ and $n_{\text{sweeps}} = n_{\text{steps}}/n = 100$ for $B/\lambda = -10, 0, 10$ and both a hot start and a cold start. Plot the history of

$$s^{(m)} = \frac{1}{n} \sum_j s_j^{(m)},$$

where $s_j^{(m)}$ is the orientation of the jth spin after m Monte Carlos sweeps. Discuss the thermalization of this observabe. How does this change, if we have $n = 1000$ spins?

(iii) Compute $\langle s \rangle$ for $n = 100$ and $\beta\lambda = 0.025, 0.1, 0.15$ for $B/\lambda = -30, -25, \ldots, 25, 3$, using your heat bath implementation. For the simulation, choose a sufficient number of thermalization sweeps. Do not measure s on every single sweep, but leave gaps of 20 sweeps between measurements. Plot $\langle s \rangle$ as a function of B and compare it to the analytical solution in the thermodynamic limit

$$\lim_{n \to \infty} \langle s \rangle = \frac{\sinh(\beta B)}{\sqrt{\sinh^2(\beta B) + e^{-4\beta\lambda}}}.$$

Interpret your results, in particular when approaching $\beta \to 0$ and $\beta \to \infty$.