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 \( s_j = \pm 1, \ j = 1, \ldots, n: \)

\[ H = -\lambda \sum_{<j,k>} s_js_k - B \sum_j s_j, \]

with coupling \( \lambda \), 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

\[ s^{(m)}_j = \frac{1}{n} \sum_j s^{(m)}_j, \]

where \( s^{(m)}_j \) is the orientation of the \( j \)th spin after \( m \) Monte Carlo sweeps. Discuss the thermalization of this observable. 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 \( \beta \to \infty \).