Introduction to Computer Simulation I

Homework 7

Due: Wednesday, 10 December 2025

13. **Relaxation time of the magnetization of the 1D Ising model**

Study the relaxation time of the magnetization of the 1D Ising model for the Glauber update algorithm. To this end use your computer code of problem 10 for *periodic* boundary consitions and start a chain of $L = 100$ spins in an initial configuration where all spins are pointing up ($s_i = +1$, $i = 1, \ldots, L$)). Determine after each of the first 200 sweeps (that is after L randomly chosen spin-flip proposals) the magnetization per spin, $m = (1/L) \sum_{i=1}^{L} s_i$. Since this curve still shows strong fluctuations, average the whole "computer experiment" over 10 000 replicas (using different random numbers). This curve should show an exponentially decaying behavior, $m(t) = m(0)e^{-t/\tau_{\mathrm{relax}}}$, from where the relation time τ_{relax} can be read off, which depends on the chosen simulation temperature.

a) Run the simulation at any rate for the case $k_B T/J = 1$ and consider also the chain lengths $L = 50, 20, 10$, and 2. Determine for each case τ_{relax} through a linear fit.

b) "Play" with the temperature in approximately the range $2/3 \leq k_B T/J \leq 2$.

c) Repeat the whole prodecure in part a) (and preferably also b)) with the Metropolis update algorithm, which can be done quite easily.

d) In principle one could determine along similar lines the relaxation time of the energy (which, in contrast to the magnetization, does not approach zero but a finite equilibrium value discussed in problem 4).

e) For more details see the original paper by:
R. J. Glauber, *Time-Dependent Statistics of the Ising Model*,
J. Math. Phys. **4** (1963) 294–307.

14. **Heat-bath update for the 2D Potts model**

Generalize your simulation program for the 2D Ising model of problem 11 (square lattice, periodic boundary conditions) to the q-state Potts model which is defined by

$$H = -J \sum_{\langle ij \rangle} \delta_{\sigma_i,\sigma_j} ,$$

where $\sigma_i = 1, \ldots, q$ and $\delta_{\sigma_i,\sigma_j}$ is the Kronecker delta symbol.

Employ for the spin updates the heat-bath algorithm and study the model for $q = 8$ on a small 10×10 lattice as a function of the inverse temperature $\beta = J/k_B T$.