Prof. Dr. Wolfhard Janke WS2025/26

Introduction to Computer Simulation I

Homework 12

Due: Wednesday, 28 January 2026

23. **Reweighting "on the flight"**

a) Use for the two-dimensional Ising model with $L = 16$ the reweighted histograms at $\beta_1 = 0.375$ and $\beta_2 = 0.475$ of problem 22 to compute the mean energy and specific heat. Compare with the exact results.

b) Use now the same simulation data at $\beta_0 = \beta_c = \ln(1 + \sqrt{2})/2$ as in problem 22 and determine for $\beta = \beta_1$ und β_2 the mean energy and specific heat "on the flight" from $(k = 1, 2)$

$$\overline{e^k} = (1/L^2) \sum_{i=1}^{N} E_i^k \exp(-(\beta - \beta_0)E_i) / \sum_{i=1}^{N} \exp(-(\beta - \beta_0)E_i)\,,$$

where E_i, $i = 1, \ldots, N$, are the energy measurements (with i in units of sweeps).

c) The energy distribution $P_\beta(e)$ $(e = E/L^2)$ at $\beta = \beta_1$ and β_2 can also be determined "on the flight", if one counts the "hits" of $E_i = E$ $(= -2L^2, \ldots, 2L^2)$ not with weight $+1$ as at the simulation point β_0 but with $\exp(-(\beta - \beta_0)E_i$. Test this statement (for a direct comprison with the histograms of problem 22 the same normalization must be used, e.g., $\sum_E P_\beta(e) = N$).

24. **Nonconserved Dynamics**

Use your code for Metropolis simulations of the 2D Ising model with nonconserved dynamics (fluctuating magnetisation) on a square lattice of size $L^2 = 32^2$ with periodic boundary conditions. Start with an initial configuration where the spins s_i take the values ± 1 with probability 0.5 such that the total magnetization almost vanishes. This mimics a configuration at infinite temperature .

a) Run your simulations at temperature $T = 0.1T_c$ up to 10^4 Monte Carlo sweeps (MCS) and plot snapshots of the spin configurations at times $t = 10, 10^2, 10^3$, and 10^4 MCS. What does one observe?

b) Now repeat the simulations 4 more times, using each time a different initial configuration and also an independent time evolution generated by using a different (pseudo-) random-number seed. Estimate the mean length $\ell(t)$ of the developing domains of "up" and "down" spins by determining the mean number of kinks along the x and y direction (at a kink the direction of the spins changes). How is the mean number of kinks related to the energy of the system? Plot $\ell(t)$, the energy, and the mean acceptance rate as a function of time (= MCS) and verify that in each case a power-law behavior develops.