Prof. Dr. Wolfhard Janke, Fabio Müller SS2025

Introduction to Computer Simulation II

Homework 6

Due: Monday, 26 May 2025

11. **2D XY model overview**

    Use your single-cluster program for the 2D XY model of problem 10 for the determination of the mean energy, specific heat and susceptibility in the range $\beta = 1/k_B T = 0, \ldots, 2$ in steps of $\Delta\beta = 0.05$. Compare the results for lattice sizes 8×8, 24×24 (and may be also 60×60), each with periodic boundary conditions.

12. **Mean cluster size and improved estimator for the susceptibility of the 2D XY model**

    For general $O(n)$ spin models it can be shown that, when employing the embedded single-cluster algorithm, the magnetic susceptibility in the high-temperature phase, $\chi = \beta V \langle m^2 \rangle$ with $m = (1/V) \sum_{i=1}^{V} \vec{s}_i$, can be estimated by the improved estimator

    $$\hat{\chi}/\beta = \frac{n}{|C|} \left(\sum_{i \in C} \vec{r} \cdot \vec{s}_i \right)^2 .$$

    Here $|C|$ is the mean cluster size, which *only* for the Ising model with $n = 1$ is directly an improved estimator for χ/β (how does that follow from above formula?). Compare for the 2D XY model with $n = 2$ (24×24 square lattice, periodic boundary conditions) the two estimators for the susceptibility, that is the standard estimator $\propto m^2$ and the improved estimator, at three points of the high-temperature phase ($\beta = 1.0, 0.8, 0.6$) and verify that $\langle |C| \rangle \approx 0.81 \chi/\beta$.