Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Computational Quantum Physics
Exercise 10

FS 16
Prof. S. Huber

Problem 10.1 Monte Carlo simulation of the classical 2D Ising model

Write a classical MC simulation of the Ising model on an $L \times L$ square lattice, defined by the Hamiltonian

$$H = -J \sum_{\langle i,j \rangle} s_i s_j, \tag{1}$$

where the sum runs over pairs of nearest neighbor sites i, j and the Ising spins can take the values $s_i \in \{+1, -1\}$. Use periodic boundary conditions in both dimensions.

1. Use local updates, measure the absolute value of the magnetization $\langle |m| \rangle = \frac{1}{L^2} |\sum_i s_i|$ and its square $\langle m^2 \rangle$ for different values of the inverse temperature β. Compute error bars with a binning analysis. You can use the Classical Monte Carlo example (1D Ising model in Python) on the lecture homepage as a starting point.

2. Local updates become inefficient at low temperature and close to phase transitions. Therefore in this part you improve your simulation by implementing Wolff cluster updates described in the Monte Carlo notes. Verify your implementation by comparing results with those from the simple updates and observe that autocorrelation effects are a lot smaller.

Problem 10.2 Continuous time Quantum Monte Carlo

Next, we will solve the $(0 + 1)$d Ising model, given by the Hamiltonian

$$H = \Gamma \sigma_x \tag{2}$$

using a continuous-time segment update Monte Carlo method as discussed in the lecture.

1. Think about good data structures to implement the domain boundaries.

2. Be careful with correctly implementing the periodic boundary conditions and with detailed balance.

3. In the end, you should be able to reproduce the magnetization curve $\langle \sigma_x \rangle = \tanh \beta\Gamma$. You can calculate the magnetization in the Monte Carlo scheme as

$$\langle \sigma_x \rangle = \frac{\#\text{ of kinks}}{\beta\Gamma} \tag{3}$$