ETH
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Computational Quantum Physics
Exercise 9

FS 12
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The aim of this exercise series is to write a quantum Monte Carlo simulation for a chain of L Ising spins in a transverse field, that is the Hamilton operator

$$\hat{H} = -\sum_{i=1}^{L} \left(J\sigma_i^z \sigma_{i+1}^z + \Gamma \sigma_i^x \right), \tag{1}$$

$\sigma_i^{x,z}$ being Pauli matrices acting on the ith spin. Periodic boundary conditions $\sigma_{L+1} \equiv \sigma_1$ are assumed throughout this exercise. We will achieve this by first writing a simulation for the *classical two-dimensional* Ising model and then adapting this code to simulate the quantum chain.

Problem 9.1 Monte Carlo simulation of the classical 2D Ising model with local updates

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

$$H = -J \sum_{\langle i,j \rangle} s_i s_j, \tag{2}$$

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 local updates, i.e. each simulation step proposes to flip a random spin, which is accepted with Metropolis acceptance probability

$$P(x \to y) = \min\left\{1, e^{-\beta(H(y)-H(x))}\right\}.$$

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 and make sure these are not reduced by autocorrelation effects.

Problem 9.2 Monte Carlo simulation of the classical 2D Ising model with cluster updates

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. Verify your implementation by comparing results with the simple updates of problem 1 and observe that autocorrelation effects are a lot smaller.

Problem 9.3 Monte Carlo simulation of the quantum 1D Ising model

Generalize your simulation to an anisotropic square lattice with $L \times M$ spins and coupling constants J_x, J_τ between horizontal and vertical neighbors, respectively. Complete the mapping to the quantum system by identifying

$$\beta_{cl} J_x = \Delta J, \qquad \beta_{cl} J_\tau = -\frac{1}{2} \log \Delta\Gamma, \tag{3}$$

where β_{cl} is the inverse temperature of the classical system and $\Delta = \beta/M$ the imaginary time discretization of the quantum system. Note that in order to get meaningful results, you have to take $\Delta \ll 1$ and hence the quantum mechanical model with $|J/\Gamma| \sim 1$ corresponds to an extremely anisotropic classical Ising model.

Run your code for different ratios of the coupling constants, plot the results vs. J/Γ and try to locate the quantum phase transition in the model. You can improve your estimate by simulating larger and larger systems. (As for the classical model, a true phase transition can only happen in the thermodynamic limit $L, M \to \infty$, i.e. for the infinite chain at zero temperature.)