ETH
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Computational Quantum Physics
Exercise 11

FS 16
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Problem 11.1 Monte Carlo simulation of the quantum 1D Ising model

In this exercise we write a quantum Monte Carlo simulation for a 1D (quantum) Ising model in a transverse field, described by the Hamiltonian

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

$\sigma_i^{x,z}$ 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 adapting the code for the *classical two-dimensional* Ising model to simulate the quantum chain.

As shown in the lecture the 1D quantum Ising model can be mapped onto an anisotropic 2D classical Ising model upon identifying

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

where β_{cl} is the inverse temperature of the classical system and $\Delta = \beta/M$ the imaginary time discretization of the quantum system.

Generalize your simulation from the last exercise to an anisotropic square lattice with $L \times M$ spins and coupling constants J_x, J_τ between horizontal and vertical neighbors, respectively. 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.)

Reasonable parameters for the simulation are: system sizes between 16 and 48 spins, J/Γ between 0.5 and 2.

Problem 11.2 Continuous time Quantum Monte Carlo

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

$$H = \Gamma \sigma_x \tag{3}$$

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

$$\langle \sigma_x \rangle = \frac{\#\text{ of kinks}}{\beta\Gamma} \tag{4}$$