LAB VIII
Simulation of a quantum transversal field Ising model

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Plan

1. Our model
2. QMC Heat Bath algorithm

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Model Hamiltonian

We want to set up a Monte Carlo simulation for the simplest quantum model of a magnet in 1D

$$H = -J \sum_i \sigma_i^z \sigma_{i+1}^z - h \sum_i \sigma_i^x .$$

The magnet is at temperature β, ferromagnetic coulpling is J, and the transversal field is h.

We mapped this TFIM to an anisotropic 2D Ising model with effective couplings ($\beta_{\text{eff}} = 1$):

$$H = -J\Delta\tau \sum_{il} s_{i,l} s_{i+1,l} - \gamma \sum_{il} s_{i,l} s_{i,l+1} ,$$

where $\Delta\tau = \beta/M$ is a unit step in the imaginary time direction and $\gamma = -\frac{1}{2}\log(\tanh \Delta\tau h)$ is the effective coupling in imaginary time.

Our task

Calculate magnetization of 1D TFIM for the parameters: $\beta = 5$, $L = 20$, $J = 1$ as a function of h. Assume $M = 30$ slices in the imaginary time direction. Compare with an analytical result (Onsager) valid for $h < J$:

$$m(h) = \left[1 - \left(\frac{\sinh(\beta h/M)}{\sinh(\beta J/M)}\right)^2\right]^{1/8}.$$

Run the heat bath code developed for a classical 2D Ising model, adapt it for our effective anisotropic 2D model.

Note: for small h our algorithm sometimes "freezes", try restart with a random configuration, or run more equilibration steps

Magnetization: we define $m = \frac{1}{LM}\sum \sigma_{il}$ and esitmate $\langle|m|\rangle$ over MC steps.

Extra task

Consider TFIM with $N = 6$ spins on a periodic chain. Using the Kronecker product definition of spin operators build the model Hamiltonian matrix.

Diagonalize the matrix, find eigenenergies and eigenvectors, and calculate directly $< Q >$ from the definition for a quantum system. Let the observable operator be $Q = (M)^2$ with $M = \frac{1}{N}\sum_i \hat{\sigma}_i^z$. Plot this quantity versus h and compare with $< m^2 >$ calculated from QMC simulation.

Kronecker product definition: $\sigma_i^z = \mathbf{1} \otimes \ldots \otimes \sigma_z \otimes \ldots \otimes \mathbf{1}$ with Pauli matrix σ_z at the position i. Kronecker product is available in NumPy: `from numpy import kron`.