Computational methods for quantum correlated systems

Project 1: Exact Diagonalization **WiSe 2022/23** **Submission: 11.11.2022**

This project has to be done individually. The solution should contain the working computer program, the outputs and clear description of what you did and why. Use figures, diagrams or tables to present and discuss you results. You can use a separate PDF file to write your discussions. The required programming languages are Python or Julia. You can upload your solution to the StudIP before 14:00 on the submission day.

If you have questions or comments about this exercise, please, contact me via

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1 Full and exact diagonalization of one-dimensional spin-$\frac{1}{2}$ Heisenberg model (20 points)

Consider a one-dimensional lattice of length L with periodic boundary conditions described by the spin-$\frac{1}{2}$ antiferromagnetic Heisenberg model

$$H = J \sum_{j=1}^{L-1} \left[\frac{1}{2} \left(S_j^+ S_{j+1}^- + S_j^- S_{j+1}^+ \right) + S_j^z S_{j+1}^z \right], \tag{1}$$

where S_j^+ (S_j^-) raise (lower) the value of S_j^z at site j with the z-axis as the quantization axis. Set $J = 1$.

1.1 Construction of Hamiltonian matrix and full diagonalization:

(a) Build a matrix for Hamiltonian (1) for arbitrary L without using any conservation law of the system.

(b) Use the available full diagonalization method in your programming languages to diagonalize the Hamiltonian for $L = 2, 4, 6, 8, 10, 12$

(c) Build another matrix for (1) for arbitrary L using the conservation of total magnetization $S^z = \sum_{j=1}^{L} S_j^z$.

(d) Use the same full diagonalization method as in 1.1(b) to diagonalize the matrices of all possible values of S^z for $L = 2, 4, 6, 8, 10, 12$.

(e) For each length L, compare the time and memory needed for the full diagonalization in 1.1(b) with the full diagonalization of the matrix with maximum size in 1.1(d).

1.2 Exact diagonalization using the Lanczos method:

(a) Use the Lanczos method to calculate the ground state eigenenergy E_0 and eigenstate $|\psi_0\rangle$ for the Hamiltonian (1) with $L = 10, 12, 14, 16, 19, 20$ without using any conservation law of the system.

(b) Use the Lanczos method to calculate the ground state eigenenergy E_0 and eigenstate $|\psi_0\rangle$ for the Hamiltonian (1) with $L = 10, 12, 14, 16, 19, 20$ for all possible values of S^z.

(c) For each length L, compare the time and memory needed to get the eigenenergy E_0 using Lanczos method in 1.2(a) with the time and memory needed to get the eigenenergy of the Hamiltonian matrix with maximum size in 1.2(b).

(d) Calculate the spin gap E_s defined as

$$E_s = E_0\left(S^z = \frac{1}{2}\right) - E_0\left(S^z = 0\right) \tag{2}$$

for $L = 6, 8, ..., 20$. Plot of E_s vs. $\frac{1}{L}$ and make linear extrapolation to get the value of E_s at $L \to \infty$ (at the thermodynamic limit).