University of Göttingen
Institute for Theoretical Physics
Methods of Computational Physics, WiSe 2022/23
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Project 6: Heisenberg chain and diagonalisation

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After a warm-up exercise, we begin this project with the simplest method of directly implementing and diagonalising the Hamiltonian of the Heisenberg chain with N spins, using periodic boundary conditions, and then successively refine first by using symmetries to order the Hamiltonian matrix into smaller blocks and then by using the Lanczos method for an approximative diagonalisation.

We will study the $S = \frac{1}{2}$ Heisenberg chain with the Hamiltonian

$$H = J \sum_{i=0}^{N-1} \mathbf{S}_i \cdot \mathbf{S}_{i+1} = J \sum_{i=0}^{N-1} \left[S_i^z S_{i+1}^z + \frac{1}{2} \left(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+ \right) \right],$$

where we label the spins $i = 0, \ldots, N-1$. The periodic boundary condition is implemented by identifying $\mathbf{S}_N = \mathbf{S}_0$. We want to study an antiferromagnetic system and therefore set $J = 1$.

1. Warm-up (3 points)

Let us first familiarise ourselves with the spin states and their bit and base-10 representations.

a) Write down the state $|\uparrow\uparrow\downarrow\uparrow\downarrow\uparrow\rangle$ in bit representation. Which base-10 integer corresponds to those bits? (1 point)

b) Write an algorithm that determines the periodicity R_a (= the minimum number of shifts needed to obtain the same state) of any state given its base-10 integer representation. Calculate the periodicity of the state $|a\rangle$, with $a = 9588514242$. (2 points)

2. Direct diagonalisation (12 points)

Implement the construction of the Hamiltonian in the spin states basis for length N. Use the bit/base-10 representations of the spin states for the construction. Then, apply a diagonalisation method of your choice (e.g. the `eigh` function of the `numpy.linalg` module) to solve for the Hamiltonian's eigensystem.

a) Report the ground-state energies E_0 for different chain lengths $N = 2, \ldots, 6$. For each E_0, give one of the corresponding eigenvectors and the quantum number m_z. (4 points)

b) Plot the time needed to diagonalise the Hamiltonian in dependence of N for $N = 2, \ldots, 11$ (feel free to include even larger N if you can). Discuss the scaling qualitatively. (3 points)

c) Plot the thermal expectation value for the specific heat C, the magnetic susceptibility χ and the correlation $S_{z,0}S_{z,2}$ for at least three N, e.g. $N = 4, 8, 12$. The observable $S_{z,i}$ is defined to measure the z-component of the ith spin. Compare the specific heat and the magnetic susceptibility to their exact high-temperature limits $C \to 3/(13T^2)$ and $\chi \to 1/(4T)$, respectively. Discuss your results. (5 points)

d) (Bonus) Set up a spin chain with $N = 5$ and plot the time evolution of $S_{z,i}$ for $i = 1, \ldots, N$ for the initial state $|\Psi(0)\rangle = |\downarrow\downarrow\uparrow\downarrow\downarrow\rangle$. The time evolution is given by $\langle\Psi(t)|S_{z,i}|\Psi(t)\rangle$, as usual. Since H is not dependent on t, we have $|\Psi(t)\rangle = \exp(-iHt)\,|\Psi(0)\rangle$, where we have set $\hbar = 1$. (4 bonus points)

3. Block-diagonalisation into m_z subspaces (6 points)

Now separate H into blocks of constant m_z. Then replace the diagonalisation of the whole H with the diagonalisation of the individual blocks. To validate your implementation, you can check that you get the same ground state energies E_0 for $N = 2, \ldots, 6$.

Plot the time needed to diagonalise the Hamiltonian in dependence of N for $N = 2$ to at least $N = 11$, comparing with the timing results of 2b). Discuss the scaling qualitatively.

4. Lanczos method (12 points)

Apply the Lanczos method to the block-diagonalised Hamiltonian of part 3 (or to the full Hamiltonian, if you did not succeed to implement the separation into blocks in part 3). To validate your implementation, you can again check that you get the same ground state energies E_0 for $N = 2, \ldots, 6$. To get exact result for this validation, you will have to use $\Lambda = M$ for each $M \times M$-sized m_z block. In the following, stop the Lanczos method either at $\Lambda = M$, or when the relative change of the ground state energy is less than $\epsilon_0 = 10^{-6}$, whatever happens first.

a) Plot the time needed to apply the Lanczos method in dependence of N for $N = 2$ to at least $N = 11$, comparing with the timing results of parts 2 and 3. Discuss the scaling qualitatively. (6 points)

b) Now we study the convergence of the Lanczos method. For $N = 10$ and $m_z = 0$, plot the four lowest energies E_n with respect to Λ, and discuss your results. (If you did not succeed with the m_z block separation, you can study the four lowest energies of the full Hamiltonian instead.) (6 points)