ETH
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Computational Quantum Physics
Exercise 4

FS 16
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Problem 4.1 Exact diagonalization

Implement exact diagonalization for the Heisenberg chain. The Heisenberg chain consists of spin-$\frac{1}{2}$ particles on a one-dimensional chain with the Hamiltonian

$$H = \sum_{\langle i,j \rangle} \mathbf{S^i} \cdot \mathbf{S^j}.$$

The sum runs over pairs of nearest neighbours and $\mathbf{S^j} = \frac{1}{2}(\sigma_x^j, \sigma_y^j, \sigma_z^j)$, where σ_α^j are the Pauli matrices acting on the spin at site j. As the dimension of the Hilbert space grows exponentially in the number of sites on the chain we will only be able to tackle small problems.

Since the total magnetization, $S_z = \sum_i S_z^i$, commutes with the Hamiltonian, $[H, S_z] = 0$, this is a symmetry of the system and all eigenstates of H are eigenstates of S_z and can be characterized according to their quantum number. In your program, make use of the resulting block structure of H to speed up your calculation. You should also use multi-spin coding, i.e. store your basis states in such a way that each site only takes up one bit of memory.

For the ground state at open boundary conditions, you can find some reference results below:

L	**Energy per site**
2	-0.375
3	$-\frac{1}{3}$
4	-0.40401
$\vdots$	$\vdots$
∞	-0.44325

Using your result, discuss the following aspects:

- Observe that the energy oscillates with system size — chains of odd length always have slightly higher energy than chains of comparable even length. This holds true both with open and periodic boundary conditions, but for different reasons. Can you explain this behaviour?

- Consider how the energy gap $\Delta E = E_1 - E_0$ scales with the system size L (for even L). For an appropriately chosen fitting range, you should find that it extrapolates to zero as $\Delta E(L) \sim L^{-1}$.