

Computational Quantum Physics Exercise 6

Problem 6.1 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

$$H = \sum_{\langle i,j \rangle} \mathbf{S}^i \cdot \mathbf{S}^j. \quad (1)$$

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	-.4025
⋮	⋮
∞	-0.44325

(2)

Using your result, discuss the following problems:

- Observe that the energy oscillates with system size – odd length chains always have slightly higher energy than even-length chains with comparable size. 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 $\Delta E(L) \sim L^{-1}$.