# **Computational Many-Body Physics**

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### Sheet 5

## **Exercise 1: Kitaev clusters**

Kitaev clusters are quantum spin models defined by the Hamiltonian

$$H = -J \sum_{ij\alpha} J^{\alpha}_{ij} S^{\alpha}_i S^{\alpha}_j ,$$

 $(i, j = 1, ..., N, \alpha = x, y, z)$  with each spin of the cluster connected to exactly three spins with different couplings (x, y, or z), see section 2.1 in the script. In the following, the couplings  $J_{ij}^{\alpha}$  of the Kitaev cluster can be set to 1.

For a given N, various different Kitaev clusters can be constructed (and the number of possible clusters increases with N, of course).

a) Show that, for N = 6, one can construct two different Kitaev clusters which have a different spectrum of eigenenergies.

One of the Kitaev clusters that can be constructed for N = 8 can be visualized as a cube, with the eight spins of the cluster corresponding to the corners of the cube, and the twelve links corresponding to the edges. This particular Kitaev cluster has a non-degenerate ground state.

b) Show that the spin correlations in the ground state of the Kitaev cube are only non-zero for nearest neighbour sites (this turns out to be a general property of all Kitaev clusters).

# Exercise 2: Entanglement entropy for the one-dimensional Heisenberg model

Here we consider the one-dimensional Heisenberg model with open boundary conditions:

$$H = -\sum_{i=1}^{N-1} J_i \, \vec{S}_i \cdot \vec{S}_{i+1} \; .$$

For an even number of sites N and  $J_i < 0$  (the anti-ferromagnetic case), the groundstate of this model is non-degenerate. The focus in this exercise is on the entanglement entropy  $S_e$ , for which the system is divided in two parts (A and B), with parts A and B comprising sites  $1, \ldots, M_A$  and  $M_A + 1, \ldots, N$ , respectively.

- a) Calculate the entanglement entropy for the ground state of the Heisenberg model for N = 10 and  $J_i = -1$  (the homogeneous case) as a function of  $M_A$ .
- b) Compare the result from a) with the maximal values of  $S_e$  that can be achieved for the entanglement between parts A and B.
- c) For  $J_i = -1$ , N = 6, and  $M_A = 3$ , the entanglement entropy  $S_e = 0.711...$  is much lower than the maximal value  $S_{e,\max} = 3\ln(2) = 2.079...$ . Find a set of *J*-values (with  $-1 \leq J_i < 0, i = 1, ..., 5$ ), such that  $S_e > 1.5$ .