Computational Many-Body Physics

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Exercise Sheet No. 6

Please upload your solutions to ILIAS until **Thursday, July 7, 16:00**.

Exercise 1: Kitaev clusters

(8 points)

Kitaev clusters are quantum spin models defined by the Hamiltonian

$$H = -J \sum_{ij\alpha} J_{ij}^{\alpha} S_i^{\alpha} S_j^{\alpha} \ ,$$

($i, j = 1, \dots, N$, $\alpha = x, y, z$) 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}^{α} 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 (by plotting the two possibilities). Calculate numerically the spectrum of eigenenergies of these two clusters. (4 points)

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 (numerically) 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). (4 points)

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

(9 points)

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. (5 points)

b) Prepare a plot of the results for S_e from part a) together with the maximal values of S_e that can be achieved for the entanglement between parts A and B. (2 points)

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 $-1 \leq J_i < 0$, $i = 1, \ldots, 5$), such that $S_e > 1.5$. (2 points)