Problem 1: Schmidt values, Area law and Boundary conditions

1. Write down an exact diagonalization code for the transverse field Ising model:

$$H = -J \sum \sigma_i^x \sigma_{i+1}^x - h \sum \sigma_i^z$$
$$\sigma_i^x = [0, 1; 1, 0]$$
$$\sigma_i^z = [1, 0; 0, -1]$$

2. Start with open boundary conditions (the first sum in the Hamiltonian runs from *i=1* to *N-1;* the second - from 1 to *N.*). Let's take the parameters J=1 and h=0.1 - this corresponds to a gapped phase with a spontaneously broken parity symmetry. Diagonalize the Hamiltonian and find the ground state for *N=16* sites (the energy of this state is -15.045031336). Reshape the ground state into a square matrix of linear size 2^8 and perform singular value decomposition. Plot singular values in a semi-log scale. How many singular values are larger than 10^{-15}; larger than 10^{-8}?

3. Repeat the step (2) for a para-magnetic phase at h=10 and then for a critical point at h=1. Plot singular values in each case on the same plot and compare all three cases. How singular values decay in gapped vs critical systems?

4. Include periodic boundary conditions into your code. Repeat step (2) for h=1 and plot singular values on top of all previous results. What is the MPS bond dimension needed to include all Schmidt values above 10^{-8}; above 10^{-15}? Compare with open boundary conditions.

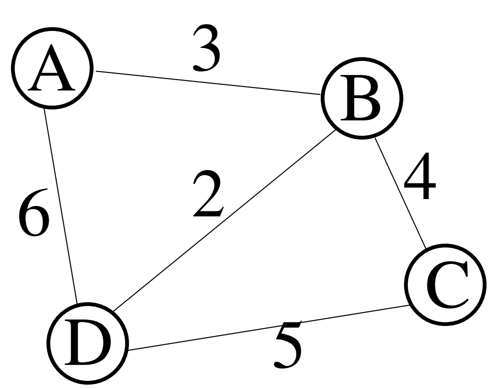
5. Open free vs Open fixed BC: Consider open boundary conditions with a boundary field in x-direction at the first and last site (e.g. hx=10). Repeat step (2) for h=0.1, 1, 10. What do you see? Why?

6. High-energy states. Let us use again open and free boundary conditions and h=1. Repeat step (2) for excited states: 2$^{\text{nd}}$, 3$^{\text{rd;}}$ 60$^{\text{th}}$.

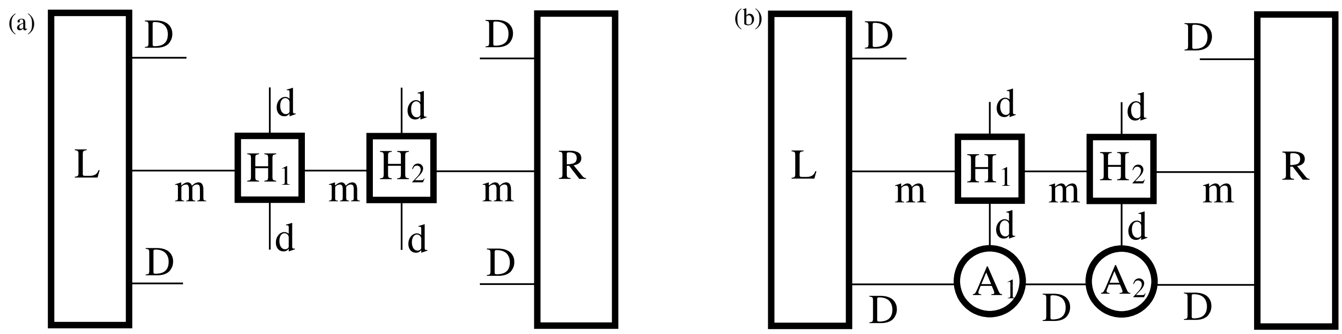
7. Random state: Define a random vector of size 2^16 and normalize it. Perform svd decomposition and compare the results with all previously obtained curves in steps (2)-(6).

Problem 2: Complexity and efficient contraction

1. Find the optimal order of contraction and the complexity of each step for the network of four tensors A, B, C and D with the specified bond dimensions.



2. The network shown in (a) is called an effective Hamiltonian – it is a full many-body Hamiltonian written in a truncated basis defined by MPS with bond dimension D. What is the complexity associated with contraction of the effective Hamiltonian shown in (a)? In practice however, we never write down the effective Hamiltonian explicitly. Instead one uses iterative algorithms, e.g. Lanczos, where the Hamiltonian is never written as a matrix but only through its action on a given state. The corresponding network is shown in (b). Find the optimal way to contract the network and an associated complexity. Typical bond dimensions: D=1000; d=2; m=5.



Problem 3. Matrix Product Operators

1. Construct the most compact form of MPO for the transverse field Ising model defined in the Problem 1. Consider both, open and periodic boundary conditions. For local Hamiltonians you may find the optimal bond dimension by performing SVD decomposition of the full Hamiltonian. For this reshape the Hamiltonian into a matrix grouping bra- and ket- indices of the first N/2 sites into matrix' rows and of the last N/2 sites into its columns. Perform SVD of the obtained matrix and see how many non-zero entries appear.

2. Construct the most compact MPO for the Majumdar-Ghosh spin-1/2 chain:

$$H = J_1 \sum \vec{S}_i \cdot \vec{S}_{i+1} + J_2 \sum \vec{S}_i \cdot \vec{S}_{i+2}$$

3. Construct the most compact MPO for the superconducting Kitaev chain:

$$H = \sum t(c_i^\dagger c_{i+1} + \mathrm{h.c.}) + s(c_i^\dagger c_{i+1}^\dagger + \mathrm{h.c.}) + \mu c_i^\dagger c_i$$

Problem 4. Infinite-size DMRG

1. Implement infinite-size DMRG for the transverse field Ising model with open boundary conditions
2. For small system sizes benchmark your code with the results from exact diagonalization
3. Study how the energy convergence vary with D
4. For h=0.1 and h=1 study how entanglement entropy in the middle of the chain changes with a system size N. For a fixed bond dimension D the entanglement entropy will, at some point, saturate. Why it saturates for h=0.1 and why for h=1? Plot entanglement entropy for various values of D and compare the results. Tip: go up to N~1000 and D=5,10,20.