DRSTP SPCTM school 2018 Introduction to tensor networks for QMBS

Exercise 1

You can skip this exercise and move directly to exercise 2! It's only added here as additional material for the interested students (the solution codes are in the dropbox).

Problem 1.1 Schmidt decomposition and entanglement entropy

The aim of this exercise is to get familiar with basic concepts of tensor network methods.

- 1. Compute the ground state of a S=1/2 Heisenberg chain with open boundary conditions with N=16 sites using a sparse matrix diagonalization like in tutorial 3. You can use the provided functions in the ex1 folder.
- 2. Split the ground state in the middle of the chain using an SVD (using the Matlab functions reshape and svd as in the tutorial). Compute the entanglement entropy and plot the distribution of the eigenvalues of the reduced density matrix p_k (= the square of the singular values). Normalize them such that their sum is equal to 1.
- 3. Create a random state in the Hilbert space and do the same as in 2. Compare the distribution of p_k to the previous one (adding it to the same plot). What can you observe?
- 4. Do the splitting of the ground state and the random state as in 2, but without keeping all the singular values. Make a plot of the relative error of the energy as a function the number of singular values (states) D kept, for a few values between $D=2\ldots 100$. Observe how the energy quickly converges to the exact solution up to machine precision for the ground state, whereas the energy of the random state converges only very slowly. Make sure you either normalize the approximated wave function or divide by its norm when computing the energy.

Problem 1.2 Decomposition of a state into an MPS using SVDs

This is a similar exercise as 1.1 but now instead of doing a single cut in the middle of the system, we do a full decomposition of a state into an MPS.

Note: If you want to try a simpler version of this exercise, simply do it for a specific case, e.g. L=4, without writing a general code which works for arbitrary L.

- 1. Write a function to decompose an arbitrary state into an MPS using a sequence of SVD's. You can use the *tensorsvd* function to do this (see tutorial 5). You can store the MPS, e.g. in a Matlab cell array. ¹
- 2. Write a function to recompute the state as a vector from an MPS by multiplying all the MPS tensors together, using *tcontract*. You can check if the two functions are correct by first decomposing a state into an MPS (keeping all singular values) and then recomputing the state from the MPS. This should give the same state (e.g. it has the same energy).²

Hint: to reshape a 2^L vector into a $2 \times 2 \cdots \times 2$ tensor you can use: T = reshape(V, ones(1, L)*2);

²Note that in practice we do not recompute the state as a vector from a given MPS since this is computationally not efficient. Instead we directly compute observables (e.g. the energy) from the MPS.

3. Do an approximate decomposition of the ground state as an MPS system keeping only a maximal bond dimension D.³ Plot the relative error of the energy of the MPS for a few values of D between $D = 2 \dots 100$, similarly as in the last exercise.

Problem 1.3 Product vs entangled states

(a) Is the following state defined on two sites an entangled or a product state?

$$|\psi\rangle = \frac{1}{\sqrt{4}} (|\uparrow\uparrow\rangle + |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle + |\downarrow\downarrow\rangle)$$

Compute the reduced density matrix $\hat{\rho}_1$ of this state (by hand). What is the value of the entanglement entropy between the two sites?

(b) Is the following state defined on two sites an entangled or a product state?

$$|\psi\rangle = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$$

Compute the reduced density matrix $\hat{\rho}_1$ of this state (by hand). What is the value of the entanglement entropy between the two sites?

³Note that at the boundary the bond dimension of the MPS will typically be smaller than the maximal D we impose. This is because the lth bond in the MPS (from the left or from the right) has a maximal Hilbert space dimension of 2^l .