

Lecture “Analytical and Numerical Methods for Quantum Many-Body Systems from a Quantum Information Perspective” — Exercise Sheet #3

1. Given a 1D state $|\Psi\rangle$ with Schmidt decompositions

$$|\Psi\rangle = \sum_k \lambda_k^s |\alpha_k^s\rangle |\beta_k^s\rangle ,$$

for the cut between sites s and $s + 1$, and tail weights of the Schmidt spectrum for a given D_{\max}

$$\epsilon_s := \sum_{k > D_{\max}} (\lambda_k^s)^2 ,$$

determine a bound on the total truncation error when truncating the bond dimension of $|\Psi\rangle$ to D_{\max} . (We discussed this in the lecture but ignored the fact that the Schmidt spectrum at a cut might be affected by previous truncations.)

There are various ways to do it:

- (a) You can come up with your very personal proof. (Highly encouraged!)
- (b) You can follow the proof given in <http://arxiv.org/abs/cond-mat/0505140>. (This is Lemma 1 in the paper.)
- (c) You can try a proof along the following lines (check all claims made in the following – no guarantee taken!):

Truncating at cut s can be achieved by acting on the sites left of s with a projector

$$P_s = \sum_{k \leq D_{\max}} |\alpha_k^s\rangle \langle \alpha_k^s| .$$

In the right gauge, it should be clear that sequentially cutting the tail of the Schmidt decomposition from right to left can be understood as acting with $P_1 P_2 \cdots P_{N-1}$ on $|\Psi\rangle$. We can then show that

$$P_{N-1} |\Psi\rangle = |\Psi\rangle + |\delta\Psi\rangle ,$$

where $|\delta\Psi\rangle$ is small (as a function of ϵ_{N-1}), and then continue by applying P_{N-2} , etc., and thereby obtain a bound on the overall error.

2. We say that $\vec{p} = (p_1, \dots, p_D)$, $p_1 \geq p_2 \geq \dots \geq 0$ majorizes $\vec{q} = (q_1, \dots, q_D)$, $q_1 \geq q_2 \geq \dots \geq 0$, and write $\vec{p} \succeq \vec{q}$, iff

$$\forall d = 1, \dots, D : \sum_{i=1}^d p_i \geq \sum_{i=1}^d q_i$$

with equality for $d = D$. (Intuitively, this says that the distribution q is more flat than p .) For a probability distribution \vec{p} with $\sum_i p_i = 1$, the α Rényi entropy, $\alpha \neq 1$, is given by

$$S_\alpha(\vec{p}) = \frac{\log \sum_i p_i^\alpha}{1 - \alpha} .$$

Prove that the Rényi entropy is *Schur concave*, i.e.,

$$\vec{p} \succeq \vec{q} \Rightarrow S_\alpha(\vec{p}) \leq S_\alpha(\vec{q}) . \tag{1}$$

Further, verify that the distribution used in the lecture to minimize the Rényi entropy majorizes all other distributions and thus has the minimum possible entropy.

3. Verify the relation of entropy scaling, truncation error, and bond dimension sketched at the end of the lecture on Nov. 23rd. (The derivation follows the proof of Lemma 2 in <http://arxiv.org/abs/cond-mat/0505140>).

4. Write a code (or modify the provided DMRG code) to implement the simple method to truncate the bond dimension discussed in the lecture. Use this to write a simple algorithm for simulating time evolution. (To this end, you have to find a tensor decomposition for $e^{-ih\delta t}$; the simplest way is to approximate it by $\mathbb{1} - ih\delta t$ and use that h can be written as a sum of tensor products. Then, apply one Trotter step, truncate the bond dimension, and iterate.) You can check how well the method works for a given time T by evolving until $t = T$, then un-evolving back to $t = 0$, and verifying if you arrive at the original state.

Use the algorithm also with imaginary time evolution to obtain an approximation to the ground state; this can be used to create an initial configuration for the DMRG algorithm.