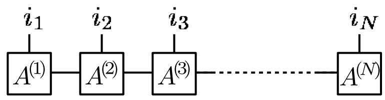
Lecture 260070 “Entanglement in quantum many-body systems” – SS 2021

— Exercise Sheet #2 —

Note: Problem 3a and 3b count as separate problems from the point of view of demonstrating one problem in the lecture.

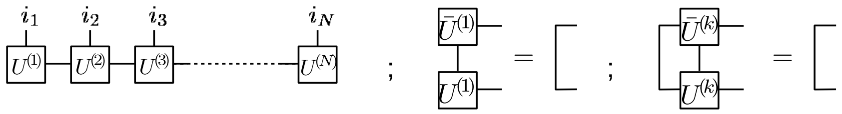
Problem 3a: Left- and right-canonical form for MPS

In this and the following problem, we will study canonical forms for MPS.
To start with, consider a general MPS with bond dimension D, i.e. a state $|\psi\rangle = \sum c_{i_1,\dots,i_N}|i_1,\dots,i_N\rangle$ such that

$$c_{i_1,\dots,i_N} = A^{(1)}_{i_1} A^{(2)}_{i_2} A^{(N-1)}_{i_{N-1}} A^{(N)}_{i_N} =$$  , (1)

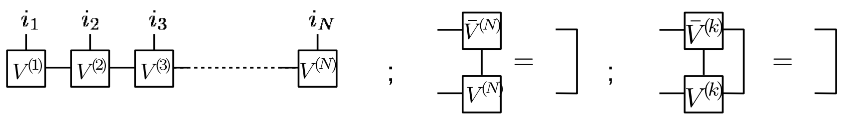
where $A^{(k)}_{i_k}$, $k = 2,\dots,N-1$ are $D \times D$ matrices, and the leftmost and rightmost A are vectors. Unlike in the derivation in the lecture, we assume no special condition on the A's, i.e., they can be *arbitrary* matrices.

1. The form discussed in the lecture, where the A's are isometries from left to right,

 (2)

is called *left-canonical form.* Show that any MPS of the form (1) can be brought into left-canonical form by a sequence of SVDs, where the size of the matrices for which the SVD has to be applied is independent of the system size (specifically, $dD \times D$ matrices.)
(*Note:* The procedure is pretty much exactly the same as the one used in the lecture to decompose a general $c_{i_1,\dots,i_N}$, but there, one had to perform SVDs of the whole $c_{i_1,(i_2,dots,i_N)}$, which scales exponentially with the system size and is thus unfeasible in practice. The point here is that once the state is presented in the form (1), this exponential scaling vanishes.)

2. Show that one can also obtain a canonical form where the tensors are isometries from the right,

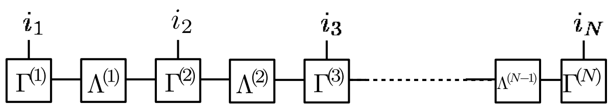
 (3)

the *right-canonical form.*

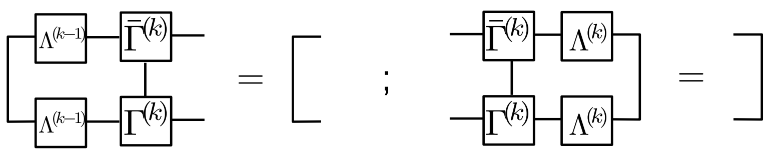
Problem 3b: The Γ-Λ-form

This problem partly builds on Problem 3a, and uses the concepts and equations discussed there.

1. A form which combines the advantages of both forms in the Γ-Λ-form

 , (4)

where

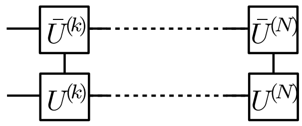
 (5)

(and correspondingly for the left-most and right-most tensor without the Λ and the outer index, as in (2) and (3)), and Λ can be chosen to be a diagonal matrix with positive entries (if Λ isn't chosen that way, then a complex conjugate $\bar{\Lambda}$ has to be used in the upper layer).

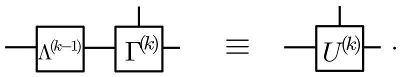
(a) Check that the form (4) allows to obtain both the left- and right-canonical form, by blocking each Γ either with the Λ to its left or to its right.

(b) Show that the matrix $\Lambda^{(k)}$ at any cut contains the Schmidt coefficients of the state at that cut. What are the Schmidt vectors?

(c) Describe an algorithm to get an MPS into the form (4,5).
(*Hint:* You can start e.g. from the left-canonical form (2), and for every cut (starting from the left) consider

$\rho :=$ 

(ρ is positive semi-definite – why?), define $\Lambda^{(k)} = \sqrt{\rho}$, and redefine



Also, it might be easier to first not restrict to Λ being diagonal, and just ensure the condition (5); in a second step, you can then consider how to make Λ diagonal).

Problem 4: Truncating Matrix Product States

In this problem, we derive a bound on the total error when truncating the bond dimension of a 1D MPS (or generally an arbitrary 1D state $|\Psi\rangle = \sum c_{i_1,\dots,i_N}|i_1,\dots,i_N\rangle$ for which we have decomposed $c_{i_1,\dots,i_N}$ as an MPS to some D.

To this end, consider 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 $s+1$. For each of these cut, there is a "tail weight" of the Schmidt spectrum for $k > D$,

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

The goal of the problem is to show that there is a way to truncate the MPS description of $|\Psi\rangle$ to bond dimension D at *all* cuts, with a total error

$$\epsilon_{\text{tot}} \le \sum_s \epsilon_s \ .$$

There are different ways in which to proceed:

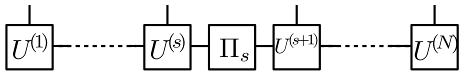
1. You can come up with your very personal proof. (Highly encouraged!)

2. You can follow the proof given in http://arxiv.org/abs/cond-mat/0505140. (This is Lemma 1 in the paper.) Good luck!

3. You can try a proof along the following lines (but make sure to check all claims made in the following!):

   (a) Work in the left-canonical gauge (the one used in the lecture when decomposing $c_{i_1,\dots,i_N}$, see Problem 3a.)

(b) Show that truncating the Schmidt decomposition at cut s can be achieved by inserting a rank-D projector Π_s in the MPS at the cut s,



(c) Show that the same truncation can also be achieved by acting on the physical sites left of the cut with a projector

$$P_s = \sum_{k \le D} |\alpha_k^s\rangle\langle\alpha_k^s| \ ,$$

i.e., by applying $P_s \equiv (P_s \otimes I)$ to $|\Psi\rangle$ – that is, applying Π_s and P_s in the left-canonical form has the same effect. Show that this only depends on the left-canonical property of the tensors *left* of the cut s.

(d) Show that inserting the aforementioned rank-D projector Π_s at all cuts at the same time yields an MPS with bond dimension D.

(e) Show that inserting the aforementioned rank-D projector Π_s at all cuts at the same time amounts to acting with $P_1 P_2 \cdots P_{N-1}$ on $|\Psi\rangle$.

(f) To bound the total error

$$\big\| |\Psi_D\rangle - |\Psi\rangle \big\| \tag{6}$$

where

$$|\Psi_D\rangle := P_1 P_2 \cdots P_{N-1} |\Psi\rangle \ ,$$

we can use that in each step,

$$P_s |\Psi\rangle = |\Psi\rangle + |\delta_s\rangle \ , \tag{7}$$

where $|\delta_s\rangle$ is small (i.e., bounded by a function of ϵ_s – which function?), and orthogonal projectors in a Hilbert space are contractive (i.e., norm-nonincreasing), and use a sequence of triangle inequalities.

(g) If you proceeded above in the straightforward way, you probably have obtained

$$\big\| |\Psi_D\rangle - |\Psi\rangle \big\| \le \sum \big\| |\delta_s\rangle \big\|$$

– that is, the norm-difference scales linearly with N, and thus, the error in measuring a physical quantity scales as N^2. Show that this can be improved to

$$\big\| |\Psi_D\rangle - |\Psi\rangle \big\|^2 \le \sum \big\| |\delta_s\rangle \big\|^2 = \sum \epsilon_s \ ,$$

i.e., a scaling where the errors in meausurements scale *linearly* in N.
(*Hint:* Use that in (7), $|\delta_s\rangle$ can be chosen such that $P_s|\delta_s\rangle = 0$, and analyze what happens when you apply $P_s(|\psi\rangle + |\delta_{s+1}\rangle) = |\psi\rangle + |\delta'_s\rangle$ – what is the norm of $|\delta'_s\rangle$?)