Matrix Product State *

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Abstract

These notes follow mathematical proofs related to matrix product states (MPS). In particular, they trace the arguments in [3].

Throughout this note the number of sites is denoted by N. The dimension of the local Hilbert space is denoted by d and is assumed to be the same at every site. Whenever singular value decomposition (SVD) or Schmidt decomposition (SD) is used, it means the compact decomposition in which singular vectors with zero singular value are omitted.

1 Derivation of MPS

A general MPS is written as

$$|\psi\rangle = \sum_{i_1,\ldots,i_N} A^{[1]}_{i_1} A^{[2]}_{i_2} \cdots A^{[N]}_{i_N} |i_1 \cdots i_N\rangle , \tag{1.1}$$

where $A^{[m]}_{i_m}$ is an $r_{m-1} \times r_m$ matrix.

- An MPS is said to be written with open boundary conditions (OBC) when $A^{[1]}_{i_1}$ and $A^{[N]}_{i_N}$ are vectors, namely when $r_0 = r_N = 1$. This is called an OBC-MPS representation.
- The number $r = \max_m r_m$ is called the bond dimension of the MPS.

Notice that "being an OBC-MPS" is a rule for the representation, not a boundary condition imposed on the physical problem. For example, the following theorem shows that any quantum state, including the ground state of a translation-invariant Hamiltonian with periodic boundary condition, admits an OBC-MPS representation. In [3] the canonical equations are written as

$$\sum_i A^{[m]}_i A^{[m]\dagger}_i = \mathbf{1}_{D_m}, \qquad \sum_i A^{[m]\dagger}_i \Lambda^{[m-1]} A^{[m]}_i = \Lambda^{[m]}.$$

That form is obtained when the Schmidt decomposition is performed from the right. Here the Schmidt decomposition is performed from the left. Following the proof in a slightly different convention is also useful for understanding the argument.

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*This English translation was generated from the original Japanese note using AI translation by ChatGPT (GPT-5).

Theorem 1.1 (Completeness and standard form [2]). *Let $|\psi\rangle \in \mathbb{C}^{d\otimes N}$ be normalized, $\langle\psi|\psi\rangle = 1$. Then $|\psi\rangle$ has an OBC-MPS representation of bond dimension $r < d^{\lfloor N/2 \rfloor}$ satisfying the following conditions:*

1. *For every $1 \le m \le N$,*
$$\sum_i A_i^{[m]\dagger} A_i^{[m]} = \mathbf{1}_{r_m}. \tag{1.2}$$

2. *For every $1 \le m \le N$,*
$$\sum_i A_i^{[m]} \Lambda^{[m]} A_i^{[m]\dagger} = \Lambda^{[m-1]}. \tag{1.3}$$

3. $\Lambda^{[0]} = \Lambda^{[N]} = 1$. *For $1 \le m \le N-1$, $\Lambda^{[m]}$ is an $r_m \times r_m$ positive diagonal matrix and* $\operatorname{tr}\Lambda^{[m]} = 1$.

Proof. Following [4], we construct the MPS by performing Schmidt decompositions successively from the left. Write the pure state as

$$|\psi\rangle = \sum_{i_1,\ldots,i_N} \psi_{i_1 i_2 \cdots i_N} |i_1 \ldots i_N\rangle . \tag{1.4}$$

First regard the wave function as a matrix with row index i_1 and column index $(i_2 \cdots i_N)$. The compact SVD gives

$$\psi_{i_1\cdots i_N} = \psi_{i_1,(i_2\cdots i_N)} = \sum_{a_1=1}^{r_1} U_{i_1,a_1} \sqrt{\Lambda^{[1]}_{a_1,a_1}}\, V^\dagger_{a_1,(i_2\cdots i_N)} \tag{1.5}$$

$$= \sum_{a_1=1}^{r_1} A^{[1]i_1}_{a_1} \psi_{a_1 i_2 \cdots i_N}, \qquad r_1 \le d, \tag{1.6}$$

where

$$A^{[1]i_1}_{a_1} = U_{i_1,a_1}, \qquad \psi_{a_1 i_2\cdots i_N} = \sqrt{\Lambda^{[1]}_{a_1,a_1}}\, V^\dagger_{a_1,(i_2\cdots i_N)}. \tag{1.7}$$

The singular values have been written as $\sqrt{\Lambda^{[1]}_{a_1,a_1}} > 0$ in order to match the convention of the theorem. Since $|\psi\rangle$ is normalized, $\operatorname{tr}\Lambda^{[1]} = 1$. Moreover, because $V^\dagger V = 1_{r_1}$,

$$\sum_{i_2\cdots i_N} \psi^*_{a_1 i_2\cdots i_N} \psi_{a_1' i_2 \cdots i_N} = \delta_{a_1 a_1'} \Lambda^{[1]}_{a_1,a_1}, \qquad \sum_{a_1 i_2 \cdots i_N} |\psi_{a_1 i_2\cdots i_N}|^2 = 1. \tag{1.8}$$

Thus the residual wave function is again normalized in the appropriate sense.

Next apply the compact SVD to the matrix with row index $(a_1 i_2)$ and column index $(i_3 \cdots i_N)$:

$$\psi_{a_1 i_2\cdots i_N} = \sum_{a_2=1}^{r_2} U_{(a_1 i_2),a_2} \sqrt{\Lambda^{[2]}_{a_2,a_2}}\, V^\dagger_{a_2,(i_3\cdots i_N)} \tag{1.9}$$

$$= \sum_{a_2=1}^{r_2} A^{[2]i_2}_{a_1 a_2} \psi_{a_2 i_3\cdots i_N}, \qquad r_2 \le r_1 d, \tag{1.10}$$

with

$$\operatorname{tr}\Lambda^{[2]} = 1, \qquad A^{[2]i_2}_{a_1a_2} = U_{(a_1i_2),a_2}, \qquad \psi_{a_2i_3\cdots i_N} = \sqrt{\Lambda^{[2]}_{a_2,a_2}}\, V^\dagger_{a_2,(i_3\cdots i_N)}. \tag{1.11}$$

Continuing in the same way, for $n = 3, \ldots, N-1$,

$$\psi_{a_{n-1}i_n\cdots i_N} = \sum_{a_n=1}^{r_n} U_{(a_{n-1}i_n),a_n} \sqrt{\Lambda^{[n]}_{a_n,a_n}}\, V^\dagger_{a_n,(i_{n+1}\cdots i_N)} \tag{1.12}$$

$$= \sum_{a_n=1}^{r_n} A^{[n]i_n}_{a_{n-1}a_n} \psi_{a_ni_{n+1}\cdots i_N}, \tag{1.13}$$

where

$$r_n \le \min(r_{n-1}d, d^{N-n}), \qquad \operatorname{tr}\Lambda^{[n]} = 1, \qquad A^{[n]i_n}_{a_{n-1}a_n} = U_{(a_{n-1}i_n),a_n}. \tag{1.14}$$

At the last site we put

$$A^{[N]i_N}_{a_{N-1}} = \psi_{a_{N-1}i_N}. \tag{1.15}$$

This gives the MPS expansion.

The first canonical equation follows from the orthonormality of the columns of each U:

$$\sum_{i_n=1}^{d} [A^{[n]i_n\dagger} A^{[n]i_n}]_{a_na'_n} = \sum_{a_{n-1}=1}^{r_{n-1}} \sum_{i_n=1}^{d} U^*_{(a_{n-1}i_n),a_n} U_{(a_{n-1}i_n),a'_n} = \delta_{a_na'_n} \tag{1.16}$$

for $n = 1, \ldots, N-1$. For $n = N$, the normalization of $\psi_{a_{N-1}i_N}$ gives the same equation. In matrix form,

$$\sum_{i_n=1}^{d} A^{[n]i_n\dagger} A^{[n]i_n} = 1_{r_n}, \qquad n = 1, \ldots, N. \tag{1.17}$$

For the second canonical equation, use the orthonormality of V. For $n = 2, \ldots, N$ one has

$$\sum_{i_n\cdots i_N} \psi^*_{a_{n-1}i_n\cdots i_N} \psi_{a'_{n-1}i_n\cdots i_N} = \Lambda^{[n-1]}_{a_{n-1},a_{n-1}} \delta_{a_{n-1}a'_{n-1}}. \tag{1.18}$$

Substituting the decomposition at the n-th step gives

$$\sum_{i_n\cdots i_N} \psi^*_{a_{n-1}i_n\cdots i_N} \psi_{a'_{n-1}i_n\cdots i_N} \tag{1.19}$$

$$= \sum_{i_n} \sum_{a_n=1}^{r_n} A^{[n]i_n*}_{a_{n-1}a_n} \Lambda^{[n]}_{a_n,a_n} A^{[n]i_n}_{a'_{n-1}a_n} \tag{1.20}$$

$$= \sum_{i_n} [A^{[n]i_n} \Lambda^{[n]} A^{[n]i_n\dagger}]_{a'_{n-1}a_{n-1}}. \tag{1.21}$$

The case $n = N$ is included by putting $\Lambda^{[N]} = 1$. For $n = 1$ a direct computation gives

$$\sum_{i_1} A^{[1]i_1} \Lambda^{[1]} A^{[1]i_1\dagger} = \sum_{a_1=1}^{r_1} \Lambda^{[1]}_{a_1,a_1} = 1. \tag{1.22}$$

Thus, with $\Lambda^{[0]} = 1$,

$$\sum_{i_n} A^{[n]i_n} \Lambda^{[n]} A^{[n]i_n\dagger} = \Lambda^{[n-1]}, \qquad n = 1, \ldots, N. \tag{1.23}$$

Finally, the bond dimension estimate follows from the rank bounds in the successive Schmidt decompositions:

$$r_n \leq \min(d^n, d^{N-n}) \leq d^{\lfloor N/2 \rfloor}. \tag{1.24}$$

Since zero singular values are omitted in the compact decomposition, one can write the strict inequality in the theorem by increasing the bound slightly if necessary. □

Remark 1.2. The standard OBC-MPS representation is unique up to the ordering of the Schmidt values and the choice of bases inside degenerate singular-value subspaces. The matrices $\Lambda^{[m]}$ are the nonzero eigenvalues of the reduced density matrix across the cut $[1, \ldots, m] : [m+1, \ldots, N]$. Indeed, from the construction,

$$|\psi\rangle = \sum_{a_m=1}^{r_m} |\phi_{a_m}^{[1,\ldots,m]}\rangle \sqrt{\Lambda_{a_m,a_m}^{[m]}} \, |\phi_{a_m}^{[m+1,\ldots,N]}\rangle \,, \tag{1.25}$$

with orthonormal Schmidt vectors on both sides. Tracing out the right subsystem gives

$$\rho_{[1,\ldots,m]} = \sum_{a_m=1}^{r_m} \Lambda_{a_m,a_m}^{[m]} \, |\phi_{a_m}^{[1,\ldots,m]}\rangle \langle \phi_{a_m}^{[1,\ldots,m]}| \,. \tag{1.26}$$

Consequently, a state admits an OBC-MPS representation of bond dimension at most D if and only if

$$\max_m \operatorname{rank} \rho_{[1,\ldots,m]} \leq D. \tag{1.27}$$

Theorem 1.3 (Matrix degrees of freedom in OBC-MPS [3]). *Let*

$$|\psi\rangle = \sum_{i_1,\ldots,i_N} B_{i_1}^{[1]} B_{i_2}^{[2]} \cdots B_{i_N}^{[N]} \, |i_1 \cdots i_N\rangle \tag{1.28}$$

be a normalized OBC-MPS representation, where $B_{i_m}^{[m]}$ *has size* $D_{m-1} \times D_m$ *and* $D_0 = D_N = 1$. *Let* r_m *be the Schmidt rank across the cut* $[1, \ldots, m] : [m+1, \ldots, N]$. *Then there are matrices* Y_m *and* Z_m *with* $Y_m Z_m = 1_{r_m}$ *such that*

$$A_i^{[m]} = Y_{m-1} B_i^{[m]} Z_m \tag{1.29}$$

is in the standard form of Theorem 1.1.

Proof. The proof is a controlled gauge transformation of the matrices $B_i^{[m]}$. It is useful to split it into three steps.

First, perform an SVD from the left. For the first site, write the span of the row vectors $B_i^{[1]}$ as

$$B_i^{[1]} = \sum_{a_1=1}^{r_1} A_{a_1}^{[1]i} Z_{a_1}^{[1]}. \tag{1.30}$$

The matrices $A^{[1]i}$ are chosen so that

$$\sum_i A^{[1]i\dagger} A^{[1]i} = 1_{r_1}. \tag{1.31}$$

Substituting this into the MPS and repeating the same decomposition at the next site gives

$$Z^{[m-1]} B_i^{[m]} = \sum_{a_m=1}^{r_m} A_{a_{m-1}a_m}^{[m]i} Z_{a_m}^{[m]}, \qquad \sum_i A^{[m]i\dagger} A^{[m]i} = 1_{r_m}. \tag{1.32}$$

After this step, the state is represented by matrices satisfying the left-isometric condition and by residual matrices $Z^{[m]}$.

Second, diagonalize the positive matrices obtained from the right contractions. The reduced density matrix across the cut is determined by the positive matrix

$$\rho_m = Z^{[m]} Z^{[m]\dagger}. \tag{1.33}$$

Let

$$Z^{[m]} Z^{[m]\dagger} = V^{[m]} \Delta^{[m]2} V^{[m]\dagger} \tag{1.34}$$

be its spectral decomposition with positive diagonal entries in $\Delta^{[m]}$. Inserting $V^{[m]\dagger} V^{[m]}$ and $\Delta^{[m]} (\Delta^{[m]})^{-1}$ between adjacent tensors produces matrices satisfying

$$\sum_i A_i^{[m]} \Lambda^{[m]} A_i^{[m]\dagger} = \Lambda^{[m-1]}. \tag{1.35}$$

Third, if some eigenvalues are zero, restrict to the support. Let P_m be the isometry from the support of $\Lambda^{[m]}$ into the original auxiliary space. Replacing the auxiliary matrices by

$$P_{m-1}^{\dagger} A_i^{[m]} P_m \tag{1.36}$$

does not change the represented state, since components in the kernel never contribute to the Schmidt expansion. The resulting diagonal matrices $\Lambda^{[m]}$ are strictly positive. The final gauge matrices can be written as

$$Y_n = P_n^{\dagger} V^{[n]\dagger} \Delta^{[n]} U^{[n]\dagger}, \qquad Z_n = U^{[n]} (\Delta^{[n]})^{-1} V^{[n]} P_n, \tag{1.37}$$

and hence

$$Y_n Z_n = P_n^{\dagger} P_n = 1_{\tilde{r}_n}. \tag{1.38}$$

□

2 Translation-Invariant MPS

We now consider MPS representations of translation-invariant pure states. The translation operator is

$$\hat{T} \left| i_1 i_2 \cdots i_N \right\rangle = \left| i_N i_1 \cdots i_{N-1} \right\rangle. \tag{2.1}$$

We consider eigenstates

$$\hat{T} \left| \psi \right\rangle = e^{iP} \left| \psi \right\rangle. \tag{2.2}$$

In this note no state with $e^{iP} \neq 1$ will be treated. A translation-invariant pure state with momentum $e^{iP} = 1$ will be called a TI state.

Theorem 2.1 (Site-independent MPS [3]). *Let $|\psi\rangle$ be a pure state satisfying $\hat{T}|\psi\rangle = |\psi\rangle$. Then $|\psi\rangle$ admits a representation*

$$\left| \psi \right\rangle = \sum_{i_1, \ldots, i_N} \operatorname{tr}\left[A_{i_1} \cdots A_{i_N} \right] \left| i_1 \cdots i_N \right\rangle, \tag{2.3}$$

where the matrices A_i do not depend on the site. This is called a TI-MPS representation. When it is obtained from an OBC-MPS of bond dimension D, the bond dimension generally increases from D to ND.

Proof. Let

$$|\psi\rangle = \sum_{i_1\cdots i_N} A^{[1]}_{i_1}\cdots A^{[N]}_{i_N}\,|i_1\cdots i_N\rangle \tag{2.4}$$

be an OBC-MPS representation. Since $|\psi\rangle$ is invariant under translations, all cyclic shifts of this representation give the same state. Define block-cyclic matrices

$$B_i = N^{-1/N}\begin{pmatrix} 0 & A_i^{[1]} & & & \\ & 0 & A_i^{[2]} & & \\ & & \ddots & \ddots & \\ & & & 0 & A_i^{[N-1]} \\ A_i^{[N]} & & & & 0 \end{pmatrix}. \tag{2.5}$$

Then only products which traverse the cycle contribute to the trace, and

$$\sum_{i_1,\ldots,i_N} \operatorname{tr}\left[B_{i_1}\cdots B_{i_N}\right]|i_1\cdots i_N\rangle \tag{2.6}$$

$$= \frac{1}{N}\sum_{j=0}^{N-1}\hat{T}^{-j}\,|\psi\rangle = |\psi\rangle\,. \tag{2.7}$$

□

Before moving to Theorem 4 of [3], we collect some facts about the transfer map. For a set of $D\times D$ matrices $\{A_i\}_{i=1}^d$, define

$$E(X) = \sum_i A_i^\dagger X A_i. \tag{2.8}$$

This map is positive, because it preserves positive semidefinite matrices. The spectral radius of E is the maximum modulus of its eigenvalues. In components,

$$E_{jk,lm} = \langle j|E(|l\rangle\langle m|)|k\rangle = \sum_i [A_i]^*_{lj}[A_i]_{mk}. \tag{2.9}$$

With respect to the Hilbert-Schmidt inner product

$$\langle X, Y\rangle = \operatorname{tr}[X^\dagger Y], \tag{2.10}$$

the adjoint map is

$$E^\dagger(X) = \sum_i A_i X A_i^\dagger. \tag{2.11}$$

The spectra of E and $E^\dagger$ are complex conjugates of one another, and their spectral radii agree. Moreover the Jordan block sizes also agree. Indeed, if $P^{-1}EP$ is a Jordan form, then $E^\dagger$ has the transposed conjugate Jordan blocks, which are similar to ordinary Jordan blocks after reversing the order of basis vectors.

Theorem 2.2. *For a finite-system TI-MPS representation, without changing the state $|\psi\rangle$, the matrices A_i can be decomposed into block-diagonal form*

$$A_i = \begin{pmatrix} A_i^1 & 0 & 0 \\ 0 & A_i^2 & 0 \\ 0 & 0 & \cdots \end{pmatrix}. \tag{2.12}$$

For each block, let λ_j be the spectral radius of $\mathcal{E}_j(X) = \sum_i A_i^{j\dagger} X A_i^j$. Then:

1. $$\sum_i A_i^{j\dagger} A_i^j = \lambda_j \mathbf{1}, \tag{2.13}$$

   and $\mathbf{1}$ *is the unique eigenvector of* $\mathcal{E}_j$ *with eigenvalue* λ_j*.*

2. *There exists a positive diagonal matrix* Λ^j *such that*

   $$\sum_i A_i^j \Lambda^j A_i^{j\dagger} = \lambda_j \Lambda^j, \tag{2.14}$$

   and Λ^j *is the unique eigenvector of* $\mathcal{E}_j^\dagger(X) = \sum_i A_i^j X A_i^{j\dagger}$ *with eigenvalue* λ_j*.*

If the initial bond dimension is D*, the resulting bond dimension is at most* D*.*

Remark: In [3], uniqueness of the eigenvector of $\mathcal{E}_j^\dagger$ is not explicitly mentioned. I add it here because I could not prove that Λ^j is positive definite without such uniqueness.

Lemma 2.3. *Let* $E : \mathbb{C}^{D\times D} \to \mathbb{C}^{D\times D}$ *be*

$$E(X) = \sum_i A_i^\dagger X A_i. \tag{2.15}$$

Assume that there is a positive definite eigenvector X *with positive real eigenvalue* $\lambda > 0$*. If there is another eigenvector* Y *with the same eigenvalue which is not a scalar multiple of* X*, then there exists a positive semidefinite, non-invertible eigenvector with the same eigenvalue. The same statement holds for* $E^\dagger(X) = \sum_i A_i X A_i^\dagger$*.*

Proof. Suppose

$$\sum_i A_i^\dagger X A_i = \lambda X, \qquad \sum_i A_i^\dagger Y A_i = \lambda Y. \tag{2.16}$$

Since $Y^\dagger$ is also an eigenvector, we may replace Y by its Hermitian part and assume that Y is Hermitian. Diagonalize

$$X^{-1/2} Y X^{-1/2} = \sum_{a=1}^{D} \lambda_a |a\rangle\langle a|, \qquad \lambda_1 \geq \cdots \geq \lambda_D. \tag{2.17}$$

If $\lambda_1 \neq 0$, then

$$X - \frac{1}{\lambda_1} Y = X^{1/2} \left(\sum_{a=1}^{D} \left(1 - \frac{\lambda_a}{\lambda_1}\right) |a\rangle\langle a| \right) X^{1/2} \tag{2.18}$$

is positive semidefinite and has a zero eigenvalue. It is also an eigenvector with eigenvalue λ. If $\lambda_1 = 0$, then $-Y$ is positive semidefinite and non-invertible. Replacing A_i by $A_i^\dagger$ gives the statement for $E^\dagger$. □

Lemma 2.4. *Let*

$$E(X) = \sum_i A_i^\dagger X A_i. \tag{2.19}$$

If E has a positive semidefinite, non-invertible eigenvector with positive real eigenvalue, then the same TI-MPS state can be represented by block-diagonal matrices. The analogous statement holds for $E^\dagger$.

Proof. Let $X \geq 0$ be such an eigenvector and let $R = \operatorname{im} X$ be its support. For $v \in \ker X$,

$$0 = \langle v|E(X)|v\rangle = \sum_i \langle A_i v|X|A_i v\rangle\,. \tag{2.20}$$

Since every term is nonnegative, $A_i v \in \ker X$ for every i. Thus $\ker X$ is invariant under all A_i. With respect to the decomposition $\mathbb{C}^D = R \oplus \ker X$, the matrices can be written in triangular block form. In a trace of a cyclic product, the off-diagonal triangular blocks do not contribute independently; the trace is the sum of the traces of the diagonal block products. Therefore the same state is obtained by replacing A_i by the direct sum of the diagonal blocks. For $E^\dagger$, the same proof with A_i and $A_i^\dagger$ interchanged gives the dual statement. □

Lemma 2.5 (Finite-dimensional Krein-Rutman, Theorem 2.5 of [7])**.** *A positive linear map on a finite-dimensional C^*-algebra has a nonzero positive semidefinite eigenvector whose eigenvalue is the spectral radius.*

Proof of Theorem 2.2. Apply Lemma 2.5 to E and to $E^\dagger$. If the eigenspace at the spectral radius has more than one independent positive definite direction, Lemma 2.3 produces a positive semidefinite non-invertible eigenvector. Then Lemma 2.4 decomposes the representation into smaller blocks without changing the state. Repeating this procedure terminates because the bond dimension is finite. In each final block, the eigenspaces of E and $E^\dagger$ at the spectral radius are one-dimensional and generated by positive definite matrices.

Let $X > 0$ be the eigenvector of E with eigenvalue λ_j in one block:

$$\sum_i A_i^\dagger X A_i = \lambda_j X. \tag{2.21}$$

The similarity transform

$$B_i = X^{1/2} A_i X^{-1/2} \tag{2.22}$$

gives

$$\sum_i B_i^\dagger B_i = \lambda_j \mathbb{1}. \tag{2.23}$$

The positive eigenvector of the adjoint map can then be diagonalized by a unitary transformation; this gives the positive diagonal matrix Λ^j and proves the second condition. □

After rescaling each block by $\sqrt{\lambda_j}$, we obtain the standard form

$$A_i = \begin{pmatrix} \sqrt{\lambda_1} A_i^1 & & \\ & \sqrt{\lambda_2} A_i^2 & \\ & & \ddots \end{pmatrix}, \tag{2.24}$$

where each block has spectral radius one and satisfies

$$\sum_i A_i^{j\dagger} A_i^j = 1, \qquad \sum_i A_i^j \Lambda^j A_i^{j\dagger} = \Lambda^j. \tag{2.25}$$

The identity is the unique fixed point of $\mathcal{E}_j(X) = \sum_i A_i^{j\dagger} X A_i^j$, and Λ^j is the unique fixed point of the adjoint channel.

Remark 2.6. In Wolf's terminology, a positive map is irreducible if it has no nontrivial invariant projection. The "one-block standard TI-MPS" condition is closely related to irreducibility, although the precise relation should be checked carefully. Even a one-block standard TI-MPS can be a superposition of macroscopically distinct wave functions. For example, take

$$A_0 = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \qquad A_1 = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}. \tag{2.26}$$

For even N, this gives the antiferromagnetic GHZ-type state

$$|0101\cdots\rangle + |1010\cdots\rangle . \tag{2.27}$$

The transfer map has eigenvalues $\{1, -1, 0, 0\}$.

Theorem 2.7 (Periodic-system decomposition [3]). *Let a TI-MPS be in one-block standard form. If the transfer map*

$$E(X) = \sum_i A_i X A_i^\dagger \tag{2.28}$$

has p eigenvalues of modulus one, then, if p divides N, the state is a sum of p periodic states of bond dimension D. If p does not divide N, the state is zero.

Proof. The detailed proof is not followed here.

$$@@@ \tag{2.29}$$

Define

$$\Gamma_L : M_D(\mathbb{C}) \to \mathbb{C}^{d^L}, \qquad X \mapsto \sum_{i_1,\ldots,i_L} \mathrm{tr}\,[X A_{i_1} \cdots A_{i_L}]\, |i_1 \cdots i_L\rangle . \tag{2.30}$$

The map Γ_L is injective if and only if the products

$$A_{i_1} \cdots A_{i_L} \tag{2.31}$$

span the whole matrix algebra $M_D(\mathbb{C})$. Indeed, if these products span all matrices, then $\mathrm{tr}\,[XY] = 0$ for all $Y \in M_D(\mathbb{C})$ implies $X = 0$. Conversely, if the products do not span the whole algebra, choose a nonzero X orthogonal to their span with respect to the trace pairing. Then $\Gamma_L(X) = 0$, so Γ_L is not injective. If Γ_L is injective, then $\Gamma_{L'}$ is injective for all $L' \geq L$.

Definition 2.8 (Condition C1). The TI-MPS satisfies condition C1 if there exists L_0 such that Γ_{L_0} is injective, equivalently, the products of length L_0 span $M_D(\mathbb{C})$.

Proposition 2.9. *Assume that a standard TI-MPS satisfies C1 with* $L_0 < N$*. Then:*

1. *The MPS is one-block standard.*
2. *For a bipartition* $[1, \dots, R] : [R+1, \dots, N]$ *with* $L_0 \leq R \leq N - R$*, the reduced density matrix has rank* D^2*.*

Proof. For the second statement, define

$$|L_{\alpha\beta}\rangle = \Gamma_R(|\beta\rangle\langle\alpha|), \qquad |R_{\alpha\beta}\rangle = \Gamma_{N-R}(|\alpha\rangle\langle\beta|). \tag{2.32}$$

Because R and $N - R$ are at least L_0, both sets are linearly independent. The state can be written as

$$|\psi\rangle = \sum_{\alpha,\beta=1}^{D} |L_{\alpha\beta}\rangle |R_{\alpha\beta}\rangle . \tag{2.33}$$

Thus the Schmidt rank across this cut is D^2. If the MPS had more than one block, the rank would be smaller than the square of the total bond dimension in a way incompatible with C1, because products would preserve the block decomposition and could not span the full matrix algebra. ☐

Lemma 2.10. *Let* T *and* S *be linear maps and let* $Y_1, \dots, Y_n$ *be vectors such that*

$$T(Y_k) = S(Y_{k+1}), \qquad k = 1, \dots, n-1. \tag{2.34}$$

Assume $Y_1, \dots, Y_{n-1}$ *are linearly independent but* $Y_1, \dots, Y_n$ *are linearly dependent. Then, for a nonzero root* x *of the corresponding dependence polynomial, there exists a nonzero vector* Y *such that*

$$T(Y) = x^{-1} S(Y). \tag{2.35}$$

Proof. Write a minimal relation as

$$Y_n + \mu_{n-1} Y_{n-1} + \cdots + \mu_1 Y_1 = 0. \tag{2.36}$$

Let x be a nonzero root of

$$x^{n-1} + \mu_{n-1} x^{n-2} + \cdots + \mu_1. \tag{2.37}$$

The vector

$$Y = Y_1 + x Y_2 + \cdots + x^{n-2} Y_{n-1} \tag{2.38}$$

then satisfies the desired equation by telescoping. ☐

Lemma 2.11. *The solutions of*

$$W(C \otimes 1_n) = (B \otimes 1_n) W \tag{2.39}$$

are precisely matrices of the form $S \otimes M_n(\mathbb{C})$*, where* S *solves*

$$SC = BS. \tag{2.40}$$

Proof. Write W as an $n \times n$ block matrix. Each block satisfies the same intertwining equation $XC = BX$. Conversely, any block matrix whose blocks satisfy this equation solves the tensor equation. ☐

Theorem 2.12 (Uniqueness of the standard form [3])**.** *Let*

$$|\psi\rangle = \sum_{i_1,\ldots,i_N} \operatorname{tr}\left[B_{i_1} \cdots B_{i_N}\right] |i_1 \cdots i_N\rangle \tag{2.41}$$

be a bond-D standard TI-MPS satisfying:

(i) Condition C1 holds.

(ii) The standard OBC-MPS representation is unique.

(iii) $N > 2L_0 + D^4$.

If another bond-D standard TI-MPS with matrices C_i represents the same state, then there exist a unitary matrix U and a phase $e^{i\theta}$ such that

$$B_i = e^{i\theta} U C_i U^\dagger. \tag{2.42}$$

Remark: The statement in [3] does not include the phase. I do not see how to prove that the phase is one. If U and θ could be chosen independently of N, then comparison for different lengths may force the phase to be trivial.

Proof. Using C1 and the previous proposition, the Schmidt rank in the middle of the chain is D^2. From the TI matrices one builds an OBC representation by vectorizing boundary matrices:

$$b_i^{[1]} = (\langle 1|\, B_i \otimes 1_D, \ldots, \langle D|\, B_i \otimes 1_D), \qquad B_i^{[m]} = B_i \otimes 1_D, \tag{2.43}$$

and similarly at the right boundary, so that the product reproduces $\operatorname{tr}\left[B_{i_1} \cdots B_{i_N}\right]$. Perform the same construction for C_i. By the uniqueness assumption for the standard OBC-MPS representation, there are invertible matrices W_k satisfying

$$W_k(B_i \otimes 1_D) = (C_i \otimes 1_D) W_{k+1}. \tag{2.44}$$

Because there are more than D^4 such matrices, they are linearly dependent. Lemma 2.10 then gives a nonzero matrix W and a nonzero scalar x such that

$$W(B_i \otimes 1_D) = x^{-1}(C_i \otimes 1_D) W. \tag{2.45}$$

By Lemma 2.11, there is a nonzero matrix R such that

$$R B_i = x^{-1} C_i R. \tag{2.46}$$

Using the standard form and the fixed positive density matrices, one shows that $|x| = 1$. Indeed, $R \Lambda_B R^\dagger$ is a fixed point of the adjoint transfer map for C up to the factor $|x|^{-2}$, and uniqueness of the fixed point forces $|x| = 1$. The same uniqueness also implies that $R^\dagger R$ is proportional to the identity. After normalizing R, it becomes unitary. Writing $x = e^{-i\theta}$ gives

$$B_i = e^{i\theta} U C_i U^\dagger. \tag{2.47}$$

☐

Definition 2.13 (Condition C2)**.** Let r be the spectral radius of

$$E(X) = \sum_i A_i^\dagger X A_i. \tag{2.48}$$

Condition C2 means that the only eigenvalue of E with absolute value r is r itself.

Conditions C1 and C2 are equivalent; see [9]. The implication C2 ⇒ C1 also appears in [1]. The estimate for the required L_0 behaves as $O(\exp(1/|\lambda_2|))$ when the second eigenvalue is close to the unit circle, and in general [9] gives a bound of order $O(D^4)$.

Theorem 2.14 (Fannes-Katsura type statement)**.** *The unitary U in Theorem 2.12 is unique up to a phase, and the phase $e^{i\theta}$ is unique.*

Proof.

$$@@@ \tag{2.49}$$

3 Equivalence of Conditions C1 and C2

We follow the proof of [9].

A trace-preserving completely positive (CP) linear map $E : \mathbb{C}^{D\times D} \to \mathbb{C}^{D\times D}$ is called a quantum channel.

If $\sum_i A_i^\dagger A_i = 1_D$, then

$$\sum_i \operatorname{tr}[A_i X A_i^\dagger] = \sum_i \operatorname{tr}[X A_i^\dagger A_i] = \operatorname{tr} X, \tag{3.1}$$

so $X \mapsto \sum_i A_i X A_i^\dagger$ is a quantum channel. Conversely, if this CP map is trace preserving, applying the condition to $X = |k\rangle\langle l|$ for all k, l gives

$$\sum_i A_i^\dagger A_i = 1_D. \tag{3.2}$$

For Kraus operators $\{A_k \in \mathbb{C}^{D\times D}\}_{k=1}^d$, write

$$\mathcal{E}_A(X) = \sum_{k=1}^d A_k X A_k^\dagger. \tag{3.3}$$

Define

$$S_n(A) = \operatorname{Span}\{A_{k_1} \cdots A_{k_n}\}_{k_1,\ldots,k_n} \subset \mathbb{C}^{D\times D}, \tag{3.4}$$

and for $|\phi\rangle \in \mathbb{C}^D$ define

$$H_n(A,\phi) = S_n(A)\,|\phi\rangle\,. \tag{3.5}$$

Because

$$\mathcal{E}_A^n(|\phi\rangle\langle\phi|) = \sum_{k_1,\ldots,k_n} A_{k_1}\cdots A_{k_n}\,|\phi\rangle\,(A_{k_1}\cdots A_{k_n}\,|\phi\rangle)^\dagger\,, \tag{3.6}$$

one has

$$\operatorname{rank}\mathcal{E}_A^n(|\phi\rangle\langle\phi|) = \dim H_n(A,\phi). \tag{3.7}$$

Definition 3.1 ((a) Primitive)**.** The quantum channel $\mathcal{E}_A$ is primitive if there exists a natural number n such that

$$H_n(A,\phi) = \mathbb{C}^D \tag{3.8}$$

for every nonzero vector $|\phi\rangle \in \mathbb{C}^D$. The smallest such n is denoted by $q(\mathcal{E}_A)$.

If $n \geq q(\mathcal{E}_A)$, then $H_n(A,\phi) = \mathbb{C}^D$ for every nonzero $|\phi\rangle$. Indeed, primitivity implies that for every nonzero $|\phi\rangle$ some $A_k\,|\phi\rangle$ is nonzero. Hence, if $S_n(A)\eta = \mathbb{C}^D$ for all nonzero η, then

$$S_n(A)A_k\,|\phi\rangle \subset S_{n+1}(A)\,|\phi\rangle \tag{3.9}$$

already spans $\mathbb{C}^D$.

If $n \geq q(\mathcal{E}_A)$, then $\mathcal{E}_A^n(\rho)$ is full-rank for every density matrix ρ. Writing $\rho = \sum_k p_k\,|k\rangle\langle k|$, each nonzero contribution $\mathcal{E}_A^n(|k\rangle\langle k|)$ is positive definite, and a positive linear combination of positive definite matrices is positive definite.

If $\mathcal{E}_A$ is primitive, then $\mathcal{E}_A^p$ is primitive for every natural number p, since

$$(\mathcal{E}_A^p)^n = \mathcal{E}_A^{np}. \tag{3.10}$$

Definition 3.2 ((b) Eventually full Kraus rank)**.** The quantum channel $\mathcal{E}_A$ has eventually full Kraus rank if there exists a natural number n such that

$$S_n(A) = \mathbb{C}^{D\times D}. \tag{3.11}$$

The smallest such n is denoted by $i(A)$.

This is condition C1. If $n \geq i(A)$, then again $S_n(A) = \mathbb{C}^{D\times D}$.

Definition 3.3 ((c) Strongly irreducible)**.** The quantum channel $\mathcal{E}_A$ is strongly irreducible if:

(i) The only eigenvalue of $\mathcal{E}_A$ with $|\lambda| = 1$ is $\lambda = 1$, including multiplicity.

(ii) An eigenvector ρ for $\lambda = 1$ is positive definite, $\rho > 0$.

This is condition C2. The positive definiteness of the eigenvector at $\lambda = 1$ is exactly the condition imposed on each block in the standard TI-MPS form.

Proposition 3.4.

$$q(\mathcal{E}_A) \leq i(A). \tag{3.12}$$

Proof. If $n \geq i(A)$, then $S_n(A) = \mathbb{C}^{D\times D}$. For any nonzero $|\phi\rangle$, choose an orthonormal basis whose first vector is proportional to $|\phi\rangle$. The matrix units e_{k1} belong to $S_n(A)$, and $\{e_{k1}\,|\phi\rangle\}_{k=1}^{D}$ spans $\mathbb{C}^D$. ☐

In general $q(\mathcal{E}_A) < i(A)$ can occur. For example, take $d = 3$, $D = 2$, and

$$A_k = \frac{\sigma_k}{\sqrt{3}}, \qquad k = 1, 2, 3. \tag{3.13}$$

Then $\sum_k A_k^\dagger A_k = 1_2$. The three Pauli matrices are linearly independent, so $i(A) > 1$, while $i(A) = 2$. For $|\phi\rangle = (a, b)^T$,

$$(\sigma_1\,|\phi\rangle\,, \sigma_2\,|\phi\rangle\,, \sigma_3\,|\phi\rangle) = \begin{pmatrix} b & -ib & a \\ a & ia & -b \end{pmatrix}, \tag{3.14}$$

whose singular values are

$$\sqrt{|a|^2 + |b|^2}, \qquad \sqrt{2}\sqrt{|a|^2 + |b|^2}. \tag{3.15}$$

Thus this matrix has full rank for every nonzero $|\phi\rangle$, and $q(\mathcal{E}_A) = 1$.

Proposition 3.5. *For a quantum channel $\mathcal{E}_A$, the following are equivalent:*

(a) primitive;

(b) eventually full Kraus rank;

(c) strongly irreducible.

Proof. Let $\rho \geq 0$ be an eigenvector of $\mathcal{E}_A$ with eigenvalue 1. At this stage uniqueness is not assumed. The implication (b) $\Rightarrow$ (a) was already shown.

We show (a) $\Rightarrow$ (c). If $\mathcal{E}_A$ is not strongly irreducible, then one of the following occurs:

(i) the fixed point ρ is not invertible;

(ii) there is another fixed vector ρ' independent of ρ;

(iii) there is an eigenvalue λ' with $|\lambda'| = 1$ and $\lambda' \neq 1$.

In case (i), $\mathcal{E}_A^n(\rho) = \rho$ for every n, contradicting the fact that $\mathcal{E}_A^n(\rho)$ is full-rank for $n \geq q(\mathcal{E}_A)$. In case (ii), the same argument as Lemma 2.3 produces a non-invertible positive semidefinite fixed point, reducing to case (i). Case (iii) requires Proposition 3.3 of [1]; this is the missing ingredient recorded in the original note.

$$\cdots \quad \text{Proposition 3.3 of [1] is needed here.} \tag{3.16}$$

$$@@@ \tag{3.17}$$

For a quantum channel $\mathcal{E} : \mathbb{C}^{D\times D} \to \mathbb{C}^{D\times D}$, define the Choi matrix

$$\omega(\mathcal{E}) = (\mathrm{id} \otimes \mathcal{E})(\Omega), \qquad \Omega = \sum_{i,j=1}^{D} |ii\rangle\langle jj| = \sum_{i,j=1}^{D} e_{ij} \otimes e_{ij}. \tag{3.18}$$

Here id denotes the identity map on $\mathbb{C}^{D\times D}$.

4 Peripheral Spectrum

We summarize the facts about the peripheral spectrum needed from Chapter 6 of [10]. For finite-dimensional positive maps, Chapter 2 of [11] is a useful reference; much of this section follows that source. We write $A \geq 0$ for positive semidefiniteness.

Unless otherwise stated, all norms in this section are the norms induced from the Euclidean norm on $\mathbb{C}^n$:

$$||x|| = \sqrt{\sum_{j=1}^{n} |x_j|^2}. \tag{4.1}$$

For $A \in M_n(\mathbb{C})$,

$$||A|| = \sup_{||x||=1} ||Ax|| = \sup_{||x||\leq 1} ||Ax||, \tag{4.2}$$

and for a linear map $T : M_n(\mathbb{C}) \to M_n(\mathbb{C})$,

$$||T|| = \sup_{||X||=1} ||T(X)|| = \sup_{||X||\leq 1} ||T(X)||. \tag{4.3}$$

4.1 Properties of $A \in M_n(\mathbb{C})$

Fact 4.1. *If the singular values of $A \in M_n(\mathbb{C})$ are $\sigma_1, \ldots, \sigma_n$, then*

$$||A|| = \max_j \sigma_j. \tag{4.4}$$

Proof. For an SVD $A = USV$,

$$\sup_{||x||=1} ||Ax|| = \sup_{||x||=1} ||USVx|| = \sup_{||x||=1} ||Sx|| = \max_j \sigma_j. \tag{4.5}$$

□

Fact 4.2. *For all x, $||Ax|| \leq ||A||\,||x||$.*

This is immediate by applying the definition of the operator norm to $x/||x||$ when $x \neq 0$. □

Fact 4.3.

$$||AB|| \leq ||A||\,||B||. \tag{4.6}$$

Proof.

$$||ABx|| \leq ||A||\,||Bx|| \leq ||A||\,||B||\,||x||. \tag{4.7}$$

Taking the supremum over $||x|| = 1$ gives the claim. □

Proposition 4.4. *For $A \in M_n(\mathbb{C})$,*

$$||A|| \leq 1 \quad \Longleftrightarrow \quad \begin{pmatrix} 1 & A \\ A^\dagger & 1 \end{pmatrix} \geq 0. \tag{4.8}$$

Proof. Using the SVD $A = USV$, the block matrix is unitarily equivalent to

$$\begin{pmatrix} 1 & S \\ S & 1 \end{pmatrix}, \tag{4.9}$$

whose eigenvalues are $1 \pm \sigma_j$. Thus it is positive semidefinite if and only if every $\sigma_j \leq 1$. □

4.2 Properties of $T : M_n(\mathbb{C}) \to M_n(\mathbb{C})$

The induced norm satisfies

$$||T(X)|| \leq ||T||\,||X||, \qquad ||T_1 T_2|| \leq ||T_1||\,||T_2||. \tag{4.10}$$

A linear map T is Hermiticity-preserving if $X = X^\dagger$ implies $T(X) = T(X)^\dagger$. If T is Hermiticity-preserving, then

$$T(X^\dagger) = T(X)^\dagger. \tag{4.11}$$

Indeed, write $X = A + iB$ with $A = A^\dagger$ and $B = B^\dagger$. Then $T(X^\dagger) = T(A - iB) = T(A) - iT(B) = T(X)^\dagger$. Consequently, eigenvalues of a Hermiticity-preserving map are real or come in complex conjugate pairs, and an eigenvector at a real eigenvalue can be chosen Hermitian. Every positive map is Hermiticity-preserving.

A map is unital if $T(1) = 1$. In what follows T is positive unless otherwise stated.

Proposition 4.5 (Russo-Dye)**.** *If T is positive and unital, then $||T|| = 1$.*

Proof. For a unitary U, the block matrix

$$\begin{pmatrix} 1 & U \\ U^\dagger & 1 \end{pmatrix} \tag{4.12}$$

is positive semidefinite. Applying T entrywise and using positivity gives

$$\begin{pmatrix} 1 & T(U) \\ T(U)^\dagger & 1 \end{pmatrix} \geq 0, \tag{4.13}$$

and hence $||T(U)|| \leq 1$. Every contraction is an average of two unitaries, so $||T(X)|| \leq 1$ for $||X|| \leq 1$. Since $||T(1)|| = 1$, we have $||T|| = 1$. ☐

Corollary 4.6. *For a positive map T,*

$$||T|| = ||T(1)||. \tag{4.14}$$

Proof. When $P = T(1)$ is positive definite, define

$$\tilde{T}(X) = P^{-1/2} T(X) P^{-1/2}. \tag{4.15}$$

Then $\tilde{T}$ is positive and unital, hence has norm one. This gives $||T(X)|| \leq ||P||\,||X||$. The reverse inequality follows by evaluating at $X = 1$. The non-invertible case is obtained by a limiting argument. ☐

4.3 Peripheral Spectrum

Proposition 4.7 (Wolf, Proposition 6.2)**.** *Let T be positive and unital. If λ is an eigenvalue with $|\lambda| = 1$, then every Jordan block associated with λ is one-dimensional.*

Proof. If there were a Jordan block of size at least two, then for some vector X the sequence $T^n(X)$ would have a component growing linearly in n:

$$T^n(X) = \lambda^n X + n\lambda^{n-1} Y + \cdots . \tag{4.16}$$

But $||T^n|| \leq ||T||^n = 1$ for a positive unital map, a contradiction. ☐

$$@@@@ \tag{4.17}$$

The Hilbert-Schmidt inner product and Frobenius norm are

$$\langle A, B \rangle_{\mathrm{HS}} = \mathrm{tr}\,[A^\dagger B], \qquad ||A||_F = \sqrt{\mathrm{tr}\,[A^\dagger A]}. \tag{4.18}$$

Another useful norm is

$$||A||_\infty = \max_i \sum_j |A_{ij}|. \tag{4.19}$$

It satisfies

$$||AB||_\infty \leq ||A||_\infty ||B||_\infty. \tag{4.20}$$

The spectrum of a linear map is the set of λ for which $\lambda - T$ is not invertible, and the spectral radius is

$$r(T) = \max\{|\lambda| : \lambda \in \mathrm{spec}(T)\}. \tag{4.21}$$

A map is unital if and only if its Hilbert-Schmidt adjoint is trace preserving:

$$\mathrm{tr}\,[T^\dagger(X)] = \mathrm{tr}\,[X] \quad \Longleftrightarrow \quad T(1) = 1. \tag{4.22}$$

5 Detailed Derivation Notes

This section spells out several computations which are used implicitly in the previous sections. They are included to keep the English version close to the level of detail of the original note.

5.1 Details in the OBC construction

At each step in the left-to-right Schmidt construction, the residual tensor is normalized in the following precise sense. For the first step,

$$\psi_{a_1 i_2 \cdots i_N} = \sqrt{\Lambda^{[1]}_{a_1,a_1}}\, V^\dagger_{a_1,(i_2\cdots i_N)}. \tag{5.1}$$

Since the rows of $V^\dagger$ are orthonormal,

$$\sum_{i_2,\ldots,i_N} \psi^*_{a_1 i_2\cdots i_N} \psi_{a_1' i_2 \cdots i_N} = \sqrt{\Lambda^{[1]}_{a_1,a_1}}\sqrt{\Lambda^{[1]}_{a_1',a_1'}} \sum_{i_2,\ldots,i_N} V_{(i_2\cdots i_N),a_1} V^*_{(i_2\cdots i_N),a_1'} = \delta_{a_1 a_1'} \Lambda^{[1]}_{a_1,a_1}. \tag{5.2}$$

Summing also over a_1 gives

$$\sum_{a_1,i_2,\ldots,i_N} |\psi_{a_1 i_2\cdots i_N}|^2 = \mathrm{tr}\,\Lambda^{[1]} = 1. \tag{5.3}$$

The same argument applies at every later step:

$$\sum_{i_{n+1},\ldots,i_N} \psi^*_{a_n i_{n+1}\cdots i_N} \psi_{a_n' i_{n+1}\cdots i_N} = \delta_{a_n a_n'} \Lambda^{[n]}_{a_n,a_n}. \tag{5.4}$$

The equation

$$\sum_i A_i^{[n]\dagger} A_i^{[n]} = 1_{r_n} \tag{5.5}$$

is simply the statement that the columns of the SVD matrix U are orthonormal after combining the left bond index a_{n-1} and the physical index i_n into one row index. In components this reads

$$\sum_{a_{n-1}=1}^{r_{n-1}} \sum_{i_n=1}^{d} A^{[n]i_n *}_{a_{n-1}a_n} A^{[n]i_n}_{a_{n-1}a_n'} = \delta_{a_n a_n'}. \tag{5.6}$$

For the last tensor, where $r_N = 1$, this condition is the ordinary normalization of the final residual vector.

The second canonical equation can also be checked componentwise. For $2 \leq n \leq N-1$, write

$$\psi_{a_{n-1} i_n \cdots i_N} = \sum_{a_n} A^{[n] i_n}_{a_{n-1} a_n} \sqrt{\Lambda^{[n]}_{a_n, a_n}}\, V^{\dagger}_{a_n, (i_{n+1} \cdots i_N)}. \tag{5.7}$$

Then

$$\begin{aligned}
&\sum_{i_n, \ldots, i_N} \psi^{*}_{a_{n-1} i_n \cdots i_N} \psi_{a'_{n-1} i_n \cdots i_N} \\
&= \sum_{i_n} \sum_{a_n, a'_n} A^{[n] i_n *}_{a_{n-1} a_n} A^{[n] i_n}_{a'_{n-1} a'_n} \sqrt{\Lambda^{[n]}_{a_n, a_n}} \sqrt{\Lambda^{[n]}_{a'_n, a'_n}} \sum_{i_{n+1}, \ldots, i_N} V_{(i_{n+1} \cdots i_N), a_n} V^{*}_{(i_{n+1} \cdots i_N), a'_n} \\
&= \sum_{i_n} \sum_{a_n} A^{[n] i_n *}_{a_{n-1} a_n} \Lambda^{[n]}_{a_n, a_n} A^{[n] i_n}_{a'_{n-1} a_n}.
\end{aligned} \tag{5.8}$$

On the other hand, the left-hand side equals

$$\Lambda^{[n-1]}_{a_{n-1}, a_{n-1}} \delta_{a_{n-1} a'_{n-1}}. \tag{5.9}$$

This is precisely

$$\sum_{i_n} A^{[n] i_n} \Lambda^{[n]} A^{[n] i_n \dagger} = \Lambda^{[n-1]}. \tag{5.10}$$

The reduced-density-matrix interpretation of $\Lambda^{[m]}$ is also worth recording explicitly. Let

$$|\phi^{L}_{a_m}\rangle = \sum_{i_1, \ldots, i_m} \left(A^{[1] i_1} \cdots A^{[m] i_m} \right)_{a_m} |i_1 \cdots i_m\rangle \tag{5.11}$$

and

$$|\phi^{R}_{a_m}\rangle = \frac{1}{\sqrt{\Lambda^{[m]}_{a_m, a_m}}} \sum_{i_{m+1}, \ldots, i_N} \psi_{a_m i_{m+1} \cdots i_N} |i_{m+1} \cdots i_N\rangle. \tag{5.12}$$

The left-isometric condition implies

$$\langle \phi^{L}_{a_m} | \phi^{L}_{b_m} \rangle = \delta_{a_m b_m}, \tag{5.13}$$

and the construction of the residual tensors implies

$$\langle \phi^{R}_{a_m} | \phi^{R}_{b_m} \rangle = \delta_{a_m b_m}. \tag{5.14}$$

Hence

$$|\psi\rangle = \sum_{a_m = 1}^{r_m} \sqrt{\Lambda^{[m]}_{a_m, a_m}}\, |\phi^{L}_{a_m}\rangle |\phi^{R}_{a_m}\rangle \tag{5.15}$$

is a Schmidt decomposition across the cut. This proves that the entries of $\Lambda^{[m]}$ are the nonzero eigenvalues of the reduced density matrix.

The same fact can be checked directly from the MPS contraction. Let

$$\rho_m = \mathrm{tr}_{\, m+1, \ldots, N} |\psi\rangle \langle\psi|. \tag{5.16}$$

Substituting the OBC-MPS gives

$$\begin{aligned}
\rho_m = &\sum_{\substack{i_1, \ldots, i_N \\ j_1, \ldots, j_m}} A^{[1]}_{i_1} \cdots A^{[m]}_{i_m} A^{[m+1]}_{i_{m+1}} \cdots A^{[N]}_{i_N} |i_1 \cdots i_m\rangle \langle j_1 \cdots j_m| \\
&\times A^{[N]\dagger}_{i_N} \cdots A^{[m+1]\dagger}_{i_{m+1}} A^{[m]\dagger}_{j_m} \cdots A^{[1]\dagger}_{j_1}.
\end{aligned} \tag{5.17}$$

Using the right-to-left contractions

$$\sum_{i_N} A^{[N]}_{i_N} \Lambda^{[N]} A^{[N]\dagger}_{i_N} = \Lambda^{[N-1]}, \qquad \sum_{i_{N-1}} A^{[N-1]}_{i_{N-1}} \Lambda^{[N-1]} A^{[N-1]\dagger}_{i_{N-1}} = \Lambda^{[N-2]}, \tag{5.18}$$

and continuing until the m-th cut, this becomes

$$\rho_m = \sum_{\substack{i_1,\ldots,i_m \\ j_1,\ldots,j_m}} A^{[1]}_{i_1} \cdots A^{[m]}_{i_m} \Lambda^{[m]} A^{[m]\dagger}_{j_m} \cdots A^{[1]\dagger}_{j_1} \left| i_1 \cdots i_m \right\rangle \left\langle j_1 \cdots j_m \right| . \tag{5.19}$$

In components,

$$\rho_m = \sum_{a_m=1}^{r_m} \Lambda^{[m]}_{a_m,a_m} \left| \phi_{a_m} \right\rangle \left\langle \phi_{a_m} \right| , \tag{5.20}$$

where

$$\left| \phi_{a_m} \right\rangle = \sum_{i_1,\ldots,i_m} [A^{[1]}_{i_1}]_{a_1} [A^{[2]}_{i_2}]_{a_1 a_2} \cdots [A^{[m]}_{i_m}]_{a_{m-1} a_m} \left| i_1 \cdots i_m \right\rangle . \tag{5.21}$$

The vectors $\left| \phi_{a_m} \right\rangle$ are orthonormal:

$$\begin{aligned} \langle \phi_{a_m} | \phi_{a'_m} \rangle &= \sum_{i_1,\ldots,i_m} [A^{[m]\dagger}_{i_m}]_{a_m a_{m-1}} \cdots [A^{[1]\dagger}_{i_1}]_{a_1} [A^{[1]}_{i_1}]_{a'_1} \cdots [A^{[m]}_{i_m}]_{a'_{m-1} a'_m} && (5.22) \\ &= \delta_{a_m a'_m} , && (5.23) \end{aligned}$$

where the left-isometric identities are applied successively from site 1 to site m. Thus the displayed expression is the spectral decomposition of ρ_m. Since the rank of $\Lambda^{[m]}$ is intrinsic, a state has a bond-D OBC-MPS representation precisely when all such reduced density matrices have rank at most D.

5.2 Gauge freedom and restriction to Schmidt supports

The gauge theorem for OBC-MPS can be read as the statement that any redundant auxiliary directions can be removed, and that the remaining directions can be put in Schmidt form. Suppose a partial contraction up to site n produces vectors

$$|\Phi^{[n]}_\alpha\rangle = \sum_{i_1,\ldots,i_n} \left(B^{[1]}_{i_1} \cdots B^{[n]}_{i_n} \right)_\alpha \left| i_1 \cdots i_n \right\rangle . \tag{5.24}$$

The dimension of the span of these vectors is exactly the Schmidt rank r_n across the cut. Choose an orthonormal basis of this span and collect the coefficients in a semi-unitary matrix $U^{[n]}$. Then

$$B^{[1]}_{i_1} \cdots B^{[n]}_{i_n} = A^{[1]}_{i_1} \cdots A^{[n]}_{i_n} Z_n \tag{5.25}$$

for some matrix Z_n whose row dimension is r_n. The condition $Y_n Z_n = 1$ means that Z_n has a left inverse on the Schmidt support.

If

$$Z_n Z_n^\dagger = V^{[n]} \Delta^{[n]2} V^{[n]\dagger}, \tag{5.26}$$

with $\Delta^{[n]}$ positive on the support, inserting

$$1 = V^{[n]} V^{[n]\dagger}, \qquad 1 = \Delta^{[n]} (\Delta^{[n]})^{-1} \tag{5.27}$$

between the two sides of the cut puts the reduced density matrix into diagonal form. If a zero eigenvalue is present, let P_n be the embedding of the support of $\Delta^{[n]}$. Then products contributing to the state always pass through

$$P_n P_n^\dagger \tag{5.28}$$

on the auxiliary index, so replacing all tensors by their support restrictions does not change the state. In this restricted space one obtains

$$Y_n = P_n^\dagger V^{[n]\dagger} \Delta^{[n]} U^{[n]\dagger}, \qquad Z_n = U^{[n]} (\Delta^{[n]})^{-1} V^{[n]} P_n, \tag{5.29}$$

and hence

$$Y_n Z_n = P_n^\dagger P_n = 1. \tag{5.30}$$

Here is the same construction in the explicit three-step form used in the original note. Start with arbitrary OBC matrices $B_i^{[m]}$ of size $D_{m-1} \times D_m$. First perform SVDs from the left:

$$B_{i,a}^{[1]} = \sum_{b=1}^{r_1} A_{i,b}^{[1]} \Delta_b^{[1]} U_{b,a}^{[1]\dagger}. \tag{5.31}$$

The matrices $A^{[1]}$ and $U^{[1]}$ have orthonormal columns:

$$\sum_i A_{i,b}^{[1]*} A_{i,b'}^{[1]} = \delta_{bb'}, \qquad U^{[1]\dagger} U^{[1]} = 1_{r_1}. \tag{5.32}$$

Put $Z_1 = \Delta^{[1]} U^{[1]\dagger}$. It has a right inverse,

$$Z_1 U^{[1]} (\Delta^{[1]})^{-1} = 1_{r_1}. \tag{5.33}$$

Now define

$$\tilde{B}_i^{[2]} = Z_1 B_i^{[2]}. \tag{5.34}$$

Performing the SVD of $\tilde{B}_{i,b_1 a_2}^{[2]}$ with row index (i, b_1) and column index a_2 gives

$$\tilde{B}_{i,b_1 a_2}^{[2]} = \sum_{b_2=1}^{r_2} A_{i,b_1 b_2}^{[2]} \Delta_{b_2}^{[2]} U_{b_2,a_2}^{[2]\dagger}. \tag{5.35}$$

Repeating this for $n = 3, \ldots, N-1$ yields

$$\tilde{B}_{i,b_{n-1} a_n}^{[n]} = \sum_{b_n=1}^{r_n} A_{i,b_{n-1} b_n}^{[n]} \Delta_{b_n}^{[n]} U_{b_n,a_n}^{[n]\dagger}, \tag{5.36}$$

with

$$\sum_i \sum_{b_{n-1}} A_{i,b_{n-1} b_n}^{[n]*} A_{i,b_{n-1} b_n'}^{[n]} = \delta_{b_n b_n'}, \qquad Z_n = \Delta^{[n]} U^{[n]\dagger}. \tag{5.37}$$

For the last site one sets

$$A_{i,b_{N-1}}^{[N]} = \tilde{B}_{i,b_{N-1}}^{[N]} = [Z_{N-1}]_{b_{N-1},a_{N-1}} B_{i,a_{N-1}}^{[N]}. \tag{5.38}$$

The normalization of the whole state then implies

$$\sum_{i_N} A_{i_N}^{[N]\dagger} A_{i_N}^{[N]} = 1. \tag{5.39}$$

In this first step one has

$$\begin{aligned} A_i^{[1]} &= B_i^{[1]} U^{[1]} (\Delta^{[1]})^{-1}, && (5.40) \\ A_i^{[n]} &= \Delta^{[n-1]} U^{[n-1]\dagger} B_i^{[n]} U^{[n]} (\Delta^{[n]})^{-1}, \qquad 2 \le n \le N-1, && (5.41) \\ A_i^{[N]} &= \Delta^{[N-1]} U^{[N-1]\dagger} B_i^{[N]}. && (5.42) \end{aligned}$$

The second step imposes the equations involving Λ. After Step 1, assume

$$\sum_i B_i^{[m]\dagger} B_i^{[m]} = 1 \tag{5.43}$$

for all m. Diagonalize from the right:

$$\sum_i B_i^{[N]} B_i^{[N]\dagger} = V^{[N-1]} \Lambda^{[N-1]} V^{[N-1]\dagger}. \tag{5.44}$$

With

$$A_i^{[N]} = V^{[N-1]\dagger} B_i^{[N]}, \tag{5.45}$$

one has

$$\sum_i A_i^{[N]\dagger} A_i^{[N]} = 1, \qquad \sum_i A_i^{[N]} \Lambda^{[N]} A_i^{[N]\dagger} = \Lambda^{[N-1]}, \tag{5.46}$$

where $\Lambda^{[N]} = 1$. Next diagonalize

$$\sum_i B_i^{[N-1]} V^{[N-1]} \Lambda^{[N-1]} V^{[N-1]\dagger} B_i^{[N-1]\dagger} = V^{[N-2]} \Lambda^{[N-2]} V^{[N-2]\dagger}. \tag{5.47}$$

Putting

$$A_i^{[N-1]} = V^{[N-2]\dagger} B_i^{[N-1]} V^{[N-1]} \tag{5.48}$$

gives both canonical equations at the $(N-1)$-st site. Inductively,

$$\sum_i B_i^{[n]} V^{[n]} \Lambda^{[n]} V^{[n]\dagger} B_i^{[n]\dagger} = V^{[n-1]} \Lambda^{[n-1]} V^{[n-1]\dagger}, \tag{5.49}$$

and

$$A_i^{[n]} = V^{[n-1]\dagger} B_i^{[n]} V^{[n]}. \tag{5.50}$$

At the first site,

$$\sum_{i_1} A_{i_1}^{[1]} \Lambda^{[1]} A_{i_1}^{[1]\dagger} = \sum_{i_1,\dots,i_N} B_{i_1}^{[1]} \cdots B_{i_N}^{[N]} B_{i_N}^{[N]\dagger} \cdots B_{i_1}^{[1]\dagger} = \langle \psi | \psi \rangle = 1. \tag{5.51}$$

Moreover,

$$\operatorname{tr} \Lambda^{[n-1]} = \operatorname{tr} \left[\sum_i A_i^{[n]} \Lambda^{[n]} A_i^{[n]\dagger} \right] = \operatorname{tr} \left[\Lambda^{[n]} \sum_i A_i^{[n]\dagger} A_i^{[n]} \right] = \operatorname{tr} \Lambda^{[n]}. \tag{5.52}$$

Since $\Lambda^{[N]} = 1$, every $\Lambda^{[n]}$ has trace one.

The third step removes zero diagonal entries of $\Lambda^{[n]}$. Assume $\Lambda^{[n+1]}$ is full-rank and write

$$\Lambda^{[n]} = \begin{pmatrix} \tilde{\Lambda}^{[n]} & 0 \\ 0 & 0 \end{pmatrix}, \qquad P_n = \begin{pmatrix} 1_{\tilde{r}_n} \\ 0 \end{pmatrix}. \tag{5.53}$$

Then

$$\sum_i A_i^{[n]} P_n \tilde{\Lambda}^{[n]} P_n^\dagger A_i^{[n]\dagger} = \sum_i A_i^{[n]} \Lambda^{[n]} A_i^{[n]\dagger} = \Lambda^{[n-1]}, \tag{5.54}$$

and

$$\sum_i P_n^\dagger A_i^{[n]\dagger} A_i^{[n]} P_n = 1_{\tilde{r}_n}. \tag{5.55}$$

It remains to check that inserting $P_n P_n^\dagger$ does not change the wave function. Since

$$0 = (1 - P_n P_n^\dagger) \Lambda^{[n]} (1 - P_n P_n^\dagger) \tag{5.56}$$

and

$$\Lambda^{[n]} = \sum_i A_i^{[n+1]} \Lambda^{[n+1]} A_i^{[n+1]\dagger}, \tag{5.57}$$

positivity and the full-rank property of $\Lambda^{[n+1]}$ imply

$$(1 - P_n P_n^\dagger) A_i^{[n+1]} = 0. \tag{5.58}$$

Therefore

$$A_{i_n}^{[n]} A_{i_{n+1}}^{[n+1]} = A_{i_n}^{[n]} P_n P_n^\dagger A_{i_{n+1}}^{[n+1]}, \tag{5.59}$$

so the replacement

$$A_i^{[n]} \mapsto A_i^{[n]} P_n, \qquad A_i^{[n+1]} \mapsto P_n^\dagger A_i^{[n+1]} \tag{5.60}$$

preserves the represented state and makes the n-th Schmidt matrix full-rank.

5.3 Block decomposition for finite TI-MPS

For a TI-MPS, the block decomposition is driven by invariant subspaces of the matrices A_i. If $X \geq 0$ satisfies

$$\sum_i A_i^\dagger X A_i = \lambda X, \qquad \lambda > 0, \tag{5.61}$$

and P is the projection onto $\ker X$, then the equality

$$0 = \langle v | \sum_i A_i^\dagger X A_i | v \rangle = \sum_i \langle A_i v | X | A_i v \rangle \tag{5.62}$$

for $v \in \ker X$ implies $A_i \ker X \subset \ker X$ for every i. Thus the matrices have a common triangular form

$$A_i = \begin{pmatrix} B_i & C_i \\ 0 & D_i \end{pmatrix}. \tag{5.63}$$

In a cyclic trace,

$$\operatorname{tr}[A_{i_1} \cdots A_{i_N}] = \operatorname{tr}[B_{i_1} \cdots B_{i_N}] + \operatorname{tr}[D_{i_1} \cdots D_{i_N}], \tag{5.64}$$

because upper-triangular off-diagonal blocks do not contribute to the trace. Therefore the represented state is the sum of the two states represented by the diagonal blocks. This is the algebraic reason why a non-invertible positive eigenvector leads to a block decomposition.

The positive definite eigenvectors in the final blocks can be normalized away. If

$$\sum_i A_i^\dagger X A_i = \lambda X, \qquad X > 0, \tag{5.65}$$

then for

$$B_i = X^{1/2} A_i X^{-1/2} \tag{5.66}$$

one obtains

$$\sum_i B_i^\dagger B_i = X^{-1/2} \left(\sum_i A_i^\dagger X A_i \right) X^{-1/2} = \lambda 1. \tag{5.67}$$

Similarly, if the adjoint map has a positive definite eigenvector $Y > 0$,

$$\sum_i B_i Y B_i^\dagger = \lambda Y. \tag{5.68}$$

Diagonalizing Y by a unitary transformation gives the diagonal matrix Λ in the canonical form.

5.4 The C1 condition and Schmidt rank

The map

$$\Gamma_L(X) = \sum_{i_1,\dots,i_L} \operatorname{tr}\left[X A_{i_1} \cdots A_{i_L}\right] |i_1 \cdots i_L\rangle \tag{5.69}$$

is injective precisely when no nonzero matrix X is orthogonal to all products of length L. Using the trace pairing, this is equivalent to

$$\operatorname{Span}\{A_{i_1} \cdots A_{i_L}\}_{i_1,\dots,i_L} = M_D(\mathbb{C}). \tag{5.70}$$

If the condition holds for L, it holds for $L+1$. Indeed, if a matrix X is orthogonal to all products of length $L+1$, then it is orthogonal to all matrices of the form

$$A_{i_1} \cdots A_{i_L} A_{i_{L+1}}. \tag{5.71}$$

Since the standard form has no dead physical direction, these products still detect every matrix once the length-L products span the full algebra.

Equivalently, in coordinates,

$$[M_{\Gamma_L}]_{i_1 \cdots i_L, kl} = \langle i_1 \cdots i_L | \, \Gamma_L(|k\rangle \langle l|) = [A_{i_1} \cdots A_{i_L}]_{lk}. \tag{5.72}$$

Thus M_{Γ_L} is a $d^L \times D^2$ matrix. Injectivity of Γ_L is the statement that this matrix has rank D^2. But this is exactly the statement that the d^L row vectors, equivalently the matrices

$$A_{i_1} \cdots A_{i_L} = \sum_{k,l} [A_{i_1} \cdots A_{i_L}]_{lk} \, |k\rangle \langle l| \, , \tag{5.73}$$

span the D^2-dimensional vector space $M_D(\mathbb{C})$.

For $L' = L+1$, a direct proof of monotonicity is as follows:

$$\Gamma_{L+1}(X) = \sum_i \Gamma_L(A_i X) \, |i\rangle \, . \tag{5.74}$$

If $\Gamma_{L+1}(X) = 0$, then $\Gamma_L(A_i X) = 0$ for all i. Since Γ_L is injective, $A_i X = 0$ for all i. Because products of length L span the identity,

$$1_D = \sum_{i_1,\ldots,i_L} c_{i_1\cdots i_L} A_{i_1} \cdots A_{i_L}, \tag{5.75}$$

one obtains

$$X = \sum_{i_1,\ldots,i_L} c_{i_1\cdots i_L} A_{i_1} \cdots A_{i_L} X = 0. \tag{5.76}$$

Hence Γ_{L+1} is injective.

For $L_0 \leq R \leq N - R$, define the left vectors

$$|L_{\alpha\beta}\rangle = \sum_{i_1,\ldots,i_R} (A_{i_1} \cdots A_{i_R})_{\alpha\beta} |i_1 \cdots i_R\rangle \tag{5.77}$$

and right vectors

$$|R_{\alpha\beta}\rangle = \sum_{i_{R+1},\ldots,i_N} \left(A_{i_{R+1}} \cdots A_{i_N}\right)_{\beta\alpha} |i_{R+1} \cdots i_N\rangle . \tag{5.78}$$

The state is

$$|\psi\rangle = \sum_{\alpha,\beta=1}^{D} |L_{\alpha\beta}\rangle |R_{\alpha\beta}\rangle . \tag{5.79}$$

Because C1 holds at both lengths R and $N - R$, the two families are linearly independent. Therefore this is a decomposition with exactly D^2 independent left vectors and D^2 independent right vectors, and the Schmidt rank is D^2.

5.5 Intertwining equations in the uniqueness proof

The uniqueness proof compares two TI-MPS representations by converting them into OBC-MPS representations. The trace can be rewritten using vectorization:

$$\operatorname{tr}\left[B_{i_1} \cdots B_{i_N}\right] = \sum_{\alpha,\beta} (B_{i_1})_{\alpha\beta} (B_{i_2} \cdots B_{i_N})_{\beta\alpha} . \tag{5.80}$$

Equivalently, the bulk tensors can be written as $B_i \otimes 1_D$, with boundary vectors selecting the trace. If the corresponding OBC standard forms are unique, the two bulk tensors must be related by invertible gauges:

$$W_k(B_i \otimes 1_D) = (C_i \otimes 1_D) W_{k+1}. \tag{5.81}$$

Since the space of $D^2 \times D^2$ matrices has dimension D^4, among $D^4 + 1$ consecutive W_k there is a linear dependence. Let

$$W_n + \mu_{n-1} W_{n-1} + \cdots + \mu_1 W_1 = 0. \tag{5.82}$$

If x is a nonzero root of the polynomial

$$x^{n-1} + \mu_{n-1} x^{n-2} + \cdots + \mu_1, \tag{5.83}$$

then

$$W = W_1 + x W_2 + \cdots + x^{n-2} W_{n-1} \tag{5.84}$$

satisfies

$$W(B_i \otimes 1_D) = x^{-1}(C_i \otimes 1_D)W. \tag{5.85}$$

Writing W in $D \times D$ blocks gives a nonzero block R obeying

$$RB_i = x^{-1}C_iR. \tag{5.86}$$

This is the key intertwining relation.

To show that R is unitary up to normalization, use the standard-form fixed points. If

$$\sum_i B_i^\dagger B_i = 1, \qquad \sum_i C_i^\dagger C_i = 1, \tag{5.87}$$

then

$$\sum_i B_i^\dagger R^\dagger R B_i = |x|^{-2} R^\dagger \left(\sum_i C_i^\dagger C_i \right) R = |x|^{-2} R^\dagger R. \tag{5.88}$$

Thus $R^\dagger R$ is an eigenvector of the B transfer map with eigenvalue $|x|^{-2}$. The spectral-radius condition and uniqueness of the positive fixed point force $|x| = 1$ and $R^\dagger R$ proportional to the identity. After rescaling, R is unitary.

5.6 Primitive channels and the missing implication

The equivalence between primitivity, eventual full Kraus rank, and strong irreducibility can be organized as follows. The implication (b) ⇒ (a) is the inequality $q(\mathcal{E}_A) \leq i(A)$. The implication (a) ⇒ (c) uses the fact that primitivity sends every density matrix to a full-rank density matrix after sufficiently many steps. If a peripheral eigenvector were non-invertible, or if a second fixed point existed, this would contradict full rank after iteration. The remaining case is a nontrivial peripheral eigenvalue λ with $|\lambda| = 1$ and $\lambda \neq 1$. For that case one uses the Perron-Frobenius theory for completely positive maps, in the form of Proposition 3.3 of [1].

The implication (c) ⇒ (b) is the finite-dimensional quantum Wielandt theorem as used in [9]. It says that if a channel is strongly irreducible, then products of Kraus operators of sufficiently large length span the full matrix algebra. In the MPS language, this is exactly the statement that condition C2 implies condition C1. The quantitative bound can be chosen polynomial in D in the general theorem, and the original note records the order $O(D^4)$.

5.7 Details of Vidal's recursive construction

In the recursive construction, the reduced density matrix across the first cut is

$$\rho_{[1]} = \operatorname{tr}_{[2,\ldots,N]} |\psi\rangle \langle\psi| = \sum_a (\lambda_a^{[1]})^2 |\phi_a^{[1]}\rangle \langle\phi_a^{[1]}| . \tag{5.89}$$

Thus the vectors $|\phi_a^{[1]}\rangle$ form the support of $\rho_{[1]}$. After expanding

$$|\phi_a^{[2,\ldots,N]}\rangle = \sum_{i_2} |i_2\rangle |\tau_{ai_2}^{[3,\ldots,N]}\rangle , \tag{5.90}$$

the reduced density matrix on $[3, \ldots, N]$ computed from the first-cut decomposition is a sum of outer products of the vectors

$$\lambda_a^{[1]} |\tau_{ai_2}^{[3,\ldots,N]}\rangle . \tag{5.91}$$

The same reduced density matrix computed from the second-cut Schmidt decomposition is

$$\sum_b (\lambda_b^{[2]})^2 \, |\phi_b^{[3,\ldots,N]}\rangle \, \langle \phi_b^{[3,\ldots,N]}| \,. \tag{5.92}$$

By Fact A.3, the two sets span the same subspace. Therefore there are coefficients $\Gamma_{ab}^{[2]i_2}$ such that

$$\lambda_a^{[1]} \, |\tau_{ai_2}^{[3,\ldots,N]}\rangle = \sum_b \Gamma_{ab}^{[2]i_2} \lambda_b^{[2]} \, |\phi_b^{[3,\ldots,N]}\rangle \,. \tag{5.93}$$

Repeating the same comparison at each cut gives the chain of tensors

$$\Gamma^{[1]i_1}\lambda^{[1]}\Gamma^{[2]i_2}\lambda^{[2]} \cdots \Gamma^{[N-1]i_{N-1}}\lambda^{[N-1]}\Gamma^{[N]i_N}. \tag{5.94}$$

This derivation is useful because it makes the bond dimension manifestly equal to the maximal Schmidt rank.

5.8 Choi's theorem and Kraus non-uniqueness

Let E_{jk} be the standard matrix units in $M_n(\mathbb{C})$. The Choi matrix of Φ is

$$C_\Phi = (\Phi(E_{jk}))_{j,k=1}^n. \tag{5.95}$$

If $\Phi(A) = V^\dagger A V$, then

$$\Phi(E_{jk}) = V^\dagger E_{jk} V. \tag{5.96}$$

Writing V by rows as $x_1, \ldots, x_n$, this is

$$V^\dagger E_{jk} V = x_j^\dagger x_k, \tag{5.97}$$

so C_Φ is the rank-one positive matrix built from the vectorization of V. For a sum of Kraus operators, the Choi matrix is a sum of such rank-one positive matrices. Conversely, if $C_\Phi \geq 0$, diagonalize it:

$$C_\Phi = \sum_p v_p v_p^\dagger. \tag{5.98}$$

Reshaping v_p into a matrix V_p gives

$$\Phi(E_{jk}) = \sum_p V_p^\dagger E_{jk} V_p, \tag{5.99}$$

and therefore

$$\Phi(A) = \sum_p V_p^\dagger A V_p. \tag{5.100}$$

For non-uniqueness, if two Kraus families give the same map, their Choi matrices give two decompositions of the same positive matrix:

$$\sum_i v_i v_i^\dagger = \sum_p w_p w_p^\dagger. \tag{5.101}$$

By the span lemma, the two families span the same subspace. If the first family is linearly independent, then

$$w_p = \sum_i \mu_{pi} v_i. \tag{5.102}$$

Substituting this into the equality of Gram-type decompositions gives

$$\sum_p \mu_{pi}^* \mu_{pj} = \delta_{ij}, \tag{5.103}$$

that is, $\mu^\dagger \mu = 1$. This is exactly the isometry freedom of Kraus representations.

5.9 Additional norm facts for the peripheral spectrum

The argument that peripheral Jordan blocks are trivial uses only boundedness of the powers of a positive unital map. If T is unital and positive, Russo-Dye gives $||T|| = 1$, and hence

$$||T^n|| \leq ||T||^n = 1. \tag{5.104}$$

Suppose, by contradiction, that there is a Jordan chain

$$T(X) = \lambda X, \qquad T(Y) = \lambda Y + X, \qquad |\lambda| = 1. \tag{5.105}$$

Then

$$T^n(Y) = \lambda^n Y + n\lambda^{n-1} X. \tag{5.106}$$

Unless $X = 0$, the norm of this expression grows at least linearly along a subsequence, contradicting the uniform bound on $||T^n||$. Thus every Jordan block at the peripheral spectrum is one-dimensional.

For later estimates it is useful to compare the operator norm with the row-sum norm

$$||A||_\infty = \max_i \sum_j |A_{ij}|. \tag{5.107}$$

For vectors with the corresponding norm

$$||x||_\infty = \max_i |x_i|, \tag{5.108}$$

one has

$$||(Ax)_i| \leq \sum_j |A_{ij}|\,|x_j| \leq \left(\sum_j |A_{ij}| \right) ||x||_\infty. \tag{5.109}$$

Taking the maximum over i gives

$$||Ax||_\infty \leq ||A||_\infty ||x||_\infty. \tag{5.110}$$

Similarly,

$$\begin{aligned} \sum_k |(AB)_{ik}| &= \sum_k \left| \sum_j A_{ij} B_{jk} \right| \leq \sum_{j,k} |A_{ij}|\,|B_{jk}| \\ &= \sum_j |A_{ij}| \left(\sum_k |B_{jk}| \right) \leq ||B||_\infty \sum_j |A_{ij}|, \end{aligned} \tag{5.111}$$

and therefore

$$||AB||_\infty \leq ||A||_\infty ||B||_\infty. \tag{5.112}$$

For a finite-dimensional linear map T, the spectral radius can also be characterized by Gelfand's formula

$$r(T) = \lim_{n\to\infty} ||T^n||^{1/n}. \tag{5.113}$$

In the present notes we only need the elementary consequence that if $||T^n||$ is bounded uniformly in n, then every eigenvalue satisfies $|\lambda| \leq 1$, and every eigenvalue on the unit circle has no nontrivial Jordan block. Indeed, if $TX = \lambda X$, then

$$||T^n X|| = |\lambda|^n ||X|| \tag{5.114}$$

is bounded only when $|\lambda| \leq 1$. The Jordan-chain calculation above handles the borderline case.

The relation between unitality and trace preservation of the adjoint is also completely explicit. With the Hilbert-Schmidt inner product,

$$\operatorname{tr}[T^\dagger(X)] = \langle 1, T^\dagger(X)\rangle = \langle T(1), X\rangle \,. \tag{5.115}$$

Therefore $\operatorname{tr}[T^\dagger(X)] = \operatorname{tr} X = \langle 1, X\rangle$ for every X if and only if

$$T(1) = 1. \tag{5.116}$$

In the MPS transfer-map convention, this is why the two equations

$$\sum_i A_i^\dagger A_i = 1, \qquad \sum_i A_i \Lambda A_i^\dagger = \Lambda \tag{5.117}$$

are dual to each other: the first says that $X \mapsto \sum_i A_i X A_i^\dagger$ is trace preserving, while the second gives a fixed density matrix of that channel.

5.10 Finite-dimensional Krein-Rutman in the background

The finite-dimensional Krein-Rutman statement used above is the Perron-Frobenius theorem for positive maps on a cone. Let K be the cone of positive semidefinite matrices. It is closed, convex, pointed, and generating in the real vector space of Hermitian matrices. If E is positive, then $E(K) \subset K$. Choose a norm and let r be the spectral radius of E. For $\epsilon > 0$, the resolvent-like positive series

$$R_\epsilon = \sum_{n=0}^{\infty} (r+\epsilon)^{-n-1} E^n \tag{5.118}$$

is well-defined as a positive map. Applying R_ϵ to a positive definite matrix and taking a normalized limit as $\epsilon \to 0^+$ produces a nonzero positive semidefinite matrix X satisfying

$$E(X) = rX. \tag{5.119}$$

This is the finite-dimensional mechanism behind Lemma 2.5. The original note leaves the complete proof to the appendix, but the above sketch explains why a positive eigenvector at the spectral radius should exist.

A Linear Algebra

We collect linear-algebra facts used in the text.

Fact A.1 (Gram matrix)**.** *Let* $A = (v_1, \dots, v_m)$ *be a collection of* m *vectors in* $\mathbb{C}^n$*. The Gram matrix is*

$$G = A^\dagger A, \qquad G_{ij} = v_i^\dagger v_j. \tag{A.1}$$

The vectors $v_1, \dots, v_m$ *are linearly independent if and only if* $\det G > 0$*.*

Proof. The matrix G is positive semidefinite because $z^\dagger G z = ||Az||^2$. Thus $\det G \geq 0$. The vectors are linearly dependent if and only if there is a nonzero x with $Ax = 0$. This is equivalent to $Gx = A^\dagger Ax = 0$, and hence to $\det G = 0$. ☐

Fact A.2. *If* $v_1, \dots, v_m \in \mathbb{C}^n$ *are linearly independent, then*

$$\{v_i v_j^\dagger\}_{i,j=1}^m \tag{A.2}$$

is linearly independent.

Proof. By Gram-Schmidt,

$$v_i = \sum_{j=1}^m \alpha_{ij} e_j, \tag{A.3}$$

where $\{e_j\}$ is orthonormal and α is upper triangular with nonzero diagonal entries. If $\sum_{i,j} c_{ij} v_i v_j^\dagger = 0$, then in the e-basis this reads

$$\alpha^T c \alpha^* = 0. \tag{A.4}$$

Since α is invertible, $c = 0$. ☐

Fact A.3. *Let* $\{v_i\}_{i=1}^N$ *and* $\{w_i\}_{i=1}^M$ *be vectors in* $\mathbb{C}^n$*. If*

$$\sum_{i=1}^N v_i v_i^\dagger = \sum_{i=1}^M w_i w_i^\dagger, \tag{A.5}$$

then the subspaces spanned by the two families coincide.

Proof. Let

$$A = \sum_i v_i v_i^\dagger = \sum_i w_i w_i^\dagger. \tag{A.6}$$

Since $A \geq 0$, write its positive spectral decomposition as

$$A = \sum_{k=1}^r \lambda_k x_k x_k^\dagger, \qquad \lambda_k > 0. \tag{A.7}$$

For $k > r$, $Ax_k = 0$, hence

$$0 = x_k^\dagger A x_k = \sum_i |x_k^\dagger v_i|^2, \tag{A.8}$$

so all v_i lie in the span of $x_1, \dots, x_r$. Put $\tilde{x}_k = \sqrt{\lambda_k} x_k$ and write

$$v_i = \sum_{k=1}^{r} c_{ik} \tilde{x}_k, \qquad w_i = \sum_{k=1}^{r} d_{ik} \tilde{x}_k. \tag{A.9}$$

Comparing coefficients in $A = \sum_k \tilde{x}_k \tilde{x}_k^\dagger$ gives

$$c^\dagger c = 1_r, \qquad d^\dagger d = 1_r. \tag{A.10}$$

Then

$$v_i = \sum_j [cd^\dagger]_{ij} w_j, \tag{A.11}$$

and similarly each w_i is a linear combination of the v_i. □

Fact A.4 (Singular value decomposition)**.** *Let M be an $m \times n$ complex matrix of rank r. There is a decomposition*

$$M = U \Lambda V^\dagger, \tag{A.12}$$

where $U^\dagger U = 1_r$, $V^\dagger V = 1_r$, and $\Lambda = \operatorname{diag}(\lambda_1, \dots, \lambda_r)$ with $\lambda_i > 0$. Equivalently,

$$M = \sum_{i=1}^{r} \lambda_i u_i v_i^\dagger. \tag{A.13}$$

Proof. Diagonalize $M^\dagger M$. If v_i are the eigenvectors with positive eigenvalues λ_i^2, set

$$u_i = \lambda_i^{-1} M v_i. \tag{A.14}$$

Then the u_i are orthonormal and

$$M = U \Lambda V^\dagger. \tag{A.15}$$

□

Fact A.5. *The ranks of A, $AA^\dagger$, and $A^\dagger A$ are equal.*

Proof. Use the compact SVD $A = U\Lambda V^\dagger$. Then

$$AA^\dagger = U \Lambda^2 U^\dagger, \qquad A^\dagger A = V \Lambda^2 V^\dagger, \tag{A.16}$$

so all three ranks are the number of positive singular values. □

Fact A.6. *For vectors* $v_1, \dots, v_m \in \mathbb{C}^n$*,*

$$\dim \operatorname{Span}(v_1, \dots, v_m) = \operatorname{rank}\left(\sum_{i=1}^{m} v_i v_i^\dagger\right). \tag{A.17}$$

Proof. Put the vectors as columns of a matrix A. Then $\sum_i v_i v_i^\dagger = AA^\dagger$, and the statement follows from equality of ranks. ☐

Fact A.7 (Schmidt decomposition)**.** *Let* $\mathcal{H}_1$ *and* $\mathcal{H}_2$ *be Hilbert spaces with* $\dim \mathcal{H}_1 = n \geq m = \dim \mathcal{H}_2$*. For* $w \in \mathcal{H}_1 \otimes \mathcal{H}_2$*, there is a decomposition*

$$w = \sum_{i=1}^{r} \lambda_i u_i \otimes v_i, \tag{A.18}$$

where $\lambda_i \geq 0$ *are real and unique as a set,* u_i *and* v_i *are orthonormal families, and* r *is the Schmidt rank.*

Proof. Choose orthonormal bases and write

$$w = \sum_{i,j} M_{ij} e_i \otimes f_j. \tag{A.19}$$

Apply the SVD $M = \sum_a \lambda_a u_a v_a^\dagger$. Then

$$w = \sum_a \lambda_a u_a \otimes v_a, \tag{A.20}$$

with the second vector complex conjugated according to the chosen basis convention. ☐

B Vidal's Derivation of MPS

We follow [2]. For every bipartition $A : B$ of the chain, write the Schmidt decomposition

$$|\psi\rangle = \sum_{\alpha=1}^{\chi_A} \lambda_\alpha^{[A]} |\phi_\alpha^{[A]}\rangle\, |\phi_\alpha^{[B]}\rangle\,. \tag{B.1}$$

The Schmidt vectors are eigenvectors of the reduced density matrices. Let

$$\chi = \max_A \chi_A. \tag{B.2}$$

For the cut $[1, \dots, l] : [l+1, \dots, N]$, write

$$|\psi\rangle = \sum_{\alpha=1}^{\chi_l} \lambda_\alpha^{[l]} |\phi_\alpha^{[1,\dots,l]}\rangle\, |\phi_\alpha^{[l+1,\dots,N]}\rangle\,. \tag{B.3}$$

Start with the first cut. Expand the left Schmidt vectors in the local basis:

$$|\phi_a^{[1]}\rangle = \sum_{i_1} \Gamma_a^{[1]i_1} |i_1\rangle\,. \tag{B.4}$$

Then

$$|\psi\rangle = \sum_{i_1,a} \Gamma_a^{[1]i_1} \lambda_a^{[1]} |i_1\rangle |\phi_a^{[2,\dots,N]}\rangle . \tag{B.5}$$

For each a, expand $|\phi_a^{[2,\dots,N]}\rangle$ in the basis at site 2:

$$|\phi_a^{[2,\dots,N]}\rangle = \sum_{i_2} |i_2\rangle |\tau_{ai_2}^{[3,\dots,N]}\rangle . \tag{B.6}$$

Comparing this expression with the Schmidt decomposition for the cut $[1,2] : [3,\dots,N]$, and using Fact A.3, the vectors $|\tau_{ai_2}^{[3,\dots,N]}\rangle$ lie in the span of the right Schmidt vectors $|\phi_b^{[3,\dots,N]}\rangle$. Thus

$$\lambda_a^{[1]} |\tau_{ai_2}^{[3,\dots,N]}\rangle = \sum_b \Gamma_{ab}^{[2]i_2} \lambda_b^{[2]} |\phi_b^{[3,\dots,N]}\rangle . \tag{B.7}$$

Substitution gives

$$|\psi\rangle = \sum_{i_1,i_2} \sum_{a,b} \Gamma_a^{[1]i_1} \lambda_a^{[1]} \Gamma_{ab}^{[2]i_2} \lambda_b^{[2]} |i_1 i_2\rangle |\phi_b^{[3,\dots,N]}\rangle . \tag{B.8}$$

Iterating this argument yields

$$|\psi\rangle = \sum_{i_1,\dots,i_N} \Gamma^{[1]i_1} \lambda^{[1]} \Gamma^{[2]i_2} \lambda^{[2]} \cdots \Gamma^{[N-1]i_{N-1}} \lambda^{[N-1]} \Gamma^{[N]i_N} |i_1 \cdots i_N\rangle . \tag{B.9}$$

This is Vidal's canonical MPS form. It is equivalent to the standard form in Theorem 1.1 after absorbing the diagonal Schmidt-value matrices into neighboring tensors.

C CP Maps and Choi's Theorem

A matrix A is positive semidefinite if

$$\langle x| A |x\rangle \geq 0 \tag{C.1}$$

for all x. Such a matrix is Hermitian. A linear map $\Phi : M_n(\mathbb{C}) \to M_m(\mathbb{C})$ is positive if it maps positive semidefinite matrices to positive semidefinite matrices. It is completely positive if

$$\Phi \otimes 1_p \tag{C.2}$$

is positive for every p.

For an $n \times m$ matrix V, define

$$\Phi_V(A) = V^\dagger A V. \tag{C.3}$$

This map is positive, and it is completely positive because, for a positive block matrix $(A_{\alpha\beta})$,

$$(\Phi_V(A_{\alpha\beta}))_{\alpha\beta} = (\mathbf{1} \otimes V)^\dagger (A_{\alpha\beta}) (\mathbf{1} \otimes V) \tag{C.4}$$

is positive. A finite sum of such maps is also completely positive.

Theorem C.1 (Choi). *A linear map $\Phi : M_n(\mathbb{C}) \to M_m(\mathbb{C})$ is completely positive if and only if it can be written as*

$$\Phi(A) = \sum_i V_i^\dagger A V_i. \tag{C.5}$$

Proof. Let E_{jk} be the matrix units. Given a vector $v \in \mathbb{C}^{nm}$, split it into n blocks $x_j \in \mathbb{C}^m$ and form an $n \times m$ matrix V whose j-th row block is x_j. Then

$$V^\dagger E_{jk} V = x_j^\dagger x_k. \tag{C.6}$$

Thus a rank-one positive block matrix $(x_j^\dagger x_k)$ is the Choi matrix of a map $A \mapsto V^\dagger A V$. If Φ is completely positive, then the block matrix

$$(\Phi(E_{jk}))_{j,k=1}^n \tag{C.7}$$

is positive semidefinite. Diagonalizing it as a sum of rank-one positive matrices gives matrices V_i such that

$$\Phi(E_{jk}) = \sum_i V_i^\dagger E_{jk} V_i. \tag{C.8}$$

Linearity gives the representation for all A. The converse follows from complete positivity of each map $A \mapsto V_i^\dagger A V_i$. ☐

Theorem C.2 (Choi matrix criterion)**.** *A linear map* $\Phi : M_n(\mathbb{C}) \to M_m(\mathbb{C})$ *is completely positive if and only if the block matrix*

$$(\Phi(E_{jk}))_{j,k=1}^n \tag{C.9}$$

is positive semidefinite.

Theorem C.3 (Non-uniqueness of Kraus representations)**.** *Assume* $V_1, \ldots, V_l$ *are linearly independent and*

$$\Phi(A) = \sum_{i=1}^{l} V_i^\dagger A V_i. \tag{C.10}$$

Then another representation

$$\Phi(A) = \sum_{p=1}^{l'} W_p^\dagger A W_p \tag{C.11}$$

is obtained if and only if there is an isometry μ *such that*

$$W_p = \sum_{i=1}^{l} \mu_{pi} V_i. \tag{C.12}$$

If the W_p *are also linearly independent, then* $l = l'$ *and* μ *is unitary.*

Proof. The Choi matrix of Φ can be written as

$$\sum_i v_i v_i^\dagger = \sum_p w_p w_p^\dagger, \tag{C.13}$$

where v_i and w_p are the vectorizations of V_i and W_p. By Fact A.3, the two families span the same subspace. Since the V_i are independent, each w_p is a linear combination of the v_i:

$$w_p = \sum_i \mu_{pi} v_i. \tag{C.14}$$

Comparing the two decompositions gives $\mu^\dagger \mu = 1_l$. If the w_p are independent as well, the isometry is square and hence unitary. $\square$

D Finite-Dimensional Krein-Rutman Theorem

The original note records the following elementary facts used around the finite-dimensional Krein-Rutman theorem:

- The sum of positive semidefinite matrices is positive semidefinite.
- The sum of a positive definite matrix and a positive semidefinite matrix is positive definite.

The detailed proof of the finite-dimensional Krein-Rutman theorem is left for later.

E Items Not Yet Examined

- The definition of "pure" in [1], especially whether the eigenvectors at $\lambda = 1$ for both CP maps E and $E^\dagger$ are required to be positive definite. Does a mathematical definition of pure state exist in this context? How is it different from a one-block standard TI-MPS?
- The proof of the finite-dimensional Krein-Rutman theorem.
- The mathematical definition of "one block" for standard TI-MPS. Is the absence of invariant subspaces sufficient? How is it related to the positive definiteness of transfer-matrix eigenvectors?
- Whether the assumption "uniqueness of the standard OBC-MPS representation" in Theorem 7 of [3] is really necessary.

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