

# On the Behavior of Transfer Matrices between MPS

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## 1 Preliminaries

I will call a collection of  $D \times D$  matrices  $\{A_i\}_{i=1}^d$ ,  $A_i \in \text{Mat}_{D \times D}(\mathbb{C})$ , an MPS. When matrix sizes  $D$  of different values are treated at the same time, I will write, for instance, a  $D$ -MPS. An MPS is called canonical if

$$\sum_i A_i A_i^\dagger = 1_D \quad (1)$$

is satisfied. An MPS is called injective if, denoting by  $\rho_A$  the spectral radius of the transfer matrix

$$T_{AA}(X) = \sum_i A_i X A_i^\dagger, \quad (2)$$

the eigenvalue  $\lambda$  with  $|\lambda| = \rho_A$  is unique, the corresponding eigenspace is one-dimensional, and the eigenvector is positive definite. For an injective MPS  $\{A_i\}_i$ , note that it can always be brought into canonical form by using the eigenvector  $X$ ,  $X > 0$ , for  $\lambda = \rho_A$  and performing

$$A_i \mapsto \frac{1}{\sqrt{\rho_A}} X^{-1/2} A_i X^{1/2}. \quad (3)$$

The following fact is known [1]. Write

$$|\{A_i\}_i\rangle_L := \sum_{i_1, \dots, i_L} \text{tr}[A_{i_1} \cdots A_{i_L}] |i_1 \cdots i_L\rangle. \quad (4)$$

For two canonical and injective  $D$ -MPS  $\{A_i\}_i$  and  $\{B_i\}_i$ , if there exist  $L \in \mathbb{N}$  and  $e^{i\phi} \in U(1)$  such that  $|\{A_i\}_i\rangle_L = e^{i\phi} |\{B_i\}_i\rangle_L$ , then there exist  $e^{i\theta} \in U(1)$  and  $V \in U(D)$  such that

$$A_i = e^{i\theta} V^\dagger B_i V. \quad (5)$$

The phase  $e^{i\theta}$  is unique, and  $V$  is unique up to a  $U(1)$  phase.

Let  $G$  be a finite group, and let  $\phi : G \rightarrow \{\pm 1\}$  be a homomorphism. The value  $\phi_g$  indicates whether the action is unitary or antiunitary. For a matrix  $X$ , introduce the notation

$$X^{\phi_g} = \begin{cases} X & (\phi_g = 1), \\ X^* & (\phi_g = -1). \end{cases} \quad (6)$$

On the Hilbert space spanned by  $\bigotimes_{x=1}^L |i_x\rangle$ , define the  $G$  action by

$$\hat{g} = \bigotimes_{x=1}^L \hat{u}_g^{[x]}, \quad \hat{u}_g^{[x]} |j_x\rangle = \sum_{i_x} |i_x\rangle [u_g]_{i_x j_x}, \quad u_g \in U(d), \quad u_g u_h^{\phi_g} = u_{gh}. \quad (7)$$

The collection  $\{u_g\}_{g \in G}$  is a linear representation of  $G$ . Define a canonical and injective MPS  $\{A_i\}_i$  to be  $G$ -symmetric if, for every  $L \in \mathbb{N}$ , there exists  $e^{i\phi_L}$  such that

$$\hat{g} |\{A_i\}_i\rangle_L = e^{i\phi_L} |\{A_i\}_i\rangle_L. \quad (8)$$

Then, by the fact stated above, for each  $g \in G$  there exist  $e^{i\theta_g} \in U(1)$  and  $V_g \in U(D)$  such that

$$\sum_j [u_g]_{ij} A_j^{\phi_g} = e^{i\theta_g} V_g^\dagger A_i V_g. \quad (9)$$

Here  $e^{i\theta_g}$  is unique, and  $V_g$  is unique up to a  $U(1)$  phase. The relation

$$e^{i\theta_g} e^{i\phi_g \theta_h} = e^{i\theta_{gh}}, \quad g, h \in G \quad (10)$$

holds. Moreover, there exists  $\omega_{g,h} \in U(1)$  such that

$$V_g V_h^{\phi_g} = \omega_{g,h} V_{gh}, \quad g, h \in G. \quad (11)$$

Then

$$(\omega_{h,k})^{\phi_g} \omega_{gh,k}^{-1} \omega_{g,hk} \omega_{g,h}^{-1} = 1, \quad (12)$$

that is,  $\omega \in Z^2(G, U(1)_\phi)$ . Under a redefinition of the phases of  $V_g$ ,  $V_g \mapsto V_g \alpha_g$ ,  $\alpha_g \in U(1)$ , one has  $\omega \mapsto \omega \delta \alpha$ . Thus  $\omega$  is classified by the group cohomology class  $[\omega] \in H^2(G, U(1)_\phi)$ .

## 2 Transfer matrices

For a canonical and injective  $D_0$ -MPS  $\{A_i^0\}_{i=1}^d$  and a  $D_1$ -MPS  $\{A_i^1\}_i$ , define the transfer matrix  $T_{A^0 A^1} \in \text{End}(\text{Mat}_{D_0 \times D_1}(\mathbb{C}))$  by

$$T_{A^0 A^1}(X) = \sum_i A_i^0 X (A_i^1)^\dagger. \quad (13)$$

The inner product between the MPS on  $L$  sites is  $\text{tr}[(T_{A^0 A^1})^L]$ . If we choose the basis  $e_{ab} = |a\rangle \langle b|$  for the space of  $D_0 \times D_1$  matrices, the matrix elements of the transfer matrix are

$$[T_{A^0 A^1}]_{ab,cd} = \text{tr} \left[ \sum_i A_i^0 e_{cd} (A_i^1)^\dagger e_{ab}^T \right] = \sum_i \langle a | A_i^0 | c \rangle \langle b | (A_i^1)^* | d \rangle. \quad (14)$$

When  $\{A_i^0\}_i$  and  $\{A_i^1\}_i$  are  $G$ -symmetric, let us examine the  $G$  symmetry of the transfer matrix  $T_{A^0 A^1}$ . Assume

$$\sum_j [u_g]_{ij} (A_j^\mu)^{\phi_g} = e^{i\theta_g^\mu} (V_g^\mu)^\dagger A_i^\mu V_g^\mu, \quad V_g^\mu (V_h^\mu)^{\phi_g} = \omega_{g,h}^\mu V_{gh}^\mu, \quad \mu \in \{0, 1\}. \quad (15)$$

Note that

$$A_i^\mu = \left( \sum_j [u_g^\dagger]_{ij} e^{i\theta_g^\mu} (V_g^\mu)^\dagger A_j^\mu V_g^\mu \right)^{\phi_g}. \quad (16)$$

Then, for  $g \in G$ ,

$$T_{A^0 A^1}(X) = \sum_i A_i^0 X (A_i^1)^\dagger \quad (17)$$

$$= \sum_i \left( \sum_j [u_g^\dagger]_{ij} e^{i\theta_g^0} (V_g^0)^\dagger A_j^0 V_g^0 \right)^{\phi_g} X \left( \left( \sum_k [u_g^\dagger]_{ik} e^{i\theta_g^1} (V_g^1)^\dagger A_k^1 V_g^1 \right)^{\phi_g} \right)^\dagger \quad (18)$$

$$= \sum_i \left( e^{i\theta_g^0} (V_g^0)^\dagger A_i^0 V_g^0 \right)^{\phi_g} X \left( \left( e^{i\theta_g^1} (V_g^1)^\dagger A_i^1 V_g^1 \right)^{\phi_g} \right)^\dagger \quad (19)$$

$$= e^{i\phi_g(\theta_g^0 - \theta_g^1)} ((V_g^0)^\dagger)^{\phi_g} \left( \sum_i A_i^0 V_g^0 X^{\phi_g} (V_g^1)^\dagger (A_i^1)^\dagger \right)^{\phi_g} (V_g^1)^{\phi_g} \quad (20)$$

$$= e^{i\phi_g(\theta_g^0 - \theta_g^1)} ((V_g^0)^\dagger)^{\phi_g} (T_{A^0 A^1} (V_g^0 X^{\phi_g} (V_g^1)^\dagger))^{\phi_g} (V_g^1)^{\phi_g}. \quad (21)$$

In other words, the following symmetry holds:

$$((V_g^0))^{\phi_g} T_{A^0 A^1}(X) ((V_g^1)^{\phi_g})^\dagger = e^{i\phi_g(\theta_g^0 - \theta_g^1)} (T_{A^0 A^1}(V_g^0 X^{\phi_g} (V_g^1)^\dagger))^{\phi_g}. \quad (22)$$

In components,

$$(\text{lhs})_{ab,cd} = \text{Tr}[(V_g^0)^{\phi_g} T_{A^0 A^1}(e_{cd}) ((V_g^1)^{\phi_g})^\dagger e_{ab}^T] \quad (23)$$

$$= \sum_{ef} [T_{A^0 A^1}]_{ef,cd} \text{Tr}[(V_g^0)^{\phi_g} e_{ef} ((V_g^1)^{\phi_g})^\dagger e_{ab}^T] \quad (24)$$

$$= \sum_{ef} [T_{A^0 A^1}]_{ef,cd} [V_g^0]_{ae}^{\phi_g} [(V_g^1)^*]_{bf}^{\phi_g}, \quad (25)$$

while

$$(\text{rhs})_{ab,cd} = \text{Tr} \left[ e^{i\phi_g(\theta_g^0 - \theta_g^1)} \left( T_{A^0 A^1}(V_g^0 e_{cd}^{\phi_g} (V_g^1)^\dagger) \right)^{\phi_g} e_{ab}^T \right] \quad (26)$$

$$= e^{i\phi_g(\theta_g^0 - \theta_g^1)} \sum_{ef} \text{Tr} \left[ \left( T_{A^0 A^1}(e_{ee} V_g^0 e_{cd}^{\phi_g} (V_g^1)^\dagger e_{ff}) \right)^{\phi_g} e_{ab}^T \right] \quad (27)$$

$$= e^{i\phi_g(\theta_g^0 - \theta_g^1)} \sum_{ef} [V_g^0]_{ec}^{\phi_g} [(V_g^1)^*]_{fd}^{\phi_g} \text{Tr}[(T_{A^0 A^1}(e_{ef}))^{\phi_g} e_{ab}^T] \quad (28)$$

$$= e^{i\phi_g(\theta_g^0 - \theta_g^1)} \sum_{ef} [V_g^0]_{ec}^{\phi_g} [(V_g^1)^*]_{fd}^{\phi_g} [T_{A^0 A^1}]_{ab,ef}^{\phi_g}. \quad (29)$$

Thus

$$\sum_{ef} [T_{A^0 A^1}]_{ef,cd}^{\phi_g} [V_g^0]_{ae} [(V_g^1)^*]_{bf} = e^{i(\theta_g^0 - \theta_g^1)} \sum_{ef} [V_g^0]_{ec} [(V_g^1)^*]_{fd} [T_{A^0 A^1}]_{ab,ef}, \quad (30)$$

and, written as

$$\sum_{ef} (V_g^0 \otimes V_g^{1*})_{ab,ef} [T_{A^0 A^1}]_{ef,cd}^{\phi_g} = e^{i(\theta_g^0 - \theta_g^1)} \sum_{ef} [T_{A^0 A^1}]_{ab,ef} (V_g^0 \otimes V_g^{1*})_{ef,cd}, \quad (31)$$

we see that this has the following matrix form:

$$(V_g^0 \otimes V_g^{1*}) [T_{A^0 A^1}]^{\phi_g} = e^{i(\theta_g^0 - \theta_g^1)} T_{A^0 A^1} (V_g^0 \otimes V_g^{1*}), \quad g \in G. \quad (32)$$

Let  $|\lambda\rangle$  be an eigenstate of  $T_{A^0 A^1}$  with eigenvalue  $\lambda$ .

If  $e^{i\theta_g^0}$  and  $e^{i\theta_g^1}$  are different one-dimensional representations of  $G$ , then there exists  $g \in G$  with  $\phi_g = 1$  such that  $e^{i(\theta_g^0 - \theta_g^1)} \neq 1$ . For such a  $g \in G$ ,  $e^{-i(\theta_g^0 - \theta_g^1)} \lambda$  is also an eigenvalue.

Suppose that  $e^{i\theta_g^0}$  and  $e^{i\theta_g^1}$  are the same one-dimensional representation of  $G$ . Then the transfer matrix  $T_{A^0 A^1}$  satisfies the symmetry

$$(V_g^0 \otimes V_g^{1*}) [T_{A^0 A^1}]^{\phi_g} = T_{A^0 A^1} (V_g^0 \otimes V_g^{1*}), \quad g \in G. \quad (33)$$

If  $[\omega^0] \neq [\omega^1]$ , then  $T_{A^0 A^1}$  is block diagonalized with respect to the irreducible decomposition of  $V^0 \otimes V^{1*}$ . Since the dimensions of the  $\omega^0 \omega^{1*}$ -irreducible representations are at least two, if  $\lambda$  is an eigenvalue, then either  $\lambda$  itself, or  $\lambda^*$ , is also an eigenvalue.

From the above, if  $e^{i\theta_g^0}$  and  $e^{i\theta_g^1}$  are different one-dimensional representations, or if  $[\omega^0] \neq [\omega^1]$ , then the absolute values of the eigenvalues of the transfer matrix  $T_{A^0 A^1}$  always appear in pairs of at least two.

In other words, when two translation-invariant and  $G$ -symmetric one-dimensional nondegenerate states  $\{A_i^0\}_i$  and  $\{A_i^1\}_i$  belong to different SPT phases, the absolute values of the eigenvalues of the transfer matrix  $T_{A^0 A^1}$  always appear in pairs of at least two.

## References

- [1] D. Perez-Garcia, F. Verstraete, M. M. Wolf, J. I. Cirac, *Matrix Product State Representations*, arXiv:quant-ph/0608197.