

# Irreducible forms of Matrix Product States: Theory and Applications

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The canonical form of Matrix Product States (MPS) and the associated fundamental theorem, which relates different MPS representations of a state, are the theoretical framework underlying many of the analytical results derived through MPS, such as the classification of symmetry-protected phases in one dimension. Yet, the canonical form is only defined for MPS without non-trivial periods, and thus cannot fully capture paradigmatic states such as the antiferromagnet. Here, we introduce a new standard form for MPS, the *irreducible form*, which is defined for arbitrary MPS, including periodic states, and show that any tensor can be transformed into a tensor in irreducible form describing the same MPS. We then prove a fundamental theorem for MPS in irreducible form: If two tensors in irreducible form give rise to the same MPS, then they must be related by a similarity transform, together with a matrix of phases. We provide two applications of this result: an equivalence between the refinement properties of a state and the divisibility properties of its transfer matrix, and a more general characterisation of tensors that give rise to matrix product states with symmetries.

## I. INTRODUCTION

The description of quantum many-body systems is not scalable due to the exponential growth of the Hilbert space dimension with the number of subsystems. The desire to develop efficient techniques to analyse strongly correlated systems has motivated the program of tensor networks, which are a theoretical and numerical tool [1, 2] to describe these systems in various settings (various physical dimensions, with various symmetries, appropriate for describing ground states of gapped or gapless Hamiltonians, etc). The simplest and most thoroughly studied type of tensor networks are Matrix Product States (MPS) [3–5], which are suitable for describing ground states of one-dimensional gapped Hamiltonians. Among many other things, they have allowed to characterise the symmetries of states in terms of the corresponding tensors [6], and have given rise to a classification of gapped phases in one-dimensional systems [7–9].

One of the most interesting features of MPS is that they allow to describe families of translationally invariant systems, even in the thermodynamic limit, in a simple and concise way. Any rank-three tensor  $A$ , with coefficients  $A_{\alpha,\beta}^i$  with  $i = 1, \dots, d$ , and  $\alpha, \beta = 1, \dots, D$ , generates a family of translationally invariant MPS,<sup>1</sup> namely

$$\mathcal{V}(A) = \left\{ |V_N(A)\rangle = \sum_{i_1, \dots, i_N=1}^d \text{Tr}(A^{i_1} \dots A^{i_N}) |i_1, \dots, i_N\rangle \in (\mathbb{C}^d)^{\otimes N} \right\}_{N \in \mathbb{N}}, \quad (1)$$

where each  $|V_N(A)\rangle$  corresponds to a state of  $N$  spins of physical dimension  $d$ , and the  $D \times D$  matrices  $A^i$  have coefficients  $A_{\alpha,\beta}^i$ . Thus, the properties of this whole family of states are completely determined by the tensor  $A$ , and therefore by a number of coefficients that is independent of  $N$ . This fact has enabled to study many-body systems by just analysing the properties of  $A$ .

Many of the results obtained for MPS rely on what is called the canonical form, together with the associated “fundamental theorem” which relates different MPS representations of a family of states [10]: Different tensors  $A$  and  $B$  can generate the same family of states,  $\mathcal{V}(A) = \mathcal{V}(B)$ , which introduces an ambiguity when analysing many-body states in terms of the tensors that generate them, being crucial e.g. in the analysis of phases under symmetries. The canonical form constitutes a specific normal form into which an MPS tensor can be brought without changing the family of states it generates, and which has a number of favorable properties. The fundamental theorem of MPS then asserts that for any two tensors  $A$  and  $B$  in canonical form for which  $\mathcal{V}(A) = \mathcal{V}(B)$ , there exists a simple local gauge transformation relating them: There exists some invertible matrix  $Y$  such that  $A^i = Y B^i Y^{-1}$ , and thus, the matrices  $A^i$  and  $B^i$  are the same up to a change of basis given by  $Y$ .

However, the canonical form is not defined for all possible tensors  $A$ . Specifically, this excludes translationally invariant MPS which are superpositions of states with non-trivial periodicity  $m > 1$ , such as the antiferromagnetic

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<sup>1</sup> Strictly speaking, this is a family of matrix product vectors [10], but we shall refer to them as matrix product states in this paper.

state  $|0, 1, 0, 1, 0, 1, \dots\rangle + |1, 0, 1, 0, 1, 0, \dots\rangle$  with period  $m = 2$ . The way to deal with such states has hitherto been to block  $m$  spins, yielding an MPS which is translationally invariant in a trivial way, at which point the canonical form and the fundamental theorem can be applied. However, the local entanglement structure relating to the non-trivial periodicity is lost in this procedure, and the physical properties of the system can change radically (e.g., the antiferromagnet becomes a ferromagnet when blocking 2 sites). It is therefore desirable to have a standard form, together with a fundamental theorem, which are directly applicable to all translational invariant MPS, including periodic ones.

In this work, we introduce a new standard form, the *irreducible form*, which is applicable to all tensors generating translationally invariant MPS, including  $m$ -periodic states. We show how to transform an arbitrary tensor  $A$  generating a family of translationally invariant MPS into a tensor  $B$  in irreducible form which generates the same family of states,  $\mathcal{V}(A) = \mathcal{V}(B)$ , without the need for blocking. We then derive a fundamental theorem for MPS in irreducible form: Given any  $A$  and  $B$  in irreducible form which generate the same family of states,  $\mathcal{V}(A) = \mathcal{V}(B)$ , there exist a unitary matrix  $Z$  and an invertible matrix  $Y$  such that  $ZA^i = YB^iY^{-1}$  for all  $i$ , with  $[Z, A^i] = 0$  and  $\mathcal{V}(A) = \mathcal{V}(ZA)$ , this is,  $A$  and  $B$  are related by a local gauge transformation.

We moreover provide some applications of this result. The first one is in the context of renormalization of MPS, and relates the possibility of refining MPS with the divisibility properties of a trace preserving completely positive map (i.e. a quantum channel) that is associated to the corresponding tensor. The second one is in the context of symmetries of MPS and extends the results of previous works to MPS which are periodic.

The rest of the paper is organized as follows. In Section II we introduce the irreducible form and show how to transform any tensor  $A$  to its irreducible form. We also study how the irreducible form behaves under blocking. In Section III we present the fundamental theorem for MPS in irreducible form. In Section IV we show some applications of our result, and in Section V we conclude. The proof of a key technical lemma is postponed to Appendix A.

## II. THE IRREDUCIBLE FORM FOR MPS

In this section we introduce the irreducible form and show its basic properties (Section II A), and then study how it behaves under blocking (Section II B).

Let us first fix some notation. We are given a tensor  $A = \{A^i \in \mathcal{M}_D\}_{i=1, \dots, d}$ , where  $\mathcal{M}_D$  denotes the set of  $D \times D$  complex matrices, and  $D$  is called the bond dimension of  $A$ . This tensor defines the family of translationally invariant MPS of Eq. (1). As in this paper we will only deal with translationally invariant MPS, we will often simply call them MPS. Given  $A$ , the completely positive (CP) map  $\mathcal{E}_A$  associated to it is defined as  $\mathcal{E}_A(\cdot) = \sum_{i=1}^d A^i \cdot A^{i\dagger}$ , and its dual map as  $\mathcal{E}_A^*(\cdot) = \sum_{i=1}^d A^{i\dagger} \cdot A^i$ .

### A. The irreducible form

The procedure that transforms  $A$  to its irreducible form is the same as the one that transforms it to its canonical form [10], with the only difference that we do not block sites together. That is, we project  $A$  onto its invariant subspaces (as explained, e.g., at the beginning of Sec. 2.3. of Ref. [10]), which allows to express  $A$  in a block diagonal form

$$A^i = \bigoplus_{j \in \tilde{J}} \tilde{A}_j^i,$$

so that the CP map associated to each block  $\mathcal{E}_{\tilde{A}_j} : \mathcal{M}_{D_j} \rightarrow \mathcal{M}_{D_j}$  is *irreducible* [11], in the sense that there exists no non-trivial hermitian projector  $P$  so that  $\mathcal{E}_{\tilde{A}_j}(P\mathcal{M}_{D_j}P) \subseteq P\mathcal{M}_{D_j}P$ . Denoting the spectral radius of  $\mathcal{E}_{\tilde{A}_j}$  by  $\varrho_j$  (recall that  $\varrho_j > 0$ ), and defining  $A_j^i := \tilde{A}_j^i / \sqrt{\varrho_j}$ , we are left with

$$A^i = \bigoplus_{j \in \tilde{J}} \mu_j A_j^i, \quad (2)$$

where  $\mu_j := \sqrt{\varrho_j} > 0$ , and every  $\mathcal{E}_{A_j}$  is an irreducible CP map of spectral radius 1. This is known to be equivalent to having 1 as a non-degenerate eigenvalue with an associated strictly positive eigenvector for both  $\mathcal{E}_{A_j}$  and  $\mathcal{E}_{A_j}^*$  [11]. There could however be other eigenvalues of modulus one. If this is not the case the map is called *primitive*, and the corresponding block or tensor is called *normal* [10]. We shall refer to the set of eigenvalues of magnitude one of a map as its peripheral spectrum, following [11].

If there are other eigenvalues of modulus one, one can show (see e.g. [11]) that they must be exactly the  $m_j$ -roots of unity for some  $m_j$ , each of them with multiplicity 1. This is why we shall call the blocks  $A_j$  in the decomposition of

Eq. (2) *periodic*, and  $m_j$  its *period* or *periodicity*. Note that normal tensors are just periodic tensors with period equal to 1.

**Definition 1** (Irreducible form). *A tensor  $A$  is in irreducible form if it is in form (2) with  $\mu_j > 0$ , and every  $\mathcal{E}_{A_j}$  is an irreducible CP map of spectral radius 1.*

We have just shown the following.

**Proposition 2.** *Given any tensor  $A$ , one can always find another tensor  $B$  in irreducible form such that  $\mathcal{V}(A) = \mathcal{V}(B)$ .*

We have also seen that if  $A$  has bond dimension  $D$ , then  $B$  has bond dimension  $\tilde{D} \leq D$ . Moreover, if all blocks in (2) are normal [10] (i.e. have period 1), then (2) is just the canonical form of  $A$  according to the definitions in [10].

The next step is to group blocks that are *essentially the same* in the following sense.

**Definition 3** (Repeated blocks). *We say that two blocks, say  $A_j$  and  $A_k$ , are repeated if there exist a phase  $\xi$  and an invertible matrix  $Y$  so that*

$$A_j^i = e^{i\xi} Y A_k^i Y^{-1}. \quad (3)$$

We say that they are equivalent if (3) holds with  $\xi = 0$ .

Clearly, a block of periodicity  $m$  cannot be repeated with one of periodicity  $n \neq m$ . Taking any minimal set  $J \subseteq \tilde{J}$  of non-repeated blocks, there is a permutation of the blocks in (2) that allows to rewrite  $A$  as

$$A^i = \bigoplus_{j \in J} (R_j \otimes A_j^i), \quad (4)$$

where  $R_j := \text{diag}(\mu_{j,1}, \dots, \mu_{j,r_j})$ , with  $\mu_{j,l} \in \mathbb{C} \setminus \{0\}$ . We shall henceforth refer to  $\{\mu_{j,l}\}_l$  as the multiplicities of block  $A_j$ .

**Definition 4** (Basis of periodic tensors). *Any set  $\{A_j\}_{j \in J}$  of non-repeated periodic tensors that allows to rewrite (up to a similarity transformation) a tensor  $A$  in irreducible form as in (4) is called a basis of periodic tensors for  $A$ . Two bases of periodic tensors are called equivalent if they have the same number of elements, and each element of one basis is equivalent to an element of the other basis. Note that the prefactors of the basis elements can always be absorbed in the multiplicities.*

If all blocks are normal in (2), then the set  $\{A_j\}_{j \in J}$  is called instead a basis of normal tensors [10].

As in the case of the canonical form, we can also impose conditions on the fixed points of the maps  $\mathcal{E}_{A_j}$ . That is, let  $\rho_j$  denote the unique (positive definite) fixed point of  $\mathcal{E}_{A_j}^*$ . Defining

$$A_j'^i := \sqrt{\rho_j} A_j^i \frac{1}{\sqrt{\rho_j}} \quad (5)$$

we have that  $\mathcal{E}_{A_j'}^*(\mathbb{1}_{D_j}) = \mathbb{1}_{D_j}$ , i.e. it is unital. (Note that this is equivalent to stating that  $\mathcal{E}_{A_j}$  is trace-preserving.) Since Eq. (5) is a similarity transform,  $\mathcal{E}_{A_j'}^*$  is still irreducible and with spectral radius 1 (Proposition 6.6. of [11]), and so is  $\mathcal{E}_{A_j'}$ . Now let  $\sigma_j$  denote the fixed point of  $\mathcal{E}_{A_j'}$ , which is again positive definite,  $\sigma_j > 0$ , and has spectral decomposition  $\sigma_j = U_j \Lambda_j U_j^\dagger$ . Defining

$$A_j''^i = U_j^\dagger A_j'^i U_j,$$

we have that  $\mathcal{E}_{A_j''}(\Lambda_j) = \Lambda_j$  where  $\Lambda_j$  is diagonal and positive definite. Moreover  $\mathcal{E}_{A_j''}^*$  is still unital.

That is, without loss of generality we can take every block in (2) (and (4)) with the additional property that the CP maps  $\mathcal{E}_{A_j}$  are trace preserving and have a diagonal positive matrix as a unique fixed point. If this is the case, by analogy with [10] we say that  $A$  is in *irreducible form II*. Note that if two blocks with associated trace-preserving CP maps are repeated, then the invertible matrix  $Y$  in Definition 3 must be unitary. Note also that one can freely change from irreducible form to irreducible form II just by a block diagonal similarity transformation. Hence one can prove the results here in either form and they will immediately apply for the other one, just by replacing appropriately “invertible map” by “unitary map”.

Finally,  $m_j$ -periodic tensors  $A_j$  are known to have [11] the following off-diagonal structure

$$A_j^i = \sum_{u=0}^{m_j-1} P_{j,u} A_j^i P_{j,u+1}, \quad \text{with } P_{j,u} P_{j,u'} = \delta_{u,u'} P_{j,u}, \quad \sum_{u=0}^{m_j-1} P_{j,u} = \mathbb{1}_{D_j}, \quad P_{j,m_j} = P_{j,0}. \quad (6)$$

If the tensors are in irreducible form II, the projectors  $P_{j,u}$  are hermitian,  $\mathcal{E}_{A_j}^*(P_{j,u}) = P_{j,u+1}$  and hence the unitary  $U_j = \sum_{u=0}^{m_j-1} \omega_j^u P_{j,u}$  verifies that

$$\mathcal{E}_{A_j}^*(U_j^l) = \omega_j^l U_j^l, \quad \text{with } \omega_j = e^{i \frac{2\pi}{m_j}}, \quad \text{for } l = 0, \dots, m_j - 1. \quad (7)$$

From (6) it follows that

$$|V_N(A_j)\rangle = \begin{cases} \sum_{u=0}^{m_j-1} \sum_{i_1, \dots, i_N} \text{Tr}(P_{j,u} A_j^{i_1} \cdots A_j^{i_N}) |i_1, \dots, i_N\rangle & \text{if } m_j \mid N \\ 0 & \text{else.} \end{cases}$$

That is, if  $m_j$  divides  $N$ , then  $|V_N(A_j)\rangle$  is a sum of  $m_j$   $m_j$ -periodic terms, and otherwise the state is 0. Thus,  $|V_N(A_j)\rangle$  is translationally invariant in a non-trivial way, since the translation operator by one site generates a cyclic permutation of the  $m_j$  terms.

## B. Blocking periodic tensors

Before proceeding, it is important to analyse how periodic tensors, and hence the irreducible form, behave under the blocking of tensors. Since blocking tensors corresponds to taking powers of the associated CP maps, the question is equivalent to studying how irreducible CP maps behave under powers. For that, the off-diagonal decomposition (6) plays a key role. In this direction, the following result is proven in [12], but we shall include here a proof for completeness. We will denote the tensor  $A$  after blocking  $p$  sites by  $A^{(p)}$ , i.e.

$$A^{(p)} = \{A^{i_1} A^{i_2} \cdots A^{i_p}\}_{i_1, \dots, i_p \in \{1, \dots, d\}}.$$

We will also denote by  $\mathbf{i}$  the multiindex that contains  $(i_1, \dots, i_p)$ .

**Lemma 5** (Blocking a single periodic block). *Let  $A$  be in irreducible form II with a single periodic block of periodicity  $m$ . If  $p$  is a multiple of  $m$ , then  $A^{(p)}$  is in canonical form II with a basis of normal tensors given by  $\{C_u = P_u A^{(p)}\}_{u=0}^{m-1}$  (with  $P_u$  as in (6), but without the block index  $j$ ).*

Note that for convenience we choose not to project out the zero blocks in  $C_u$ , this is,  $C_u$  consists of the actual normal tensor, supported on the range of  $P_u$ , padded with zeros. We will stick to this convention in the following. In addition, we will also assume gauge transformations acting between different  $C_u$  and  $C_v$  to be only defined on the respective supports, and being zero outside.

*Proof.* Without loss of generality we can assume that  $p = m$ . We first want to see that  $\{C_u\}_{u=0}^{m-1}$  forms a basis of normal tensors. We will first show that each  $C_u$  is a normal tensor, which amounts to seeing that  $\mathcal{E}_{C_u}$  is primitive. Note first that since  $A$  is a periodic block,  $\mathcal{E}_A$  is irreducible with peripheral spectrum  $\{\omega^r\}_{r=0}^{m-1}$ , where  $\omega = e^{i2\pi/m}$ . The CP map associated to  $A^{(m)}$  is  $\mathcal{E}_A^m$  (which denotes the  $m$ -fold application of the map  $\mathcal{E}_A$ ), and it can be expressed as

$$\mathcal{E}_A^m(\rho) = \sum_{u, u'=0}^{m-1} P_u \mathcal{E}_A^m(P_u \rho P_{u'}) P_{u'}.$$

This map has 1 (with multiplicity  $m$ ) as a unique eigenvalue of magnitude one. Denote the fixed point of  $\mathcal{E}_A$  by  $\Lambda_A$ . Then it is immediate to see that the set of fixed points of  $\mathcal{E}_A^m$  is given by  $\{P_u \Lambda_A P_u\}_u$ , the set of fixed points of  $\mathcal{E}_A^{*m}$  is given by  $\{P_u\}_u$ , that  $P_u \Lambda_A P_u$  and  $P_u$  are the fixed points of  $\mathcal{E}_{C_u}$  and  $\mathcal{E}_{C_u}^*$ , respectively, and that  $\mathcal{E}_{C_u}$  does not have any other eigenvalue of magnitude 1. Therefore  $\mathcal{E}_{C_u}$  is primitive, and  $C_u$  is a normal tensor in canonical form II, for all  $u$ .

It only remains to be seen that the  $C_u$ 's are non-repeated. So imagine that there were a  $C_u$  and a  $C_v$  related to each other by

$$C_u^{\mathbf{i}} = e^{i\xi} U C_v^{\mathbf{i}} U^\dagger. \quad (8)$$

As mentioned above, we choose  $U$  such that it is only non-zero on the respective supports,  $U = P_u U P_v$ , where it acts like a unitary (i.e.  $U U^\dagger = P_u$  and  $U^\dagger U = P_v$ ). We have that

$$\mathcal{E}_A^m(U) = \sum_{\mathbf{i}} C_u^{\mathbf{i}} U C_v^{\mathbf{i}\dagger} = e^{i\xi U} \sum_{\mathbf{i}} C_v^{\mathbf{i}} C_v^{\mathbf{i}\dagger}.$$

Noting that  $\mathcal{E}_{C_v}(\mathbb{1}) = \mathcal{E}_{C_v}(P_v) = P_v$  we obtain that  $\mathcal{E}_A^m(U) = e^{i\xi U}$ . But we established above that  $\{P_u \Lambda_A P_u\}_{u=1}^m$  are the only fixed points of  $\mathcal{E}_A^m$ , and that  $\mathcal{E}_A^m$  has no other eigenvalues of modulus 1. Hence relation (8) cannot hold.  $\square$

As a consequence, if a tensor  $A$  is in irreducible form (irreducible form II) and  $m = \text{lcm}(\{m_j\}_{j \in J})$ , the tensor  $A^{(m)}$  is in canonical form (canonical form II).

Lemma 5 can be easily generalised to an arbitrary  $p$ .

**Lemma 6.** *Let  $A$  be in irreducible form II with a single periodic block of periodicity  $m$ . Take  $p \in \mathbb{N}$  and let  $r = \text{gcd}(m, p)$ . Then  $A^{(p)}$  is in irreducible form II, with  $r$  periodic tensors of periodicity  $m/r$ , given by  $C_\alpha = \tilde{P}_\alpha A^{(p)}$ ,  $\alpha = 0, \dots, r-1$ , where*

$$\tilde{P}_\alpha = \sum_{k=0}^{m/r-1} P_{[\alpha+pk]_m},$$

where the notation  $[s]_m$  stands for  $(s \bmod m)$ .

Though we will not need it here, the tensors  $C_\alpha$  are non-repeated. The argument is essentially the same as in the previous lemma. We just need the following trivial observation.

**Lemma 7.** *For each  $u \in \{0, \dots, m-1\}$  there exists a unique  $\alpha_u \in \{0, \dots, r-1\}$  and a unique  $k_u \in \{0, \dots, (m/r)-1\}$  so that  $u = [\alpha_u + pk_u]_m$ .*

This implies that in Lemma 6,  $\tilde{P}_\alpha \tilde{P}_\beta = \delta_{\alpha,\beta} \tilde{P}_\alpha$  and  $\sum_{\alpha} \tilde{P}_\alpha = \mathbb{1}_{\mathcal{M}_D}$ . Moreover, by their definition,  $C_\alpha = \tilde{P}_\alpha A^{(p)} = \tilde{P}_\alpha A^{(p)} \tilde{P}_\alpha$  for all  $\alpha$ . Hence, each of the  $C_\alpha$  defines a new block. We are thus only left to show that each of them is periodic of periodicity  $m/r$ . Since we know that the peripheral spectrum of  $\mathcal{E}_A^p$  is  $\{\omega^l\}_{l=0}^{m/r-1}$ , with  $\omega = e^{i\frac{2\pi}{m}}$ , and each eigenvalue has multiplicity  $r$ , to finish the proof of Lemma 6, it is enough to see that the peripheral spectrum of each  $\mathcal{E}_{C_\alpha}$  is  $\{\omega^l\}_{l=0}^{m/r-1}$ . This, however, follows immediately using Eq. (7) since

$$\mathcal{E}_{C_\alpha}^*(P_{[\alpha+pk]_m}) = P_{[\alpha+p(k+1)]_m}.$$

### III. THE FUNDAMENTAL THEOREM FOR MPS

In this section we present the fundamental theorem for MPS in irreducible form. In Section III A we will present some preliminary results, in Section III B we will present the theorem in the proportional case (i.e. when  $|V_N(A)\rangle$  is proportional to  $|V_N(B)\rangle$  for all  $N$ ), and in Section III C the theorem in the equal case (i.e. when  $\mathcal{V}(A) = \mathcal{V}(B)$ ).

#### A. Preliminary results

We start by recalling the fundamental theorem for MPS in canonical form in the proportional case and in the equal case.

**Theorem 8** (Theorem 2.10. of [10]). *Let  $A$  and  $B$  be two tensors in canonical form with basis of normal tensors  $\{A_j^i\}_{j \in J}$  and  $\{B_k^i\}_{k \in K}$ . If  $|V_N(A)\rangle$  and  $|V_N(B)\rangle$  are proportional to each other for all  $N$ , then  $|J| = |K|$ , and for each  $j$  there exists a  $k$ , a phase  $\xi_k$ , and an invertible matrix  $Y_k$  such that  $A_j^i = e^{i\xi_k} Y_k B_k Y_k^{-1}$ . That is, any two tensors in canonical form giving proportional MPS for all  $N$  have equivalent bases of normal tensors.*

**Theorem 9** (Corollary 2.11. of [10]). *Let  $A$  and  $B$  be two tensors in canonical form so that  $\mathcal{V}(A) = \mathcal{V}(B)$ . Then  $A$  and  $B$  have equivalent bases of normal tensors with exactly the same multiplicities. In particular, there is an invertible  $Y$  such that  $A^i = Y B^i Y^{-1}$ .*

This fundamental theorem is a direct consequence of the fact that normal tensors are essentially *equal or orthogonal* in the following sense.

**Proposition 10** (Lemma A.2. of [10]). *Let  $A_1$  and  $A_2$  denote two normal tensors with bond dimensions  $D_1, D_2$ , and generating MPS  $|V_N(A_1)\rangle, |V_N(A_2)\rangle$ , respectively. Then*

$$\lim_{N \rightarrow \infty} \langle V_N(A_1) | V_N(A_1) \rangle = 1, \quad (9a)$$

$$\lim_{N \rightarrow \infty} |\langle V_N(A_1) | V_N(A_2) \rangle| = 0 \text{ or } 1. \quad (9b)$$

In the latter case,  $D_1 = D_2$  and there exists an invertible matrix  $Y$  and a phase  $\phi$  so that  $A_1^i = e^{i\phi} Y A_2^i Y^{-1}$ .

We will also require the following trivial result, as well as some results about moments of numbers that are presented below.

**Lemma 11.** *Given  $g \in \mathbb{N}$ , there exists  $\varepsilon > 0$  such that for any  $m \geq g$ , any  $g$  vectors  $|w_1\rangle, \dots, |w_g\rangle \in \mathbb{R}^m$  fulfilling*

$$1. |\langle w_i | w_j \rangle| \leq \varepsilon \text{ if } i \neq j, \text{ and}$$

$$2. |\langle w_i | w_i \rangle| \geq 1 - \varepsilon$$

*must be linearly independent.*

**Lemma 12.** *Consider two sets of non-zero complex numbers  $\{\mu_l\}_{l=1}^s, \{\nu_l\}_{l=1}^t$ . If*

$$\sum_{l=1}^s \mu_l^N = \sum_{l=1}^t \nu_l^N, \quad 1 \leq N \leq \max(s, t),$$

*then  $s = t$ , and there is a permutation  $\pi$  such that  $\mu_l = \nu_{\pi(l)}$  for all  $l$ .*

The proof of this lemma can be found e.g. in [13].

**Lemma 13.** *Consider two sets of non-zero complex numbers  $\{\mu_l\}_{l=1}^s, \{\nu_l\}_{l=1}^t$ . If there exists an  $N_0$  such that*

$$\sum_{l=1}^s \mu_l^N = \sum_{l=1}^t \nu_l^N, \quad \forall N \geq N_0, \quad (10)$$

*then  $s = t$ , and there is a permutation  $\pi$  such that  $\mu_l = \nu_{\pi(l)}$  for all  $l$ .*

*Proof.* We fix an arbitrary  $k \geq N_0$  and consider Eq. (10) for  $N = nk$  with  $n = 1, \dots, \max(s, t)$ . By Lemma 12,  $s = t$ , and there is a permutation  $\pi_k$  such that  $\mu_l^{nk} = \nu_{\pi_k(l)}^{nk}$  for all  $l$ . Since the number of possible permutations is finite, there must exist one permutation  $\pi$  so that for two  $k_1, k_2 \geq N_0$  with  $\gcd(k_1, k_2) = 1$ ,

$$\mu_l^{k_1} = \nu_{\pi(l)}^{k_1}, \quad \mu_l^{k_2} = \nu_{\pi(l)}^{k_2} \quad \forall l. \quad (11)$$

(For example we could consider all prime  $k$ , and consider the permutations associated to them.) By Bezout's identity, there exist integer numbers  $a, b \in \mathbb{Z}$  so that  $ak_1 + bk_2 = 1$ . From this and Eq. (11) it follows that  $\mu_l = \nu_{\pi(l)}$  for all  $l$ .  $\square$

## B. The fundamental theorem for MPS – proportional case

In this section we present the fundamental theorem for MPS in irreducible form in the proportional case. Throughout this section and the following one, we will denote the irreducible form of a tensor  $B$  by

$$B^i = \bigoplus_{k \in \tilde{K}} \nu_k B_k^i.$$

Additionally,  $\{B_k\}_{k \in \tilde{K}}$  will denote a basis of periodic tensors for  $B$ , leading to

$$B^i = \bigoplus_{k \in \tilde{K}} (S_k \otimes B_k^i), \quad (12)$$

where  $S_k := \text{diag}(\nu_{k,1}, \dots, \nu_{k,s_k})$  with  $\nu_{k,l} \in \mathbb{C} \setminus \{0\}$ . As in the case of Theorem 8, the fundamental theorem of MPS in irreducible form will be a consequence of the following generalisation of Proposition 10.

**Proposition 14.** Consider two periodic tensors,  $A$  and  $B$ , with corresponding bond dimension  $D_a, D_b$ , periods  $m_a, m_b$  and generating MPS  $|V_N(A)\rangle, |V_N(B)\rangle$ . Then

$$\lim_{N \rightarrow \infty} \langle V_N(A) | V_N(A) \rangle = m_a$$

(where the limit is restricted to multiples of  $m_a$ ), and similarly for  $B$ . Moreover, either

$$\lim_{N \rightarrow \infty} |\langle V_N(A) | V_N(B) \rangle| = 0,$$

(again with the limit restricted to common multiples of  $m_a$  and  $m_b$ ) or  $D_a = D_b$  and there exist a phase  $\phi$  and an invertible matrix  $Y$  so that  $A^i = e^{i\phi} Y B^i Y^{-1}$ ; the latter can only happen if  $m_a = m_b$ . As a consequence of this and Lemma 11, given a basis of periodic tensors  $\{A_j\}_{j \in J}$  for  $A$ , there exists an  $N_0$  so that for all  $N \geq N_0$ , the set of non-zero vectors in  $\{|V_N(A_j)\rangle\}_{j \in J}$  is linearly independent and spans linearly  $|V_N(A)\rangle$ .

Note that this last property is the one that justifies the name *basis of periodic vectors*. The proof of this result is postponed to Appendix A. We are now ready to present the main theorem in the proportional case. The proof mimics the one of Theorem 8 given in [10].

**Theorem 15** (Fundamental theorem for MPS – proportional case). Let  $A$  and  $B$  be in irreducible form with basis of periodic tensors  $\{A_j\}_{j \in J}$  and  $\{B_k\}_{k \in K}$ , respectively, and assume that for all  $N$ ,  $|V_N(A)\rangle$  and  $|V_N(B)\rangle$  are proportional to each other. Then for every  $j \in J$  there is exactly one  $k \in K$  (with the same period), a phase  $\xi_k$ , and an invertible matrix  $Y_k$  such that

$$A_j^i = e^{i\xi_k} Y_k B_k^i Y_k^{-1}.$$

That is, any two tensors in irreducible form giving proportional MPS for all  $N$  have equivalent bases of periodic tensors.

In the case of irreducible form II, both in Proposition 14 and Theorem 15 the invertible matrix must be unitary. Notice that this theorem only relates the bases of periodic tensors of  $A$  and  $B$ , but it does not relate  $A$  and  $B$  themselves, as the latter requires relating their multiplicities. This will only be possible in the equal case (Theorem 16).

*Proof.* Let us first consider  $B_k$  for some given  $k \in K$ . It is not possible that  $\langle V_N(B_k) | V_N(A_j) \rangle \rightarrow 0$  as  $N \rightarrow \infty$  for all  $j$ , since otherwise the MPS generated by  $A$  and  $B$  could not be proportional for all  $N$  (see Lemma 11). Thus, according to Proposition 14, there must exist one  $j_k \in J$  such that  $B_k = e^{i\phi_k} Y_k A_{j_k} Y_k^{-1}$  for some phase  $\phi_k$  and invertible matrix  $Y_k$ . We thus conclude that  $|K| \leq |J|$ . But if we had considered  $A_k$  to start with, we would obtain  $|J| \leq |K|$ , so that  $|J| = |K|$ , and we are done.  $\square$

### C. The fundamental theorem for MPS – equal case

We are now ready to present the fundamental theorem for MPS in irreducible form in the equal case.

**Theorem 16** (Fundamental theorem for MPS – equal case). Let  $A$  and  $B$  be in irreducible form. If  $\mathcal{V}(A) = \mathcal{V}(B)$ , then  $A$  and  $B$  have equivalent bases of periodic tensors  $\{A_j\}_{j \in J}$  and  $\{B_j\}_{j \in J}$ . Moreover, for each  $j$ , with periodicity  $m_j$ , there exists a diagonal unitary matrix  $Z_j$  with  $Z_j^{m_j} = \mathbb{1}_{r_j}$  (i.e. all diagonal entries are  $m_j$ -roots of unity), so that the diagonal matrices  $R_j$  and  $S_j$  associated to  $A_j$  and  $B_j$  in equations (4) and (12), respectively, are related by  $Z_j R_j = S_j$  after a reordering of the diagonal entries of  $S_j$ . Denoting  $Z = \bigoplus_{j \in J} Z_j \otimes \mathbb{1}_{D_j}$ , this implies that

$$Z A^i = Y B^i Y^{-1}$$

for all  $i$ , with  $[A^i, Z] = 0$  and  $\mathcal{V}(A) = \mathcal{V}(ZA)$ .

Note that any such  $Z$  is a gauge degree of freedom in the MPS generated by the tensor  $A$ , since the vector generated by block  $A_j$ ,  $|V_N(A_j)\rangle$ , is non-zero only for  $N$  multiple of  $m_j$ , and hence any  $m_j$ -root of unity in the multiplicities of  $A_j$  has no effect on the state  $|V_N(A)\rangle$ .

*Proof.* By Theorem 15 we know that both tensors have equivalent bases of periodic tensors, so that for all  $j \in J$ , there is an invertible  $Y_j$  such that  $B_j^i = Y_j A_j^i Y_j^{-1}$  (the phase can be absorbed in  $S_j$ ). We thus have that  $|V_N(A_j)\rangle = |V_N(B_j)\rangle$ . By assumption,

$$\sum_j \text{tr}(R_j^N) |V_N(A_j)\rangle = \sum_j \text{tr}(S_j^N) |V_N(B_j)\rangle = \sum_j \text{tr}(S_j^N) |V_N(A_j)\rangle,$$

and since by Proposition 14, there is an  $N_0$  such that the non-zero elements of  $\{|V_N(A_j)\}_j$  are linearly independent for  $N \geq N_0$ , we have that  $\text{Tr}(R_j^N) = \text{Tr}(S_j^N)$  for all  $N \geq N_0$  such that  $m_j \mid N$ . From Lemma 13 we conclude that  $r_j = s_j$  and that there is a permutation  $\pi$  such that  $\mu_{j,l}^{m_j} = \nu_{j,\pi(l)}^{m_j}$  for all  $l$ , and thus

$$Z_j R_j = T_j S_j T_j^\dagger,$$

where  $T_j$  is the matrix that implements the permutation  $\pi$ , and  $Z_j$  has the desired properties.  $Y$  is then constructed as  $Y = \bigoplus T_j \otimes Y_j$  (and possibly permutations of blocks), and  $Z = \bigoplus Z_j \otimes \mathbb{1}$ .  $\square$

#### IV. APPLICATIONS

We now present some applications of the new fundamental theorem for MPS (Theorem 16). Namely, we first show an equivalence between the refinement properties of a state and the divisibility of its transfer matrix (Section IV A), and then a more general characterisation of the tensors that give rise to MPS with symmetries (Section IV B).

##### A. The refinement of a state and the divisibility of its transfer matrix

In Ref. [14], certain continuum limits of translationally invariant matrix product states are studied. An indispensable tool for this study is a relation between the refinement of a state and the divisibility properties of its transfer matrix (both concepts to be defined below), which we establish in Theorem 17 with the help of the new fundamental theorem for MPS (Theorem 16).

We first need a couple of definitions. A trace-preserving CP map  $\mathcal{E}$  is called *p-divisible* if there is another trace-preserving CP map  $\mathcal{E}'$  such that  $\mathcal{E} = \mathcal{E}'^p$  (where the latter denotes the  $p$ -fold application of the map). Given a tensor  $B$ , we say that  $\mathcal{V}(B)$  can be *p-refined* if there exists another tensor  $A$  and an isometry  $W : \mathbb{C}^d \rightarrow (\mathbb{C}^d)^{\otimes p}$  such that

$$|V_{pN}(A)\rangle = W^{\otimes N} |V_N(B)\rangle \quad \forall N. \quad (13)$$

**Theorem 17** (*p-refinement and p-divisibility*). *Let  $B$  be in irreducible form II. Then  $\mathcal{V}(B)$  can be p-refined if and only if  $\mathcal{E}_B$  is p-divisible.*

*Proof.* We first show that if  $\mathcal{V}(B)$  can be  $p$ -refined, then  $\mathcal{E}_B$  is  $p$ -divisible. Our initial assumption is thus that for all  $N$

$$|V_{pN}(A)\rangle = W^{\otimes N} |V_N(B)\rangle = |V_N(C)\rangle,$$

where we have defined the tensor  $C$  through

$$C^{i_1, \dots, i_p} := \sum_{i=1}^d W^{(i_1, \dots, i_p), i} B^i.$$

If we see  $i_1, \dots, i_p$  as a single physical index, it is clear that  $C$  is also in irreducible form II. Our goal is now to find an  $\tilde{A}$  with  $|V_{pN}(\tilde{A})\rangle = |V_{pN}(A)\rangle$  such that  $\mathcal{E}_{\tilde{A}}^p = \mathcal{E}_C = \mathcal{E}_B$ ; in fact, we will construct an  $\tilde{A}$  for which even  $\tilde{A}^{(p)} = C$ .

First, by Proposition 2, we can assume without loss of generality that  $A$  is in irreducible form II. Following Lemma 6,  $A^{(p)}$  is then in irreducible form II as well. Theorem 16 then implies that

$$Z A^{i_1} \dots A^{i_p} = Z A^{(p), i_1, \dots, i_p} = U C^{i_1, \dots, i_p} U^\dagger.$$

In order to construct an  $\tilde{A}$  such that  $\tilde{A}^{(p)} = C$ , we thus would like to distribute  $Z$  evenly across all  $A$ 's and absorb it in  $A$  ( $U$  is easily taken care of), which is subtle since  $Z$  only commutes with  $A^{(p)}$ .

So, to this end, consider a periodic block  $A_j$  with periodicity  $m_j$  in the irreducible decomposition (2) of  $A$ , and let  $r_j = \text{gcd}(p, m_j)$ . From Lemma 6, we know that the blocks that arise from  $A_j$  in the irreducible decomposition of  $A^{(p)}$  are precisely  $\tilde{P}_{j,\alpha} A_j^{(p)}$ , with  $\alpha = 0, \dots, r_j - 1$ , where

$$\tilde{P}_{j,\alpha} = \sum_{k=0}^{\frac{m_j}{r_j} - 1} P_{j, [\alpha + pk]_{m_j}},$$

with  $P_{j,\alpha}$  defined in Eq. (6). Further,  $Z$  (restricted to the support of  $A_j$ ) acts on them as

$$Z\tilde{P}_{j,\alpha}A_j^{(p)} = c_{j,\alpha}\tilde{P}_{j,\alpha}A_j^{(p)}, \quad (14)$$

where  $c_{j,\alpha}^{m_j/r_j} = 1$ . We now define

$$A_j^i = \sum_{u=0}^{m_j-1} d_{j,u} P_{j,u} A_j^i,$$

where  $d_{j,u} = c_{j,\alpha_{u+1}}^{k_{u+1}}/c_{j,\alpha_u}^{k_u}$ , with  $\alpha_u \in \{0, \dots, r_j - 1\}$  and  $k_u \in \{0, \dots, \frac{m_j}{r_j} - 1\}$  such that  $u = [\alpha_u + pk_u]_m$  (those are unique, cf. Lemma 7). It follows that

$$A_j^{(p)} = \sum_{u=0}^{m_j-1} \left( \prod_{k=0}^{p-1} d_{j,u+k} \right) P_{j,u} A_j^{(p)} = \sum_{u=0}^{m_j-1} c_{j,\alpha_u} P_{j,u} A_j^{(p)}, \quad (15)$$

where we have used  $\prod d_{j,u+k} = c_{j,\alpha_{u+p}}^{k_{u+p}}/c_{j,\alpha_u}^{k_u} = c_{j,\alpha_u}$  (since by definition  $k_{u+p} = k_u + 1$  and  $\alpha_{u+p} = \alpha_u$ ). Comparing Eqs. (14) and (15), we find that for  $A' := \bigoplus_{j \in \bar{J}} \mu_j A_j'$  (cf. (2)), we have that  $A'^{(p)} = ZA'^{(p)}$ , and thus, defining  $\tilde{A} = U^\dagger A' U$ , we have that  $\tilde{A}^{(p)} = C$  and thus  $\mathcal{E}_A^p = \mathcal{E}_C = \mathcal{E}_B$ , completing the proof.

The proof of the converse is straightforward: If  $\mathcal{E}_B$  is  $p$ -divisible, there exists an  $A$  such that  $\mathcal{E}_B = \mathcal{E}_A^p$ . Different Kraus representations of the same channel are related by an isometry  $W$  through

$$A^{i_1} \dots A^{i_p} = \sum_{i=1}^d W^{(i_1, \dots, i_p), i} B^i,$$

which immediately implies (13). □

The consequences of this theorem will be explored in [14].

## B. Characterization of symmetries

For MPS in canonical form, the characterisation of the tensors that give rise to MPS with symmetries was studied in [6]. An extension of this characterisation to general MPS follows immediately from our new fundamental theorem (Theorem 16).

**Corollary 18** (Symmetries). *Let  $A$  be in irreducible form II. If there is a local unitary matrix  $u$  such that  $|V_N(A)\rangle = u^{\otimes N} |V_N(A)\rangle$  for all  $N$ , then there is a diagonal unitary  $Z$  such that  $[A^i, Z] = 0$  for all  $i$  and  $\mathcal{V}(A) = \mathcal{V}(ZA)$ , and another unitary  $U$  such that for all  $i'$*

$$\sum_i u^{i', i} A^i = ZUA^{i'}U^\dagger. \quad (16)$$

In (16)  $u^{i', i}$  denotes the components of  $u$ . The consequences of this result will be explored elsewhere.

## V. CONCLUSIONS

In this paper, we have introduced a new standard form for tensors generating Matrix Product States, the *irreducible form*. The irreducible form generalizes the canonical form for MPS and is directly applicable to general MPS, including those with non-trivial periodicity. We have provided a constructive way to transform any MPS tensor  $A$  into a tensor  $A'$  in irreducible form which generates the same family of MPS. We have then derived a fundamental theorem for MPS in irreducible form — namely, we have shown that if two tensors  $A$  and  $B$  in irreducible form give rise to the same family of translationally invariant MPS,  $\mathcal{V}(A) = \mathcal{V}(B)$ , then these two tensors must be related by a similarity transform  $Y$  and a diagonal matrix of phases  $Z$ , namely  $ZA^i = YB^iY^{-1}$ , where  $Z$  commutes with  $A$ , and is “invisible” to the state,  $\mathcal{V}(A) = \mathcal{V}(ZA)$ . This result generalizes the fundamental theorem for MPS in canonical form, which yields the same statement but without the  $Z$ .

We have then presented two applications of this result. The first is a theorem that proves that the refinement properties of a state are equivalent to the divisibility properties of its associated quantum channel. The second is a characterisation of tensors that give rise to matrix product states with symmetries. Finally, our findings could also be applicable to further scenarios where the fundamental theorem of MPS in canonical form has proven useful, such as in the characterisation of 2D topological order through Matrix Product Operators [15], or in the classification of symmetry protected phases in one dimension [7, 8].

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### Appendix A: Proof of Proposition 14

Here we prove Proposition 14 in the case of irreducible form II.

First note that since  $\langle V_N(A)|V_N(A)\rangle = \text{tr}(E_A^N)$ , with  $E_A = \sum_{i=1}^d A^i \otimes \bar{A}^i$  the Choi matrix of  $\mathcal{E}_A$  which has the same spectrum as  $\mathcal{E}_A$ , it is clear that

$$\lim_{N \rightarrow \infty} \langle V_N(A)|V_N(A)\rangle = m_a,$$

for  $N \in m_a\mathbb{N}$ , and a similar equation holds for  $B$ .

For the rest, the first thing to prove is that if  $A$  and  $B$  have different periods  $m_a \neq m_b$ , then

$$\lim_{N \rightarrow \infty} |\langle V_N(A)|V_N(B)\rangle| = 0.$$

Clearly, if  $N$  is not a multiple of both  $m_a$  and  $m_b$ , then  $|\langle V_N(A)|V_N(B)\rangle| = 0$ . So let us consider  $N$  of the form  $kp$  with  $p = \text{lcm}(m_a, m_b)$ . By Lemma 5, it is enough to show that  $P_u A^{(p)}$  and  $Q_v B^{(p)}$  cannot be related by

$$P_u A^{(p)} = e^{i\xi} U Q_v B^{(p)} U^\dagger. \quad (\text{A1})$$

For simplicity, we will present the argument for the case in which  $m_a = 1, m_b > 1$  (in which case  $P_u = \mathbb{1}$ ). The general case is analogous.

Eq. (A1) implies that

$$\sum_{i_1 \dots i_{pN}} \text{Tr}(A^{i_1} \dots A^{i_{pN}}) |i_1 \dots i_{pN}\rangle = e^{i\xi N} \sum_{i_1 \dots i_{pN}} \text{Tr}(Q_v B^{i_1} \dots B^{i_{pN}}) |i_1 \dots i_{pN}\rangle$$

for all  $N$ . Applying the translation operator by one site to both sides of the equation, and using that the left hand side is translationally invariant and that  $Q_v B^i = B^i Q_{v+1}$ , we obtain that

$$\sum_{i_1 \dots i_{pN}} \text{Tr}(Q_v B^{i_1} \dots B^{i_{pN}}) |i_1 \dots i_{pN}\rangle = \sum_{i_1 \dots i_{pN}} \text{Tr}(Q_{v+1} B^{i_1} \dots B^{i_{pN}}) |i_1 \dots i_{pN}\rangle$$

for all  $N$ . But by Lemma 5,  $Q_v B^{(p)}$  and  $Q_{v+1} B^{(p)}$  are non-repeated blocks, and thus they cannot generate states equal to each other for all  $N$ , which is the desired contradiction.

So assume that the periods of  $A$  and  $B$  are both  $m$ . We consider two separate cases. In the first case, there do not exist  $u, v$  such that

$$P_u A^{(m)} = e^{i\xi} U Q_v B^{(m)} U^\dagger.$$

In this case, using Proposition 10 we obtain that

$$\lim_{N \rightarrow \infty} |\langle V_N(A) | V_N(B) \rangle| = 0.$$

So we are only left with the case in which there exist  $\tilde{u}, \tilde{v} \in \{1, \dots, m\}$ , a phase  $\lambda_{\tilde{v}}$  and a unitary  $V$  such that

$$P_{\tilde{u}} A^{(m)} = e^{i\lambda_{\tilde{v}}} V Q_{\tilde{v}} B^{(m)} V^\dagger. \quad (\text{A2})$$

In the rest of the proof we will show that, in this case, there is a phase  $\xi$  and a unitary matrix  $U$  so that  $A^i = e^{i\xi} U B^i U^\dagger$ . This will finish the proof of Proposition 14.

First note that since  $P_{\tilde{u}}$  and  $Q_{\tilde{v}}$  are projectors, Eq. (A2) implies that we can choose  $V = P_{\tilde{u}} V Q_{\tilde{v}}$ . (As earlier,  $V$  is a unitary if restricted to its support and range.) Eq. (A2) also implies that for all  $N$

$$\sum_{i_1, \dots, i_{mN}} \text{Tr}(P_{\tilde{u}} A^{i_1} \dots A^{i_{mN}}) |i_1, \dots, i_{mN}\rangle = e^{i\lambda_{\tilde{v}} N} \sum_{i_1, \dots, i_{mN}} \text{Tr}(Q_{\tilde{v}} B^{i_1} \dots B^{i_{mN}}) |i_1, \dots, i_{mN}\rangle. \quad (\text{A3})$$

If  $T$  is the translation operator, applying  $T^l$  for  $l = 1, 2, \dots, m-1$  on both sides of Eq. (A3), we obtain that

$$\sum_{i_1, \dots, i_{mN}} \text{Tr}(P_{\tilde{u}+l} A^{i_1} \dots A^{i_{mN}}) |i_1, \dots, i_{mN}\rangle = e^{i\lambda_{\tilde{v}} N} \sum_{i_1, \dots, i_{mN}} \text{Tr}(Q_{\tilde{v}+l} B^{i_1} \dots B^{i_{mN}}) |i_1, \dots, i_{mN}\rangle.$$

We have by Lemma 5 that  $P_{\tilde{u}+l} A^{(m)}$  and  $Q_{\tilde{v}+l} B^{(m)}$  are normal tensors, and thus from Theorem 8 it follows that for every  $l = 1, \dots, m-1$  there is a phase  $\lambda_{\tilde{v}+l}$  and a unitary  $U_{\tilde{v}+l} = P_{\tilde{u}+l} U_{\tilde{v}+l} Q_{\tilde{v}+l}$  such that

$$P_{\tilde{u}+l} A^{i_1} \dots A^{i_m} = e^{i\lambda_{\tilde{v}+l}} U_{\tilde{v}+l} Q_{\tilde{v}+l} B^{i_1} \dots B^{i_m} U_{\tilde{v}+l}^\dagger. \quad (\text{A4})$$

Thus, for any  $u = \tilde{u} + l$  and  $v = \tilde{v} + l$ , we have that  $v - u = \tilde{v} - \tilde{u} =: q$ , i.e.,  $u$  and  $v$  are related through a cyclic permutation. Thus, throughout the rest of the proof we will use that

$$v = u + q \pmod{m}. \quad (\text{A5})$$

Now, define the tensors

$$A_u^i := P_u A^i P_{u+1}, \quad (\text{A6})$$

$$B_v^i := U_v Q_v B^i Q_{v+1} U_{v+1}^\dagger, \quad (\text{A7})$$

so that Eq. (A4) reads

$$A_u^{i_1} A_{u+1}^{i_2} \dots A_{u+m-1}^{i_m} = e^{i\lambda_v} B_v^{i_1} B_{v+1}^{i_2} \dots B_{v+m-1}^{i_m}, \quad \text{for } u = 1, \dots, m. \quad (\text{A8})$$

By Lemma 5,  $A_u^{i_1} \dots A_{u+m-1}^{i_m}$  is normal for every  $u$ , and thus there is some length  $N_0$  at which it becomes injective [10]. Consider the tensor

$$F_u^{\mathbf{i}} := A_u^{i_1} A_{u+1}^{i_2} \dots A_{u+m-1}^{i_m}, \quad (\text{A9})$$

where  $\mathbf{i} = (i_1, \dots, i_m)$ . Since on the right hand side of Eq. (A9),  $A_u^{i_1} \dots A_{u+m-1}^{i_m}$  is repeated  $N_0$  times,  $F_u^{\mathbf{i}}$  is injective. Thus there is an inverse  $\Omega_u$  such that

$$\sum_{\mathbf{i}} (\Omega_u^{\mathbf{i}})_{\alpha, \beta} (F_u^{\mathbf{i}})_{\alpha', \beta'} = \delta_{\alpha, \alpha'} \delta_{\beta, \beta'}, \quad u = 1, \dots, m. \quad (\text{A10})$$

Now consider the concatenation of tensors

$$A_u^{i_1} F_{u+1}^{\mathbf{i}_1} A_{u+1}^{i_2} F_{u+2}^{\mathbf{i}_2} \dots A_{u+m-1}^{i_{m-1}} F_u^{\mathbf{i}_{m-1}}.$$

Note that this is simply the tensor  $A_u^{i_1} \dots A_{u+m-1}^{i_m}$  repeated  $mN_0 + 1$  times, which by Eq. (A8) equals  $e^{i\lambda_v(mN_0+1)}$  times  $(B_v^{i_1} \dots B_{v+m-1}^{i_m})$  repeated  $mN_0 + 1$  times. We apply the inverses

$$\Omega_{u+1}^{\mathbf{i}_1} \otimes \Omega_{u+2}^{\mathbf{i}_2} \otimes \dots \otimes \Omega_{u+m-1}^{\mathbf{i}_{m-1}}$$

to it. Using (A10) we obtain  $A_u^{i_1} \otimes A_{u+1}^{i_2} \otimes \dots \otimes A_{u+m-1}^{i_m}$ , and using Eq. (A8), we obtain  $e^{i\eta_v} B_v^{i_1} \otimes B_{v+1}^{i_2} \otimes \dots \otimes B_{v+m-1}^{i_m}$ , where

$$\eta_v := \lambda_v(mN_0 + 1) - N_0 \sum_{l=1}^m \lambda_l.$$

That is, we have found that

$$A_u^{i_1} \otimes A_{u+1}^{i_2} \otimes \dots \otimes A_{u+m-1}^{i_m} = e^{i\eta_v} B_v^{i_1} \otimes B_{v+1}^{i_2} \otimes \dots \otimes B_{v+m-1}^{i_m} \quad \text{for } u = 1, \dots, m. \quad (\text{A11})$$

Applying the translation operator  $l$  times to both sides of Eq. (A11), for  $l = 1, \dots, m-1$ , and using that Eq. (A11) is valid for all  $i_1, \dots, i_m$ , we obtain that  $\eta_v$  is independent of  $v$ , which we will henceforth call  $\eta := \eta_v$ . Now, (A11) gives

$$A_u^i = \kappa_v e^{i\eta/m} B_v^i, \quad \text{for } u = 1, \dots, m, \quad (\text{A12})$$

with

$$\prod_{v=1}^m \kappa_v = 1. \quad (\text{A13})$$

Using now that the operator norm  $\|\sum_i A_u^{i\dagger} A_u^i\| = \|\sum_i B_v^{i\dagger} B_v^i\| = 1$ , we obtain that  $|\kappa_v| = 1$  for all  $v$ . Thus  $\kappa_v$  can be written as  $\kappa_v = e^{i\theta_v}$  with  $\theta_v \in \mathbb{R}$ .

Therefore, recalling the definitions of  $A_u$  (Eq. (A6)) and  $B_v$  (Eq. (A7)), Eq. (A12) can be written as

$$P_u A^i P_{u+1} = e^{i\theta_v} e^{i\eta/m} U_v Q_v B^i Q_{v+1} U_{v+1}^\dagger, \quad \text{for } u = 1, \dots, m. \quad (\text{A14})$$

Additionally, from Eq. (A13) we have that  $\sum_{v=1}^m \theta_v = 0 \pmod{2\pi}$ . Thus there are some other phases  $\{\phi_v\}_{v=1}^m$  such that  $\theta_v = \phi_v - \phi_{v+1} \pmod{2\pi}$  for  $v = 1, \dots, m$ , where the sum  $v+1$  is modulo  $m$ . These can be chosen as

$$\phi_1 = 0, \quad \phi_v = -\sum_{l=1}^{v-1} \theta_l, \quad \text{for } v = 2, \dots, m. \quad (\text{A15})$$

With this definition, we have that

$$P_u A^i P_{u+1} = e^{i\eta/m} e^{i\phi_v} U_v Q_v B^i Q_{v+1} U_{v+1}^\dagger e^{-i\phi_{v+1}}, \quad \text{for } u = 1, \dots, m. \quad (\text{A16})$$

Thus, finally, defining  $U = \sum_{u=1}^m e^{i\phi_{u+q}} P_u U_{u+q} Q_{u+q}$  (where we have used the definition of  $v$ , Eq. (A5)), and the form of  $A$  and  $B$ ), Eq. (A16) can be written as

$$A^i = e^{i\xi} U B^i U^\dagger, \quad (\text{A17})$$

where  $\xi = \eta/m$ .

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