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PAPER: Quantum statistical physics, condensed matter, integrable systems

Fermionic quantum cellular automata and generalized matrix-product unitaries

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Abstract. In this paper, we study matrix-product unitary operators (MPUs) for fermionic one-dimensional chains. In stark contrast to the case of 1D qudit systems, we show that (i) fermionic MPUs (fMPUs) do not necessarily feature a strict causal cone and (ii) not all fermionic quantum cellular automata (QCA) can be represented as fMPUs. We then introduce a natural generalization of the latter, obtained by allowing for an additional operator acting on their auxiliary space. We characterize a family of such generalized MPUs that are locality-preserving, and show that, up to appending inert ancillary fermionic degrees of freedom, any representative of this family is a fermionic QCA (fQCA) and vice versa. Finally, we prove an index theorem for generalized MPUs, recovering the recently derived classification of fQCA in one dimension. As a technical tool for our analysis, we also introduce a graded canonical form for fermionic matrix product states, proving its uniqueness up to similarity transformations.

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1. Introduction

Among the achievements of tensor network (TN) theory, several results stand out in the context of the classification of topological phases of matter, now a pillar in modern quantum many-body physics [1]. For one-dimensional (1D) systems, this problem can naturally be formulated in terms of matrix product states (MPSs) [2, 3], and consists, loosely speaking, of determining all the possible equivalence classes under suitably defined smooth deformations. Arguably, the case where such a problem is best understood is that of 1D bosonic symmetry-protected topological (SPT) phases [4–7], where they have been completely classified by the second cohomology group [8–10] using the previously-derived results for the canonical forms (CFs) of MPSs [3, 11].

Recently, increasing attention has been devoted to the classification of topological systems far from equilibrium. This was also motivated by experimental advances in atomic, molecular and optical physics, which now make it possible to probe quantum many-body dynamics in exquisite detail [12–17]. The classification of periodically driven Floquet systems, in particular, has attracted a lot of theoretical work in the past few years [18–31].

In this context, a relevant problem pertains to the study of matrix product unitary operators (MPUs) [10, 32–35] in one dimension, namely, matrix product operators (MPOs) that are also unitary. This is intimately connected with the classification of two-dimensional (2D) Floquet SPT phases [36]: indeed, given a 2D Floquet system which exhibits many-body localization in the bulk, its edge dynamics are well described by an MPU [32, 37–39].

The theory of MPUs was first developed in [33, 34] for 1D qudit systems (see also [40], for a recent generalization in higher spatial dimensions). As a nontrivial result, it was shown that all MPUs are in fact quantum cellular automata (QCA) and vice versa [41, 42], i.e. MPUs feature a causal cone, strictly propagating information over a finite distance only. This observation is particularly interesting, because it allows one to address the analysis of QCA by means of the powerful tools developed within the theory of MPSs. For example, based on the latter, it was proven that, in the absence of symmetries, the equivalence classes of MPUs under smooth deformations are labeled by an index which can be computed directly from their local tensors. This index quantifies

the net quantum information flow through the MPU, and was shown to be equivalent to the Gross, Nesme, Vogts, and Werner (GNVW) index introduced in [43]. Later, the same problem was addressed in the presence of a local symmetry in [35], where it was shown that a complete classification can be obtained by also taking into account the cohomology class of the symmetry group, thus proving a conjecture raised earlier by Hastings [44].

While, so far, MPUs have been exclusively studied for qudit systems, 1D fermionic QCA (fQCA) have recently been analyzed in [45, 46]. In particular, it was shown that while one can develop an index theory along the lines of [43], the fermionic index need not be a rational number, as for qudits, but can also include a factor of the square root of two. Furthermore, such a classification is only complete if we allow for a more general notion of the *stable equivalence* of QCA, which involves enlarging the Hilbert space by appending inert ancillary fermionic degrees of freedom (d.o.f.) [46]. We note that the emergence of a richer picture might have been expected, based on previous studies on fermionic SPT phases in one dimension [47–49]. In that case, by mapping fermions onto qudits via the Jordan–Wigner (JW) transformation [50], it was shown that the fermionic classification problem can be reduced to a bosonic one, in the presence of an additional \mathbb{Z}_2 -symmetry, corresponding to conserved fermionic parity [10, 49].

At this point, a fundamental question is whether fQCA are also equivalent to fermionic MPUs (fMPUs), similarly to the case for qudits. For this problem, it is not natural to reduce ourselves to the latter case via a JW transformation, since it typically generates nonlocal terms for periodic boundary conditions (PBC). In fact, it is more convenient to work using a genuinely fermionic formalism [51, 52], where the definition of MPSs and MPOs can be generalized in a straightforward way. This is the approach that we take in this work, where we provide a thorough study of fMPUs and their connections to fQCA. Our results show that the picture is much richer with respect to the case of qudits, as we outline in the following.

1.1. Summary of our results

1.1.1. fMPUs are not equivalent to fQCA. Based on [33, 34], one could expect that any fMPU is automatically a quantum cellular automaton, i.e. it displays a strict causal cone. Our first result is to show that this is not the case. In particular, in section 5.1 we exhibit an example of an fMPU with PBCs which is not locality-preserving. In fact, the inverse statement is also untrue, and we find that the most natural generalization of MPUs to fermionic d.o.f. is not enough to capture all fQCA. This is discussed in section 5.2, where we built an MPO implementing a translation of Majorana modes. This is a quantum cellular automaton [46], but we show that it cannot be written in the expected form.

1.1.2. Characterization of locality-preserving fMPUs. As a second main result, we introduce a class of ‘generalized’ fMPUs, and identify a condition on the corresponding local tensors such that any representative of this family is an fQCA and vice versa. This is discussed in section 6, where generalized fMPUs are defined by allowing for an additional operator acting on the corresponding auxiliary space, and further characterized in section 6.1. The condition guaranteeing a strictly causal cone is

expressed in equation (62); it generalizes the simplicity condition introduced for qudits [33]. In addition, we find that any tensor generating an fMPU with antiperiodic boundary conditions (ABC) is necessarily simple after blocking, while this is not true in the periodic case.

1.1.3. Index theory from fMPUs. Third, we show that for the class of locality-preserving fMPUs, one can define an index based on the local tensors, which coincides with that of [46]. Although our construction is analogous to the one carried out for qudits [33, 34], there are some practical differences, and the definition for the index contains additional signs, as discussed in section 7. Here, our main result is the Index theorem 7.1, which states that the fermionic index displays all the expected stability properties that are present in the case of qudits, and correctly classifies fMPUs with respect to smooth deformations preserving unitarity.

1.1.4. Graded canonical form for fMPSs. Finally, as a byproduct of our work, we introduce and study a new graded canonical form (GCF) for fMPSs, which is based on the definition of irreducible fermionic tensors recently presented in [53]. This is detailed in appendix D, where we prove the existence and uniqueness of the GCF in the case of ABCs. This is a technical result which allows us to directly generalize some derivations of [33], but which is also interesting *per se* and might have applications in other problems.

1.2. Structure of the paper

The rest of this work is organized as follows. We begin in section 2, where we briefly recall the definition of QCA, and review some key results obtained in the recent literature. We proceed with section 3, where we introduce the basic aspects of TNs in qudit systems, and review some of the main results derived in [33] for MPUs. We move on to section 4, where we introduce the standard language of fermionic TNs using the so-called fiducial state formalism. In section 5, we discuss our first results for fMPUs, while generalized fMPUs are finally introduced and analyzed in section 6. The corresponding index theory is then developed in section 7, which represents the most technical part of our work, and is carried out using the formalism of graded TNs. Finally, we report our conclusions in section 8.

2. QCA and index theory

Before embarking on the study of fMPUs, we briefly recall some known facts about QCA. While they are usually defined in terms of the automorphisms of the C^* algebra of local operators in infinite systems [43], one can also define them as unitary operators acting on finite systems, which is the point of view taken in this work. Specifically, if we first consider a 1D qudit system associated with the Hilbert space $\mathcal{H} = \bigotimes_j \mathcal{H}_j$, with $\mathcal{H}_j \simeq \mathbb{C}_j^d$, a QCA of range r is a unitary operator U such that for any local operator \mathcal{O}_j acting non-trivially only on \mathcal{H}_j , the transformed operator $U^\dagger \mathcal{O}_j U$ acts non-trivially only on the qudits $k = j - r, j - r + 1, \dots, j + r$. A completely analogous definition can be given for fermionic d.o.f.

QCA have been completely characterized for 1D qudit systems in [43]. There, it was shown that any quantum cellular automaton is obtained by composing a finite number of shift operators, and ‘finite depth’ quantum circuits, which are obtained by applying a finite number of ‘layers’ of two-site local unitary gates acting on disjoint sets of qudits. Moreover, QCA can be classified according to a rational index (denoted by GNVW in this work), which measures the net quantum information flow through the system. Two QCA have the same index if and only if they can be continuously deformed into one another, or, equivalently, are related by the application of a finite-depth quantum circuit. For instance, a one-site shift of qubits on a ring has a GNVW index of 2, and is thus in a different class from a finite-depth quantum circuit, which has a GNVW index of 1. Finally, it was shown that this index is multiplicative with respect to composition.

These results were generalized for 1D fermionic systems in [46]. In these works, it was shown that one can define a similar index, although technical complications arise due to the structure of the local fermionic algebra. Physically, the main result was the discovery that the classification of fQCA is richer than in the case of qudits: indeed, the fermionic index is not necessarily a rational number, but also includes factors of the square root of two. This is due to the existence of a special fermionic quantum cellular automaton: the Majorana-shift operator, which consists of the translation of Majorana modes (rather than physical fermions). A physical picture of this fermionic quantum cellular automaton was already given in [45], where it was shown that this shift can be understood as a unitary operator that exchanges the topological phases of the 1D complex fermion chain [47]. For PBC, the latter have different parity, implying that the Majorana-shift fermionic quantum cellular automaton with PBC necessarily does not preserve parity.

The above picture provides a strong motivation for the study of fMPUs. In particular, since ‘plain’ fermionic MPOs (i.e. with no additional operator acting on the auxiliary space) are by construction parity-preserving, cf section 4.1, one could expect that the most natural generalization of MPUs defined for qudits [33] would not adequately capture the Majorana-shift fQCA. Furthermore, a natural question is whether the fermionic index can be extracted from the local tensors of fermionic MPOs defining the associated unitary operators, by analogy with the case of qudit MPUs [33]. These issues will be addressed in the rest of this work.

3. Basics of matrix product states

In this section, we recall some basic definitions and results of MPSs, following the treatment in [54].

We consider a Hilbert space \mathcal{H}_d of dimension d , with an orthonormal basis denoted by $\{|i\rangle\}_{i=0}^{d-1}$. We introduce the tensor \mathcal{A} , which is defined by its elements $A_{\alpha,\beta}^n$, with $n = 0, \dots, d-1$, and $\alpha, \beta = 0, \dots, D-1$. We define n and α, β as the physical and bond (auxiliary) indices, respectively. The tensor \mathcal{A} defines a family of translation-invariant states $|V^{(N)}\rangle \in \mathcal{H}_d^{\otimes N}$

$$|V^{(N)}\rangle = \sum_{n_1, \dots, n_N=0}^{d-1} c_{n_1, \dots, n_N} |n_1\rangle \otimes \cdots \otimes |n_N\rangle, \quad (1)$$

where

$$c_{n_1, \dots, n_N} = \text{tr} [A^{n_1} \dots A^{n_N}], \tag{2}$$

and where A^n denotes the $D \times D$ matrix with elements $A^n_{\alpha, \beta}$. We call $|V^{(N)}\rangle$ the MPS generated by the tensor \mathcal{A} .

MPSs admit a convenient graphical representation [54], as we now briefly recall. First, the individual tensors are denoted by

$$\mathcal{A} = \text{---} \bigcirc \text{---} \quad , \tag{3}$$

where the horizontal (vertical) lines represent the bond (physical) indices. The MPS $|V^{(N)}\rangle$ is then represented as

$$|V^{(N)}\rangle = \underbrace{\text{---} \bigcirc \text{---} \bigcirc \text{---} \dots \text{---} \bigcirc \text{---}}_N \quad . \tag{4}$$

Here, the lines that join different tensors indicate that the corresponding indices are contracted, while the vertical lines represent the physical indices. The curvy lines at the end indicate that the last and first tensors are also contracted, mimicking the presence of the trace in equation (2).

An important object in the theory of MPSs is the so-called transfer matrix (TM), which can be defined as

$$E = \sum_{n=0}^{d-1} A^n \otimes \bar{A}^n, \tag{5}$$

and which admits the graphical representation

$$E = \text{---} \bullet \text{---} \quad \text{---} \bigcirc \text{---} \quad . \tag{6}$$

In equation (5), \bar{A}^n is the complex-conjugated matrix of A^n , and corresponds to a black circle in equation (6). In the following, we will let λ_E denote the spectral radius of E , i.e. its eigenvalue with the largest absolute value.

A fundamental result is that MPSs of the form (2) can be brought into a CF [3, 54], which is particularly important when comparing the MPSs generated by different tensors. We recall here the precise definition, which we will refer to later on.

Definition 3.1. We say that a tensor \mathcal{A} generating an MPS is in CF if: (i) the matrices are of the form $A^n = \bigoplus_{k=1}^r \mu_k A_k^n$, where $\mu_k \in \mathbb{C}$ and the spectral radius of the TM, E_k , associated with A_k^n is equal to one; (ii) for all k , there exists no projector, P_k , such that $A_k^n P_k = P_k A_k^n P_k$ for all n .

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Loosely speaking, this means that the matrices A^n are written in a block-diagonal form, and that the blocks cannot be decomposed into smaller ones. It is also useful to recall the following

Definition 3.2. We say that a tensor \mathcal{A} generating an MPS is irreducible if there exists no projector, P , such that $A^n P = P A^n P$ for all n . Furthermore, we say that \mathcal{A} is normal if it is irreducible and its associated TM has a unique eigenvalue of magnitude (and value) equal to its spectral radius, which is equal to one.

Given two tensors \mathcal{A} and \mathcal{B} , it is straightforward to show that they generate the same MPS if they are related to one another by a *gauge* transformation, namely $B^n = X A^n X^{-1}$, for some invertible $D \times D$ matrix, X . One can also see that for a normal tensor it is always possible to find a gauge transformation defining a new normal tensor that is in canonical form II (CFII).

Definition 3.3. Let \mathcal{A} be a normal tensor, and Φ and ρ be the left and right eigenvectors of E corresponding to the eigenvalue 1. We say that \mathcal{A} is in CFII if

$$(\Phi| = \sum_{n=0}^{D-1} \langle n, n|, \tag{7a}$$

$$|\rho\rangle = \sum_{n=0}^{D-1} \rho_n |n, n\rangle, \tag{7b}$$

where $\rho_n > 0$ and $(\Phi|\rho\rangle = 1$.

Note that in equation (7) we have used round brackets, to indicate that the bra and ket states correspond to the auxiliary space. Note also that Φ and ρ can be considered as $D \times D$ matrices or as vectors in $\mathcal{H}_D \otimes \mathcal{H}_D$, and by definition, we have the graphical equations



$$\text{Diagram} = (, \tag{8}$$



$$\text{Diagram} =), \tag{9}$$

where a rectangle denotes the tensor corresponding to ρ (while Φ corresponds to the identity operator, simply denoted by a continuous line).

When discussing notions of locality and renormalization procedures, a natural concept is that of *blocking*. In essence, this consists of grouping k neighboring sites to form

a single one, which we can associate with a blocked tensor \mathcal{A}_k . This is formalized in the following.

Definition 3.4. Given the tensor \mathcal{A} generating an MPS, we denote the blocked tensor by \mathcal{A}_k , which is defined by the graphical representation

$$\mathcal{A}_k = \underbrace{\text{---} \bigcirc \text{---} \bigcirc \text{---} \cdots \text{---} \bigcirc \text{---}}_k . \tag{10}$$

Note that the physical and auxiliary dimensions of the blocked tensor \mathcal{A}_k are $d_k = d^k$ and D , respectively. We recall that the blocking procedure is important because, after blocking, for any tensor \mathcal{B} it is always possible to obtain another one, \mathcal{A} , in CF that generates the same MPS [54].

While the above definitions have been given for MPSs, they can be straightforwardly extended to MPOs. To this end, we recall that an MPO $M^{(N)}$ admits the graphical representation

$$M^{(N)} = \underbrace{\text{---} \bigcirc \text{---} \bigcirc \text{---} \cdots \text{---} \bigcirc \text{---}}_N , \tag{11}$$

where the lower and upper vertical lines correspond to the input and output qudits, respectively. Any MPO can then be trivially mapped onto an MPS by grouping both input and output lines to form a single physical index (corresponding to a local space with dimension d^2), with a graphical identification

$$\text{---} \bigcirc \text{---} \mapsto \text{---} \bigcirc \text{---} . \tag{12}$$

In this way, the definitions of TM, CF, and blocking can also be naturally extended to MPOs.

3.1. MPUs in qudit systems

Let us consider a tensor \mathcal{U} that generates a family of MPOs $U^{(N)}$ of the form in equation (11), such that $U^{(N)}$ is a unitary operator for all non-negative integers N . The resulting MPOs $U^{(N)}$ are called matrix product unitaries, and were investigated in [33, 34]. In preparation for the fermionic case, we now review some of their properties, and present the main results derived in [33].

First, by viewing \mathcal{U} as a tensor generating an MPS as in equation (12), we can define the normalized TM

$$E_{\mathcal{U}} = \frac{1}{d} \text{---} \overset{\bullet}{\bigcirc} \text{---} , \tag{13}$$

which plays an important role in the analysis of MPUs. In particular, the starting point of [33] is the observation that $E_{\mathcal{U}}$ has just one nonzero eigenvalue, which is equal to

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one, and that \mathcal{U}/\sqrt{d} is a normal tensor. This follows simply from the unitarity condition $U^{(N)\dagger}U^{(N)} = \mathbb{1}$, and

$$\frac{1}{d^N} \text{tr} [U^{(N)\dagger}U^{(N)}] = \text{tr} [E_{\mathcal{U}}^N]. \quad (14)$$

Using this observation, it was possible to prove that for any tensor \mathcal{U} generating an MPU, there exists some $k \leq D^4$ such that the blocked tensor \mathcal{U}_k is *simple*. In general, we define a tensor \mathcal{U} to be simple, if two tensors a, b exist, such that



$$(15a)$$



$$(15b)$$

It is also clear, using a graphical proof, that any simple tensor generates an MPU, making the characterization of [33] complete.

The simplicity condition also made it possible to derive a standard form for the tensor \mathcal{U} , by means of which a fundamental theorem of MPUs was proven in [33]. The latter stated that two tensors \mathcal{U} and \mathcal{V} generate the same MPU for all non-negative integers N iff they have the same standard form (up to single-site gauge transformations).

Importantly, a simple corollary of these results is that for qudit systems, any MPU (with finite bond dimensions) is a 1D quantum cellular automaton, and vice versa. This means that any MPU $U^{(N)}$ maps any operator \mathcal{O} supported on a finite region into another one, $U^{(N)\dagger}\mathcal{O}U^{(N)}$, which is also supported on a finite spatial region. Such an identification between MPUs and QCA is based on the classification of [43], according to which any given quantum cellular automaton can be represented by a finite number of layers of finite-depth circuits and translations.

The aim of the rest of this work is to explore if and how such a picture generalizes to fermionic 1D systems. As we have already anticipated, significant differences emerge, as we lay out in the following. We begin our study in the next section, by introducing fermionic 1D TNs.

4. Fermionic tensor networks

We consider a chain of N sites, and in each site we have n_F fermionic modes with (physical) annihilation operators $a_{x,j}$, $x = 1, \dots, N$, $j = 1, \dots, n_F$. The creation and annihilation operators satisfy canonical anticommutation relations

$$\{a_{x,j}, a_{y,k}^\dagger\} = \delta_{x,y} \delta_{j,k}, \quad (16a)$$

$$\{a_{x,j}, a_{y,k}\} = 0. \quad (16b)$$

In the following, we denote the physical vacuum by $|\Omega\rangle$, with $a_{x,j}|\Omega\rangle = 0$, while we introduce the short-hand notation

$$(a_x^\dagger)^n = (a_{x,1}^\dagger)^{n^{(1)}} \cdots (a_{x,n_F}^\dagger)^{n^{(n_F)}}, \tag{17}$$

where $(n^{(1)}, \dots, n^{(n_F)})$ is the binary decomposition of n . We can define a fermionic parity operator \mathcal{P} satisfying $\mathcal{P}|\Omega\rangle = |\Omega\rangle$, and

$$\mathcal{P}(a_{x,1}^\dagger)^{n^{(1)}} \cdots (a_{x,n_F}^\dagger)^{n^{(n_F)}} = (-1)^{|n|} (a_{x,1}^\dagger)^{n^{(1)}} \cdots (a_{x,n_F}^\dagger)^{n^{(n_F)}} \mathcal{P} \tag{18}$$

where

$$|n| = \sum_{j=1}^{n_F} n^{(j)} \pmod{2}. \tag{19}$$

Using the above notations, any state in the system can be represented as

$$|\Psi\rangle = \sum_{n_1, \dots, n_N=0}^{d-1} c_{n_1, \dots, n_N} a_1^{\dagger n_1} \cdots a_N^{\dagger n_N} |\Omega\rangle, \tag{20}$$

where $d = 2^{n_F}$. In the following, we will always work with states that have well-defined parity, namely

$$\mathcal{P}|\Psi\rangle = (-1)^{|\Psi|} |\Psi\rangle. \tag{21}$$

This implies that c_{n_1, \dots, n_N} is zero unless $\sum_{j=1}^N |n_j| \equiv |\Psi| \pmod{2}$.

Before discussing fMPSs, it is useful to recall that, in the case of fermions, there are two natural types of boundary condition to be considered: periodic and antiperiodic. Accordingly, one can define two types of translation operator. If PBCs are assumed, we define T_P by its action

$$T_P|\Omega\rangle = |\Omega\rangle, \tag{22a}$$

$$T_P a_{x,j}^\dagger T_P^{-1} = a_{x+1,j}^\dagger, \quad 1 \leq x \leq N-1, \tag{22b}$$

$$T_P a_{N,j}^\dagger T_P^{-1} = a_{1,j}^\dagger, \tag{22c}$$

while for ABCs, we define T_{AP} by

$$T_{AP}|\Omega\rangle = |\Omega\rangle, \tag{23a}$$

$$T_{AP} a_{x,j}^\dagger T_{AP}^{-1} = a_{x+1,j}^\dagger, \quad 1 \leq x \leq N-1, \tag{23b}$$

$$T_{AP} a_{N,j}^\dagger T_{AP}^{-1} = -a_{1,j}^\dagger. \tag{23c}$$

Using equations (22) and (23), one can easily find a condition of the coefficients c_{n_1, \dots, n_N} for which the state (20) is invariant under T_P or T_{AP} . Specifically

$$\begin{aligned} T_P|\Psi\rangle = |\Psi\rangle &\Leftrightarrow c_{n_1, \dots, n_N} = (-1)^{|n_1|(|\Psi|+1)} c_{n_2, \dots, n_N, n_1}, \\ T_{AP}|\Psi\rangle = |\Psi\rangle &\Leftrightarrow c_{n_1, \dots, n_N} = (-1)^{|n_1||\Psi|} c_{n_2, \dots, n_N, n_1}. \end{aligned} \tag{24}$$

We stress that both types of boundary condition appear frequently when working with fermionic systems. For instance, using equation (24), one can easily see that a state obtained by occupying each fermionic mode (with $n_F = 1$) is invariant under translations with PBCs or ABCs, depending on whether N is odd or even. Accordingly, both types of boundary condition will be studied in this work.

4.1. Fermionic MPSs

Up until now, several equivalent formulations have been developed for fermionic TNs [51–53, 55–60]. Here, we will focus on the fiducial-state formalism introduced in [51, 52], whose appeal lies mainly in its physically motivated construction. In the second, more technical part of the paper, however, we will also make use of the formalism of graded TNs recently introduced in [53, 59] (see also [61, 62]), which is reviewed in appendix B.

For qudit systems, one can think of MPSs (or, more generally of projected-entangled-pair states (PEPS)) as being obtained from a sequence of local projections onto maximally entangled pairs of auxiliary qudits [63]. The idea described in [51, 52] is that the same construction can be carried out for fermionic systems, provided that the auxiliary d.o.f. are taken to be fermionic particles themselves. As a technical point, it is convenient to choose auxiliary particles such as Majorana fermions. Furthermore, one needs to enforce a given fermionic parity on the local projectors, in order to ensure that the fMPS itself has well-defined parity.

A detailed discussion of this construction is provided in appendix A, while here we only report the final result for the coefficients in equation (20). The explicit form of the latter depend on whether PBCs or ABCs are assumed. In particular, we have, respectively,

$$c_{n_1, \dots, n_N} = \text{tr}(Z A^{n_1} \dots A^{n_N}), \quad (\text{PBC}) \quad (25)$$

$$c_{n_1, \dots, n_N} = \text{tr}(A^{n_1} \dots A^{n_N}) \quad (\text{APB}) \quad (26)$$

Here we have introduced the parity operator Z

$$Z = \begin{pmatrix} \mathbb{1}_e & 0 \\ 0 & -\mathbb{1}_o \end{pmatrix}, \quad (27)$$

where $\mathbb{1}_e, \mathbb{1}_o$ are identity operators acting on the even and odd subspaces of dimensions D_e and D_o , with $D_e = D_o = D/2$, and $D = 2^{N_F}$, for some positive integer N_F . Furthermore, in order to ensure that the fMPS has well-defined parity, we require that the matrices A^n satisfy⁵

$$Z A^n = (-1)^{|n|} A^n Z, \quad (28)$$

where $|n|$ is defined in equation (19). In the following, we will thus define a periodic (antiperiodic) fMPS to be a state taking the form of (20), where the coefficients can be cast as in equation (25) (equation (26)), and where the local tensors satisfy (28).

⁵We note that equation (28) implies that \mathcal{A} is an even tensor. One could also consider fMPSs built out of odd local tensors, which would lead to states with well-defined parity for each non-negative integer N . However, choosing \mathcal{A} to be even is not a restriction, since blocking an odd tensor twice yields an even one.

Note that it is straightforward to verify that the coefficients (25) and (26) satisfy equation (24).

The parity operator, Z^c allows us to assign a \mathbb{Z}_2 -grading structure to the auxiliary space \mathbb{C}^D , which simply means that \mathcal{H}_D can be divided into two complementary subspaces of even and odd states. Here we define a state to be even or odd if it is a superposition of Z -eigenstates with eigenvalues $+1$ or -1 , respectively. If $|\alpha\rangle$ is an eigenstate of Z , we will denote the corresponding eigenvalue by $(-1)^{|\alpha|}$, with $|\alpha| = 0$ ($|\alpha| = 1$) for even (odd) states, namely

$$Z|\alpha\rangle = (-1)^{|\alpha|}|\alpha\rangle. \tag{29a}$$

The observations above also allow us to define the parity of tensors acting on both the auxiliary and physical spaces in a natural way. In particular, let $A_{\alpha,\beta}^n \neq 0$ be an element of the tensor \mathcal{A} . We can then define the parity of \mathcal{A} as

$$|\mathcal{A}| = |n| + |\alpha| + |\beta| \pmod{2}. \tag{30}$$

Clearly, this definition only makes sense if it is independent from the choice of n , α and β . This is the case if A^n satisfies equation (28), which in fact implies that \mathcal{A} is an even tensor.

Given the parity operator (27), it is possible to write down the general form of the matrices A^n satisfying equation (28). In particular, it is easy to show that, in the basis where Z is written as in equation (27), A^n must have the following block structure

$$A^n = \begin{pmatrix} B^n & 0 \\ 0 & C^n \end{pmatrix}, \quad |n| = 0, \tag{31}$$

$$A^n = \begin{pmatrix} 0 & B^n \\ C^n & 0 \end{pmatrix}, \quad |n| = 1, \tag{32}$$

where B^n, C^n are arbitrary matrices.

So far, we have considered $D = 2^{N_F}$, $d = 2^{N_F}$. However, this can be naturally relaxed as the tensor \mathcal{A} can have many zeros and thus we can compress its dimensions. This happens when for some values of n , $A_{\alpha,\beta}^n = 0$ for all α, β or, alternatively, for some α , $A_{\alpha,\beta}^n = A_{\beta,\alpha}^n = 0$ for all n and β . In this case we can restrict ourselves to subspaces of \mathbb{C}^d and \mathbb{C}^D with dimensions d' and D' , respectively. We can also call Z' and \mathcal{P}' the projection of Z and \mathcal{P} onto these subspaces: importantly, they remain diagonal with diagonal elements ± 1 , meaning that the reduced spaces maintain the \mathbb{Z}_2 -grading structure. In the following, we will consider that this is the case and drop the primes in the notation, so that d and D can take arbitrary values.

It is straightforward to also employ the fiducial-state formalism to treat fMPOs. In general, any fermionic operator $U^{(N)}$ can be written in the form

$$U^{(N)} = \sum_{\substack{n_1, \dots, n_N=0 \\ m_1, \dots, m_N=0}}^{d-1} c_{m_1, \dots, m_N}^{n_1, \dots, n_N} f_1^{n_1, m_1} \dots f_N^{n_N, m_N}. \tag{33}$$

Here, we introduce the operators $f_j^{n,m}$, defined by $f_j^{n,m}|\Omega\rangle = \delta_{m,0}(a_j^n)^\dagger|\Omega\rangle$, and

$$f_j^{n,m}(a_k^\dagger)^p = (-1)^{(|n|+|m|)|p|} (a_k^\dagger)^p f_j^{n,m}, \quad j \neq k, \tag{34a}$$

$$f_j^{n,m}(a_j^\dagger)^p = \delta_{m,p} (a_j^\dagger)^n, \tag{34b}$$

where $(a_j^\dagger)^n$ was defined in equation (17). Note that from these equations it also follows that

$$[f_j^{n,m}]^\dagger = f_j^{m,n}. \tag{35}$$

For example, in the case $n_F = 1$, we have $f_j^{0,0} = a_j a_j^\dagger$, $f_j^{0,1} = a_j$, $f_j^{1,0} = a_j^\dagger$ and $f_j^{1,1} = a_j^\dagger a_j$.

Analogously to fMPSs, fMPOs are defined by a specific form for the coefficients $c_{m_1, \dots, m_N}^{n_1, \dots, n_N}$, which is obtained by following the construction outlined in appendix A. Once again, we have to distinguish between PBCs and ABCs, for which we obtain, respectively,

$$c_{m_1, \dots, m_N}^{n_1, \dots, n_N} = \text{tr}(ZU^{n_1, m_1} \dots U^{n_N, m_N}), \quad (\text{PBC}) \tag{36}$$

$$c_{m_1, \dots, m_N}^{n_1, \dots, n_N} = \text{tr}(U^{n_1, m_1} \dots U^{n_N, m_N}) \quad (\text{ABC}) \tag{37}$$

Here, Z is defined as in equation (27), while $U^{n,m}$ are $D \times D$ matrices which must satisfy

$$ZU^{n,m} = (-1)^{|n|+|m|} U^{n,m} Z. \tag{38}$$

It is important to note that elementary operations with fMPSs and fMPOs, such as blocking or composition, in general result in additional signs for the corresponding tensors. Since these signs are at the root of some qualitative differences arising in the case of fMPUs, we discuss them in some detail in appendix A.2.

5. Fermionic matrix product unitaries

We now finally introduce the fMPUs. There are two main results in this section: the construction of a translation-invariant fMPO which is unitary but not a QCA (cf section 5.1), and the derivation of the TN form of the Majorana-shift operator for open and PBCs, cf equations (52), and (54).

Based on the formalism of fermionic TNs, we can formulate a very natural generalization of the definition of MPUs (presented in section 3.1) to fermionic systems. Namely, we call $U^{(N)}$ an fMPU if it is an fMPO and $[U^{(N)}]^\dagger U^{(N)} = \mathbb{1}$ for all $N \geq 1$. Furthermore, as opposed to the case for qudits, it makes sense to define fMPUs both for PBCs and ABCs, corresponding to the coefficients (36) and (37), respectively.

Arguably, one of the most important questions regarding fMPUs is whether they are all locality-preserving. We find that this is not the case for periodic fMPUs, in stark contrast with the case of qudits. We show this in the next subsection, by providing an explicit example of such a non-locality-preserving fMPU. Technically, this qualitative difference between fermions and qudits arises because of the presence of the operator Z in the trace in equation (36), which makes it possible for the TM of periodic fMPUs to display a nontrivial spectrum, cf also equation (A33).

5.1. Non-locality-preserving fMPUs

We now provide an explicit example of a periodic fMPU which is not locality-preserving. Once again, we use the fiducial-state formalism, but our example can be straightforwardly translated into the language of graded TNs, cf appendix B.

Let us consider a chain of N sites, with two fermionic modes per site, $n_F = 2$, corresponding to the annihilation operators $a_{x,1}, a_{x,2}$, $x = 1, \dots, N$. Let $U^{(N)}$ be a periodic fMPO of the form given in (33), with the coefficients given in equation (36). In order to construct our example, we choose $D = 3$, so that

$$Z = \begin{pmatrix} +1 & 0 & 0 \\ 0 & +1 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \tag{39}$$

We stress, once again, that the bond-dimension can be taken to be a power of two, by simply appending arbitrarily many lines and columns filled with zeros. We now define the local tensor \mathcal{U} , by specifying its non-zero matrix elements $U_{\alpha,\beta}^{m,n}$, which are

$$U_{\alpha,\beta}^{0,0} = \delta_{\alpha,\beta}, \quad \alpha, \beta = 0, 1, 2, \tag{40}$$

$$U_{\alpha,\beta}^{n,m} = \delta_{\alpha,n-1} \delta_{\beta,m-1}, \quad \alpha, \beta = 0, 1, 2, \quad n, m = 1, 2, 3. \tag{41}$$

For completeness, we also tabulate the explicit matrices $U^{n,m}$ in appendix C.1, from which it is possible to verify that they satisfy equation (38), and thus generate a legitimate periodic fMPO. In the following, we prove the unitarity of $U^{(N)}$, and analyze its properties.

5.1.1. Spectral properties of the TM. First of all, it is interesting to note that the spectrum of the TM (defined in equation (A32) for fMPOs), denoted by \mathcal{S}_E , is nontrivial. In particular, a direct calculation gives $\mathcal{S}_E = \{\lambda_j\}_{j=0}^8$, with $\lambda_0 = 1$ and $\lambda_j = 1/4$, for $j = 1, \dots, 8$. This is already a point of departure with respect to the case of qudits, where the TM of an MPU has a single nonzero eigenvalue, which is equal to one. By further inspection, one can see that the eigenvector of E associated with $\lambda_0 = 1$ is also an eigenstate of $Z \otimes Z$ with eigenvalue $+1$. Analogously, one can see that the rest of the eigenvectors associated with λ_j , $j > 0$, are also eigenstates of $Z \otimes Z$: four of them have the eigenvalue $+1$, and the other four have the eigenvalue -1 . Thus, we obtain from equation (A33), $(1/d^N) \text{tr} U^{(N)\dagger} U^{(N)} = 1 + (4/4^N) - (4/4^N) = 1$, as should be the case for a unitary operator.

5.1.2. Proof of unitarity. Next, we show that $U^{(N)}$ is unitary. One could do this by checking that the fMPO generated by the tensor $\mathbb{U}^{(N)}$ defined in equation (A31) is an identity. Here, we follow a different strategy, which is based on the action of $U^{(N)}$ on basis states. In particular, from the explicit form of the local tensors, we show in appendix C.1 that

$$U^{(N)}|\Omega\rangle = |\Omega\rangle, \tag{42}$$

and, $\forall P = 1, \dots, N$, $\{j_\ell\}_{\ell=1}^P \in \{1, 2, 3\}^P$,

$$U^{(N)} a_{i_1}^{j_1\dagger} a_{i_2}^{j_2\dagger} \dots a_{i_P}^{j_P\dagger} |\Omega\rangle = (-1)^\gamma a_{i_1}^{j_P\dagger} a_{i_2}^{j_1\dagger} \dots a_{i_P}^{j_{P-1}\dagger} |\Omega\rangle. \tag{43}$$

Here $\{i_k\}_{k=1}^P$ is a strictly increasing sequence of integers, with $1 \leq i_k \leq N$, which label the site at which the creation operators act. Furthermore, $(-1)^\gamma$ is a sign which depends on the specific state. Note that in equation (43), j_ℓ takes a value in the set $\{1, 2, 3\}$, namely $j_\ell \neq 0$, and that $U^{(N)}$ does not act as a translation operator, but only shifts the creation operators at fixed positions. From equations (42) and (43), it is clear that $U^{(N)}$ maps two orthonormal bases one onto another, and it is thus unitary.

5.1.3. Proof of non-locality. Finally, we explicitly prove that the operator $U^{(N)}$ is not locality-preserving, i.e. there exists a local operator \mathcal{O}_j , acting only on site j , such that the support of $U^\dagger \mathcal{O}_j U$ is not contained in any finite region. In order to see this, consider the state $|\Psi_{j,k}\rangle = a_{j,1}^\dagger a_{k,1}^\dagger |\Omega\rangle$ and choose the operator $\mathcal{O}_j = a_{j,2}^\dagger a_{j,1}$. Then, using the explicit action in equation (43), we have

$$\begin{aligned} U^\dagger \mathcal{O}_j U |\Psi_{j,k}\rangle &= (-1)^\gamma U^\dagger \mathcal{O}_j |\Psi_{j,k}\rangle \\ &= (-1)^\gamma U^\dagger a_{j,2}^\dagger a_{k,1}^\dagger |\Omega\rangle = (-1)^{\gamma'} a_{j,1}^\dagger a_{k,2}^\dagger |\Omega\rangle, \end{aligned} \tag{44}$$

where we chose $j \neq k$ and where $(-1)^\gamma, (-1)^{\gamma'}$ are signs that are irrelevant for our discussion. We see that the operator $U^\dagger \mathcal{O}_j U$ induces a modification of the mode at site k , which can be taken arbitrarily far away from j , and thus it is not localized in the neighborhood of site j .

In conclusion, we have exhibited an example of an fMPU with PBCs which is not locality-preserving. The choice of PBCs was important: indeed, as we discuss in the next section, fMPUs with ABCs are necessarily QCA.

5.2. The Majorana-shift operator

The results of the previous subsection show that, in general, fMPUs are not QCA. On the other hand, it is also true that fMPUs with coefficients in the form of either equation (36) or equation (37) do not exhaust all the possible QCA (even after blocking), once again in stark contrast to the case of qudits. This was already mentioned in section 2, where we anticipated the special role played by the translation of Majorana modes [45, 46]. We review it explicitly in this subsection, where we also derive the corresponding TN representation.

Let us consider a chain of N sites, with one fermionic mode per site, $n_F = 1$, associated with the fermionic annihilation operators a_n . We can introduce the $2N$ Majorana modes γ_n by

$$a_n = \frac{1}{2} (\gamma_{2n-1} + i\gamma_{2n}), \tag{45}$$

$$a_n^\dagger = \frac{1}{2} (\gamma_{2n-1} - i\gamma_{2n}). \tag{46}$$

We now consider two automorphisms of the operator algebra α_P, α_{AP} , defined by the following action

$$\alpha_P(\gamma_j) = \gamma_{j+1}, \quad j = 1, \dots, 2N - 1, \tag{47}$$

$$\alpha_P(\gamma_{2N}) = \gamma_1, \tag{48}$$

and

$$\alpha_{\text{AP}}(\gamma_j) = \gamma_{j+1}, \quad j = 1, \dots, 2N - 1, \quad (49)$$

$$\alpha_{\text{AP}}(\gamma_{2N}) = -\gamma_1. \quad (50)$$

Clearly, α_{P} and α_{AP} implement an fQCA, which we will refer to as the Majorana shift (or translation).

Importantly, both α_{P} and α_{AP} can be represented by a unitary operator. Namely there exist $M_{\text{P}}^{(N)}$, $M_{\text{AP}}^{(N)}$, such that $M_{\text{P}}^{(N)} M_{\text{P}}^{(N)\dagger} = M_{\text{AP}}^{(N)} M_{\text{AP}}^{(N)\dagger} = \mathbb{1}$, and $\alpha_{\text{P}}(\mathcal{O}) = M_{\text{P}}^{(N)} \mathcal{O} M_{\text{P}}^{(N)\dagger}$, $\alpha_{\text{AP}}(\mathcal{O}) = M_{\text{AP}}^{(N)} \mathcal{O} M_{\text{AP}}^{(N)\dagger}$, for all operators \mathcal{O} . Let us focus, for instance, on the case of ABCs. After a bit of guesswork, it is not difficult to arrive at the following explicit expression for the operator $M_{\text{AP}}^{(N)}$ ⁶

$$M_{\text{AP}}^{(N)} = \frac{(1 - \gamma_1 \gamma_2)}{\sqrt{2}} \frac{(1 - \gamma_2 \gamma_3)}{\sqrt{2}} \dots \frac{(1 - \gamma_{2N-1} \gamma_{2N})}{\sqrt{2}}. \quad (51)$$

Note that the order of the factors is important here, since they do not all commute with one another. Starting from equation (51), one can rewrite $M_{\text{AP}}^{(N)}$ as in equation (33), where the coefficients read

$$c_{m_1, \dots, m_N}^{n_1, \dots, n_N} = \frac{1}{\sqrt{2}} \text{tr} (M^{n_1, m_1} \dots M^{n_N, m_N}) \quad (\text{ABC}). \quad (52)$$

Here the trace is over a 2D space, and we introduced

$$M^{n, m} = \frac{1}{\sqrt{2}} i^m \sigma_x^{n+m}, \quad n, m = 0, 1, \quad (53)$$

in terms of the Pauli matrix σ^x . A proof of equation (52) is reported in appendix C.2. Note that the matrices $M^{n, m}$ satisfy (28), with $Z = \text{diag}(1, -1)$, so that (52) admits a fiducial-state representation. Note also that the local tensor of the inverse shift can be obtained using equation (A21).

In order to obtain M_{P} , one could be tempted to simply insert the operator $Z = \text{diag}(1, -1)$ into the trace in equation (52). However, due to the specific form of the tensors $M^{n, m}$, the resulting coefficients are all vanishing. In fact, as we show in appendix C.2, it turns out that a unitary operator with PBCs is obtained if the matrix $X = \sigma^x$ is inserted instead. In particular, the unitary operator $M_{\text{P}}^{(N)}$ can be represented as shown in equation (33), where the coefficients are given by

$$c_{m_1, \dots, m_N}^{n_1, \dots, n_N} = \frac{1}{\sqrt{2}} \text{tr} (X \tilde{M}^{n_1, m_1} \dots \tilde{M}^{n_N, m_N}) \quad (\text{PBC}), \quad (54)$$

with

$$\tilde{M}^{n, m} = \frac{1}{\sqrt{2}} (-i)^m \sigma_x^{n+m}, \quad n, m = 0, 1. \quad (55)$$

⁶ Interestingly, in [46] it was shown that $M_{\text{AP}}^{(N)}$ can also be written as a Gaussian operator, namely as the exponential of an expression which is quadratic in the Majorana modes. This provides an alternative representation to the one given here in terms of fermionic TNs. We also note that an equation similar to (51) has appeared recently in [64] for PBCs.

Crucially, viewing the auxiliary space as a graded space with parity $Z = \text{diag}(1, -1)$, the operator X is odd, namely $|X| = 1$. Furthermore, $[X, M^{n,m}] = 0$ for all n, m . Thus, using equation (24), we immediately see that M_P is indeed invariant under translation with PBCs.

Although they appear different, a legitimate question is whether the coefficients (52) and (54) can be cast in the forms (36) and (37). In fact, this is not the case, and for PBCs this can be seen very easily. Indeed, the presence of X in the trace (54) implies that $M_P^{(N)}$ is an odd operator (namely, it maps even states into odd ones, and vice versa), while any fMPU defined by (36) is necessarily even. The same conclusion holds for ABCs, as can be seen by an inspection of the corresponding CF, discussed in the next section.

Finally, it is instructive to apply a JW transformation to $M_{AP}^{(N)}$. In fact, starting from equation (51) and using standard techniques, it is possible to rewrite it as a qubit ($d = 2$) MPO with open boundaries. A crucial point, however, is that the bulk tensors of this MPO do not generate an MPU when PBCs are imposed. This example shows that fQCA cannot be simply understood in terms of periodic MPUs on qudit chains.

6. Generalized fermionic MPUs

In this section, we present our second main result; i.e. we introduce a class of ‘generalized’ fMPUs (section 6.1), and identify a condition on the corresponding local tensors such that any representative of this family is an fQCA and vice versa (sections 6.2, and 6.3).

The main motivation for generalized fMPUs is to have a class of fMPOs that also includes the Majorana-shift operators (52) and (54). A natural way to do this is to allow for an additional operator acting on the auxiliary space, such that it has well-defined parity and that it implements the correct boundary conditions. More precisely, we say that $U^{(N)}$ is a generalized fMPU if it is unitary for $N \geq 1$, and can be written as in (33), with coefficients of the form

$$c_{m_1, \dots, m_N}^{n_1, \dots, n_N} = \text{tr}(S U^{n_1, m_1} \dots U^{n_N, m_N}). \quad (56)$$

As usual, we require that all the local tensors have well-defined parity. Namely, the trace in equation (56) is over a graded space with the parity operator, Z defined in equation (27), and where the matrices $U^{n,m}$ satisfy equation (28). Furthermore, the operator S must also have well-defined parity, and satisfy particular commutation relations with $U^{n,m}$. Since these depend on the boundary conditions chosen, it is convenient to separate the periodic and antiperiodic cases. For PBCs, we allow for S to be even or odd, but we require that

$$S U^{n,m} = (-1)^{(|S|+1)(|n|+|m|)} U^{n,m} S \quad (\text{PBC}). \quad (57)$$

On the other hand, it can be shown, using equation (24), that there are no odd states or operators that are invariant under translations with ABCs. Therefore, in the latter case we require that S is even, and satisfies

$$[S, U^{m,n}] = 0, \quad |S| = 0 \quad (\text{ABC}). \quad (58)$$

The conditions imposed above constitute the minimal requirement in order to have an fMPO with well-defined parity that is invariant under translations with PBCs and ABCs, respectively.

It is immediately visible that the Majorana-shift operators are indeed generalized fMPUs. In particular, for PBCs and ABCs, we see from equations (52) and (54) that $S = X/\sqrt{2}$ and $S = \mathbb{1}/\sqrt{2}$, respectively. On the other hand, we know from section 5.1 that not all generalized fMPUs are QCA, so a natural question is to ask which conditions of S and $U^{n,m}$ guarantee that $U^{(N)}$ is locality-preserving.

To address this problem, we need to introduce some technical definitions that generalize those presented in section 3 for irreducible and normal tensors. These are inspired by the work described in [53], where it was pointed out that the notion of an irreducible tensor should be modified in the fermionic case, due to the requirement that all the tensors are even. We begin with the following

Definition 6.1. Let V be a graded Hilbert space, with a parity operator Z , and $W \subset V$ with an associated orthogonal projector P_W . We say that W is a graded subspace if $[P_W, Z] = 0$. Accordingly, an even tensor \mathcal{A} is said to be graded irreducible (GI) if there is no proper graded subspace which is left invariant by all the matrices A^n .

Clearly, if \mathcal{A} is GI, there are two possibilities: either there is no invariant subspace, or there is an invariant subspace that is non-graded. In the latter case, we prove in appendix D (see also [53]) that there exists a quite precise characterization of the matrices A^n , which, up to an even gauge transformation, takes the form

$$A^n = (\sigma^x)^{|n|} \otimes B^n, \quad (59)$$

where B^n are $D/2 \times D/2$ matrices, and where the parity operator is $Z = \sigma^z \otimes \mathbb{1}$. Note that in this case, the auxiliary space splits into even and odd subspaces with the same dimensions.

Next, we generalize the notion of normal tensors and CF, which will be of great importance for the classification of fMPUs.

Definition 6.2. We say that an even tensor \mathcal{A} is a graded normal tensor (GNT) if (i): there is no non-trivial graded invariant subspace; (ii) the corresponding TM has either exactly one or two eigenvalues of magnitude and value equal to its spectral radius which is equal to 1. In the first case we say that the GNT is non-degenerate, while in the second case we say that it is degenerate.

Definition 6.3. We say that an even tensor \mathcal{A} generating an fMPS is in GCF if: (i): the matrices are of the form $A^n = \bigoplus_{k=1}^r \mu_k A_k^n$, where $\mu_k \in \mathbb{C}$ and the spectral radius of the TM E_k associated with A_k^n is equal to one; (ii): the parity operator Z has the same block structure as A^n and, for all k , \mathcal{A}_k is a GNT.

Here, it is useful to mention that for ABCs, we can always change the sign of the parity operator, Z^c in the auxiliary space without modifying the state. This is because Z does not enter into the trace defining the fMPS coefficients (26) and, if $ZA^i = (-1)^{|i|} A^i Z$, we also have $\tilde{Z}A^i = (-1)^{|i|} A^i \tilde{Z}$ with $\tilde{Z} = -Z$. Furthermore, if \mathcal{A} is in GCF, we have the freedom to changing the sign of the parity for each graded normal block independently, without modifying the state.

The GCF is discussed in detail in appendix D, where it is shown that, in the case of ABCs, it is possible to derive a series of results that nontrivially generalize those for the CF of MPSs. In particular, we prove the following fundamental theorems.

Theorem 6.4. *After blocking, for any even tensor, \mathcal{A} , it is always possible to obtain another even tensor, \mathcal{A}_{GCF} , in GCF and generating the same fMPS with ABCs.*

Theorem 6.5. *Consider two (even) tensors \mathcal{A} and \mathcal{B} in GCF, with diagonal parity operators in the auxiliary space Z_a, Z_b . If they generate the same fMPS with ABCs for all N then: (i) the dimensions of the matrices A^i and B^i coincide; (ii) there exists an invertible matrix X , and a permutation matrix Π such that $A^i = X\Pi B^i \Pi^{-1} X^{-1}$, and $[X, Z_a] = 0$.*

6.1. Type-I and type-II generalized fMPUs

The definition of GNTs gives us a hint of the reason why fMPUs of the form (36) and (37) are not enough to capture all fQCA. In the case of PBCs, for instance, one can see from equation (59) that a degenerate normal tensor yields vanishing coefficients when plugged into equation (36). On the other hand, the additional operator S in the definition (56) allows us to ‘close the trace’ in such a way that degenerate normal tensors give non-vanishing contributions. In fact, this is exactly what happens for the Majorana-shift operator (54).

Motivated by this discussion, we define two special classes of generalized fMPUs. These provide a ‘minimal’ subset of the operators (56) which allow for both degenerate and non-degenerate normal tensors. In particular, for PBCs, we say that $U^{(N)}$ is a generalized fMPU of the first kind (or type I) if it can be cast in the form (56) with $S = e^{i\alpha} Z$, while it is of the second kind (or type II) if

$$S = \frac{e^{i\alpha}}{\sqrt{2}} \sigma^x \otimes \mathbb{1} \quad \text{and} \quad U^{m,n} = (\sigma^x)^{|n|+|m|} \otimes N^{n,m}, \tag{60}$$

for $\alpha \in \mathbb{R}$ and arbitrary $N^{n,m}$, and with a parity operator $Z = \sigma^z \otimes \mathbb{1}$. Analogously, for ABCs, we say that $U^{(N)}$ is a generalized fMPU of the first kind if it can be cast in the form (56) with $S = e^{i\alpha} \mathbb{1}$, while it is of the second kind if

$$S = \frac{e^{i\alpha}}{\sqrt{2}} \mathbb{1} \quad \text{and} \quad U^{m,n} = (\sigma^x)^{|n|+|m|} \otimes N^{n,m}, \tag{61}$$

for $\alpha \in \mathbb{R}$ and arbitrary $N^{n,m}$, and with a parity operator $Z = \sigma^z \otimes \mathbb{1}$. We note that, for fMPUs of the second kind, the boundary tensors bear a normalization constant $1/\sqrt{2}$, which takes into account the fact that degenerate normal tensors have two eigenvalues equal to one.

We are now in a position to address the relation between fMPUs and QCA. At this point, it is convenient to distinguish between PBCs and ABCs, since the emerging picture is quite different.

6.2. FMPUs and QCA: antiperiodic boundary conditions

We begin our discussion with the case of ABCs, where a quite strong statement holds: namely, all type-I and type-II fMPUs introduced in section 6.1 are 1D fQCA and vice versa. This section is devoted to establishing this equivalence. For clarity, we will report here only the main statements, while we refer the reader to appendix E for all the technical proofs. As a first step, it is useful to characterize the GCF for tensors generating type-I and type-II fMPUs.

Proposition 6.6. *Let \mathcal{U} be in GCF, and suppose \mathcal{U} generates a type-I (type-II) fMPU $U^{(N)}$ with ABCs. Then, \mathcal{U}/\sqrt{d} is graded normal non-degenerate (degenerate).*

We report the proof in appendix E. This proposition is a direct generalization of the one given in [33] for MPUs in qudit systems. In fact, one could push the analogy further, and show that, after blocking, any tensor \mathcal{U} generating a type-I or type-II fMPU is *simple*, where one also needs to generalize the notion of simplicity as follows:

Definition 6.7. We say that an even tensor \mathcal{U} with a TM $E_{\mathcal{U}}$ is simple if

$$\text{Diagram (62a)} \tag{62a}$$

$$\text{Diagram (62b)} \tag{62b}$$

and $E_{\mathcal{U}}^2 = E_{\mathcal{U}}$, where we denote the TM $E_{\mathcal{U}}$ by a square, and where we use the graphical notation explained in appendix A.2 for fermionic TNs.

Note that for type-I fMPUs, this condition coincides with equation (15) because, after blocking, the TM reads $E = |r\rangle\langle l|$, where $|l\rangle, |r\rangle$ are the left and right eigenvectors associated with the eigenvalue 1. However, for type-II fMPUs the simplicity condition is different, because the TM has two eigenvectors associated with 1. In appendix E, we prove the following.

Proposition 6.8. *Suppose that the tensor \mathcal{U} generates a type-I (type-II) fMPU $U^{(N)}$ with ABCs. Then, there exists a $k \leq D^4$ such that \mathcal{U}_k is simple (according to definition 6.7).*

Given a tensor \mathcal{U} , the simplicity condition VI.7 clearly implies that $U^{(N)}$ is locality-preserving. In order to establish an equivalence between fMPUs and fQCA, it remains to be shown that the latter can always be represented as a type-I or type-II fMPU. This is proved in appendix E, and we arrive at the main result of this section.

Proposition 6.9. *Up to appending inert ancillary fermionic d.o.f., any type-I or type-II fMPU with ABCs is a 1D fermionic quantum cellular automaton and vice versa.*

6.3. FMPUs and QCA: periodic boundary conditions

As we have seen in section 5.1, fMPUs with PBCs are not necessarily locality-preserving and in this case, we need to impose further conditions on the tensors. An important point is that any tensor \mathcal{U} (in GCF) generating a type-I or type-II fMPU with ABCs also generates one in the periodic case. Indeed, let \mathcal{U} be a non-degenerate normal tensor generating a type-I fMPU $U_A^{(N)}$ with ABCs. Then, by blocking a finite number of times, we can assume that it is simple. Let $U_P^{(N)}$ be the fMPU with PBCs, obtained by inserting the operator Z into the trace. In order to show that $U_P^{(N)}$ is unitary, we can apply the simplicity condition to $U_P^{(N)\dagger}U_P^{(N)}$, and obtain

$$U_P^{(N)\dagger}U_P^{(N)} = \begin{array}{c} \blacksquare \bullet \\ \blacksquare \circ \\ \hline \blacksquare \bullet \\ \blacksquare \circ \end{array} \begin{array}{c} \hline \hline \hline \hline \end{array} \begin{array}{c} \bullet \\ \circ \end{array}, \tag{63}$$

where we denote the parity operator, Z , by a small black box. Now, because each tensor is even, and $Z^2 = \mathbb{1}$, we have

$$\begin{array}{c} \blacksquare \bullet \\ \blacksquare \circ \end{array} = \begin{array}{c} \bullet \blacksquare \\ \circ \blacksquare \end{array}. \tag{64}$$

Finally, as is shown in appendix E, for a normal non-degenerate tensor, the right eigenvector associated with the eigenvalue 1 of the TM E is even, which implies $(Z \otimes Z)E_{\mathcal{U}} = E_{\mathcal{U}}$. Thus, since $Z^2 = \mathbb{1}$, we have $U_P^{(N)\dagger}U_P^{(N)} = \mathbb{1}$. In a similar way, one can show that if \mathcal{U} is a normal degenerate tensor generating a type-II fMPU with ABCs, then it also generates a type-II fMPU in the periodic case. To see this, one has to use the fact that $X = \sigma^x \otimes \mathbb{1}$ commutes with $U^{i,j} = (\sigma^x)^{|i|+|j|} \otimes N^{i,j}$ for all i, j , and that $(X \otimes X)E_{\mathcal{U}} = E_{\mathcal{U}}$, which follows from the properties of the TM $E_{\mathcal{U}}$ associated with a graded normal degenerate tensor, cf appendix E.

The above discussion, together with the results of the previous subsection, tells us that any fQCA can be represented as an fMPU with PBCs. It also allows us to identify which properties we need to require in order for periodic fMPUs to be locality-preserving. In particular, if $U^{(N)}$ is a type-I fMPU, then we require that the corresponding tensor \mathcal{U} is simple, and that $(Z \otimes Z)E_{\mathcal{U}} = E_{\mathcal{U}}$, while if $U^{(N)}$ is a type-II fMPU, we require that $(X \otimes X)E_{\mathcal{U}} = E_{\mathcal{U}}$ (in addition to the simplicity condition). With these additional constraints, we finally have an identification between fMPUs and fQCA in the case of PBCs. We can summarize the results of this section in the following theorem.

Theorem 6.10. *Up to appending an inert ancillary fermionic d.o.f., any fQCA can be represented as an fMPU of type I or type II with either PBCs or ABCs. Furthermore*

- (a) *any type-I or type-II fMPU with ABC is necessarily a fermionic quantum cellular automaton;*
- (b) *any type-I fMPU with PBC is a fermionic quantum cellular automaton if it is generated by a simple tensor \mathcal{U} , and the TM $E_{\mathcal{U}}$ satisfies $(Z \otimes Z)E_{\mathcal{U}} = E_{\mathcal{U}}$, $\text{tr}(E_{\mathcal{U}}) = 1$;*

(c) any type-II fMPU with PBC is a fermionic quantum cellular automaton if it is generated by a simple tensor \mathcal{U} , and the TM $E_{\mathcal{U}}$ satisfies $(X \otimes X)E_{\mathcal{U}} = E_{\mathcal{U}}$, $\text{tr}(E_{\mathcal{U}}) = 2$.

Note that the fMPU discussed in section 5.1 is not simple, and, accordingly, is not locality-preserving.

7. Index theory for generalized fMPUs

In this section, we finally discuss how to extract an index to classify the locality-preserving fMPUs defined in section 6.1, thus recovering the results recently derived in [46], where the GNVW index [43] was generalized to the case of fermionic systems. Our logic is very similar to the one employed in [33], but there are non-trivial practical differences, due once again to the fermionic nature of the elementary d.o.f.

First of all, we recall the definition of the index for qudits. Let \mathcal{U} be a tensor generating an MPU, and we denote the corresponding elements using $U_{\alpha,\beta}^{n,m}$. One can define two maps $\mathcal{M}_{1,2}: \mathbb{C}^d \otimes \mathbb{C}^D \rightarrow \mathbb{C}^d \otimes \mathbb{C}^D$, as

$$\mathcal{M}_1: |m\rangle \otimes |\alpha\rangle \mapsto U_{\alpha,\beta}^{n,m} |n\rangle \otimes |\beta\rangle, \quad (65a)$$

$$\mathcal{M}_2: |m\rangle \otimes |\beta\rangle \mapsto U_{\alpha,\beta}^{n,m} |n\rangle \otimes |\alpha\rangle. \quad (65b)$$

Denoting the rank of these maps by r , and ℓ , respectively, the MPU index was defined in [33] as $\text{ind} = (1/2)[\log_2(r) - \log_2(\ell)]$, where it was also shown to coincide with the index first introduced in [43].

Let us now consider the fermionic case. First of all, we need to consider only the class of locality-preserving fMPUs, namely tensors \mathcal{U} that become simple after blocking for a sufficient number of times. Now, if \mathcal{U} is an even tensor, with elements denoted again by $U_{\alpha,\beta}^{n,m}$, generating a type-I or type-II fMPU, one could be tempted to define the index as is defined for qudits, in terms of the maps $\mathcal{M}_{1,2}$ introduced above. However, this turns out *not* to be a valid definition for the fermionic index. In order to see the reason why not, consider a depth-two quantum circuit, with an elementary two-site gate defined by

$$U_{j,j+1} = \frac{1}{\sqrt{2}} (\mathbb{1} - Y_j X_{j+1}), \quad (66)$$

with $Y_j = -i(a_j - a_j^\dagger)$, $X_j = (a_j + a_j^\dagger)$. It is straightforward to construct the corresponding fMPU, which is characterized by local and physical dimensions $d = D = 2$. The associated tensor \mathcal{U} is normal, non-degenerate and simple. However, one can see that a definition based on equation (65) would yield a non-vanishing index, which is the wrong result for a quantum circuit (cf [46]). Furthermore, we note that blocking does not remedy this problem⁷.

In fact, it turns out that the construction for qudits must be modified by introducing additional signs in the definition of the maps $\mathcal{M}_{1,2}$. In particular, in the fermionic case,

⁷Importantly, we recall that in order to obtain the blocked tensors of fMPOs, one needs to introduce additional signs, as specified by equation (A37). These signs are crucial, since in general they modify the ranks of the operators defined when discussing the fermionic index.

we define

$$\mathcal{M}_1^f : |m\rangle \otimes |\alpha\rangle \mapsto (-1)^{|n||m|} U_{\alpha,\beta}^{n,m} |n\rangle \otimes |\beta\rangle, \quad (67a)$$

$$\mathcal{M}_2^f : |m\rangle \otimes |\beta\rangle \mapsto U_{\alpha,\beta}^{n,m} |n\rangle \otimes |\alpha\rangle. \quad (67b)$$

where the label f , specifying that we are dealing with the fermionic case, will be omitted when it does not generate confusion. We are now in a position to define the fermionic index.

Definition 7.1. Let \mathcal{U} be a tensor in GCF generating a type-I or type-II locality-preserving fMPU. Take k such that the blocked tensor \mathcal{U}_k is simple, and define r, ℓ as the ranks of the maps $\mathcal{M}_1^f, \mathcal{M}_2^f$ in equation (67), respectively. The (fermionic) index of \mathcal{U} is defined as $\text{ind}_f = (1/2)(\log_2(r) - \log_2(\ell))$, while we denote the exponentiated index using $\mathcal{I}_f = \sqrt{r/\ell}$.

For clarity, we first state our main result for the fermionic index, which will be proved in the rest of this technical section.

Theorem 7.1 (fermionic index theorem). *Let \mathcal{U} be an even tensor in GCF generating a locality-preserving fMPU. Then:*

- (a) *the exponentiated index \mathcal{I}_f is a rational number for type-I fMPUs, while $\mathcal{I}_f = \sqrt{2}(p/q)$ for type-II fMPUs, with $p, q \in \mathbb{N}$ and coprime;*
- (b) *the index does not change by blocking;*
- (c) *the index is additive by tensoring and composition;*
- (d) *the index is robust, i.e. by continuously changing \mathcal{U} (and remaining in the class of locality-preserving fMPUs), one cannot change it;*
- (e) *two tensors have the same index iff they are equivalent.*

Here, we have introduced the notion of equivalence, which will be defined in a precise way later on. Loosely speaking, two tensors are equivalent if they can be transformed continuously into one another, by blocking and attaching ancillas, respectively. The proof of theorem 7.1 is carried out in the rest of this section, which represents the most technical part of our work. While one could carry out the discussion using the fiducial-state formalism employed so far, the notation becomes significantly simpler when the language of graded TNS is exploited, as recently developed in [53, 59]. The latter is reviewed in appendix B, where it is shown to be in one-to-one correspondence with the fiducial-state formalism.

Finally, from now on, we will focus on the case of ABCs, where any generalized fMPU is guaranteed to be locality-preserving. On the technical level, this allows us to exploit the uniqueness of the GCF (cf appendix D), which is needed in order to carry out some proofs, and to exclude *a priori* the possibility of non-locality-preserving fMPUs. We stress, however, that this is not a restriction, because we have shown in the previous section that tensors generating locality-preserving fMPUs in the periodic case, are also fMPUs with ABCs.

7.1. Standard form for type-I fMPUs

We begin by showing that any type-I fMPU admits a standard form, analogous to the form of the qudit MPUs defined in [33]. Unless specified otherwise, in the rest of this section we will assume that \mathcal{U}/\sqrt{d} is graded, normal, and non-degenerate, where the left and right eigenvectors of the TM $E_{\mathcal{U}}$ corresponding to the eigenvalue 1, $(\Phi|$ and $|\rho\rangle$, are of the form

$$\langle \Phi| = \sum_{n=1}^D (n, n|, \tag{68a}$$

$$|\rho\rangle = \sum_{n=1}^D \rho_n |n, n\rangle. \tag{68b}$$

This can be done without loss of generality, as it follows from the results in appendices D and E.

We recall that, in the graded TN formalism (cf appendix B), a given local tensor \mathcal{U} is represented as

$$\mathcal{U} = \sum_{n,m,\alpha,\beta} U_{\alpha,\beta}^{n,m} |\alpha\rangle|n\rangle\langle m|(\beta| = \alpha \text{---} \bigcirc \text{---} \beta \begin{matrix} | \\ n \\ | \\ m \\ | \end{matrix}, \tag{69}$$

where $|\alpha\rangle|n\rangle\langle m|(\beta|$ is a shorthand notation for $|\alpha\rangle \otimes_{\mathfrak{g}} |n\rangle \otimes_{\mathfrak{g}} \langle m| \otimes_{\mathfrak{g}} (\beta|$, and $\otimes_{\mathfrak{g}}$ is the graded tensor product. Analogously, the tensor $\bar{\mathcal{U}}$ generating the conjugate transposed operator, reads

$$\bar{\mathcal{U}} = \sum_{n,m,\alpha,\beta} (-1)^{|\beta|+|\alpha||\beta|} (\bar{U}_{\alpha,\beta}^{n,m} |\alpha\rangle|n\rangle\langle m|(\beta|. \tag{70}$$

By simply using the contraction rules for graded TNs explained in appendix B, one could immediately write down the transfer operator

$$\mathbb{E}_{\mathcal{U}} = \frac{1}{d} \sum_{j,k} \bar{U}_{\gamma,\delta}^{j,k} U_{\alpha,\beta}^{j,k} |\alpha\rangle|\gamma\rangle(\delta|(\beta|, \tag{71}$$

where the repeated indices are summed over. Note that the order of the bra and ket vectors on the right-hand side is important.

Following [33], we now consider two different singular value decompositions of \mathcal{U} . Since this requires us to rearrange its indices, this procedure introduces additional non-trivial signs w.r.t. the qudit case, as we now explain. Our goal is to rewrite

$$\alpha \text{---} \bigcirc \text{---} \beta \begin{matrix} | \\ n \\ | \\ m \\ | \end{matrix} = \alpha \text{---} \begin{matrix} | \\ n \\ | \\ r \\ | \\ m \end{matrix} \text{---} \beta = \alpha \text{---} \begin{matrix} | \\ n \\ | \\ \ell \\ | \\ m \end{matrix} \text{---} \beta. \tag{72}$$

Importantly, every diagram here corresponds to an *even*-graded tensor. Specifically, we define

$$\mathcal{X}_1 = \begin{array}{c} n \\ | \\ \diagdown \quad \beta \\ | \\ \vdots \\ i \end{array} = X_1^{n,\beta,i} |n\rangle \langle \beta| \langle i|, \tag{73a}$$

$$\mathcal{Y}_1 = \alpha \begin{array}{c} \vdots \\ i \\ | \\ \diagup \\ | \\ m \end{array} = Y_1^{i,\alpha,m} |i\rangle \langle \alpha| \langle m|, \tag{73b}$$

$$\mathcal{X}_2 = \alpha \begin{array}{c} n \\ | \\ \diagdown \quad i \\ | \\ i \end{array} = X_2^{\alpha,n,i} |\alpha\rangle \langle n| \langle i|, \tag{73c}$$

$$\mathcal{Y}_2 = \begin{array}{c} i \\ | \\ \diagup \quad \beta \\ | \\ m \end{array} = Y_2^{i,m,\beta} |i\rangle \langle m| \langle \beta|. \tag{73d}$$

We show that we can always decompose \mathcal{U} as in equation (72), with $\mathcal{X}_i, \mathcal{Y}_i$ even tensors. First, we note that \mathcal{U} defines the linear function

$$|\beta\rangle \otimes_{\mathfrak{g}} |m\rangle \mapsto \mathcal{C}(\mathcal{U}|\beta\rangle \otimes_{\mathfrak{g}} |m\rangle) = U_{\alpha,\beta}^{n,m} |\alpha\rangle \otimes_{\mathfrak{g}} |n\rangle, \tag{74}$$

where \mathcal{C} is the contraction map introduced in appendix B. This map can be represented as a matrix, \mathcal{M}_2^f , with elements $U_{\alpha,\beta}^{n,m}$. Using a singular value decomposition, we can write

$$\mathcal{M}_2^f = V_2^\dagger D_2 W_2, \tag{75}$$

where V_2, W_2 are isometries, fulfilling $V_2 V_2^\dagger = W_2 W_2^\dagger = \mathbb{1}$, while D_2 is a diagonal positive matrix of dimension ℓ . Crucially, we can choose these matrices to be even, when they are seen as operators acting on graded spaces. Indeed, let us consider the matrix \mathcal{M}_2^f in the basis associated with the elements $U_{\alpha,\beta}^{n,m}$. We reorder the basis vectors, in such a way that the even vectors come first. Since \mathcal{U} is even, \mathcal{M}_2^f is now a block diagonal, with two blocks corresponding to the even and odd subspaces, respectively. We can then apply a singular value decomposition to each block individually, yielding isometries $V_2^{e,o}, W_2^{e,o}$ and diagonal matrices $D_2^{e,o}$. The desired decomposition in terms of even matrices is simply obtained by choosing $V_2 = V_2^e \oplus V_2^o, W_2 = W_2^e \oplus W_2^o$ and $D_2 = D_2^e \oplus D_2^o$. Next, defining the matrices $X_2 = V_2^\dagger$ and $Y_2 = D_2 W_2$, we have

$$\mathcal{U} = \mathcal{X}_2 \mathcal{Y}_2, \tag{76}$$

where appropriate contractions are implied. Since the matrices X_2, Y_2 are even, $\mathcal{X}_2, \mathcal{Y}_2$ are even-graded tensors, and the second decomposition in equation (72) is established.

The first decomposition in equation (72) can be derived in a similar way, but we need to be careful with the signs arising from the reordering of the graded tensors. Rewriting

$$\mathcal{U} = (-1)^{|n||m|+|\alpha|+|m|} U_{\alpha,\beta}^{n,m} |n\rangle \langle \beta| \otimes_{\mathfrak{g}} |\alpha\rangle \langle m|, \tag{77}$$

we see that, in order to arrive at a decomposition of the form $\mathcal{U} = \mathcal{X}_1 \mathcal{Y}_1$, with $\mathcal{X}_1, \mathcal{Y}_1$ as in equations (73a) and (73b), we need to apply a singular value decomposition to the matrix \mathcal{M}_1^f with elements $(-1)^{|n||m|+|\alpha|+|m|} U_{\alpha,\beta}^{n,m}$. Once again, this can be done by choosing even matrices, so that $\mathcal{M}_1^f = V_1^\dagger D_1 W_1$, where V_1, W_1 are isometries, and D_1 is a diagonal positive matrix of dimension r . Now we choose $X_1 = V_1^\dagger [V_1 (\mathbb{1} \otimes \rho) V_1^\dagger]^{-1/2}$, so that

$$X_1^\dagger (\mathbb{1} \otimes \rho) X_1 = \mathbb{1}, \tag{78}$$

where ρ is the positive matrix corresponding to the right eigenstate (68b). Since all the matrices involved are even, X_1 is also even, and similarly for $Y_1 = [V_1 (\mathbb{1} \otimes \rho) V_1^\dagger]^{1/2} D_1 W_1$. Thus, we have established the first decomposition in equation (72).

Importantly, the dimensions of the diagonal matrices $D_{1,2}$ introduced above, r and ℓ , coincide, by construction, with the ranks of the maps $\mathcal{M}_{1,2}^f$ in equation (67). For the map in equation (77), this follows from the fact that the factor $(-1)^{|\alpha|+|m|}$ clearly does not change the rank, r . Next, in terms of the previous decomposition, we introduce



$$u = \text{diagram}, \tag{79a}$$



$$v = \text{diagram}, \tag{79b}$$

where, as usual, joined legs denote the contraction of the corresponding graded spaces. Following [33], we can now prove two important statements

Lemma 7.2. *For any tensor \mathcal{U} , $u^\dagger u = \mathbb{1}$ and hence $r\ell \geq d^2$.*

Proof. The proof follows the same steps as given for lemma III.7 in [33]. We present it for completeness here, to show how to deal with the additional fermionic signs. First, we have



$$\text{diagram} = \text{vertical line}, \tag{80}$$

which follows from the fact that $U^{(N)}$ is unitary for all N . Given the order of bra and ket states in equation (71), the left eigenstate is

$$\left(\begin{array}{c} \alpha \\ \beta \end{array} \right) = \sum_{\alpha,\beta} \delta_{\alpha,\beta} \langle \alpha | \otimes_{\mathfrak{g}} \langle \beta |, \tag{81}$$

while the right eigenstate is

$$\left(\begin{array}{c} \alpha \\ \beta \end{array} \right) \rho = \sum_{\alpha,\beta} \delta_{\alpha,\beta} \rho_{\alpha} |\beta\rangle \otimes_{\mathfrak{g}} |\alpha\rangle, \tag{82}$$

where, once again, the order of the bra and ket states is important. With these definitions, we can explicitly perform the contractions on the left-hand side, keeping track of the signs as we move the ket and bra states close together. Note that this procedure is well-defined because all individual tensors have well-defined parity. Using $X_2^\dagger X_2 = \mathbb{1}$ and equation (78), a direct calculation shows that the left-hand side is simply $u^\dagger u$, where u is the graded operator defined in equation (79). Thus, $u^\dagger u = \mathbb{1}$, and the statement is proved. \square

Note that this lemma implies that u is an isometry. Next, we can also prove the following proposition.

Proposition 7.3. *The following are equivalent for an even tensor \mathcal{U} generating an fMPU:*

- (a) \mathcal{U} is simple;
- (b) $rl = d^2$;
- (c) u is unitary;
- (d) v is unitary.

We omit the proof of this statement, because it follows the one presented in the reference without modification [33]. Note that this result allows us introduce a standard form for type-I fMPUs. In particular, by blocking a simple tensor twice, we have

$$\begin{array}{c} \circ \\ | \\ | \\ | \end{array} = \begin{array}{c} \begin{array}{c} \diagup \quad \diagdown \\ \diagdown \quad \diagup \end{array} \\ \boxed{u} \\ | \\ | \end{array}, \tag{83}$$

where u is unitary, and we use the notation introduced in equation (79) for the unitary v . As for the case of qudits [33], the standard form is essentially unique, up to single-site unitary invertible matrices acting on the legs defining u or v .

Proposition 7.4. *Two simple tensors, \mathcal{U} and \mathcal{W} with standard forms*

$$\mathcal{U} = \begin{array}{c} \begin{array}{c} \diagup \quad \diagdown \\ \diagdown \quad \diagup \end{array} \\ \boxed{u} \\ | \\ | \end{array}, \quad \mathcal{W} = \begin{array}{c} \begin{array}{c} \diagdown \quad \diagup \\ \diagup \quad \diagdown \end{array} \\ \boxed{w} \\ | \\ | \end{array}, \tag{84}$$

generate the same type-I fMPU, i.e. $U^{(N)} = V^{(N)}$ for all N , iff even unitaries x, y and z exist, such that

$$\begin{array}{c} | \\ \vdots \\ \boxed{w} \\ | \\ | \end{array} = \begin{array}{c} \boxed{x} \quad \boxed{y} \\ \vdots \\ \boxed{u} \\ | \\ | \end{array}, \tag{85a}$$

$$\begin{array}{c} \begin{array}{c} \diagdown \quad \diagup \\ \diagup \quad \diagdown \end{array} \\ | \\ \vdots \end{array} = \begin{array}{c} \boxed{z} \\ \begin{array}{c} \diagdown \quad \diagup \\ \diagup \quad \diagdown \end{array} \\ \boxed{x^\dagger} \end{array}, \quad \begin{array}{c} \begin{array}{c} \diagup \quad \diagdown \\ \diagdown \quad \diagup \end{array} \\ | \\ \vdots \end{array} = \begin{array}{c} \boxed{z^\dagger} \\ \begin{array}{c} \diagup \quad \diagdown \\ \diagdown \quad \diagup \end{array} \\ \boxed{y^\dagger} \end{array}. \tag{85b}$$

7.2. Standard form for type-II fMPUs

Let us now consider a type-II fMPU $U^{(N)}$, generated by a graded degenerate normal tensor \mathcal{U} . It follows from corollary E.3 in appendix E that the local graded space \mathcal{H}_j has even dimensions d , with even and odd subspaces of the same dimension, $d_e = d_o = d/2$. Hence, we can assume without loss of generality that $\mathcal{H}_j \simeq \mathcal{H}_j^1 \otimes_{\mathfrak{g}} \mathcal{H}_j^2$, with $\dim(\mathcal{H}_j^2) = d/2$ while $\mathcal{H}_j^1 \simeq \mathbb{C}^{\uparrow 1}$, namely \mathcal{H}_j^1 is isomorphic to the 2D complex coordinate space with parity operator $\mathcal{P} = \text{diag}(1, -1)$. We can then introduce a type-II fMPU $M_A^{(N)}$ implementing a Majorana translation (defined in equation (52)) on the local spaces \mathcal{H}_j^1 , and acting as the identity on \mathcal{H}_j^2 . Finally, we define

$$\tilde{U}^{(N)} = U^{(N)} M_A^{(N)\dagger}, \tag{86}$$

which is clearly a unitary operator for all N . Now, $\tilde{U}^{(N)}$ is the product of two type-II fMPUs, so that it follows from proposition E.4 that it can be represented as a type-I fMPU, generated by a graded normal non-degenerate tensor $\tilde{\mathcal{U}}$. Inverting the above relation, we get the following form for type-II fMPUs

$$U^{(N)} = \tilde{U}^{(N)} M_A^{(N)}. \tag{87}$$

By blocking for a sufficient number of times, the tensor $\tilde{\mathcal{U}}$ becomes simple and we can cast it in standard form. This gives us a standard form for the tensor \mathcal{U} itself and, due to proposition 7.4, this is also unique up to single-site (even) invertible matrices. Note, however, that the tensor \mathcal{U} obtained by composing $\tilde{\mathcal{U}}$ and \mathcal{M} , corresponding to the Majorana shift, is not necessarily in GCF.

7.3. Index

Based on the constructions carried out so far, we are now in a position to prove theorem 7.1, which is the main result of this section. Before doing so, however, we need to precisely state the definition of equivalent graded tensors. Let us consider two even tensors, \mathcal{U} and \mathcal{V} generating fMPUs, of physical dimensions $d_{a,b}$ (with even/odd subspaces $d_{a,b}^{e/o}$), and let us denote two coprimes by $p_{a,b}$, such that $p_a d_a = p_b d_b$. We also denote by $\mathbb{1}_x$ the identity operator acting on a (graded Hilbert) space of dimension x , and by $\mathcal{U}^{(x)} = \mathcal{U} \otimes_{\mathfrak{g}} \mathbb{1}_x$, i.e. the tensor generating the fMPU $U^{(N)} \otimes_{\mathfrak{g}} \mathbb{1}_x^{\otimes N}$.

Definition 7.5. Two even tensors \mathcal{U} and \mathcal{V} , with auxiliary parity operators Z_U, Z_V and in GCF are strictly equivalent if $d_a^{e/o} = d_b^{e/o}$ and there exists a continuous path $\mathcal{W}(p)$ of even tensors with respect to parity $Z_{\mathcal{W}}(p)$, not necessarily in GCF, with $p \in [0, 1]$ such that $\mathcal{W}(0) = \mathcal{U}$, $\mathcal{W}(1) = \mathcal{V}$, and $Z_{\mathcal{W}}(0) = Z_U$, $Z_{\mathcal{W}}(1) = Z_V$.

Definition 7.6. Two even tensors \mathcal{U} and \mathcal{V} are equivalent if $k, p_a, p_b \in \mathbb{N}$ exist, such that $\mathcal{U}_k^{(p_a)}$ and $\mathcal{V}_k^{(p_b)}$ are strictly equivalent.

Here, it is important to stress that in the above definitions we allow for the ancilla to be a graded space where the dimensions of the even and odd subspaces are arbitrary.

As we have seen in section 7.1, type-I fMPUs admit the same kind of standard form as qudit MPUs. For this reason, their indices can be analyzed in the exact same way as

shown in [33]. In particular, following the same steps therein, the properties of stability of the index for type-I fMPUs can be established without additional difficulties. Then, one arrives at the following result, for which we omit the proof (since, once again, it is completely analogous to the one for qudit MPUs).

Proposition 7.7. *For type-I fMPUs the exponentiated index \mathcal{I}_f is a rational number, and*

- (a) *the index does not change by blocking; furthermore, if k is such that \mathcal{U}_k is simple and $q > k$, then $r_q = r_k d^{q-k}$, $\ell_q = \ell_k d^{q-k}$, where $r_{k,q}$, $\ell_{k,q}$ are the right and left ranks of $\mathcal{U}_{k,q}$, while d is the local physical dimension;*
- (b) *the index is additive by tensoring and composition;*
- (c) *the index is robust, i.e. by changing \mathcal{U} continuously, one cannot change it;*
- (d) *two tensors have the same index iff they are equivalent.*

Even though the proof of the above proposition is the same for fermions and qudits, it is useful to stress one difference between the two cases, which was already pointed out in [46]. Let us consider two even simple tensors $\mathcal{U}_A, \mathcal{U}_B$ generating type-I fMPUs, and suppose that they both have an index of 0, with the same local dimension, d . Both fMPUs admit a standard form in terms of the unitaries $u_{A,B}, v_{A,B}$ introduced in equation (79), and since both tensors have vanishing indices all input and output legs are associated with the same dimension, d . Now, in the case of qudits, this would imply that a continuous path of unitaries exists, connecting u_A, v_A with u_B, v_B . However, this is not always true for fermions, if we also require that all unitaries have well-defined parity, because graded spaces of the same dimension are not necessarily isomorphic. Specifically, using $\mathcal{H}_j^A, \mathcal{H}_j^B$ to denote the local spaces associated with the output of u_A, u_B in the above example, we can only conclude that $\mathcal{H}_j^A \simeq \mathbb{C}^{p_A|q_A}$, $\mathcal{H}_j^B \simeq \mathbb{C}^{p_B|q_B}$ with $p_A + q_A = p_B + q_B = d$. At this point, however, a continuous path of even unitaries can always be constructed by appending an ancillary space $\tilde{\mathcal{H}}_j \simeq \mathbb{C}^{1|1}$, since $\mathcal{H}_j^{A,B} \otimes_{\mathfrak{g}} \tilde{\mathcal{H}}_j \simeq \mathbb{C}^{\tilde{p}_{A,B}|\tilde{q}_{A,B}}$ and $\tilde{p}_A = \tilde{q}_A = \tilde{p}_B = \tilde{q}_B = d$.

Next, in order to complete the proof of theorem 7.1, we analyze the index for type-II fMPUs. In fact, this can be done quite easily based on their standard form introduced in section 7.2. However, at this point we need two additional lemmas, that are proved in the following.

Lemma 7.8. *Let \mathcal{M} be the tensor associated with the Majorana shift (53), and consider $\mathcal{M}^{(x)} = \mathcal{M} \otimes_{\mathfrak{g}} \mathbb{1}_x$. Using $d = 2x$ to denote the dimension of the associated physical local space, the right and left ranks for the tensor $\mathcal{M}_k^{(x)}$, obtained by blocking k times, are $r_k = 2d^k$, $\ell_k = d^k$.*

Proof. Let us first consider the right rank r . Clearly, $\mathcal{M}^{(x)}$ and \mathcal{M} have the same bond dimension, and (normalized) TM $E_{\mathcal{M}}$. Now, recalling that for any operator A ,

$\text{rank}(A) = \text{rank}(A^\dagger A)$, we have

$$\text{rank} \left(\underbrace{\text{---} \circ \text{---} \text{---} \circ \text{---} \text{---}}_k \right) = \text{rank} \left(\underbrace{\begin{matrix} \bullet & \dots & \bullet \\ \text{---} \circ \text{---} & \dots & \text{---} \circ \text{---} \end{matrix}}_k \right), \tag{88}$$

where we separated input and output with a gray dotted line. Note that the pictures on both sides of this equation define linear maps on graded spaces, and the rank refers to these maps. Next, for the Majorana shift tensor $\mathcal{M}^{(x)}$, we have

$$\begin{matrix} \bullet & \bullet \\ \text{---} \circ \text{---} & \text{---} \circ \text{---} \\ \text{---} \circ \text{---} & \text{---} \circ \text{---} \end{matrix} = \begin{matrix} \bullet \\ \text{---} \circ \text{---} \\ \text{---} \circ \text{---} \end{matrix} \Big| . \tag{89}$$

Here, we used the fact that the identity operator corresponds to the even eigenstate of the TM with an eigenvalue of 1, while σ^x corresponds to the odd eigenstate with the same eigenvalue, and

$$\begin{matrix} \bullet \\ \sigma^x \\ \text{---} \circ \text{---} \\ \text{---} \circ \text{---} \end{matrix} = 0. \tag{90}$$

Using the simplicity condition, we can simplify the right-hand side of equation (88) by iterating equation (89) $k - 1$ times. In the resulting diagram, we have $k - 1$ identities, whereas in the leftmost site we have the same tensor appearing on the left of the right-hand side of equation (89). For this tensor, the rank can be computed directly, obtaining $2d$, which yields $r_k = 2d^k$. Applying a similar procedure for the left rank, we can also show that $\ell = d^k$, thus completing the proof. Note that it is crucial to keep track of the signs arising from rearranging the tensors in the different diagrams as they are contracted, since these are at the root of the difference between the right and left ranks. \square

Lemma 7.9. *Let $U^{(N)}$ be a type-II fMPU in the standard form (87), and use $\tilde{\mathcal{U}}, \mathcal{M}$ to denote the tensors in GCF associated with $\tilde{U}^{(N)}$ and $M_A^{(N)}$, respectively. \mathcal{U} defines the tensor obtained by composing $\tilde{\mathcal{U}}$ and \mathcal{M} , and let k be such that $\tilde{\mathcal{U}}_k$ is simple. Then, the exponentiated index for \mathcal{U}_q with $q \geq 2k$ is $\mathcal{I}_f = \sqrt{2} \tilde{\mathcal{I}}_f$, where $\tilde{\mathcal{I}}_f$ is the index of $\tilde{\mathcal{U}}_k$.*

Proof. We use d to denote the local physical dimension, and use the following notations for the tensors blocked k and $k' = q - k \geq k$ times (where k is such that \mathcal{U}_k is simple)

$$\tilde{\mathcal{U}}_k = \text{---} \square \text{---} , \quad \mathcal{M}_k = \text{---} \circ \text{---} , \tag{91a}$$

$$\tilde{\mathcal{U}}_{k'} = \text{---} \blacksquare \text{---} , \quad \mathcal{M}_{k'} = \text{---} \bullet \text{---} . \tag{91b}$$

Here, \mathcal{M}_k denotes the tensor obtained by blocking the tensor associated with the Majorana shift appearing in equation (87) k times. Finally, d_k denotes the physical

By now combining proposition 7.7 with lemma 7.9 it is straightforward to prove the following proposition:

Proposition 7.10. *For type-II fMPUs the exponentiated index is in the form $\mathcal{I}_f = \sqrt{2}(p/q)$, with $p, q \in \mathbb{N}$ and coprime. Furthermore*

- (a) *the index does not change by blocking;*
- (b) *the composition (or tensor product) of two type-II fMPUs is a type-I fMPU, and the index of the latter is obtained by summing the indices of the former two;*
- (c) *the index is robust, i.e. by continuously changing \mathcal{U} , one cannot change it;*
- (d) *two tensors have the same index iff they are equivalent.*

Note that in order to prove point 4, one needs to use the fact that if \mathcal{U} is a tensor generating an fMPU, then it can be deformed continuously to a tensor in GCF generating the same fMPU, which is easily proved based on the fact that \mathcal{U} has a single block in the GCF. Now, putting together propositions 7.7 and 7.10, we finally arrive at the statement of theorem 7.1, anticipated at the beginning of this section.

8. Conclusions

In this work, we have studied matrix product unitaries for fermionic 1D chains, and highlighted several qualitative differences with respect to the case of qudits. In particular, we have shown that (i) fMPUs are not necessarily locality-preserving and (ii) not all fQCA can be represented as standard fMPUs, with either PBCs or ABCs. Next, we have defined the class of generalized fMPUs, and identified a subset of the latter that are equivalent to the family of fQCA. Finally, we have shown how the index for fQCA [46] can be extracted directly from the tensors generating fMPUs. As a technical byproduct of our work, we have also introduced a GCF for fermionic MPSs, which might be useful for more general problems. Overall, our work shows that fMPUs display significantly richer features compared to the case of MPUs.

There are several interesting questions that remain open. For example, we have shown that fMPUs of the second kind are always generated by a tensor that is obtained by composing a Majorana shift and another tensor \mathcal{U} , generating an fMPU of the first kind, cf equation (87). However, one could wonder whether a more explicit standard form exists for GNTs generating type-II fMPUs, by analogy with equation (83) for type-I fMPUs.

Clearly, another natural question pertains to the classification of fMPUs in the presence of additional symmetries, which was recently addressed for the case of qudits [35]. While the tools introduced in this work allow us to tackle this problem, based on the case of qudits we expect that additional difficulties will arise, and we leave this question for future investigations.

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Appendix A. Fiducial-state formalism

A.1. General definitions

In this appendix, we develop a fiducial-state formalism for 1D fermionic systems, following the construction introduced in [52] for two spatial dimensions. The latter is a natural generalization to that carried out for qudits, and consists of performing a sequence of projections onto maximally entangled auxiliary fermionic modes. While in [51], this was done by associating each lattice site with two auxiliary real fermions, a slightly simpler formulation can be obtained by considering maximally entangled Majorana modes instead [52]. Here we follow the latter approach, which is detailed in the following.

As in the main text, we consider a chain of N sites labeled by $x = 1, \dots, N$. We associate each site with n_F fermionic modes with (physical) annihilation operators $a_{x,j}$. Furthermore, we introduce two sets of auxiliary Majorana operators $\{\ell_{x,\mu}\}$ and $\{r_{x,\mu}\}$ with $x = 1, \dots, N$, and $\mu = 1, \dots, N_F$, where N_F is some non-negative integer, while ℓ and r stand for left and right, respectively. The Majorana operators are self-adjoint and satisfy

$$\{r_{x,\mu}, \ell_{y,\nu}\} = 0, \tag{A1}$$

$$\{r_{x,\mu}, r_{y,\nu}\} = \{\ell_{x,\mu}, \ell_{y,\nu}\} = 2\delta_{x,y}\delta_{\mu,\nu}. \tag{A2}$$

As a starting point, we introduce the local fermionic tensors acting on one physical site, and two adjacent auxiliary Majorana modes:

$$F_x = \sum_{\alpha,\beta=0}^{D-1} \sum_{n=0}^{d-1} A_{\alpha,\beta}^n \ell_x^\alpha (a_x^\dagger)^n r_x^\beta \quad x = 1, \dots, N, \tag{A3}$$

where $A_{\alpha,\beta}^n$ are complex numbers, and $D = 2^{N_F}$, $d = 2^{n_F}$. Here, we have used the shorthand notation introduced in equation (17) for $(a_x^\dagger)^n$, and also

$$\ell_x^\alpha = \ell_{x,1}^{\alpha^{(1)}} \dots \ell_{x,N_F}^{\alpha^{(N_F)}}, \tag{A4}$$

$$r_x^\beta = r_{x,N_F}^{\beta^{(N_F)}} \dots r_{x,1}^{\beta^{(1)}}, \tag{A5}$$

where $(n^{(1)}, \dots, n^{(N_F)})$ is the binary representation of n , and analogously for α and β . Importantly, the order of the factors in the product of equation (A5) is reversed with respect to (A4). While this is just a convention, it simplifies some of the subsequent algebraic manipulations.

For our construction, it is crucial that F_x has a well-defined fermionic parity (with respect to all physical and auxiliary modes). As in the main text, we can define

$$|n| = \sum_{i=1}^{n_F} n^{(i)}, \quad |\alpha| = \sum_{j=1}^{N_F} \alpha^{(j)}, \quad |\beta| = \sum_{j=1}^{N_F} \beta^{(j)}. \quad (\text{A6})$$

Then, saying that F_x has well-defined fermionic parity means that $A_{\alpha,\beta}^n = 0$ if

$$|n| + |\alpha| + |\beta| \pmod{2} \quad (\text{A7})$$

is 1 or 0, depending on whether F_j is even or odd. As we have already mentioned in the main text, in the following we will always assume F_x to be even, which is not a restriction if we are allowed to perform blocking. Next, we introduce a projection onto the neighboring Majorana modes

$$\eta_{x,y} = \prod_{\mu=0}^{D-1} \eta_{x,y,\mu}, \quad (\text{A8})$$

where

$$\eta_{x,y,\mu} = \frac{1}{2} (1 + i r_{x,\mu} \ell_{y,\mu}). \quad (\text{A9})$$

We note that, after interacting with $\eta_{x,y,\mu}$, the Majorana fermions $r_{x,\mu}$, $\ell_{y,\mu}$ become maximally entangled, forming a pure fermionic state.

Now, an fMPS is obtained in two steps. First, we act on the fermionic vacuum (with respect to all modes) with the operators F_x , $x = 1, \dots, N$. Second, we ‘concatenate’ them by projecting neighboring Majorana modes onto maximally entangled pairs with $\eta_{x,y}$ [52]. Importantly, using this procedure we can generate fermionic states that are invariant under translation with either PBCs or ABCs. Let us consider the former case. Then, applying the prescription above, we obtain

$$|\Psi\rangle = \langle \eta_{N,1} \eta_{1,2} \dots \eta_{N-1,N} F_1 \dots F_N \rangle_a |\Omega\rangle. \quad (\text{A10})$$

Here, the expectation value is expressed with respect to the auxiliary vacuum $|\Omega_a\rangle$, defined by

$$(r_{x-1,\mu} - i \ell_{x,\mu}) |\Omega_a\rangle = 0, \quad (\text{A11})$$

while we use $|\Omega\rangle$ to denote the physical one, $a_x^n |\Omega\rangle = 0$ for $n \neq (0, \dots, 0)$. Since we always have an even number of auxiliary operators, we can associate a tensor product structure between the spaces of the real and auxiliary fermions, and the expression above is well defined.

It is not difficult to see that $|\Psi\rangle$ is invariant with respect to translations with PBCs, due to the presence of the projector $\eta_{N,1}$. If one is instead interested in the case of ABCs, it is sufficient to replace it with $\eta_{1,N}$. Since, for the sake of our present discussion, both types of boundary conditions can be treated analogously, in the following we only focus on the periodic case.

By taking the expectation value with respect to the auxiliary vacuum, one can cast the state (A10) into the form (20), where the coefficients are written as in equation (25). This can be seen as follows. We first rewrite equation (A10) as

$$|\Psi\rangle = A_{\alpha_1, \beta_1}^{n_1} \dots A_{\alpha_N, \beta_N}^{n_N} \langle \Omega_a | \eta_{N,1} \dots \eta_{N-1,N} \times \ell_1^{\alpha_1} \left(a_1^\dagger \right)^{n_1} r_1^{\beta_1} \dots \ell_N^{\alpha_N} \left(a_N^\dagger \right)^{n_N} r_N^{\beta_N} | \Omega_a \rangle \otimes | \Omega \rangle, \tag{A12}$$

where repeated indices are summed over. Moving $r_N^{\beta_N}$ to the left and using the anticommutation relations, we obtain

$$|\Psi\rangle = A_{\alpha_1, \beta_1}^{n_1} \dots A_{\alpha_N, \beta_N}^{n_N} \langle \Omega_a | \eta_{N,1} \dots \eta_{N-1,N} (-1)^{p|\beta_N|} \times r_N^{\beta_N} \ell_1^{\alpha_1} \left(a_1^\dagger \right)^{n_1} r_1^{\beta_1} \dots \ell_N^{\alpha_N} \left(a_N^\dagger \right)^{n_N} | \Omega_a \rangle \otimes | \Omega \rangle, \tag{A13}$$

where

$$p = \sum_{j=1}^N |n_j| + \sum_{j=1}^N |\alpha_j| + \sum_{j=1}^{N-1} |\beta_j| \pmod{2}. \tag{A14}$$

We can now move each $\eta_{j,j+1}$ to the right until it acts on $|\Omega\rangle$. This procedure yields zero unless $\beta_j = \alpha_{j+1}$ (with the identification $\alpha_{N+1} = \alpha_1$). Furthermore, for the non-vanishing terms, we have

$$(-1)^{p|\beta_N|} = (-1)^{|\alpha_1||\beta_N|} = (-1)^{|\alpha_1|}. \tag{A15}$$

Next, we can move each remaining product to the right $r_j^{\alpha_j} \ell_{j+1}^{\alpha_j}$, which gives $(-i)^{N_F}$ when acting on $|\Omega_a\rangle$. Finally, we can rearrange the product of the elements $A_{\alpha, \beta}^n$ into a trace over an auxiliary graded space, which is generated by the basis vectors $|\alpha\rangle$, with parity $|\alpha|$. Putting all this together, we get

$$|\Psi\rangle = (-i)^{N_{N_F}} \text{tr} \left[\tilde{Z} A^{n_1} \dots A^{n_N} \right] \left(a_1^\dagger \right)^{n_1} \dots \left(a_N^\dagger \right)^{n_N} | \Omega \rangle. \tag{A16}$$

Here \tilde{Z} is a diagonal matrix with entries $+1$ and -1 which acts as the parity operator on the auxiliary space. As a last step, we perform a gauge transformation corresponding to a reordering of the basis vectors, and absorbing the factor $(-i)^{N_{N_F}}$ into the matrices A^n we arrive at the form in equation (36). Note that the commutation relations (28) follow from the parity of the tensor F_x in equation (A3).

It is straightforward to extend this formalism to define fMPOs. In this case, we consider the same setting as that used for fMPSs, but the local tensors (A3) must be replaced by

$$G_x = \sum_{\alpha, \beta=0}^{D-1} \sum_{n, m=0}^{d-1} M_{\alpha, \beta}^{n, m} \ell_x^\alpha f_x^{n, m} r_x^\beta \quad x = 1, \dots, N, \tag{A17}$$

where $f^{n, m}$ are the fermionic operators introduced in equation (34). We can then define fMPOs as

$$M = \langle \eta_{N,1} \eta_{1,2} \dots \eta_{N-1,N} G_1 \dots G_N \rangle_a, \tag{A18}$$

where the expectation value is with respect to the auxiliary vacuum, as in equation (A10). Repeating the derivation above, it is straightforward to cast M as in equation (33), with the coefficients in the form (36).

A.2. Elementary operations with fMPOs

As for the case of qudits, one can see that the family of fMPOs is closed with respect to elementary operations such as sum, conjugate transposition or composition. However, some differences arise when computing the corresponding local tensors, as we now discuss. Let us first consider the case of the conjugate transposition of a given fMPO $U^{(N)}$. From equation (33), we have

$$[U^{(N)}]^\dagger = \sum_{\substack{n_1, \dots, n_N=0 \\ m_1, \dots, m_N=0}}^{d-1} \bar{c}_{m_1, \dots, m_N}^{n_1, \dots, n_N} [f_N^{n_N, m_N}]^\dagger \dots [f_1^{n_1, m_1}]^\dagger. \tag{A19}$$

We would like to rewrite this expression as in equation (33), with the coefficients $c_{m_1, \dots, m_N}^{n_1, \dots, n_N}$ in the form of (36) or (37). In fact, this can easily be done by making use of the identities

$$[f_j^{n, m}]^\dagger = f_j^{m, n}, \tag{A20a}$$

$$f_x^{m, n} f_y^{p, q} = (-1)^{(|p|+|q|)(|m|+|n|)} f_y^{p, q} f_x^{m, n}, \tag{A20b}$$

$$f_x^{m, n} f_x^{p, q} = \delta_{n, p} f_x^{m, q}, \tag{A20c}$$

which can be established by computing the matrix elements of both sides of the equations on basis (Fock) states. As a final result, we find that $[U^{(N)}]^\dagger$ is an fMPO with local tensors defined by⁸

$$\tilde{U}_{\alpha, \beta}^{i, j} = (-1)^{|\beta|+|\alpha||\beta|} \bar{U}_{\alpha, \beta}^{j i}, \tag{A21}$$

where, as usual, we use \bar{x} to denote the complex conjugate of $x \in \mathbb{C}$.

Next, let us consider two fMPOs $U^{(N)}$, $V^{(N)}$, and define $W^{(N)} = U^{(N)}V^{(N)}$. By exploiting the fiducial-state formalism, $W^{(N)}$ can again be written as an fMPO, where the local tensors are now defined by

$$W_{(\alpha, \gamma), (\beta, \delta)}^{k, i} = \sum_j (-1)^{|\gamma|(|k|+|j|)} U_{\alpha, \beta}^{k, j} V_{\gamma, \delta}^{j, i}. \tag{A22}$$

This formula is similar to the corresponding one for qudits, but additional signs appear. In order to prove equation (A22), it is convenient to exploit the fiducial-state representation (A18). Define

$$U^{(N)} = \langle \eta_{N,1}^U \eta_{1,2}^U \dots \eta_{N-1,N}^U G_1^U \dots G_N^U \rangle_a, \tag{A23}$$

$$V^{(N)} = \langle \eta_{N,1}^V \eta_{1,2}^V \dots \eta_{N-1,N}^V G_1^V \dots G_N^V \rangle_a, \tag{A24}$$

⁸ More generally, if an additional operator X is inserted into the trace, for instance as in equation (54), one also needs to replace $X \rightarrow \tilde{X}$, with $\tilde{X}_{\alpha, \beta} = (-1)^{|\beta|(|\alpha|+|\beta|)} \bar{X}_{\alpha, \beta}$.

where

$$G_x^U = \sum_{\alpha,\beta=0}^{D-1} \sum_{n,m=0}^{d-1} U_{\alpha,\beta}^{n,m} (\ell_x^U)^\alpha f_x^{n,m} (r_x^U)^\beta, \quad (\text{A25})$$

$$\eta_{x,y}^U = \prod_{\mu=0}^{D-1} \frac{1}{2} (1 + i r_{x,\mu}^U \ell_{y,\mu}^U), \quad (\text{A26})$$

and analogously for $G_x^V, \eta_{x,y}^V$. Note that here, we consider two different sets of Majorana operators, labeled by U, V . Defining $W^{(N)} = U^{(N)}V^{(N)}$, and exploiting the parity of the local tensors, we have

$$W^{(N)} = \langle \eta_{N,1}^{UV} \eta_{1,2}^{UV} \dots \eta_{N-1,N}^U G_1^{UV} \dots G_N^{UV} \rangle_{\bar{a}}. \quad (\text{A27})$$

The expectation value is now taken with respect to the vacuum $|\Omega_{\bar{a}}\rangle$ of all auxiliary Majorana fermions, satisfying

$$(r_{x-1,\mu}^U - i \ell_{x,\mu}^U) |\Omega_{\bar{a}}\rangle = (r_{x-1,\mu}^V - i \ell_{x,\mu}^V) |\Omega_{\bar{a}}\rangle = 0. \quad (\text{A28})$$

Furthermore, we introduce $\eta_{x,y}^{UV} = \eta_{x,y}^U \eta_{x,y}^V$, and

$$\begin{aligned} G_x^{UV} &= G_x^U G_x^V = U_{\alpha,\beta}^{k,j} V_{\gamma,\delta}^{j',i} (\ell_x^U)^\alpha f_x^{k,j} (r_x^U)^\beta (\ell_x^V)^\gamma f_x^{j',i} (r_x^V)^\delta \\ &= (-1)^{|\gamma|(|k|+|j|)} U_{\alpha,\beta}^{k,j} V_{\gamma,\delta}^{j',i} (\ell_x^U)^\alpha (\ell_x^V)^\gamma f_x^{k,i} (r_x^V)^\delta (r_x^U)^\beta, \end{aligned} \quad (\text{A29})$$

where the repeated indices are summed over. Note that in the last line, we have moved $(r_x^U)^\beta$ to the left, for consistency with the conventions (A4) and (A5).

From equations (A27) and (A29), we see that $W^{(N)}$ is already written in the form (A18). Thus, repeating the derivation in the last subsection, we find that the local tensors appearing in (36) can be read directly from equation (A29), thus proving equation (A22).

Using the results above, it is also straightforward to derive the local tensor associated with $\mathbb{U}^{(N)} = [U^{(N)}]^\dagger U^{(N)}$. In particular, up to an even gauge transformation of the form

$$G_{(\alpha,\gamma),(\beta,\delta)} = (-1)^{|\alpha||\gamma|} \delta_{\alpha,\beta} \delta_{\gamma,\delta}, \quad (\text{A30})$$

a direct computation yields

$$\mathbb{U}_{(\alpha,\gamma),(\beta,\delta)}^{k,i} = \sum_j (-1)^{|\beta|(|k|+|i|)} \bar{U}_{\alpha,\beta}^{j,k} U_{\gamma,\delta}^{j,i}. \quad (\text{A31})$$

Accordingly, by taking $k = i$ and summing over i , we can also define the fermionic TM E , whose elements simply read

$$E_{(\alpha,\gamma),(\beta,\delta)} = \frac{1}{d} \sum_{i,j} \bar{U}_{\alpha,\beta}^{j,i} U_{\gamma,\delta}^{j,i}, \quad (\text{A32})$$

completely analogously to the case of qudits. This definition allows us to write down a relation similar to equation (14) for fermionic MPOs, which is important when discussing

fMPUs. In particular, in the case of PBCs, we immediately derive

$$\frac{1}{d^N} \text{tr} [U^{(N)\dagger} U^{(N)}] = \text{tr} [(Z \otimes Z) E_{\mathcal{U}}^N], \tag{A33}$$

while for ABCs we simply have

$$\frac{1}{d^N} \text{tr} [U^{(N)\dagger} U^{(N)}] = \text{tr} [E_{\mathcal{U}}^N]. \tag{A34}$$

Finally, one can also define the blocking procedure for fermionic TNs. Consider the fMPO (33), and suppose that we are interested in blocking pairs of neighboring sites. The annihilation operators associated with the ‘doubled site’ at position j are

$$\tilde{a}_j^{(n,m)} = a_{2j}^n a_{2j+1}^m. \tag{A35}$$

Now, it is easy to verify that

$$\tilde{f}_j^{(n,m),(q,p)} = (-1)^{|m|(|p|+|q|)} f_{2j}^{m,n} f_{2j+1}^{q,p}, \tag{A36}$$

satisfy equation (34), with the replacement $a_j^n \rightarrow \tilde{a}_j^{(n,m)}$. Accordingly, blocking leads to an fMPO, where the local tensor \mathcal{U}_B is defined by

$$\left(U_B^{(n,m),(p,q)} \right)_{\alpha,\beta} = U_{\alpha,\gamma}^{n,m} U_{\gamma,\beta}^{p,q} (-1)^{|m|(|p|+|q|)}. \tag{A37}$$

Based on these formulas, one can extend the graphical notation introduced in the case of qudits to fermionic TNs, where it is always understood that one should multiply the elements of the local tensors by the correct signs, as specified by the above equations. We note that a similar discussion can be carried out using the formalism of graded TNs, which has the advantage of offering a more transparent way to translate the algebraic formulation into a graphical one (and vice versa), cf appendix B.

Appendix B. Graded tensor networks

In this appendix we review the formalism of graded TNs, as introduced recently in Refs. [53, 59]. Here, we only sketch the main definitions, and the interested reader is referred to the latter works for a more systematic treatment.

Given a Hilbert space V , we say that V is \mathbb{Z}_2 -graded if there is a parity operator \mathcal{P} and a decomposition

$$V = V^e \oplus V^o, \tag{B1}$$

such that $\mathcal{P}|v\rangle = |v\rangle$ for all $|v\rangle \in V^e$, and $\mathcal{P}|v\rangle = -|v\rangle$ for all $|v\rangle \in V^o$. We say that V^e, V^o are the even and odd sectors of the graded space V , respectively. Let us now introduce a set of local \mathbb{Z}_2 -graded Hilbert spaces \mathcal{H}_j , with decomposition

$$\mathcal{H}_j = \mathcal{H}_j^e \oplus \mathcal{H}_j^o. \tag{B2}$$

We use $\{|i\rangle\}_{i=0}^{d-1}$ to denote a local basis, and $|i\rangle \in \{0, 1\}$ to denote the parity of each basis vector, so that $\mathcal{P}|i\rangle = (-1)^{|i|}|i\rangle$. In the following we will use d_e and d_o for the dimensions

of \mathcal{H}_j^e and \mathcal{H}_j^o , respectively. Next, we introduce the notion of a graded tensor product, denoted by $\otimes_{\mathfrak{g}}$. This is a tensor product equipped with a canonical isomorphism \mathcal{F} between different orderings of the local spaces. Specifically, given the graded spaces V , W , the canonical isomorphism \mathcal{F} is defined by

$$\mathcal{F}: V \otimes_{\mathfrak{g}} W \rightarrow W \otimes_{\mathfrak{g}} V, \tag{B3}$$

$$|i\rangle \otimes_{\mathfrak{g}} |j\rangle \rightarrow (-1)^{|i||j|} |j\rangle \otimes_{\mathfrak{g}} |i\rangle. \tag{B4}$$

Making use of \mathcal{F} , we can identify states in different ordered tensor products of the same local spaces.

Importantly, the \mathbb{Z}_2 -grading structure is inherited by the dual space V^* , generated by the basis $\{|i\rangle\}_{i=0}^{d-1}$, and the isomorphism \mathcal{F} can naturally be extended to tensor products also containing local dual spaces. Furthermore, a state in $V^* \otimes V$ can be naturally mapped onto \mathbb{C} via the linear map

$$\mathcal{C}: V^* \otimes_{\mathfrak{g}} V \rightarrow \mathbb{C}: \langle \psi | \otimes_{\mathfrak{g}} | \phi \rangle \rightarrow \langle \psi | \phi \rangle. \tag{B5}$$

Note that \mathcal{C} acts on the ordered graded tensor product $V^* \otimes V$. However, one can extend the action of \mathcal{C} to a different ordering, by first applying the canonical isomorphism \mathcal{F} . For instance, using this prescription, we can compute

$$\mathcal{C}(|i\rangle \otimes_{\mathfrak{g}} \langle j|) = (-1)^{|i||j|} \mathcal{C}(\langle j| \otimes_{\mathfrak{g}} |i\rangle) = (-1)^{|i|} \delta_{i,j}. \tag{B6}$$

The above definitions allow us to generalize the construction of MPSs to graded Hilbert spaces. In particular, we can define the local tensors \mathcal{A} as

$$\mathcal{A}[j] = \sum_{i,\alpha,\beta} A_{\alpha,\beta}^i |\alpha\rangle_{j-1} \otimes_{\mathfrak{g}} |i\rangle_j \otimes_{\mathfrak{g}} \langle \beta|_j \in V_j \otimes_{\mathfrak{g}} \mathcal{H}_j \otimes_{\mathfrak{g}} (V_{j+1})^*, \tag{B7}$$

where round kets and bras correspond to the bases of the auxiliary space $V_j \simeq \mathbb{C}^{D_j}$ and its dual. An fMPS is then constructed by concatenating local tensors, and gluing them together by applying the contraction map \mathcal{C} [53, 59]. In the case of PBCs, for instance, this leads to

$$\langle \psi | = \mathcal{C}(\mathcal{A}[1] \otimes_{\mathfrak{g}} \mathcal{A}[2] \otimes_{\mathfrak{g}} \dots \otimes_{\mathfrak{g}} \mathcal{A}[N]). \tag{B8}$$

A crucial requirement is that the local tensors \mathcal{A} have well-defined parity, which we can assume to be even without loss of generality. This ensures that the fMPS have well-defined parity and that no ambiguity arises in the definition of some useful constructions to manipulate them [53].

As in the case of qudits, we can introduce a natural graphical representation for graded TNs. For instance, local tensors \mathcal{A} are depicted by

$$\mathcal{A} = \sum_{i,\alpha,\beta} A_{\alpha,\beta}^i |\alpha\rangle \otimes_{\mathfrak{g}} |i\rangle \otimes_{\mathfrak{g}} \langle \beta| = \alpha \overset{i}{\circlearrowleft} \beta. \tag{B9}$$

When different tensors are joined together, it is always understood that the linear map \mathcal{C} is applied to the corresponding spaces. As usual, before applying \mathcal{C} , the local spaces in the graded tensor product must be reordered using the canonical isomorphism \mathcal{F} .

Clearly, the above formalism can be applied directly to also treat MPOs in graded spaces. To this end, we simply replace the local tensor (B7) with

$$\mathcal{M}[j] = \sum_{i,\alpha,\beta} M_{\alpha,\beta}^{m,n} |\alpha\rangle_{j-1} \otimes_{\mathfrak{g}} |m\rangle_j \otimes_{\mathfrak{g}} \langle n|_j \otimes_{\mathfrak{g}} (\beta|_j. \quad (\text{B10})$$

Finally, the contraction in equation (B8) can easily be performed using the parity of the local tensors, leading to the more explicit form

$$|\psi\rangle = \sum_{i_1, \dots, i_N=0}^{d-1} \text{tr} (\mathcal{P}_D A^{i_1} \dots A^{i_N}) |i_1\rangle \otimes_{\mathfrak{g}} \dots \otimes_{\mathfrak{g}} |i_N\rangle. \quad (\text{B11})$$

Here, \mathcal{P}_D is the parity operator acting on the auxiliary graded space with dimensions D . Note that, due to the parity of \mathcal{A} , we have $\mathcal{P}_D A^n = (-1)^{|n|} A^n \mathcal{P}_D$.

Based on equation (B11), we now see an explicit correspondence between the fiducial-state and graded TN formalisms for fermionic MPSs. Indeed, the coefficients in equation (B11) are the same as those appearing in equation (25) (up to an even gauge transformation, corresponding to a reordering of the basis vectors in auxiliary space). Furthermore, using the above prescription for the contraction of graded tensors, it is straightforward to derive, e.g. equations (A21) and (A22) for the adjoint and composition of fMPOs. In fact, the fermionic operators $f^{n,m}$ introduced in equation (34) simply correspond to $|n\rangle \otimes_{\mathfrak{g}} \langle m|$.

Appendix C. Examples of fMPUs

C.1. Non-locality-preserving fMPUs

In this appendix, we provide further details for the fMPU constructed in section 5.1. First, for completeness, we tabulate all 16 matrices $U^{n,m}$ corresponding to the elements $U_{\alpha,\beta}^{n,m}$ in (40) and (41). They read

$$U^{0,0} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad U^{0,1} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad U^{0,2} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad U^{0,3} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad (\text{C1a})$$

$$U^{1,0} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad U^{1,1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad U^{1,2} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad U^{1,3} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad (\text{C1b})$$

$$U^{2,0} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad U^{2,1} = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad U^{2,2} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad U^{2,3} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix},$$

(C1c)

$$U^{3,0} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad U^{3,1} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad U^{3,2} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \quad U^{3,3} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (\text{C1d})$$

Next, we prove equation (42). We have

$$U|\Omega\rangle = \left(\sum \text{tr} [ZU^{n_1, m_1} \dots U^{n_N, m_N}] f_1^{n_1, m_1} \dots f_N^{n_N, m_N} \right) |\Omega\rangle. \quad (\text{C2})$$

The vacuum is annihilated by f^{n_j, m_j} , unless $m_j = 0$. Since $U^{n_j, 0}$ is non-vanishing only if $n_j = 0$, there is a single non-vanishing term in the sum, corresponding to $n_j = m_j = 0$ for all j and

$$U|\Omega\rangle = \left(\text{tr} [Z (\mathbb{1}_3)^N] \right) |\Omega\rangle = (1 + 1 - 1) |\Omega\rangle = |\Omega\rangle. \quad (\text{C3})$$

Now, let us prove equation (43). We have

$$U a_{i_1}^{j_1 \dagger} a_{i_2}^{j_2 \dagger} \dots a_{i_P}^{j_P \dagger} |\Omega\rangle = \left(\sum \text{tr} [ZU^{n_1, m_1} \dots U^{n_N, m_N}] f_1^{n_1, m_1} \dots f_N^{n_N, m_N} \right) \times a_{i_1}^{j_1 \dagger} a_{i_2}^{j_2 \dagger} \dots a_{i_P}^{j_P \dagger} |\Omega\rangle. \quad (\text{C4})$$

Now, consider $r \neq i_k$, for $k = 1, 2, \dots, P$. Arguing as before, we find that the only non-vanishing terms in the sum correspond to $m_r = n_r = 0$, for which $U^{n_r, m_r} = \mathbb{1}_3$. Thus, the above expression simplifies to

$$U a_{i_1}^{j_1 \dagger} a_{i_2}^{j_2 \dagger} \dots a_{i_P}^{j_P \dagger} |\Omega\rangle = \left(\sum \text{tr} [ZU^{n_{i_1}, m_{i_1}} \dots U^{n_{i_P}, m_{i_P}}] f_{i_1}^{n_{i_1}, m_{i_1}} \dots f_{i_P}^{n_{i_P}, m_{i_P}} \right) \times a_{i_1}^{j_1 \dagger} a_{i_2}^{j_2 \dagger} \dots a_{i_P}^{j_P \dagger} |\Omega\rangle, \quad (\text{C5})$$

where the sum is now restricted over all the sequences $\{n_{i_\ell}\}_{\ell=1}^P$, $\{m_{i_\ell}\}_{\ell=1}^P$ with $n_{i_\ell}, m_{i_\ell} = 1, 2, 3$. From the explicit form of the local tensors, we see that this expression is, up to a sign, a translation of the fermionic modes on an effective chain of P sites, where each site is associated with three possible fermionic modes $a^1 = a_2$, $a^2 = a_1$, $a^3 = a_1 a_2$. This shows that equation (43) is proven. We stress that we do not need to specify the sign $(-1)^\gamma$ appearing in equation (43), because this does not affect unitarity.

C.2. Majorana-shift operator

In this appendix, we show that the fMPO $M_{\text{AP}}^{(N)}$ defined by equation (52) provides a valid representation for the translation of Majorana modes.

First of all, it is straightforward to verify that the fMPO corresponding to (52) is unitary. This can be seen, for instance, by constructing the matrices $\mathbb{U}^{k,i}$ in (A31), and observing that they generate the identity operator. Next, we show

$$M_{\text{AP}}^{(N)} \gamma_{2n} = \gamma_{2n+1} M_{\text{AP}}^{(N)}, \quad n \neq N, \quad (\text{C6})$$

$$M_{\text{AP}}^{(N)} \gamma_{2n-1} = \gamma_{2n} M_{\text{AP}}^{(N)}, \tag{C7}$$

$$M_{\text{AP}}^{(N)} \gamma_{2N} = -\gamma_1 M_{\text{AP}}^{(N)}, \tag{C8}$$

where

$$\gamma_{2n-1} = a_n^\dagger + a_n = \tilde{\delta}_{i,j+1} f_n^{i,j}, \tag{C9}$$

$$\gamma_{2n} = i(a_n^\dagger - a_n) = i(-1)^j \tilde{\delta}_{i,j+1} f_n^{i,j} \tag{C10}$$

are the Majorana modes introduced in equation (46), and where $f_n^{i,j}$ are given in equation (34). Here, we introduce the function

$$\tilde{\delta}_{a,b} = \begin{cases} 1 & a \equiv b \pmod{2}, \\ 0 & \text{otherwise.} \end{cases} \tag{C11}$$

In order to prove equations (C6)–(C8) we can use the explicit form

$$c_{j_1, \dots, j_N}^{i_1, \dots, i_N} = \frac{2}{\sqrt{2}} \frac{1}{2^{N/2}} i^J \tilde{\delta}_{I,J}, \tag{C12}$$

where $|I| = |i_1| + \dots + |i_N|$, $|J| = |j_1| + \dots + |j_N|$. For instance, using the latter, the left-hand side of (C6) can be written as (repeated indices are summed over)

$$\begin{aligned} M_{\text{AP}}^{(N)} \gamma_{2n} &= \frac{2}{\sqrt{2}} \frac{1}{2^{N/2}} i^{|j_1| + \dots + |\ell_n| + \dots + |j_N|} \tilde{\delta}_{I, |j_1| + \dots + |\ell_n| + \dots + |j_N|} f^{i_1, j_1} \dots f^{i_n, \ell_n} \dots f^{i_N, j_N} \\ &\quad \times \tilde{\delta}_{\ell_n, j_n+1} i(-1)^{j_n} f^{\ell_n, j_n} \\ &= \frac{2}{\sqrt{2}} \frac{1}{2^{N/2}} i^J (-i)^{|\ell_n| - |j_n|} \tilde{\delta}_{\ell_n, j_n+1} i(-1)^{j_n} (-1)^{\sum_{m>n} (|i_m| + |j_m|)} \\ &\quad \times \tilde{\delta}_{I, J+1} f^{i_1, j_1} \dots f^{i_N, j_N} \\ &= -\frac{2}{\sqrt{2}} \frac{1}{2^{N/2}} \tilde{\delta}_{I, J+1} i^J (-1)^{\sum_{m>n} (|i_m| + |j_m|)} f^{i_1, j_1} \dots f^{i_N, j_N}, \end{aligned} \tag{C13}$$

while, in the same way, one can compute

$$\gamma_{2n+1} M_{\text{AP}}^{(N)} = -\frac{2}{\sqrt{2}} \frac{1}{2^{N/2}} \tilde{\delta}_{I, J+1} i^J (-1)^{\sum_{m>n} (|i_m| + |i_n|)} f^{i_1, j_1} \dots f^{i_N, j_N}, \tag{C14}$$

yielding (C6). Equations (C7) and (C8) can be proved in the same way. Thus, using unitarity, we obtain $M_{\text{AP}}^{(N)} \gamma_n M_{\text{AP}}^{(N)\dagger} = \gamma_{n+1}$ for $n \neq 2N$ and $M_{\text{AP}}^{(N)} \gamma_{2N} M_{\text{AP}}^{(N)\dagger} = -\gamma_1$.

Similarly, we can analyze the operator $M_{\text{P}}^{(N)}$ corresponding to the coefficients in (54). First, constructing the fMPO representation for $M_{\text{P}}^{(N)} M_{\text{P}}^{(N)\dagger}$, and paying attention to the boundary operator X , it is easy to show that $M_{\text{P}}^{(N)}$ is unitary. Next, rewriting the coefficients in (54) as

$$c_{j_1, \dots, j_N}^{i_1, \dots, i_N} = \frac{2}{\sqrt{2}} \frac{1}{2^{N/2}} (-i)^J \tilde{\delta}_{I, J+1}, \tag{C15}$$

and by means of calculations similar to those reported in equations (C13) and (C14), we can also show

$$M_P^{(N)} \gamma_n = \gamma_{n+1} M_P^{(N)}, \quad (\text{C16})$$

with the identification $\gamma_{2N+1} = \gamma_1$. Putting all these together, we find that the fMPO corresponding to the coefficients in (54) provides a valid representation for the Majorana shift with PBCs.

Appendix D. The graded canonical form for antiperiodic boundary conditions

In this section, we provide all the proofs needed to establish the existence and uniqueness of the GCF for ABCs. Throughout this section, we will always work with even tensors, unless specified otherwise, and use $|V^{(N)}(\mathcal{A})\rangle$ to denote the fMPS with ABCs generated by \mathcal{A} . Furthermore, we will use Z to denote the parity operator acting on the space of the matrices A^i .

First, recalling definition 6.1 for GI tensors, we introduce the graded irreducible form (GIF) as follows.

Definition D.1. We say that an even tensor \mathcal{A} generating an fMPS is in GIF if: (i): the matrices are of the form $A^n = \bigoplus_{k=1}^r \mu_k A_k^n$, where $\mu_k \in \mathbb{C}$ and the spectral radius of the TM E_k associated with A_k^n is equal to one; (ii) the parity operator, Z has the same block structure as A^n and, for all k , \mathcal{A}_k is a GI (even) tensor.

Proposition D.2. *Given any even tensor \mathcal{A} , one can always find another even tensor \mathcal{B} in GIF that generates the same fMPS with ABCs.*

Proof. Let Z be the parity operator on the auxiliary space. First, if there are no non-trivial invariant graded subspaces, \mathcal{A} is a GI tensor, and thus already in GIF. Otherwise, take P to be the orthogonal projector onto an invariant graded subspace that does not contain any other non-trivial invariant graded subspace, and define $Q = \mathbb{1} - P$. Since $[P, Z] = 0$, setting $Z_P = PZP$ and $Z_Q = QZQ$ we have $Z_P(PA^iP) = (-1)^{|i|}(PA^iP)Z_P$, $Z_Q(QA^iQ) = (-1)^{|i|}(QA^iQ)Z_Q$. Furthermore, $Z_P^2 = P$, $Z_Q^2 = Q$. Thus, it is easy to see that the tensors A^i and $PA^iP + QA^iQ$ generate the same state, and both PA^iP and QA^iQ generate valid fMPSs, with the parity operators on the auxiliary spaces given by Z_P and Z_Q , respectively. We can now consider QA^iQ and decompose it into smaller blocks using the same steps. This procedure can be iterated until we end up with a tensor in GIF. \square

The following statement already appeared in [53], but here we give a detailed proof.

Proposition D.3. *Let \mathcal{A} be a GI tensor, such that a non-graded invariant subspace exists for all A^i . D denotes the dimension of the matrices A^i , and using D_e , D_o to denote the dimensions of the even and odd subspaces, we have $D = 2D_e$, and an even gauge transformation exists such that*

$$A^i = \begin{pmatrix} B^i & 0 \\ 0 & B^i \end{pmatrix} = \mathbb{1} \otimes B^i \quad \text{if } |i| = 0 \quad (\text{D1a})$$

$$A^i = \begin{pmatrix} 0 & B^i \\ B^i & 0 \end{pmatrix} = \sigma^x \otimes B^i \quad \text{if } |i| = 1, \tag{D1b}$$

and $Z = \sigma^z \otimes \mathbb{1}$. Furthermore, the following are true:

- (a) an index i exists, such that $|i| \equiv 1$ and $B^i \neq 0$;
- (b) there is no projector P such that

$$B^{i_1} \dots B^{i_p} P = P B^{i_1} \dots B^{i_p} P \quad \forall \{i_k\}_{k=1}^p, \tag{D2}$$

namely there is no invariant subspace for the algebra generated by the matrices B^i ;

- (c) there is no projector P_e such that

$$B^{i_1} \dots B^{i_p} P_e = P_e B^{i_1} \dots B^{i_p} P_e \tag{D3}$$

$$\forall \{i_k\}_{k=1}^p : \sum_{r=1}^p |i_r| \equiv 0,$$

namely there is no invariant subspace for the even subalgebra generated by the matrices B^i .

Proof. Let P be the orthogonal projector onto a proper non-graded invariant subspace of A^j , \mathcal{S}_1 , containing no smaller non-trivial invariant subspace. Defining $Q = ZPZ$ we have $[P, Z] \neq 0$, and thus, if Q projects onto $\mathcal{S}_2 = Z\mathcal{S}_1$, we have $\mathcal{S}_1 \neq \mathcal{S}_2$. If Y is an even invertible matrix, then $A^j_Y = Y A^j Y^{-1}$ leave the subspaces $Y\mathcal{S}_1, Y\mathcal{S}_2$ invariant with the corresponding orthogonal projectors P_Y, Q_Y . Note that $P_Y \neq Y P Y^{-1}$, since $Y P Y^{-1}$ is non-Hermitian and that, since Y is even, $Q_Y = Z P_Y Z$. We claim that it is always possible to find an even Y such that $P_Y Q_Y = P_Y Z P_Y Z = 0$.

To show this, it is useful to construct a Jordan decomposition of the Hilbert space for P, Q into 1D and 2D orthogonal graded subspaces that are invariant under both P and Q . To this end, we note that $\Pi = P + Q$ is Hermitian and commutes with Z . Hence, there is a common basis for eigenstates. Let $|\phi\rangle$ be an element of this basis, so that $\Pi|\phi\rangle = \lambda|\phi\rangle$ and $Z|\phi\rangle = \pm|\phi\rangle$. If $P|\phi\rangle \in \text{span}(|\phi\rangle)$, then $\text{span}(|\phi\rangle)$ is a 1D invariant graded subspace for both P and Q . Otherwise, it is easy to see that $|\phi\rangle, P|\phi\rangle$ generate a 2D space left invariant by P and Q . If $\lambda \neq 0$, this space is generated by $P|\phi\rangle$ and $ZP|\phi\rangle$, and taking the even and odd combination of these, we see that the subspace is graded. Otherwise $P|\phi\rangle = \pm ZP|\phi\rangle$ so that $P|\phi\rangle$ also has well-defined parity, and so in any case the subspace is graded. This procedure gives us a basis for the Hilbert space $\mathcal{B} = \{|v_1\rangle, |w_1\rangle, \dots, |v_r\rangle, |w_r\rangle, |u_1\rangle, \dots, |u_k\rangle\}$, where $(|v_j\rangle, |w_j\rangle)$ and $|u_j\rangle$ generate 2D and 1D invariant graded subspaces, respectively. Note that this basis is not orthogonal, since $\langle v_j | w_j \rangle \neq 0$.

Now, let R_i be the orthogonal projector onto a graded invariant subspace for P, Q of dimension 2. Since $[R_i, Z] = 0$, we have that $R_i P R_i = |v_i\rangle\langle v_i|$ and $R_i Q R_i = |w_i\rangle\langle w_i|$, with $|w_i\rangle = Z|v_i\rangle$, and $|v_i\rangle = \alpha_i|a_i\rangle + \beta_i|b_i\rangle$, where $|a_i\rangle$ ($|b_i\rangle$) is even (odd). It must be the case that $\alpha_i, \beta_i \neq 0$, otherwise $|v_i\rangle, |w_i\rangle$ are proportional. Then, we can define the 2D matrix $Y_i = \text{diag}(\beta_i, \alpha_i)$ which is invertible. Next, for all 1D blocks we define $Y_i = \mathbb{1}$. We claim that $Y = \oplus_i Y_i$ is the desired gauge matrix. Indeed, consider the basis

$\mathcal{B}_Y = \{Y|v_1\rangle, Y|w_1\rangle, \dots, Y|v_r\rangle, Y|w_r\rangle, |u_1\rangle, \dots, |u_k\rangle\}$. By construction, this is an orthogonal (although not normalized) basis: indeed, $\langle v_j|Y^\dagger Y|w_j\rangle = |\alpha_i\beta_i|^2 - |\alpha_i\beta_i|^2 = 0$, while the other orthogonality relations are immediate. Furthermore, in this basis P_Y , and Q_Y are diagonal matrices, with elements that are only 0 or 1. Thus, since $P_Y \neq P_Q$, necessarily $P_Y Q_Y = 0$: if this were not the case, then since P_Y , and P_Q have the same rank, $P_Y Q_Y$ would project onto an invariant subspace of \mathcal{S}_1 with strictly smaller dimensions, which is a contradiction.

Thus, up to an even gauge transformation, we can assume that $PQ = 0$. Now, since $P + Q$ is an invariant subspace projector that commutes with Z , it must be equal to the identity, because \mathcal{A} is GI. In the basis where Z has the form (27), this imposes the following structure on P and $Q = \mathbb{1} - P = ZPZ$

$$P = \frac{1}{2} \begin{bmatrix} \mathbb{1} & U \\ U^\dagger & \mathbb{1} \end{bmatrix}, \quad Q = \frac{1}{2} \begin{bmatrix} \mathbb{1} & -U \\ -U^\dagger & \mathbb{1} \end{bmatrix}, \tag{D4}$$

where idempotence requires $UU^\dagger = U^\dagger U = \mathbb{1}$. Hence, this is only possible if $D_e = D_o$ and U is a unitary matrix. Now, the condition $A^i P = P A^i P$ implies that the matrices A^i are of the following form

$$\begin{aligned} A^i &= \begin{pmatrix} C^i & 0 \\ 0 & U^\dagger C^i U \end{pmatrix} & \text{if } |i| = 0 \\ A^i &= \begin{pmatrix} 0 & C^i \\ U^\dagger C^i U^\dagger & 0 \end{pmatrix} & \text{if } |i| = 1. \end{aligned} \tag{D5}$$

We can then map this to the form (D1) using an even-parity gauge $\mathbb{1} \oplus U$.

Next, condition (b) follows from (c), so we only need to prove the former. We do this by contradiction. We use $S^{(e)}(B^i)$ to denote the even subalgebras generated by B^i , while we define $S^{(o)}(B^i)$ to be the linear space generated by the odd products $B^{i_1} \dots B^{i_k}$ with $\sum_j |i_j| \equiv 1 \pmod{2}$ (note that $S^{(o)}(B^i)$ is not an algebra, since it is not closed under the product). Let P_e be the projector onto an invariant subspace for $S^{(e)}(B^i)$, denoted by \mathcal{S}_e , containing no smaller invariant subspace, and define the linear space

$$\mathcal{S}_o = \{|w\rangle = B^{(o)}|v_e\rangle : |v_e\rangle \in \mathcal{S}_e, B^{(o)} \in S^{(o)}(B^i)\}. \tag{D6}$$

Specifically, \mathcal{S}_o is the space generated by applying all possible odd products to \mathcal{S}_e . P_o denotes the orthogonal projector onto \mathcal{S}_o . By definition

$$B^i P_e = P_o B^i P_e, \quad \forall |i| = 1, \tag{D7}$$

and also

$$B^i P_o = P_e B^i P_e, \quad \forall |i| = 1. \tag{D8}$$

To see this, we note that $|w\rangle \in \mathcal{S}_o \Rightarrow |w\rangle = B^{(o)}|v_e\rangle$, with $|v_e\rangle \in \mathcal{S}_e$, and $B^{(o)} \in S^{(o)}(B^i)$, and thus, $B^i|w\rangle = B^i B^{(o)}|v_e\rangle$. Since $|i| = 1$, $B^i B^{(o)}$ is in the even algebra, and thus $B^i B^{(o)}|v_e\rangle \in \mathcal{S}_e$ due to equation (D3). In the same way, we also have

$$B^i P_o = P_o B^i P_o, \quad \forall |i| = 0. \tag{D9}$$

Indeed, if $|w\rangle \in \mathcal{S}_o$, then $|w\rangle = B^{(o)}|v_e\rangle$, with $|v_e\rangle \in \mathcal{S}_e$, and $B^{(o)} \in S^{(o)}(B^i)$, and thus $B^i|w\rangle = B^i B^{(o)}|v_e\rangle$. Since $|i| = 0$, $B^i B^{(o)}$ is odd, and thus by the definition of \mathcal{S}_o , $B^i|w\rangle \in \mathcal{S}_o$. Now, consider the projector

$$\tilde{P} = \begin{pmatrix} P_e & 0 \\ 0 & P_o \end{pmatrix}. \tag{D10}$$

Clearly, $[\tilde{P}, Z] = 0$. Furthermore, $A^i \tilde{P} = \tilde{P} A^i \tilde{P}$, because this condition is equivalent to

$$\begin{aligned} B^i P_e &= P_e B^i P_e, & \forall |i| = 0, & & B^i P_o &= P_o B^i P_o, & \forall |i| = 0, \\ B^i P_e &= P_o B^i P_e, & \forall |i| = 1, & & B^i P_o &= P_e B^i P_o, & \forall |i| = 1. \end{aligned} \tag{D11}$$

The first equation is verified by definition, while the others correspond to (D7)–(D9). The existence of \tilde{P} contradicts the assumptions, and we thus conclude that also property (c) is true. \square

Corollary D.4. *Let \mathcal{A} be an even tensor in the form of (D1). Then, \mathcal{A} is GI iff there is no projector P_e such that*

$$\begin{aligned} B^{i_1} \dots B^{i_p} P_e &= P_e B^{i_1} \dots B^{i_p} P_e \\ \forall \{i_k\}_{k=1}^p : \sum_{r=1}^p |i_r| &\equiv 0. \end{aligned} \tag{D12}$$

Proof. Due to proposition D.3, we only need to prove that if there is no such P_e then \mathcal{A} is GI. Suppose this is not true, and take a projector P with $A^i P = P A^i P$, and $[P, Z] = 0$. From the latter condition, we can write P in the form

$$P = \begin{pmatrix} P_e & 0 \\ 0 & P_o \end{pmatrix}. \tag{D13}$$

Using the explicit matrix representation for A^i , it is easy to see that P_e is an invariant projector for the even matrix subalgebra generated by B_i , which is the desired contradiction. \square

We can now proceed to characterize GNTs, introduced in the definition 6.2. We begin with a simple observation.

Lemma D.5. *Let \mathcal{A} be a graded normal degenerate tensor. Then, up to an even gauge transformation, A^i are in the form (D1), and two indices i, j exist with $|i| = 1, |j| = 0$, such that $B^i \neq 0, B^j \neq 0$.*

Proof. Since the TM associated with \mathcal{A} has two eigenvalues equal to 1, then necessarily there are invariant subspaces for A^i which, by definition, can only be non-graded. Thus, due to proposition D.3, there is an even gauge transformation mapping A^i into the form (D1), and there is an i , with $|i| = 1$, such that $B^i \neq 0$. Hence, we only need to prove that one index i exists, with $|i| = 0$, such that $B^i \neq 0$. Suppose that there is no such i , and take A^i in the form (D1). Then, $A^j = \sigma^x \otimes B^j$ for all j . Using E_A and E_B to denote the transfer matrices associated with A^j and B^j , respectively, this implies

$E_A = \sigma^x \otimes \sigma^x \otimes E_B$, in a suitable basis. It follows that the spectral radii of E_A and E_B coincide. Thus, an eigenstate of E_B exists that is associated with an eigenvalue, λ , with $|\lambda| = 1$, and hence there are four eigenstates of E_A associated with an eigenvalues μ_j with $|\mu_j| = 1$. This contradicts the fact that \mathcal{A} is a graded normal degenerate tensor. \square

Next, we introduce the completely positive map associated with a tensor \mathcal{A} , which is of great importance for the study of normal tensors.

Definition D.6. For any tensor \mathcal{A} , we define the CPM

$$\mathcal{E}_{\mathcal{A}}(X) = \sum_j A^j X A^{j\dagger}. \tag{D14}$$

Analogously to the case of qudits, it is possible to characterize the fixed points of the CPM associated with GNTs.

Lemma D.7. *Let \mathcal{A} be a GNT. If \mathcal{A} is non-degenerate, then the unique fixed point of $\mathcal{E}_{\mathcal{A}}$ is an even operator, which is strictly positive. If \mathcal{A} is degenerate, then one can choose the two fixed points to be a pair consisting of an even and an odd operator. Furthermore, in the standard graded basis where $Z = \mathbb{1} \oplus (-\mathbb{1})$, they can be chosen in the form of*

$$\rho^e = \begin{pmatrix} \rho & 0 \\ 0 & \rho \end{pmatrix}, \quad \rho^o = \begin{pmatrix} 0 & \rho \\ \rho & 0 \end{pmatrix}, \tag{D15}$$

where ρ is a strictly positive operator.

Proof. First, we note that one can always choose the fixed points of the map (D14) to have a well-defined parity. Now, if \mathcal{A} is non-degenerate, then its unique fixed point X is a strictly positive operator [65]. This implies $\text{tr}[X] > 0$. On the other hand, the trace of any odd operator is vanishing. Hence, X is even.

Suppose now that \mathcal{A} is a degenerate GNT. Then, we can assume w.l.o.g. that A^j is in the form of (59). Define the unitary matrix

$$u = \frac{1}{\sqrt{2}} \begin{pmatrix} \mathbb{1} & \mathbb{1} \\ -\mathbb{1} & \mathbb{1} \end{pmatrix}. \tag{D16}$$

Note that u does not commute with the parity, Z . We have

$$\tilde{A}^j = u A^j u^\dagger = \begin{pmatrix} B^i & 0 \\ 0 & C^i \end{pmatrix}, \tag{D17}$$

where

$$C^i = \begin{cases} B^i & |i| \equiv 0, \\ -B^i & |i| \equiv 1. \end{cases} \tag{D18}$$

Defining the CPM

$$\mathcal{E}_{\tilde{\mathcal{A}}}(X) = \sum_j \tilde{A}^j X \tilde{A}^{j\dagger}, \tag{D19}$$

we have $\mathcal{E}_{\tilde{\mathcal{A}}}(X) = u\mathcal{E}_{\mathcal{A}}(u^\dagger Xu)u^\dagger$, so that $\mathcal{E}_{\mathcal{A}}$ and $\mathcal{E}_{\tilde{\mathcal{A}}}$ have the same spectrum and the eigenstates are related by a similarity transformation. Next, due to proposition D.3, the tensor \mathcal{B} defined by B^i is irreducible. Furthermore, the map $\mathcal{E}_{\mathcal{B}}$ cannot have eigenvalues λ with $\lambda \neq 1$ and $|\lambda| = 1$, otherwise they would be also eigenvalues of $\mathcal{E}_{\mathcal{A}}$. Hence, \mathcal{B} is normal, and the map $\mathcal{E}_{\mathcal{B}}$ has a unique fixed point $\rho > 0$. Furthermore, the maps $\mathcal{E}_{\mathcal{B}}$ and $\mathcal{E}_{\mathcal{C}}$ clearly coincide (where the tensor \mathcal{C} is defined by the matrices C^i). Accordingly

$$\rho_1 = \begin{pmatrix} \rho & 0 \\ 0 & 0 \end{pmatrix}, \quad \rho_2 = \begin{pmatrix} 0 & 0 \\ 0 & \rho \end{pmatrix}, \tag{D20}$$

are two eigenvectors of $\mathcal{E}_{\tilde{\mathcal{A}}}(\cdot)$ with $\lambda = 1$. Since \mathcal{A} is normal, these must be the only fixed points of $\mathcal{E}_{\tilde{\mathcal{A}}}(\cdot)$. Now taking the inverse similarity transformation with respect to u , we find that the eigenspace associated with $\lambda = 1$ of the map $\mathcal{E}_{\mathcal{A}}(\cdot)$ is spanned by the matrices

$$\rho^e = \begin{pmatrix} \rho & 0 \\ 0 & \rho \end{pmatrix}, \quad \rho^o = \begin{pmatrix} 0 & \rho \\ \rho & 0 \end{pmatrix}. \tag{D21}$$

□

Definition D.8. For graded normal non-degenerate tensors, we say that \mathcal{A} is in graded canonical form II (GCFII) if $\Phi = \mathbb{1}$ is the only fixed point of

$$\mathcal{E}'_{\mathcal{A}}(X) = \sum_j A^{\dagger j} X A^j, \tag{D22}$$

while the fixed point of the CPM (D14) is a diagonal positive and full-rank matrix ρ . For graded normal degenerate tensors, we say that \mathcal{A} is in GCFII if

$$\Phi_1 = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & \mathbb{1} \end{pmatrix}, \quad \Phi_2 = \begin{pmatrix} 0 & \mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix} \tag{D23}$$

are the only fixed points of the CPM (D22), while the fixed points of (D14) are given in (D15), where ρ is a diagonal positive and full-rank matrix.

From lemma D.7 it is easy to show that for any normal tensor there is always an even gauge transformation mapping it into GCFII.

Proposition D.9. Let \mathcal{A} be an even tensor, and denote by $E_{\mathcal{A}}$, $\mathcal{E}_{\mathcal{A}}$ the corresponding TM and the associated completely positive map, respectively. Then

- (a) \mathcal{A} is normal and non-degenerate iff (i) $\mathcal{E}_{\mathcal{A}}$ has a unique eigenvalue λ with $|\lambda| = 1$; (ii) the corresponding left and right eigenvectors Φ , ρ of the TM are positive definite operators $\rho, \Phi > 0$;
- (b) \mathcal{A} is normal and degenerate iff (i) $\mathcal{E}_{\mathcal{A}}$ has exactly two eigenvectors associated with the eigenvalue $\lambda = 1$, and no other eigenvalue μ with $|\mu| = 1$; (ii) the corresponding right (left) eigenvectors ρ_1, ρ_2 (Φ_1, Φ_2) of the TM are even and odd, respectively; (iii) the even eigenvectors Φ_1, ρ_1 are positive definite operators $\rho > 0$.

Proof. Point (a) follows directly from proposition 3 in [66]. Let us prove point (b), along similar lines. We only need to prove that conditions (i), (ii), (iii) imply that \mathcal{A}

is normal and degenerate, because the inverse statement follows directly from lemma D.7. First, we assume w.l.o.g. that \mathcal{A} is in the form of (D1) (with the parity operator $Z = \sigma^z \otimes \mathbb{1}$) and in GCFII. This means that the channel (D14) is trace preserving. We use D_e, D_o to denote the dimensions of the even and odd subspaces, and $D = D_e + D_o$. We use $\{|j\rangle\}_{j=1}^D$ to denote a basis of vectors with well-defined parity. Following [66], we define $S_n(A) \subseteq \mathcal{M}_{D \times D}$ as the linear space spanned by all the possible products of exactly n matrices A^j , where $\mathcal{M}_{D \times D}$ is the space of complex $D \times D$ matrices. Similarly, we define $S_n^e(A) \subseteq \mathcal{M}_{D \times D}$ as the linear space spanned by all possible even products of $A^j, A^{j_1} \dots A^{j_n}$, with $\sum_k |j_k| \equiv 0 \pmod{2}$. Finally, given the map \mathcal{E} , we introduce the Choi matrix $\omega(\mathcal{E}) := (\mathcal{E} \otimes \mathbb{1})(\Omega)$, where $\Omega = \sum_{i,j=1}^D |ii\rangle\langle jj|$. Since the channel is trace-preserving, the eigenvalues of the TM $E_{\mathcal{A}}$ with $|\lambda| = 1$ have trivial Jordan blocks (see proposition 6.2 of [67]). Then, from (i) we have

$$\lim_{n \rightarrow \infty} \mathcal{E}_A^n = \mathcal{E}_A^\infty, \tag{D24}$$

and

$$\mathcal{E}_A^\infty(X) = \rho_1 \text{tr}(X) + \rho_2 \text{tr}(\Phi_2 X), \tag{D25}$$

where Φ_2 is given in equation (D23).

We need to show that no proper graded subspace exists which is left invariant by all A^j . First, we note that each element, $A^e \in S_n^e(A)$ is a block diagonal matrix

$$A^e = \begin{pmatrix} A_1^e & 0 \\ 0 & A_2^e \end{pmatrix}, \tag{D26}$$

where $A_1^e \in \mathcal{M}_{D_e \times D_e}, A_2^e \in \mathcal{M}_{D_o \times D_o}$. We claim that there exists some n such that $P_e S_n^e(A) P_e = \mathcal{M}_{D_e \times D_e}$, where P_e is the projector onto the even subspace of dimension D_e . This amounts to showing that the matrices A_1^e span $\mathcal{M}_{D_e \times D_e}$. Suppose that this is not the case. Then, an

$$F_n = \begin{pmatrix} G_n & 0 \\ 0 & 0 \end{pmatrix}, \tag{D27}$$

exists, such that $\text{tr}(A_k^{(n)} F_n) = 0$, for all $A_k^{(n)} \in S_n^{(e)}(A)$ (and this is so for all $A_k^{(n)} \in S_n(A)$, since F_n is even). Thus

$$\begin{aligned} |\text{tr}(\rho_1 F_n^\dagger F_n)| &= \left| \sum_{k_1, \dots, k_n} |\text{tr}(A_{k_1} \dots A_{k_n} F_n)|^2 - \text{tr}(\rho_1 F_n^\dagger F_n) \right| \\ &= \left| \text{tr} \left[\Omega (\mathcal{E}_A^n \otimes \mathbb{1}) (\tilde{F}_n \Omega \tilde{F}_n^\dagger) \right] - \text{tr}(\rho_1 F_n^\dagger F_n) \right|, \end{aligned} \tag{D28}$$

where $\tilde{F}_n = F_n \otimes \mathbb{1}$. We claim

$$\text{tr}(\rho_1 F_n^\dagger F_n) = \text{tr} \left[\Omega (\mathcal{E}_A^\infty \otimes \mathbb{1}) (\tilde{F}_n \Omega \tilde{F}_n^\dagger) \right]. \tag{D29}$$

Indeed, using equation (D25), we have

$$\text{tr} \left[\Omega (\mathcal{E}_A^\infty \otimes \mathbb{1}) \left(\tilde{F}_n \Omega \tilde{F}_n^\dagger \right) \right] = \text{tr} (\rho_1 F_n^\dagger F_n) + \text{tr} (\rho_2 F_n^\dagger \Phi_2 F_n). \tag{D30}$$

Now, using the fact that ρ_2 and Φ_2 are odd operators, it is straightforward to show $\text{tr} (\rho_2 F_n^\dagger \Phi_2 F_n) = 0$, which follows from (D27) and the fact that odd matrices are block off-diagonal in this basis. Then, from equation (D28), we have

$$\left| \text{tr} (\rho_1 F_n^\dagger F_n) \right| \leq c_n \|\Omega\|_\infty \text{tr} \left(\tilde{F}_n \Omega \tilde{F}_n^\dagger \right) = D c_n \text{tr} (F_n F_n^\dagger), \tag{D31}$$

where $\lim_n c_n = 0$. On the other hand, using the fact that if ρ is full rank, then $\text{tr}(\rho X) \geq \frac{1}{\|\rho^{-1}\|} \text{tr}(X)$ for all $X \geq 0$, we have

$$\left| \text{tr} (\rho_1 F_n^\dagger F_n) \right| \geq \frac{1}{\|\rho_1^{-1}\|} \left| \text{tr} (F_n^\dagger F_n) \right|, \tag{D32}$$

and we obtain a contradiction. In the same way, we can prove that some n exists such that $P_o S_n^e(A) P_o = \mathcal{M}_{D_o \times D_o}$, where P_o is the projector onto the odd subspace of dimension D_o .

Now, suppose that a graded subspace $V \simeq \mathbb{C}^{D'} \subset \mathbb{C}^D$ exists, with $D' < D$, which is left invariant by all matrices A^i . Since V is graded, we can take a basis for V of the form $\{|v_1\rangle, \dots, |v_r\rangle, |w_1\rangle, \dots, |w_s\rangle\}$, where $|v_j\rangle$ are even and $|w_j\rangle$ are odd. Furthermore, since $D' < D$, either $r < D_e$, or $s < D_o$. Suppose w.l.o.g. that the former is true, and choose $|u\rangle$ to be even with $\langle u | v_j \rangle = 0$ for all j . Now taking n such that $P_e S_n^e(A) P_e = \mathcal{M}_{D_e \times D_e}$, $A_k^{(n)} \in S_n^{(e)}(A)$ exists such that $\langle u | A_k^{(n)} | v_1 \rangle \neq 0$. This is a contradiction, since we assumed that V was left invariant by all matrices A^j . \square

Corollary D.10. *Let \mathcal{A} be a degenerate (non-degenerate) GNT. Then, the blocked tensor \mathcal{A}_k is still a degenerate (non-degenerate) GNT.*

We are finally in a position to prove the existence and uniqueness of the GCF introduced in definition 6.3. We begin with the following theorem, which provides a procedure for casting any even tensor \mathcal{A} into GCF.

Theorem D.11. *After blocking, for any even tensor, \mathcal{A} , it is always possible to obtain another even tensor, \mathcal{A}_{GCF} , in GCF that generates the same fMPS with ABCs.*

Proof. By proposition D.2 we can assume w.l.o.g. that \mathcal{A} is in GIF. Furthermore, from corollary D.10, any graded normal block remains so after blocking, so that we can restrict ourselves to the study of the case where tensor \mathcal{A} has a single block in its GIF. We can also assume w.l.o.g. that the spectral radius of $\mathcal{E}_\mathcal{A}$ is one. There are only two possibilities for the tensor \mathcal{A} : (i) there is no invariant subspace for the matrices A^j or (ii) there are non-graded invariant subspaces for the matrices A^j .

Consider case (i). If there is a single eigenvalue with $|\lambda| = 1$, then $\lambda = 1$ and we are done. Otherwise, there are p eigenvalues $e^{i2\pi q/p}$, with $\text{gcd}(q, p) = 1$, where p divides the bond dimension D [65]. We can then block p times and consider the blocked tensor \mathcal{A}_p . Now, the CPM associated with \mathcal{A}_p has exactly $p > 1$ eigenvalues equal to 1. Accordingly, there is necessarily an invariant subspace for A_p^i . If there are invariant graded subspaces,

we can decompose the block further with a projector P , such that $[P, Z] = 0$ and restart the procedure for each block. Otherwise we fall into case (ii), detailed below.

Now we consider case (ii), namely suppose that \mathcal{A} has a single block in the GIF, with non-graded invariant subspaces for the matrices A^j . If A^j is a degenerate GNT we are finished. If this is not the case, we show below that the matrices A^j can be strictly decomposed into smaller blocks after blocking. Since the bond dimension D is finite, this is enough to conclude the proof.

From proposition D.3, we can assume without loss of generality that A^j has the form (D1). Since there is no invariant subspace for the matrices B^i , cf proposition D.3, the CPM

$$\mathcal{E}_{\mathcal{B}}(X) = \sum_j B^j X B^{j\dagger} \tag{D33}$$

can either have a single eigenvalue λ with $|\lambda| = 1$, (we call this case (j)) or exactly p eigenvalues $e^{i2\pi q/p}$, with $\gcd(q, p) = 1$, where p divides the bond dimension $D/2$ (we call this case (jj)). Consider case (jj) and take the tensor \mathcal{A}_p obtained by blocking p times. The matrices corresponding to \mathcal{A}_p are

$$A_p^I = \begin{pmatrix} B_p^I & 0 \\ 0 & B_p^I \end{pmatrix} = \mathbb{1} \otimes B_p^I \quad \text{if } |I| = 0, \tag{D34a}$$

$$A_p^I = \begin{pmatrix} 0 & B_p^I \\ B_p^I & 0 \end{pmatrix} = \sigma^x \otimes B_p^I \quad \text{if } |I| = 1. \tag{D34b}$$

where $I = (i_1, \dots, i_p)$, $|I| = |i_1| + \dots + |i_p|$ and

$$B_p^I = B^{i_1} \dots B^{i_p}. \tag{D35}$$

Now, since $\mathcal{E}_{\mathcal{B}_p}$ has $p > 1$ eigenvalues equal to one, there must be an invariant subspace for all B_p^I . Thus, from proposition D.3 the matrices A_p^I can be decomposed further into smaller blocks with projectors commuting with Z . Now consider (j) . In this case, the tensor \mathcal{B} is normal. Repeating the construction of lemma D.7, we consider the tensor $\tilde{\mathcal{A}}$ in equation (D17), which is related to \mathcal{A} via the similarity transformation u in equation (D16). It is clear from the diagonal structure of (D17) that $\mathcal{E}_{\tilde{\mathcal{A}}}$ (and thus $\mathcal{E}_{\mathcal{A}}$) have at least two eigenvalues equal to one. Since we are assuming that $\tilde{\mathcal{A}}$ is not normal, there must be other eigenvalues with an absolute value of one. It follows from lemma A.2 in [33] that this is only possible if there is a non-singular matrix S and a phase ϕ such that

$$B^i = e^{i\phi} S C^i S^{-1}, \tag{D36}$$

specifically, using equation (D18),

$$B^i = e^{i\phi} S B^i S^{-1}, \quad |i| = 0 \tag{D37a}$$

$$B^i = -e^{i\phi} S B^i S^{-1}, \quad |i| = 1. \tag{D37b}$$

Since S is invertible, there are $\mu \neq 0$ and $|v\rangle \neq 0$ such that

$$S|v\rangle = \mu|v\rangle. \tag{D38}$$

Since \mathcal{B} is normal, for any n there are $B^{i_1} \dots B^{i_n}$ such that $B^{i_1} \dots B^{i_n}|v\rangle \neq 0$. By making repeated use of equation (D37), we get

$$SB^{i_1} \dots B^{i_n}|v\rangle = (-1)^{\sum_j |i_j|} e^{i\phi n} \mu B^{i_1} \dots B^{i_n}|v\rangle \tag{D39}$$

namely, S has an eigenvalue of the form $\pm e^{i\phi n} \mu$ for all n . Since S is a finite-dimensional matrix, this is only possible if $\phi = 2\pi q/p$ with $p, q \in \mathbb{N}$ and $\text{gcd}(q, p) = 1$. Blocking p times, we now obtain a new tensor in the form of (D34), where now

$$B^I = SB^I S^{-1}, \quad |I| = 0 \tag{D40a}$$

$$B^I = -SB^I S^{-1}, \quad |I| = 1. \tag{D40b}$$

Next, we prove by contradiction that the even subalgebra generated by the matrices B^I has invariant subspaces, so that the blocked tensor \mathcal{A}_p can be decomposed further by proposition D.3. If this is not true, then by Burnside’s theorem [68] the even subalgebra coincides with the full matrix algebra. On the other hand, from equation (D40), we know that S must commute with any element of the even algebra, and thus $S = \alpha \mathbb{1}$, where w.l.o.g. $\alpha \neq 0$. Thus

$$B^I = -B^I \quad \forall |I| = 1 \Rightarrow B^I = 0, \quad \forall |I| = 1. \tag{D41}$$

By proposition D.3, this means that \mathcal{A}_p has invariant graded subspaces, and using corollary D.4, we arrive at a contradiction. \square

Having established the existence of the CGF for any even tensor \mathcal{A} , we now prove that the GCF is essentially unique. Our strategy closely follows the one for qudits [54].

Definition D.12. The even tensors \mathcal{A}_j ($j = 1, \dots, g$) form the basis of graded normal tensors (BGNT) of a tensor \mathcal{A} if: (i) \mathcal{A}_j are graded and normal (degenerate or non-degenerate); (ii) for each N , $|V^{(N)}(\mathcal{A})\rangle$ can be written as a linear combination of $|V^{(N)}(\mathcal{A}_j)\rangle$; (iii) some N_0 exists such that for all $N > N_0$, $|V^{(N)}(\mathcal{A}_j)\rangle$ are linearly independent.

Lemma D.13. Let $|V_{a,b}\rangle$ be two fMPSs (with ABCs) generated by two graded NTs $\mathcal{A}_{a,b}$, with $D_a \times D_a$ matrices A_α^i and parity Z_α . Then

$$\lim_{N \rightarrow \infty} \langle V_\alpha | V_\alpha \rangle = c_\alpha, \tag{D42a}$$

$$\lim_{N \rightarrow \infty} |\langle V_b | V_a \rangle| = 0 \text{ or } c_a, \tag{D42b}$$

where $c_a = 1$ if \mathcal{A}_a is non-degenerate, and $c_a = 2$ if it is degenerate. In the case where the limit (D42b) is non-vanishing, $\mathcal{A}_{a,b}$ are either both non-degenerate or both degenerate. Furthermore, an invertible matrix X , a permutation matrix Π and a phase ϕ exist, such that $A_a^i = e^{i\phi} X \Pi A_b^i \Pi^{-1} X^{-1}$, with $[X, Z_a] = 0$, and $\Pi^{-1} Z_a \Pi = \pm Z_b$.

Proof. Equation (D42a) is obvious, so we only need to prove (D42b). Suppose that $\mathcal{A}_{a,b}$ are both non-degenerate, and that the limit (D42b) is non-vanishing. Then, it follows from lemma A.2 in [54] that $D_a = D_b$, and a phase ϕ and a non-singular matrix Y exist,

such that $A_a^i = e^{i\phi} Y A_b^i Y^{-1}$. Now, define $\zeta_a = Y Z_b Y^{-1}$, and $S_a = Z_a \zeta_a$. It can be seen at once that S_a commutes with A_a^i for all i . Hence, since A_a^i is normal, $S_a = \alpha \mathbb{1}$, namely

$$Z_a = \alpha Y Z_b Y^{-1}. \tag{D43}$$

Since $Z_a^2 = Z_b^2 = \mathbb{1}$ we have $\alpha = \pm 1$. Furthermore, since Z_a and αZ_b are both diagonal and related by a similarity transformation, they have the same number of 1's and 0's on the diagonal and a permutation matrix Π exists, such that $\alpha Z_b = \Pi^{-1} Z_a \Pi$. Plugging this into (D43), we get $[Z_a, Y \Pi^{-1}] = 0$, and the statement follows.

Suppose now that \mathcal{A}_a is a graded normal degenerate tensor, so that w.l.o.g. A_a^i are in the form (D1). First, we prove by contradiction that if \mathcal{A}_b is non-degenerate, then $\lim_{N \rightarrow \infty} |\langle V_b | V_a \rangle| = 0$. Suppose that this is not true, and that $\lim_{N \rightarrow \infty} |\langle V_b | V_a \rangle| = c \neq 0$. Using a similarity transformation that does not have well-defined parity, \mathcal{A}_a can be brought into the block-diagonal form (D17). Then, it follows from lemma A.2 in [54] that an invertible matrix X and a phase ϕ exist, such that

$$A_b^i = e^{i\phi} X B^i X^{-1} \quad \text{or} \quad A_b^i = e^{i\phi} X (-1)^{|i|} B^i X^{-1}. \tag{D44}$$

Since \mathcal{A}_a is a normal degenerate tensor, the even algebra generated by B^i does not have invariant subspaces, and so the same is true for A_b^i due to equation (D44). On the other hand, we have $[Z_b, A_b^{j_1} \dots A_b^{j_n}] = 0$ for all products $A_b^{j_1} \dots A_b^{j_n}$ with $\sum_k |j_k| \equiv 0 \pmod{2}$. Since there are no invariant subspaces for the even algebra, this implies $Z_b = \pm \mathbb{1}$. By the parity of the tensor \mathcal{A}_b , it must be the case that $A_b^{|i|} \equiv 0$ for all i with $|i| \equiv 0 \pmod{2}$, or $A_b^{|i|} \equiv 0$ for all i with $|i| \equiv 1 \pmod{2}$. Using equation (D44) and lemma D.5, we arrive at a contradiction.

Finally, suppose that both \mathcal{A}_a and \mathcal{A}_b are degenerate normal tensors, and that the limit (D42b) is non-vanishing. Applying a permutation and an even gauge transformation, we can cast both tensors in the form of equation (D1), namely $A_{a,b}^i = (\sigma^x)^{|i|} \otimes B_{a,b}^i$. Reasoning as before, it follows that either $B_b^i = e^{i\phi} Y B_a^i Y^{-1}$, or $B_b^i = e^{i\phi} (-1)^{|i|} Y B_a^i Y^{-1}$ for some invertible matrix Y and $\phi \in \mathbb{R}$. In both cases, the statement easily follows. \square

Remark D.14. Note that permutations do not necessarily have a well-defined parity. However, they leave the parity operator Z in a diagonal form, which is a necessary condition in order to represent a state defined by (26) as an fMPSs. In fact, it is straightforward to show that, if G is a gauge transformation such that $G Z G^{-1}$ is diagonal, then $G = \Pi X$, where $[X, Z] = 0$, and Π is a permutation.

We have now all the necessary ingredients to state the following fundamental theorem for fMPSs.

Theorem D.15. *Let \mathcal{A} and \mathcal{B} be two tensors in GCF, with BGNT $A_{k_a}^i, B_{k_b}^i$ ($k_{a,b} = 1, \dots, g_{a,b}$), and corresponding parity operators $Z_{k_a}^a$ and $Z_{k_b}^b$, respectively. If, for all N , \mathcal{A} and \mathcal{B} generate fMPSs that are proportional to each other, then: (i) $g_a = g_b = :g$; (ii) for all k there are j_k, ϕ_k , an invertible matrix X_k , and a permutation Π_k such that $B_k^i = e^{i\phi_k} X_k \Pi_k A_{j_k}^i \Pi_k^{-1} X_k^{-1}$, with $[X_k, Z_k^b] = 0$, $\Pi_k^{-1} Z_k^b \Pi_k = \pm Z_{j_k}^a$.*

Equipped with lemma D.13, the proof of this statement follows the one presented in [54] for theorem 2.10 without modification. Finally, theorem 6.5 follows as a simple

corollary. Note that, using the same notation as that used in the statement of theorem 6.5, we know that Z_a and $\Pi Z_b \Pi^{-1}$ have the same block-diagonal structure as \mathcal{A} , and in each block they coincide up to a global minus sign.

Appendix E. fMPUs with antiperiodic boundary conditions

E.1. GCF of fMPUs with ABC

In this appendix, we provide the technical proofs of the statements presented in section 6. We begin with the characterization of the GCF of tensors generating fMPUs with ABCs.

Proposition E.1. *Let \mathcal{U} be in GCF, and suppose \mathcal{U} generates a type-I (type-II) fMPU $U^{(N)}$ with ABCs. Then, \mathcal{U}/\sqrt{d} is graded normal non-degenerate (degenerate).*

Proof. Let us first consider the case where $U^{(N)}$ is an fMPU of the first kind, i.e. as shown in equation (56) with $S = e^{i\alpha} \mathbb{1}$, $\alpha \in \mathbb{R}$. W.l.o.g., we can assume that the tensor \mathcal{U} is in GCF. We show that \mathcal{U}/\sqrt{d} is necessarily graded, normal, and non-degenerate. Indeed, since $U^{(N)}$ is unitary for all N , $(1/d)^N \text{tr}(U^{(N)\dagger}U^{(N)}) = 1$, specifically, using equation (A34), $\text{tr} E_{\mathcal{U}}^N = 1$ for all $N > 1$. Using lemma A.5 in [54], it follows that there is only one nonzero eigenvalue of $E_{\mathcal{U}}$, which is 1, and thus the GCF of \mathcal{U}/\sqrt{d} contains only one normal non-degenerate block.

Next, suppose $U^{(N)}$ is an fMPU of the second kind. Then, repeating the above argument, we get $\text{tr} E_{\mathcal{U}}^N = 2$ for all $N > 1$, where the factor 2 comes from the normalization $1/\sqrt{2}$ in equation (61). Again, using again lemma A.5 in [54], we have only two possibilities: the GCF of \mathcal{U}/\sqrt{d} has two normal non-degenerate blocks or only a single normal degenerate block. Let us assume that the former is true, and arrive at a contradiction. In this case, we can decompose $\mathcal{U} = \mathcal{V} \oplus \mathcal{W}$, where both \mathcal{V} and \mathcal{W} are even, and thus $U^{(N)} = (V^{(N)} + W^{(N)})e^{i\alpha}/\sqrt{2}$, where $V^{(N)}$ and $W^{(N)}$ are standard fMPOs with ABCs. Thus

$$\mathbb{1} = U^{(N)\dagger}U^{(N)} = \frac{1}{2}V^{(N)\dagger}V^{(N)} + \frac{1}{2}W^{(N)\dagger}W^{(N)} + \frac{1}{2}V^{(N)\dagger}W^{(N)} + \frac{1}{2}W^{(N)\dagger}V^{(N)}. \tag{E1}$$

Let us fix the value of N . We have the formal expansion

$$V^{(N)\dagger}V^{(N)} = c_1 \mathbb{1} + \sum c_{i_1, \dots, i_j}^{\alpha_1, \dots, \alpha_j} A_{i_1}^{\alpha_1} \dots A_{i_j}^{\alpha_j}. \tag{E2}$$

Here, A_j^α are traceless local operators (with well-defined parity) that, together with $\mathbb{1}/\sqrt{d}$, form an orthonormal basis of local operators corresponding to site j , namely $\text{tr}(A_j^{\alpha\dagger}A_k^\beta) = \delta_{\alpha,\beta}\delta_{j,k}$, while $c_1, c_{i_1, \dots, i_j}^{\alpha_1, \dots, \alpha_j}$ are some complex coefficients. Note that, since $V^{(N)\dagger}V^{(N)}$ is even, the sum in equation (E2) is over all possible sequences $\{\alpha_j\}, \{i_j\}$ such that $\sum_j |\alpha_j| \equiv 0 \pmod{2}$, where $|\alpha_j|$ is the parity of A^{α_j} . Similar expansions hold for $W^{(N)\dagger}W^{(N)}, V^{(N)\dagger}W^{(N)}, W^{(N)\dagger}V^{(N)}$. Now, we can multiply equation (E1) by $1/d^N$ and take the trace: using the fact that $\mathcal{V}/\sqrt{d}, \mathcal{W}/\sqrt{d}$ are normal and non-degenerate with a spectral radius equal to 1, and lemma A.5 in [54], we immediately obtain $(1/d^N)\text{tr}[V^{(N)\dagger}V^{(N)}] = 1, (1/d^N)\text{tr}[W^{(N)\dagger}W^{(N)}] = 1, (1/d^N)\text{tr}[W^{(N)\dagger}V^{(N)}] = 0,$

and $(1/d^N)\text{tr} [V^{(N)\dagger}W^{(N)}] = 0$. In particular $c_1 = 1$ in equation (E2). Next, we show that $c_{i_1, \dots, i_j}^{\alpha_1, \dots, \alpha_j}$ in equation (E2) are all vanishing. To this end, we multiply both sides of equation (E1) by $A_{i_j}^{\alpha_j \dagger} \dots A_{i_1}^{\alpha_1 \dagger}$, with $\sum_j |\alpha_j| \equiv 0 \pmod{2}$, and take the trace, obtaining

$$0 = \text{tr} [M_{V,V}] + \text{tr} [M_{W,W}] + \text{tr} [M_{W,V}] + \text{tr} [M_{V,W}]. \tag{E3}$$

Here, $M_{V,V}$ is a product of matrices $\tilde{V}[i_j, \alpha_j]$ with elements $\tilde{V}_{\beta, \gamma}[i_j, \alpha_j] = \sum_{n,m} b_{\beta}^{n,m}[i_j, \alpha_j] \mathbb{V}_{\beta, \gamma}^{n,m}$, where $\mathbb{V}_{\beta, \gamma}^{n,m}$ corresponds to the tensor generating $V^{(N)\dagger}V^{(N)}$, as defined in equation (A31), while $b_{\beta}^{n,m}[i_j, \alpha_j]$ are complex numbers, determined by the choice of $A_{i_j}^{\alpha_j \dagger}$. The matrices $M_{W,W}$, $M_{W,V}$, $M_{V,W}$ are defined similarly. Note that there is no additional parity operator Z in the trace, which is due to the fact that $A_{i_j}^{\alpha_j \dagger} \dots A_{i_1}^{\alpha_1 \dagger}$ is even. Note also that $\text{tr} [M_{V,V}] = c_{i_1, \dots, i_j}^{\alpha_1, \dots, \alpha_j}$. Now, we consider a chain of kN sites, for $k \geq 1$. We repeat the steps above, but multiply by

$$A_{i_{j+(k-1)M}}^{\alpha_j \dagger} \dots A_{i_1+(k-1)M}^{\alpha_1 \dagger} A_{i_{j+(k-2)M}}^{\alpha_j \dagger} \dots A_{i_1+(k-2)M}^{\alpha_1 \dagger} \dots A_{i_j}^{\alpha_j \dagger} \dots A_{i_1}^{\alpha_1 \dagger}. \tag{E4}$$

We get

$$0 = \text{tr} [M_{V,V}^k] + \text{tr} [M_{W,W}^k] + \text{tr} [M_{W,V}^k] + \text{tr} [M_{V,W}^k], \tag{E5}$$

for all $k \geq 1$. Once again, using lemma A.5 in [54], we conclude that each trace in equation (E3) is vanishing, and thus $c_{i_1, \dots, i_j}^{\alpha_1, \dots, \alpha_j}$ in equation (E2) is zero, as anticipated. In conclusion, the operators $V^{(N)}$ and $W^{(N)}$ satisfy

$$V^{(N)\dagger}V^{(N)} = W^{(N)\dagger}W^{(N)} = \mathbb{1}, \tag{E6}$$

$$V^{(N)\dagger}W^{(N)} = W^{(N)\dagger}V^{(N)} = 0, \tag{E7}$$

where the second equality follows from the argument above, and the fact that $\text{tr} [V^{(N)\dagger}W^{(N)}] = \text{tr} [W^{(N)\dagger}V^{(N)}] = 0$. However, equations (E6) and (E7) are inconsistent with each other, and we have arrived at the desired contradiction. \square

We are now in a position to prove that any tensor \mathcal{U} generating one of the fMPUs introduced in section 6.1 is necessarily simple, according to definition 6.7.

Proposition E.2. *Suppose that the tensor \mathcal{U} generates a type-I (type-II) fMPU $U^{(N)}$ with ABCs. Then, $k \leq D^4$ exists, such that \mathcal{U}_k is simple (according to definition 6.7).*

Proof. The case for type-I fMPUs can be treated by following the same steps as in the proof of proposition III.3 in [33], so here we will only consider type-II fMPUs. Furthermore, in order to simplify the notation, we will make use of the formalism of graded TNs, explained in appendix B.

Let us consider a tensor \mathcal{U} generating a type-II fMPU with ABCs. Due to proposition E.1, we can assume w.l.o.g. that \mathcal{U} is a degenerate GNT. Using the graphical notation explained in appendix B, we can write



$$\text{Diagram} = E \otimes_{\mathfrak{g}} \mathbb{1} + \sum_{\alpha} \mathbb{S}_{\alpha} \otimes_{\mathfrak{g}} \sigma_{\alpha}. \tag{E8}$$

We stress that here and throughout this proof, pictures correspond to graded operators, and not to matrix elements. In particular, in the right-hand side, the first part of the graded tensor products acts on the auxiliary indices, whereas the second part acts on the physical ones. Furthermore, E is the TM associated with \mathcal{U} . Finally, we choose σ_α and \mathbb{S}_α to be traceless operators with well-defined parity, and with mutually orthogonal σ_α . By lemma D.7, the TM E has two eigenvalues equal to 1. Furthermore, there are no Jordan blocks associated with the eigenvalue 1, whereas there may be one or several Jordan blocks associated with the zero eigenvalues. Using $J < D^2$ to denote the largest size of all the Jordan blocks of E , we can block J sites and consider \mathcal{U}_J . Since \mathcal{U}_J also generates a type-II fMPU, we can use the decomposition (E8) for it, where we will denote the new operators by E' and \mathbb{S}'_α .

Next, we multiply both sides of $\mathbb{1} = U^{(N)\dagger}U^{(N)}$ by $(\sigma_1^{\alpha_1} \otimes_{\mathfrak{g}} \dots \otimes_{\mathfrak{g}} \sigma_m^{\alpha_m})^\dagger$, with $\sum_j |\alpha_j| \equiv 0 \pmod{2}$, where $|\alpha_j|$ is the parity of the operator $\sigma_m^{\alpha_m}$. We obtain

$$\text{tr}(E' S'_{\alpha_1} \dots S'_{\alpha_m}) = 0, \tag{E9}$$

where S'_α is the matrix associated with \mathbb{S}'_α , namely

$$\mathbb{S}'_\alpha = (S_\alpha)_{x,y} |x\rangle \otimes_{\mathfrak{g}} |y\rangle. \tag{E10}$$

Note that there is no additional parity operator Z in equation (E9), since $\sum_j |\alpha_j| \equiv 0 \pmod{2}$. Now, we can assume w.l.o.g. that \mathcal{U}_J is in GCFII, namely that the TM associated with \mathcal{U}_J is in the form

$$E' = |\rho^{(1)}\rangle (\Phi^{(1)}| + |\rho^{(2)}\rangle (\Phi^{(2)}|, \tag{E11}$$

where

$$|\Phi^{(1)}\rangle = \sum_{n=0}^{D-1} |n, n\rangle, \quad |\Phi^{(2)}\rangle = \sum_{n=0}^{D-1} |n, D-1-n\rangle, \tag{E12}$$

$$|\rho^{(1)}\rangle = \sum_{n=0}^{D-1} \rho_n |n, n\rangle, \quad |\rho^{(2)}\rangle = \sum_{n=0}^{D-1} \rho_n |n, D-1-n\rangle, \tag{E13}$$

with $\rho_n > 0$. We show that

$$(\Phi^{(a)} | S'_{\alpha_1} \dots S'_{\alpha_m} | \rho^{(b)}) = 0, \quad \text{for } a \neq b, \tag{E14}$$

for all sequences $\{\alpha_j\}$. Note that we also prove this for $\sum_j |\alpha_j| \equiv 1 \pmod{2}$. In particular, equation (E14) can be established using the explicit representation (E8). First, we note

$$\mathbb{S}'_\alpha = \sum_{\{i_n, k_n\}} c(\{i_n, k_n\}) \begin{array}{c} \bullet \quad \dots \quad \bullet \\ | \quad \dots \quad | \\ \text{---} \quad \dots \quad \text{---} \\ | \quad \dots \quad | \\ \circ \quad \dots \quad \circ \\ | \quad \dots \quad | \\ i_1 \quad \dots \quad i_J \end{array}. \tag{E15}$$

Here $c(\{i_n, k_n\})$ are numerical coefficients arising from expanding σ_α in equation (E8) in terms of the operators $|l\rangle \otimes_{\mathfrak{g}} |m\rangle$ and reordering. Next, recall that, due to equation (61),

$U^{j,k} = (\sigma^x)^{|j|+|k|} \otimes B^{j,k}$, and

$$\begin{array}{c}
 k \\
 | \\
 \bullet \\
 | \\
 \alpha \text{---} \beta \\
 | \\
 j \\
 | \\
 \circ \\
 | \\
 \gamma \text{---} \delta \\
 | \\
 i
 \end{array}
 = \mathbb{U}_{(\alpha,\gamma),(\beta,\delta)}^{k,i} |\gamma\rangle|\alpha\rangle|k\rangle\langle i| \langle\beta| \langle\delta|,$$
(E16)

where $\mathbb{U}_{(\alpha,\gamma),(\beta,\delta)}^{k,i}$ was defined in equation (A31), and corresponds to the matrix

$$\mathbb{U}^{k,i} = \sum_j (U^{*j,k} \otimes U^{j,i}) (Z^{(|i|+|k|)} \otimes \mathbb{1}),$$
(E17)

where $Z = \sigma^z \otimes \mathbb{1}$. We can now expand $(\Phi^{(a)}|S'_{\alpha_1} \dots S'_{\alpha_m} |\rho^{(b)})$ using the above expressions, arriving at

$$\begin{aligned}
 (\Phi^{(a)}|S'_{\alpha_1} \dots S'_{\alpha_m} |\rho^{(b)}) &= \sum_{\{i_n, j_n, k_n\}} \Lambda(\{i_n, j_n, k_n\}) \text{tr} \\
 &\times \left[(\sigma^x)^{a+1} (\sigma^x)^{\sum_s (|i_s|+|k_s|)} (\sigma^z)^{\sum_s (|i_s|+|k_s|)} (\sigma^x)^{b+1} \right],
 \end{aligned}$$
(E18)

where $\Lambda(\{i_n, j_n, k_n\})$ is a coefficient that does not depend on a and b , and whose exact form is irrelevant for our discussion. Here, we used the fact that the eigenstates $(\Phi^{(a)}|$ and $|\rho^{(a)}\rangle$, when viewed as operators, correspond to the matrices $(\sigma^x)^{a+1} \otimes \mathbb{1}$ and $(\sigma^x)^{a+1} \otimes \rho$ (importantly, ρ does not depend on a). Now, if $a \neq b$ then the traces on the right-hand side are all zero, because they are either proportional to $\text{tr}(\sigma^x)$ or $\text{tr}(\sigma^z)$, and equation (E14) follows immediately. Furthermore, since $\Lambda(\{i_n, j_n, k_n\})$ does not depend on a and b , we also have

$$(\Phi^{(1)}|S'_{\alpha_1} \dots S'_{\alpha_m} |\rho^{(1)}) = (\Phi^{(2)}|S'_{\alpha_1} \dots S'_{\alpha_m} |\rho^{(2)}).$$
(E19)

It now follows from equations (E9), (E14) and (E19) that

$$E' S'_{\alpha_1} \dots S'_{\alpha_m} E' = 0,$$
(E20)

if $\sum_j |\alpha_j| \equiv 0 \pmod{2}$. On the other hand, equation (E20) is also true if $\sum_j |\alpha_j| \equiv 1 \pmod{2}$. This is because equation (E14) still holds, and $\langle \Phi^{(j)} | \mathcal{O} | \rho^{(j)} \rangle = 0$ if \mathcal{O} is odd, since $\langle \Phi^{(j)} |$ and $|\rho^{(j)}\rangle$ are either both even or both odd.

Now, any element, S , in the algebra generated by S'_α must have zero eigenvalues. Indeed, whether S is even or odd, S^2 is even, and thus $\text{tr}(S^{2N}) = \sum_j \lambda_j^{2N} = 0$ for all N , where λ_j are the eigenvalues of S . This means that $\lambda_j^2 = 0$ for all j , and thus $\lambda_j = 0$ for all j . Accordingly, any element, S , in the algebra generated by S'_α is nilpotent. It follows then, from a result by Nagata and Higman [69, 70], improved later by Razmyslov [71], that some $J' < D^2$ exists, such that

$$S'_{\alpha_1} \dots S'_{\alpha_{J'}} = 0,$$
(E21)

for any set of α 's. At this point the proof can be completed by following the one of proposition III.3 in [33] without modification. □

Corollary E.3. *Let \mathcal{U} be a type-II fMPU, and d , d_e and d_o denote the dimensions of the local physical space, and the corresponding even and odd subspaces, respectively. Then, d is even, and $d_e = d_o$.*

Proof. We prove this by contradiction. First, note that if $d_e \neq d_o$, then the same is true by blocking arbitrarily many times. This can be simply proven by induction on the number of blocked sites, k , and using the rearrangement inequality. Then, take k such that \mathcal{U}_k is simple, and assume w.l.o.g. that \mathcal{U}_k is in the form (D1). Due to the structure of the eigenstates of the TM associated with eigenvalue 1, one can construct an fMPU $U_p^{(N)}$ with PBCs by adding an operator $X = \sigma^x \otimes \mathbb{1}$ into the trace (unitarity follows from simplicity and the fact that $(X \otimes X)E_{\mathcal{U}} = E_{\mathcal{U}}$). It is immediately clear that $U_p^{(N)}$ is an odd operator. However, this is a contradiction, because for any N the dimensions of the even and odd subspaces are different, and there can be no odd invertible operator. \square

Next, we show that the fMPUs introduced in section 6.1 feature a \mathbb{Z}_2 structure with respect to composition. In fact, it is obvious that the product of two type-I fMPUs is still a type-I fMPU. Analogously, using proposition 6.6, we know that the product of a type-I and a type-II fMPU is still a type-II fMPU. In the following, we also show that the product of two type-II fMPUs can be represented as a type-I fMPU. The proof closely follows the logic of similar derivations presented in [53], and shows that the class of fMPUs introduced in section 6.1 is closed with respect to composition.

Proposition E.4. *Let \mathcal{U} and \mathcal{V} be two degenerate GNTs, generating type-II fMPUs $U^{(N)}$, $V^{(N)}$. Then, a representation of $U^{(N)}V^{(N)}$ exists as a type-I fMPU $\forall N$.*

Proof. We use Z_U and Z_V to denote the parity operators acting on the auxiliary space for \mathcal{U} and \mathcal{V} , respectively, and assume w.l.o.g. that they are in the form of (27). Let \mathcal{W} be the tensor obtained by composing \mathcal{U} and \mathcal{V} . Up to an even similarity transformation, we have

$$\begin{aligned} W_{(\alpha,\gamma),(\beta,\delta)}^{k,i} &= \sum_j (-1)^{|\gamma|(|k|+|j|)} U_{\alpha,\beta}^{k,j} V_{\gamma,\delta}^{j,i}, \\ \Rightarrow W^{k,i} &= \sum_j (\mathbb{1} \otimes Z_V)^{|k|+|j|} (U^{k,j} \otimes V^{j,i}), \end{aligned} \tag{E22}$$

while the parity operator associated with \mathcal{W} is $Z_W = Z_U \otimes Z_V$. Since \mathcal{U} and \mathcal{V} are degenerate, we can write

$$U^{k,j} = (\sigma^x)^{|k|+|j|} \otimes B^{k,j}, \tag{E23}$$

$$V^{j,i} = (\sigma^x)^{|j|+|i|} \otimes C^{j,i}, \tag{E24}$$

and $Z_{U,V} = \sigma^z \otimes \mathbb{1}$, so that permuting the basis elements, we have

$$W^{k,i} = \sum_j [(\sigma^x)^{|k|+|j|} \otimes (\sigma^z)^{|k|+|j|} (\sigma^x)^{|j|+|i|}] \otimes B^{k,j} \otimes C^{j,i}. \tag{E25}$$

In this basis, the parity operator is $Z_W = \sigma^z \otimes \sigma^z \otimes \mathbb{1} \otimes \mathbb{1}$. We now define the permutation operator acting non-trivially only on the tensor product of the first two spaces,

$\Pi = \tilde{\Pi} \otimes \mathbb{1} \otimes \mathbb{1}$, where

$$\tilde{\Pi} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \quad (\text{E26})$$

We have $\tilde{\Pi}(\sigma^z \otimes \sigma^z)\tilde{\Pi}^{-1} = \sigma^z \otimes \mathbb{1}$, and also

$$\tilde{\Pi}(\sigma^x)^{|k|+|j|} \otimes (\sigma^z)^{|k|+|j|} (\sigma^x)^{|j|+|i|} \tilde{\Pi}^{-1} = (\sigma^x)^{|k|+|i|} \otimes r_{|k|,|i|,|j|}, \quad (\text{E27})$$

where

$$r_{0,0,0} = r_{1,1,1} = \mathbb{1}, \quad r_{0,0,1} = r_{1,1,0} = y, \quad (\text{E28})$$

$$r_{0,1,0} = r_{1,0,1} = \sigma^x, \quad r_{0,1,1} = r_{1,0,0} = \sigma^z, \quad (\text{E29})$$

and

$$y = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \quad (\text{E30})$$

Accordingly, using Π as a similarity transformation, we end up with a parity operator in the form of (27) and

$$W^{k,i} = (\sigma^x)^{|k|+|i|} \otimes D^{k,i}, \quad (\text{E31})$$

where

$$D^{k,i} = \sum_j r_{|k|,|i|,|j|} \otimes B^{k,j} \otimes C^{j,i}, \quad (\text{E32})$$

From equations (E28), (E29), (E31) and (E32), we see that the even subalgebra generated by $D^{k,i}$ commutes with the matrix $y \otimes \mathbb{1} \otimes \mathbb{1}$, and is thus reducible. Accordingly, there must be a graded invariant subspace for the matrix $W^{k,i}$. In particular, we can write the corresponding projectors as

$$P = \begin{pmatrix} \tilde{P} & 0 \\ 0 & \tilde{Q} \end{pmatrix} \quad Q = \mathbb{1} - P = \begin{pmatrix} \tilde{Q} & 0 \\ 0 & \tilde{P} \end{pmatrix} \quad (\text{E33})$$

where

$$\tilde{P} = \frac{(1 - iy)}{2} \otimes \mathbb{1}, \quad \tilde{Q} = \frac{(1 + iy)}{2} \otimes \mathbb{1}. \quad (\text{E34})$$

Now, $[P, Z_W] = 0$, and $W^{k,i}P = PW^{k,i}P$, so that we can replace the tensors $W^{k,i}$ with $W^{k,i} = PW^{k,i}P + QW^{k,i}Q$, and the product $U^{(N)}V^{(N)}$ decomposes as the sum of two fMPOs. It is easy to see that these are exactly the same. This can be seen as follows. First we rewrite

$$W^{k,i} = \begin{pmatrix} D^{k,i} & 0 \\ 0 & D^{k,i} \end{pmatrix}, \quad |i| + |k| = 0 \quad (\text{E35a})$$

$$W^{k,i} = \begin{pmatrix} 0 & D^{k,i} \\ D^{k,i} & 0 \end{pmatrix}, \quad |i| + |k| = 1, \quad (\text{E35b})$$

so that

$$PW^{k,i}P = \begin{pmatrix} \tilde{P}D^{k,i}\tilde{P} & 0 \\ 0 & \tilde{Q}D^{k,i}\tilde{Q} \end{pmatrix}, \quad |i| + |k| = 0 \quad (\text{E36a})$$

$$PW^{k,i}P = \begin{pmatrix} 0 & \tilde{P}D^{k,i}\tilde{Q} \\ \tilde{Q}D^{k,i}\tilde{P} & 0 \end{pmatrix}, \quad |i| + |k| = 1, \quad (\text{E36b})$$

and

$$QW^{k,i}Q = \begin{pmatrix} \tilde{Q}D^{k,i}\tilde{Q} & 0 \\ 0 & \tilde{P}D^{k,i}\tilde{P} \end{pmatrix}, \quad |i| + |k| = 0 \quad (\text{E37a})$$

$$QW^{k,i}Q = \begin{pmatrix} 0 & \tilde{Q}D^{k,i}\tilde{P} \\ \tilde{P}D^{k,i}\tilde{Q} & 0 \end{pmatrix}, \quad |i| + |k| = 1. \quad (\text{E37b})$$

It is now straightforward to see that $PW^{k,i}P = SQW^{k,i}QS^{-1}$, where $S = \sigma^x \otimes \mathbb{1}$, and $PZ_W P = -SQZ_W QS^{-1}$. Since the overall sign of the parity does not play any role, and recalling the overall factor $1/2$ coming from the product of the prefactors $1/\sqrt{2}$, we find that $U^{(N)}V^{(N)}$ can be represented as a type-I fMPU generated by the (even) tensor $PW^{k,i}P$. \square

Finally, we can now prove the main result of Section 6.2, namely the equivalence between fQCA and fMPUs of the first and second kinds.

Proposition E.5. *Up to appending an inert ancillary fermionic d.o.f., any type-I or type-II fMPU with ABCs is a 1D fQCA and vice versa.*

Proof. Any simple tensor obviously generates a locality-preserving fMPU, so we only need to show that any fQCA can be represented as a type-I or type-II fMPU. In fact, this is almost trivial if we recall that one of the main results derived in [46], states that, after blocking and appending a finite number of fermionic ancillas, any 1D fQCA can be obtained by composing a finite number of the following elementary operations: (i) translations of fermionic modes (as defined in equations (22) and (23)); (ii) translations of Majorana modes; (iii) depth-two quantum circuits made of unitaries u and v acting on neighboring sites (importantly, u and v must have well-defined parity, which we can assume to be even w.l.o.g.). In section 5.2, we have already shown that Majorana-shift operators can be represented by type-II fMPUs. Furthermore, it is straightforward to verify that translations of fermionic modes are implemented by type-I fMPUs, with equal bond and physical dimensions and tensors $T_{\alpha,\beta}^{i,j} = \delta_{j\beta}\delta_{i\alpha}$. It is also simple to see that quantum circuits can be represented by type-I fMPUs. This can be done by following the construction for qudits, as explicitly carried out, e.g. in [34], and showing that one can always decompose the unitaries u and v in terms of even tensors. As a last step, one needs to show that an arbitrary product of type-I and type-II fMPUs can be represented as an fMPU of type I or type II. This follows from proposition E.5, so that, putting all these together, the statement is proven. \square

E.2. Index theory for fMPUs with ABC

Let $U^{(N)}$ be a type-II fMPU in the standard form (87), and use $\tilde{\mathcal{U}}$ and \mathcal{M} to denote the tensors in GCF associated with $\tilde{U}^{(N)}$ and $M_A^{(N)}$, respectively. \mathcal{U} denotes the tensor obtained by composing $\tilde{\mathcal{U}}$ and \mathcal{M} , and let k be such that $\tilde{\mathcal{U}}_k$ is simple. Then, it is shown in lemma 7.9 that the exponentiated index for \mathcal{U}_q with $q \geq 2k$ is $\mathcal{I}_f = \sqrt{2}\tilde{\mathcal{I}}_f$, where $\tilde{\mathcal{I}}_f$ is the index of $\tilde{\mathcal{U}}_k$. Now, the tensor \mathcal{U}_q , obtained by composing $\tilde{\mathcal{U}}_q$ and \mathcal{M}_q , is not necessarily in GCF, so that one needs to make sure that the index of \mathcal{U}_q coincides with that computed in the corresponding GCF. In the following, we show that this is true if we block \tilde{q} times, with $\tilde{q} \geq 4k$.

Lemma E.6. *Using the previous notations, the index of the tensor $\mathcal{U}_{\tilde{q}}$ is the same as the one computed in the corresponding GCF, where $\tilde{q} \geq 4k$.*

Proof. First, from the explicit graphical representation, it can immediately be shown that $\mathcal{W} = \mathcal{U}_{\tilde{q}}$ is simple, and that the TM reads $E_{\mathcal{W}} = |\rho_1\rangle\langle\Phi_1| + |\rho_2\rangle\langle\Phi_2|$, where $|\rho_1\rangle, |\phi_1\rangle$ are even, when seen as operators acting in the auxiliary space, and $|\rho_2\rangle, |\phi_2\rangle$ are odd. Let P and Q be the orthogonal projectors onto the support of Φ_1 and ρ_1^* , respectively, where ρ_1^* is the complex conjugate of ρ_1 . We claim that $\mathcal{W}P = \mathcal{W}$ (where matrix multiplication is intended from right to left, as usual). To this end, we need to show that if $|v\rangle$ is a state in the auxiliary space, such that $P|v\rangle = 0$ and $P^\perp|v\rangle = |v\rangle$, then

$$|w\rangle = W_{\alpha,\beta}^{n,m} |\alpha\rangle |n\rangle \langle m| (\beta|v) = 0, \tag{E38}$$

where $W_{\alpha,\beta}^{n,m}$ denotes the matrix elements associated with \mathcal{W} . First, we note that since Φ_1 is even, its support is a graded subspace, and P is an even operator. Then, we can assume w.l.o.g. that v is even, and compute

$$(w|w) = \text{tr}_{\mathcal{W}} \left(\begin{array}{c} \text{---} \\ \text{---} \end{array} \right)_{E_{\mathcal{W}}} \begin{array}{c} |v\rangle \\ |v\rangle \end{array} = \text{tr}_{\mathcal{W}} \left(\begin{array}{c} \text{---} \\ \text{---} \end{array} \right)_{\rho_2|\Phi_2} \begin{array}{c} |v\rangle \\ |v\rangle \end{array}, \tag{E39}$$

where we used the fact that $\Phi_1|v\rangle = 0$ (since $P|v\rangle = 0$, and P projects onto the support of Φ_1). We see now that the right-hand side of equation (E39) is zero, because it is proportional to the trace of ρ_2 . Indeed, the latter is zero, since ρ_2 an odd operator. In the same way, one can see that $Q\mathcal{W} = \mathcal{W}$. Then, it is easy to show that $\Phi_2P = \Phi_2$, and $Q\rho_2 = \rho_2$. Now, following the proof of proposition IV.5 in [33], we show how to obtain the GCF of \mathcal{W} using P and Q . To this end, we use Jordan’s lemma, which guarantees a decomposition of the space $\mathbb{C}^D = (\bigoplus_i \mathbb{C}^2) \oplus \mathbb{C}^k$ such that, in that basis, $P = \bigoplus_i |0\rangle\langle 0|_i \oplus R$, $Q = \bigoplus_i |v_i\rangle\langle v_i| \oplus S$, where R and S are commuting projectors on \mathbb{C}^k . We can choose $|0\rangle\langle 0|_i, |v_i\rangle\langle v_i|, R, S$ to be all even operators. Let us now define the (even) projector $\tilde{P} := \bigoplus_i |0\rangle\langle 0|_i \oplus RS$. We have the following properties:

- (a) $P\tilde{P} = \tilde{P}$;
- (b) $PQ = \tilde{P}Q$;
- (c) $QP = Q\tilde{P}$;
- (d) There exists an invertible Y such that $\tilde{P}QY = \tilde{P}$.

We claim that $\tilde{\mathcal{W}} := \tilde{P}\mathcal{W}\tilde{P}$ is the GCF of \mathcal{W} , when restricted to the range of \tilde{P} . First, using the properties above, it is straightforward to see that $\tilde{\mathcal{W}}$ and \mathcal{W} define the same fMPU for all N . Next, we need to show that $\tilde{\mathcal{W}}$ is a degenerate GNT. To this end, we observe that the transfer operator of $\tilde{\mathcal{W}}$ is $X \mapsto \text{tr}(\tilde{P}\Phi_1\tilde{P}X)\tilde{P}\rho_1\tilde{P} + \text{tr}(\tilde{P}\Phi_2\tilde{P}X)\tilde{P}\rho_2\tilde{P}$. Using the properties of the projector \tilde{P} , it can immediately be seen that $\tilde{P}\rho_i\tilde{P}$ and $\tilde{P}\Phi_i\tilde{P}$ are the left and right eigenvectors. Furthermore, they are even (odd) for $i = 1$ ($i = 2$), since \tilde{P} is even, and using the properties of \tilde{P} one can easily see that both $\tilde{P}\rho_1\tilde{P}$ and $\tilde{P}\Phi_1\tilde{P}$ are full rank in the range of \tilde{P} . Invoking proposition D.9 in appendix E, we find that $\tilde{\mathcal{W}}$ is a degenerate GNT.

Next, we show that $\tilde{\mathcal{W}}$ has the same left and right ranks as the tensor $\hat{\mathcal{W}} = \sqrt{\Phi_1}\mathcal{W}\sqrt{\rho_1^*}$, where, again, matrix multiplication is intended from right to left. For this, we take invertible matrices X, Y , and Z such that $X\sqrt{\Phi_1} = P$, $\sqrt{\rho_1^*}Z = Q$ (this can always be done: taking Z' invertible such that $Z'\sqrt{\rho_1^*} = Q$, we have $Z = Z'^{\dagger}$) and $PQY = \tilde{P}$. Then, it is simple to show that $Z\hat{\mathcal{W}}ZY = \tilde{\mathcal{W}}$, which proves the claim.

Finally, we show that the rank of $\mathcal{U}_{\tilde{q}}$ is the same as $\hat{\mathcal{W}}$. Using that fact that for any operator $\text{rank}(A) = \text{rank}(A^{\dagger}A)$, we have

$$\text{rank} \left(\begin{array}{c} \text{---} \\ | \\ \boxed{\mathcal{U}_{\tilde{q}}} \\ | \\ \text{---} \end{array} \begin{array}{c} \text{---} \\ \circlearrowright \sqrt{\rho_1} \\ \text{---} \end{array} \right) = \text{rank} \left(\begin{array}{c} \text{---} \\ | \\ \boxed{\mathcal{U}_{\tilde{q}}} \\ | \\ \text{---} \end{array} \begin{array}{c} \text{---} \\ \circlearrowright \rho_1 \\ \text{---} \end{array} \right) \tag{E40}$$

where we separate input and output with a gray dotted line, and where we denote the tensor $\mathcal{U}_{\tilde{q}}$ by a black box. Note that the cut determines the order of multiplication of the matrices involved. Next, define

$$\mathcal{V}_{\tilde{q}} = \begin{array}{c} \boxed{\mathcal{U}_{\tilde{q}}} \\ | \\ \circlearrowright \tilde{\rho} \\ | \\ \boxed{\mathcal{M}_{\tilde{q}}} \end{array} \tag{E41}$$

where $\tilde{\rho}$ is the right eigenstate associated with eigenvalue 1 of the TM $E_{\tilde{\mathcal{U}}}$. Since $\tilde{\mathcal{U}}$ is in GCF, the rank of $\tilde{\rho}$ is maximum, and clearly the left and right ranks for $\mathcal{V}_{\tilde{q}}, \mathcal{U}_{\tilde{q}}$ coincide. Finally, using once again the fact that $\text{rank}(A) = \text{rank}(A^{\dagger}A)$, we also have

$$\text{rank} \left(\begin{array}{c} \text{---} \\ | \\ \boxed{\mathcal{V}_{\tilde{q}}} \\ | \\ \text{---} \end{array} \right) = \text{rank} \left(\begin{array}{c} \text{---} \\ | \\ \boxed{\mathcal{V}_{\tilde{q}}} \\ | \\ \text{---} \end{array} \begin{array}{c} \text{---} \\ \circlearrowright \rho_1 \\ \text{---} \end{array} \right) \tag{E42}$$

Now, it is straightforward to verify that

$$\rho_1 = \begin{array}{c} \text{---} \\ | \\ \boxed{E_{\mathcal{U}}} \\ | \\ \text{---} \end{array} \begin{array}{c} \text{---} \\ \circlearrowright \tilde{\rho} \\ \text{---} \end{array} \tag{E43}$$

Here, we have used the fact that the right even eigenvector associated with the TM $E_{\tilde{\mathcal{M}}}$ is simply the identity. We can now plug this expression into the right-hand side of equation (E40), and express $\mathcal{U}_{\tilde{q}}$ in terms of \mathcal{U} . Finally, recalling that \mathcal{U}_k is simple, and making use of equation (89) for the Majorana shift operator, after a straightforward

calculation we obtain the right-hand side of equation (E42), so that the left-hand sides of equations (E40) and (E42) also coincide. Hence, since the ranks for $\mathcal{V}_{\bar{q}}$ and $\mathcal{U}_{\bar{q}}$ are the same, we have just proved that multiplying on the right by $\sqrt{\rho_1}$ does not change the rank. In a similar way, using the fact that $\text{rank}(A) = \text{rank}(AA^\dagger)$, we can show that the rank does not change by multiplying the input auxiliary space by $\sqrt{\Phi_1^*}$. Finally, the same argument can be used for the NE–SW cut, thus completing the proof. \square

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