One-dimensional SPT phases protected by frieze symmetries

Bram Van Craeynest-de Cuiper, Nicolas Dewolf, Jutho Haegeman, and Frank Verstraete

Department of Physics and Astronomy, Ghent University, Krijgslaan 281, 9000 Gent, Belgium
KERMIT, Department of Data Analysis and Mathematical Modelling, Ghent University, Belgium

We undertake a systematic study of symmetry-protected topological gapped phases of quantum spin chains in the presence of the quasi-one-dimensional frieze space groups. Here, the spatial symmetries of the one-dimensional lattice are considered together with an additional ‘vertical reflection’, which we take to be an on-site $Z_2$ symmetry. We identify seventeen distinct non-trivial phases and define canonical forms. If time-reversal is combined with a shift over one site, then no new topological phases arise. We furthermore construct explicit renormalization-group fixed point wavefunctions for symmetry-protected topological phases with global on-site symmetries, and demonstrate how group cohomology can be computed using the Smith normal form.

I. INTRODUCTION

Even though there is no intrinsic topological order in gapped one-dimensional quantum spin chains, the phase diagram becomes non-trivial when symmetry constraints are taken into account [1–9]. This gives rise to so-called symmetry protected topological (SPT) order. The intuition behind the lack of topological order in 1D is the following. Starting from the ground state of a gapped local Hamiltonian, subsequent renormalization group (RG) transformations do not alter the phase of the system [10]. After sufficiently many steps independent of system size, the state flows towards an RG fixed point that is of a valence bond structure [5, 9, 10]. A tensor product of unitaries on the state then turns this state in a trivial product state, ultimately proving that the state we started from is adiabatically connected to a product state with no topological order. This procedure can be made explicit by writing the state as a matrix product state (MPS) [11, 12]. In this formalism one RG step is equivalent to blocking two sites and acting with an isometry on the blocked site that maximally removes local entanglement inside the block while retaining the entanglement with the rest of the system [10]. When symmetries are taken into account, the RG flow should not break the symmetry. The picture that arises is that the phase diagram, which in the absence of symmetries is simply connected, falls apart in distinct classes that cannot be connected by adiabatic transformations due to topological obstructions.

Chen et al. showed that the topological obstructions that prohibit connecting different such SPT phases originate from the fact that physical symmetries can be implemented by projective representations of the symmetry group acting on the entanglement degrees of freedom [5–7]. This crucial insight led Chen et al. to a classification of SPT phases in terms of group cohomology. More specifically, the SPT classification corresponds to the second cohomology group $H^2$ of $\mathbb{G} \times U(1)$, where $\mathbb{G}$ denotes the symmetry group and can contain a global on-site symmetry subgroup, time-reversal, parity or combinations thereof. A folklore example is the case where the global on-site symmetry group is $Z_2 \times Z_2$. Since the second cohomology group of $Z_2 \times Z_2$ is $H^2 (Z_2 \times Z_2, U(1)) = Z_2$, $Z_2 \times Z_2$ can protect one non-trivial symmetry protected Haldane phase [2, 3, 13, 14]. In translation invariant systems, the classification is refined to $H^1 (\mathbb{G}, U(1)) \times H^2 (\mathbb{G}, U(1))$ where $H^1$ denotes the first cohomology group [4].

In this paper, we demonstrate that SPT phases can also be protected by quasi one-dimensional lattice symmetries. The symmetry groups we consider are the seven so-called frieze groups [15]. These are defined as being the infinite discrete subgroups of the isometries of a strip, $\text{Isom}(\mathbb{Z} \times \mathbb{R})$. Apart from translations, the generators of the frieze groups are reflections in the horizontal or vertical direction, $\pi$-rotations (equivalent to the composition of a horizontal and vertical reflection) and glide reflections. The seven distinct frieze groups these generators give rise to are denoted by $F_0$ (only translation), $F_V$ (translation + vertical reflection), $F_H$ (translation + horizontal reflection), $F_{HR}$ (translation + $\pi$-rotation), $F_G$ (translation + glide reflection), $F_{HRG}$ (translation + $\pi$-rotation + glide reflection) and $F_{VH}$ (translation + two reflections). In case there is a glide reflection, doing this glide reflection twice is equivalent to the action of the translation generator.

We derive the SPT classification corresponding to these symmetries by imposing the symmetry on a general injective MPS and identifying topologically distinct ways in which this symmetry can be implemented. Here, the vertical reflection corresponds to an on-site $Z_2$ symmetry of the system, which we represent explicitly as a swap between two physical degrees of freedom associated with every site. In this way, we obtain seventeen non-trivial phases. We construct explicit canonical representative MPS ansätze that belong to each of these phases and give an interpretation of these phases in terms of group cohomology.

Outline: We begin by providing a review of matrix product states, recapitulating the concepts of MPS injectivity, gauge transformations, the transfer matrix and the fundamental theorem of MPS. After a small review of
the implementation of symmetries in MPS and how this leads to the SPT classification of Chen et al., we present explicit MPS tensors transforming according to given cohomology classes characterizing an SPT phase. In Section IV we derive the SPT classification for frieze symmetric MPS and construct canonical forms for all of these phases. We reconsider the problem of imposing time-reversal symmetry in MPS in Section V and combine time-reversal with shifts over one site. A brief review of group cohomology is provided in Appendix A and in Appendix B we provide a method to compute group cohomology using the Smith normal form.

Summary of results

In Table I below we give an overview of the symmetry groups we consider and the SPT classification they give rise to.

Translation symmetry in itself does not give rise to non-trivial SPT phases. It can be shown that every translational invariant MPS admits a uniform representation [12]. The reflection in the \( F_V \) symmetry group can be thought of as an on-site \( \mathbb{Z}_2 \) symmetry. We find one non-trivial phase and show that there always exists a gauge in which the MPS tensors have definite \( V \)-parity. The reflection in \( F_H \) is equivalent to the parity considered in [5]. Three non-trivial SPT phases are found, in accordance with [5], and a canonical form is found in which the tensors have definite \( H \)-parity, possibly at the cost of introducing non-trivial bond tensors [16]. The same result is found for \( F_R \)-symmetric MPS. \( F_G \) symmetry admits only the trivial phase and we show that every \( F_G \)-symmetric MPS can be brought in a manifestly \( F_G \)-invariant form. In case of the larger symmetry groups \( F_{RG} \) and \( F_{VH} \) there are respectively three and seven non-trivial phases.

| Symmetry | SPT classification |
|----------|--------------------|
| \( F_0 \) | \( \mathbb{Z}_2 \) |
| \( F_V \) | \( \mathbb{Z}_2 \times 2 \) |
| \( F_H \) (Parity) | \( \mathbb{Z}_2 \times 2 \) |
| \( F_R \) | \( \mathbb{Z}_2 \) |
| \( F_G \) | \( \mathbb{Z}_2 \times 2 \) |
| \( F_{RG} \) | \( \mathbb{Z}_2 \times 3 \) |
| \( F_{VH} \) | \( \mathbb{Z}_2 \) |
| \( F_{V}^{T_i} \) | \( \mathbb{Z}_2 \) |
| \( F_{2}^{T_i/r} \) | \( \mathbb{Z}_2 \) |

TABLE I. \( F_i^{T_j} \): translation invariance over one site and a linear implementation of time reversal, \( F_i^{T_i/r} \): translation invariance over two sites and a linear - or projective implementation of time-reversal

II. REVIEW OF MATRIX PRODUCT STATES

In this paper we consider bosonic spin systems. The Hilbert space is simply the tensor product of the local \( d \)-dimensional Hilbert spaces of the constituent spins, \( \mathcal{H} \cong (\mathbb{C}^d)^{\otimes N} \). A matrix product representation of a state in \( \mathcal{H} \) with periodic boundary conditions is of the form

\[
|\psi\rangle = \sum_{\{i_k\}} \text{Tr} (A_{i_1}^{i_1} A_{i_2}^{i_2} \ldots A_{i_N}^{i_N}) |i_1\rangle |i_2\rangle \ldots |i_N\rangle. \tag{1}
\]

A periodic MPS can be pictorially represented as:

\[
\begin{array}{c}
\cdots \rightarrow A_1 \rightarrow A_2 \rightarrow \cdots \rightarrow A_N.
\end{array} \tag{2}
\]

The variational degrees of freedom are contained in the local tensors \( (A_i^j)_{\alpha\beta} \in \mathbb{C}^D \otimes \mathbb{C}^D \otimes \mathbb{C}^d \), where \( D \) is called the bond dimension. Every state in \( \mathcal{H} \) can be represented with a bond dimension that scales exponentially in the system size, but the power of matrix product states lies in the fact that ground states of gapped Hamiltonians can be well approximated by MPS with a bond dimension that scales polynomially in the number of spins. An MPS representation of a state \( |\psi\rangle \) is never unique: a gauge transformation \( A_i^j \rightarrow X_i A_i^j X_{i+1}^{-1} \) clearly leaves the state invariant because the gauge tensors \( X_i \) cancel on the bonds.

In case of translation invariance, it can be shown that one can always carry out a gauge transformation that brings the translationally invariant MPS in a canonical uniform form in which \( A_i \equiv A, \forall i [12] \):

\[
|\psi(A)\rangle = \cdots \rightarrow A \rightarrow A \rightarrow \cdots. \tag{3}
\]

Gauge transformations can furthermore be used to bring the MPS parameterization in a left- or right-canonical form, characterized respectively by:

\[
\sum_i (A_i^i)^\dagger A_i^i = 1, \quad \begin{array}{c}
\cdots \rightarrow A \rightarrow A \rightarrow \cdots.
\end{array} \tag{4}
\]

\[
\sum_i A_i^i (A_i^i)^\dagger = 1, \quad \begin{array}{c}
\cdots \rightarrow A \rightarrow A \rightarrow \cdots.
\end{array} \tag{5}
\]

We define the transfer matrix \( \mathcal{E} \) as

\[
\mathcal{E} = \sum_i A_i^i \otimes A_i^i \rightarrow A \rightarrow A. \tag{6}
\]

The transfer matrix captures all the relevant information about the entanglement and correlations of the
state. Moreover, the transfer matrix determines the MPS uniquely up to a local change in basis. This follows from the observation that the transfer matrix defines a completely positive (CP) map where the local MPS tensors play the role of Kraus operators, combined with the fact that a Kraus decomposition of a CP map is unique up to unitary equivalence [17]. If the matrices \( \{ A^i | i = 1, ..., d \} \) generate (via linear combinations and products) the entire \( D \times D \) matrix algebra, the MPS is said to be injective. In that case, the transfer matrix (interpreted as an \( D^2 \times D^2 \) matrix from the left pair of indices to the right pair) has a unique eigenvalue of largest magnitude that in an appropriate normalization of the MPS tensors can be taken to be one. Moreover, when the MPS is in a left - or right canonical form, the corresponding eigenvector is \( 1 \) as follows from (4-5).

By far the most important property of injective MPS is that it satisfies the requirements of the fundamental theorem of MPS: two injective uniform MPS defined by local tensors \( A^i \) and \( B^i \) describe the same state \( | \psi(A) \rangle \sim | \psi(B) \rangle \) if and only if there is a gauge transformation \( X \) and a phase \( \exp(i\theta) \) that intertwines the two tensors: \( A^i = e^{i\theta} X B^i X^{-1} \). If \( A \) and \( B \) are simultaneously in left (or right) canonical form, then \( X \) can be chosen unitary. Furthermore, \( e^{i\theta} \) is uniquely defined, whereas \( X \) is only defined up to an overall scaling. Put differently, for \( B = A \), the relation \( A^i = e^{i\theta} X A^i X^{-1} \) implies \( \theta = 0 \mod 2\pi \) and \( X = e^{i\theta} \) for some \( \theta \in \mathbb{C} \), as follows readily from the definition of injectivity.

### III. EXPLICIT SYMMETRIC TENSORS

If an injective translation-invariant MPS \( | \psi(A) \rangle \) is invariant under the action of a unitary on-site symmetry transformation, i.e. \( U_g^N | \psi(A) \rangle \sim | \psi(A) \rangle \) for all \( g \in G \), there must exist, for every \( g \in G \), a phase \( \varphi(g) \) and a gauge transform \( X_g \) such that

\[
\sum_j (U_g)_{ij} A^j = e^{i\varphi(g)} X^{-1}_g A^i X_g. \tag{7}
\]

This equation can only admits solutions if \( U_g \) forms a linear unitary representation of the on-site symmetry group \( G \). If \( A \) is either left or right canonical form, the gauge matrices \( X_g \) can be chosen unitary. Because of the overall scale freedom in how they are determined, it follows that they only need to constitute a projective representation of \( G \), i.e. they form a representation of \( G \) up to phase:

\[
X_g X_h = e^{i\omega(g,h)} X_{gh}. \tag{8}
\]

Here, the phases \( \omega(g,h) \) satisfy the well-known 2-cocycle equations (A2), expressing associativity of the multiplication of the \( X_g \). Solutions to this stringent constraint are called 2-cocycles. The phase \( \varphi(g) \), on the other hand, constitutes a one-dimensional linear representation of the symmetry group:

\[
\varphi(g) + \varphi(h) = \varphi(gh) \mod 2\pi. \tag{9}
\]

The scale freedom in determining gauge transforms implies that the matrices \( X_g \) can be replaced with an equivalent choice of the form \( X_g \mapsto e^{i\gamma(g)} X_g \). Hence, in the classification of projective representations labeled by 2-cocycles, these redefinitions have to be modded out, giving rise to equivalence classes of projective representations. These equivalence classes are exactly classified by the second cohomology group of \( G \) with respect to \( U_1, H^2(\mathbb{G}, U_1) \). In the context of group cohomology, the one-dimensional linear representation \( \varphi(g) \) is referred to as a 1-cocycle and is correspondingly characterized by \( H^1(\mathbb{G}, U_1) \) (Appendix A). Chen et al. showed that every choice of a 1-cocycle \( \varphi \in H^1(\mathbb{G}, U_1) \) and cohomology class \( [\omega] \in H^2(\mathbb{G}, U_1) \) gives rise to a distinct SPT phase [5].

In case of a finite symmetry group, the second cohomology group is always \( \mathbb{Z}_2 \times \mathbb{Z}_2 \times \ldots \times \mathbb{Z}_{d_N} \) for integers \( d_1, d_2, ..., d_N \), giving rise to a finite number of SPT phases. Explicit representative 2-cocycles can be obtained by writing the 2-cocycle condition as a linear system modulo \( 2\pi \) and solving it using the Smith normal form (Appendix B).

In case the symmetry group contains time-reversal or parity transformations, the above picture has to be modified as follows. Since the \( \mathbb{Z}_2 \) time-reversal is implemented anti-unitarily [18], the time-reversal operator can be written as a \( T = USK \), where \( K \) denotes complex conjugation in some basis and \( U \) is a unitary satisfying \( U^T = \pm 1 \) depending on whether time-reversal is implemented linearly or projectively (Section V A). Hence, on the MPS tensors, a symmetry \( g \in G = H \times \mathbb{Z}_2 \), \( H \) denoting the global on-site symmetry group, acts according to

\[
\sum_j (U_j)_{ij} C_g(A^j) = X_g^{-1} A^i X_g. \tag{10}
\]

The action of \( C_g \) on \( A^i \) is taking a complex conjugate only if \( g \) contains a time-reversal. From acting with time-reversal twice on the MPS tensor, it follows that in this case the matrices \( X_g \) form a generalized projective representation of the symmetry group, as their multiplication also contains the action \( C_g \):

\[
X_g C_g(X_h) = e^{i\omega(g,h)} X_{gh}, \tag{11}
\]

whereas the phases \( \exp(i\varphi(g)) \) obey

\[
e^{i\varphi(g)} C_g(e^{i\varphi(g)}) = e^{i\varphi(gh)}. \tag{12}
\]

Hence, \( \varphi(g) \) and \( \omega(g,h) \) satisfy the 1- and 2-cocycle constraints with a non-trivial group action that takes the conditioned complex conjugation \( C_g \) into account. The SPT classification in this case is given by \( H^1_G(\mathbb{G}, U_1) \times H^2_B(\mathbb{G}, U_1) \), where the subscripts \( \alpha \), \( \beta \) refer to the
non-trivial group actions originating from $C_g$. We refer to Appendix A for further details.

In case the symmetry group contains global on-site symmetries combined with parity, $G = H \times \mathbb{Z}_2^P$, we have that

$$\sum_j (U_g)_{ij} T_g (A^j) = X_g^{-1} A^j X_g,$$

(13)

where $T_g$ denotes taking the transpose if $g$ contains the parity transformation. Similarly as in the case of time-reversal, the gauge matrices multiply according to a generalized projective representation. Note, however, that if $g$ contains the parity transformation, $X_g$ can in general not be chosen unitary. As the conditioned transpose does not affect the phases $\phi$, they form a one-dimensional linear representation. The SPT classification for $H \times \mathbb{Z}_2^P$ is thus in terms of $H^1(G, U_1) \times H_2^p(G, U_1)$ (see Appendix A for further details).

Given some SPT phase characterized by $(\varphi, [\omega]) \in H^1(G, U_1) \times H_2^p(G, U_1)$, it is possible to explicitly construct zero-correlation-length MPS tensors that transform according to (7), (10) or (13). Firstly, a projective representation $X_g$ in the class $[\omega]$ can be constructed with dimension $|G|$, by modifying the (left or right) regular representation of $G$ (see Appendix A). The dimension of the local physical Hilbert space is then chosen as $|G|^2$. Concretely, this representative state and the regular representation is given by:

$$\begin{align*}
(X_g)_{g_1, g_2} &= \delta_{g_1, g_2} e^{i\varphi(g_2)} \\
(A^{h_1, h_2})_{g_1, g_2} &= \frac{1}{|G|} \delta_{h_1, g_1} \delta_{h_2, g_2} e^{i\varphi(h_2) + i\omega(h_2, h_2^{-1} h_1)}.
\end{align*}$$

(14)

(15)

Furthermore, the physical group action $U_g$ is given by $L_g \otimes L_g$, with $L_g$ the left regular representation. Hence, $(U_g)_{k_1 k_2, h_1 h_2} = \delta_{k_1, g_1} \delta_{k_2, h_2}$. Note that the Kronecker delta in the definition of the MPS tensor indicate its valence bond structure, which is modified only by a unitary diagonal transformation. Hence, it follows readily that the transfer matrix $E = \sum_{h_1, h_2} (A^{h_1, h_2})_{g_1, g_2} \otimes (A^{h_1, h_2})_{g_1', g_2'}$ is idempotent, $E^2 = E$, implying that the ansatz (15) has zero correlation length and thus defines an RG fixed point [10].

**IV. FRIEZE SYMMETRIC MPS**

In this section we derive the SPT classification of MPS invariant under frieze symmetries. We do so from starting from a general injective MPS and invoking the symmetry, which ultimately leads to topological indices that cannot be changed by a symmetry-preserving constant depth quantum circuit.

We introduce following notation:

$$\mathbb{1}_{n,m} = \mathbb{1}_n \oplus \mathbb{1}_m.$$  

(16)

This matrix satisfies $\mathbb{1}_{n,m} \mathbb{1}_{n,m}^\top = \mathbb{1}_{n,m}^{-1}$. Furthermore:

$$\Gamma = \mathbb{1}_n \otimes \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = -\Gamma^\top = -\Gamma^{-1}.$$  

(17)

And finally:

$$\sqrt{\Gamma} = \mathbb{1}_n \otimes \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}, \quad \sqrt{\Gamma}^\top = \sqrt{\Gamma}^{-1}.$$  

(18)

**F0** As mentioned in the introduction, every translationally invariant MPS can be brought in a uniform form by an appropriate gauge transformation [12]. There are no topological obstructions to do so and hence there are no non-trivial SPT phases.

**FV** Reflection around the horizontal axis can be thought of as an internal $\mathbb{Z}_2$ transformation of the MPS tensors. In order to impose such a reflection, we consider a uniform MPS with two physical legs that mimic some internal structure of the local degrees of freedom,

$$\cdots \quad A \quad A \quad A \quad \cdots.$$

(19)

Under the reflection the tensor $A$ transforms according to

$$A^{ji} = e^{i\theta} X A^{ij} X^{-1}.$$  

(20)

After applying this symmetry transformation twice we obtain

$$A^{ij} = e^{2i\theta} X^2 A^{ij} X^{-2}.$$  

(21)

From the fundamental theorem it follows that $\theta$ is a topological index, $\theta = 0, \pi \mod 2\pi$, and $X^2 = e^{i\chi} \mathbb{1}$, however this phase can be absorbed in $X$ such that $X$ squares to the identity. $F_V$ can thus protect one non-trivial SPT phase characterized by $\theta = \pi$.

If the MPS is in left canonical form, it can be shown that $X$ is unitary, which together with $X^2 = \mathbb{1}$ implies that $X$ can be written as $X = U_1^\dagger \mathbb{1}_{n,m} U$ for some unitary $U$ and $n + m = D$. With the gauge transformation $A^{ij} \rightarrow \tilde{A}^{ij} = U A^{ij} U^\dagger$ the MPS tensors $\tilde{A}$ have definite $V$-parity:

$$\tilde{A}^{ji} = \pm \mathbb{1}_{n,m} \tilde{A}^{ij} \mathbb{1}_{n,m},$$  

(22)

thus tremendously reducing the variational degrees of freedom. The signature of $\mathbb{1}_{n,m}$—that is to say, $n$ and $m$—is irrelevant for the classification of SPT orders. Indeed, notice that the $F_V$ symmetry can be thought of as an on-site $\mathbb{Z}_2$ symmetry acting on the physical level that is implemented by $\sum_{(j_1, j_2)} (U_1)_{(j_1, j_2)}^{(i_1, i_2)} A^{i_1, j_2}$ with
For some complex matrix $C$. From substitution in (25) it immediately follows that defining $A^i \mapsto \tilde{A}^i = CA^iC^{-1}$ yields a uniform MPS generated by $\tilde{A}^i$ in which the tensors $A^i$ have a definite $H$-parity given by the topological index $\theta$.

Now assume that $X$ is skew-symmetric. In that case we similarly can write $X = C^\dagger TC$ using the Youla normal form [19]. Again substituting this in (25), we can identify $A^i \mapsto \tilde{A}^i = \sqrt{TCP^\dagger \sqrt{T}}$ as the transformation to construct local tensors with a well-defined $H$-parity. However, this transformation is no actual gauge transformation in the aforementioned sense since, in order to bring the MPS in the desired form, we should insert $\mathbb{I} = C^{-1}\sqrt{T}P^\dagger \sqrt{T}$ between the $A$-tensors, which after making the transformation $A^i \mapsto \tilde{A}^i$ leaves us with residual bond tensors $\Gamma^\dagger$:

\begin{equation}
\cdots \quad \tilde{A}^i \Gamma^\dagger \tilde{A}^i \Gamma^\dagger \quad \cdots
\end{equation}

The SPT classification for $F_H$ corresponds to $H^1_\rho(Z_2, U_1) \times H^1_\rho(Z_2, U_1) = Z_2 \times Z_2$, where the first $Z_2$ factor corresponds to $\theta = 0, \pi$ and the second $Z_2$ corresponds to the phase appearing in the generalized projective representation $X$ of the parity symmetry group $Z_2^d$ (A10).

$F_G$ The $F_G$ symmetry group contains a generator of translations $T$ and a glide reflection $G$ which are related through $G^2 = T$. Therefore, we will consider an MPS ansatz which is translationally invariant under shifts over two sites. The glide reflection will then be implemented as a shift over one site followed by a reflection around the horizontal axis. Hence, without loss of generality we can take this MPS ansatz to be

\begin{equation}
\cdots \quad \tilde{A} \Gamma^\dagger \tilde{A} \Gamma^\dagger \quad \cdots
\end{equation}

Invariance under glide reflections relates the tensors $A$ and $B$ up to a gauge transformation which can in general be different on the $A - B$ and $B - A$ bonds:

\begin{equation}
\begin{aligned}
A^{ij} &= e^{i\theta_A} XB^{ij} Y^{-1} \\
B^{ij} &= e^{i\theta_B} YA^{ij} X^{-1}
\end{aligned}
\end{equation}

Carrying out this transformation twice then results in

\begin{equation}
\begin{aligned}
A^{ij} &= e^{i(\theta_A + \theta_B)} XY A^{ij} X^{-1} Y^{-1} \\
B^{ij} &= e^{i(\theta_A + \theta_B)} YX B^{ij} Y^{-1} X^{-1}
\end{aligned}
\end{equation}

Blocking two sites and using the fundamental theorem of MPS yields following conditions on the phases and gauge matrices:

\begin{equation}
\begin{aligned}
2(\theta_A + \theta_B) &= 0 \pmod{2\pi} \\
X &= e^{i\chi} Y^{-1}
\end{aligned}
\end{equation}
By absorbing a phase factor $e^{-i\frac{\pi}{2}}$ in both $X$ and $Y$, $X$ and $Y$ are each other inverses. Substituting $2(\theta_A + \theta_B) = 0 \mod 2\pi$ in (31) shows that only the case $\theta_A = 0 \mod 2\pi$ can survive. We are free to choose eg. $\theta_A = 0$. From this it then follows that $B^{ij} = YA^{ij}Y$ such that after redefining $A^{ij} \mapsto \tilde{A}^{ij} = A^{ij}Y$ the MPS can be brought in following canonical form:

$$\cdots \tilde{A} \tilde{A} \cdots \tilde{A} \cdots$$  \hspace{1cm} (33)

In case of glide reflection symmetry there are thus no non-trivial SPT phases.

$\textbf{F}_R$ Starting from a two-legged uniform MPS ansatz (19), we impose the rotation symmetry as

$$(A^{ij})^\top = e^{i\theta} X A^{ij} X^{-1}. \hspace{1cm} (34)$$

Applying this symmetry twice and using the fundamental theorem, it immediately follows that $\theta = 0, \pi \mod 2\pi$ and $X^{-1} = e^{i\pi} X$, exactly what was found in case of $F_H$ symmetry. The canonical form of an $F_R$ invariant MPS is thus again one in which the tensors have definite $R$-parity, again at the cost of introducing extra bond tensors between neighboring sites if $X$ is skew-symmetric.

$\textbf{F}_{2R}$ Without loss of generality we can start from the ansatz (33). Imposing $\pi$-rotation invariance leads to

$$(A^{ij})^\top = e^{i\theta} X A^{ij} X^{-1}. \hspace{1cm} (35)$$

Rotating twice and applying the fundamental theorem results in the same $\mathbb{Z}_2 \times \mathbb{Z}_2$ classification as in the case of $F_H$ symmetry. Again, the canonical form is one in which the tensors have definite $R$-parity defined by the topological index $\theta$, with bond tensors in case of $X = -X^\top$ and where the glide reflection symmetry is manifest:

$$\cdots \tilde{A} \tilde{A} \cdots \tilde{A} \cdots$$  \hspace{1cm} (36)

where $\tilde{A}^{ij} = CA^{ij}C^{-1}$, $X = C^\top C$,

$$\cdots \tilde{A} \tilde{T} \tilde{A} \tilde{T} \cdots \hspace{1cm} (37)$$

where $\tilde{A}^{ij} = \sqrt{T}CA^{ij}C^{-1}\sqrt{T}$, $X = C^\top\Gamma C$.

$\textbf{F}_{2H}$ We consider again the two-legged uniform ansatz (19). First imposing reflection around the horizontal axis yields

$$A^{ij} = e^{i\theta_v} X A^{ij} X^{-1}. \hspace{1cm} (38)$$

Unsurprisingly, doing this symmetry operation twice results in the same conditions on $\theta_v$ and $X$ as in the case of $F_{v}$: $\theta_v = 0, \pi \mod 2\pi$, $X^2 = 1$. $X$ is again unitary and again we can write $X = U^\dagger 1_{n,m} U$ for some unitary $U$. As was explained, the signature of $1_{n,m}$ is irrelevant. Imposing the second reflection, one obtains

$$(A^{ij})^\top = e^{i\theta_H} Y A^{ij} Y^{-1}, \hspace{1cm} (39)$$

which implies that $\theta_H = 0, \pi \mod 2\pi$, $Y = \pm Y^\top$. In this way an $\mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2$ classification is obtained.

The cohomological classification corresponds to $H^1(\mathbb{Z}_2 \times \mathbb{Z}_2 \times U_1) \times H^3_{tr}(\mathbb{Z}_2 \times \mathbb{Z}_2 \times U_1) = \mathbb{Z}_2^2 \times \mathbb{Z}_2$ [20]. The $\mathbb{Z}_2^2$ corresponds to $\theta_v$ and $\theta_H$ and the last $\mathbb{Z}_2$ corresponds to the generalized projective representation of the $H$-parity generator.

**V. TIME REVERSAL & LATTICE SYMMETRIES**

In this section we study time-reversal symmetry and time-reversal combined with translations within the MPS framework [18]. The most important feature of time-reversal is that it is an anti-unitary transformation and can hence be written as $T = UK$ where $U$ is a unitary and $K$ denotes complex conjugation in a certain basis. $T$ can be represented linearly or projectively, depending on whether $U = \pm 1$.

We revisit the work by Chen et al. on the linear implementation of time-reversal in MPS and identify the corresponding SPT classification [5]. We demonstrate that injective MPS can not be invariant under the projective representation of $T$, a tensor network manifestation of the Lieb-Schultz-Mattis theorem [21]. Finally we prove that time-reversal combined with a shift over one lattice site does not give rise to non-trivial SPT order and construct a canonical form for the trivial phase.

**A. Time reversal in TI systems**

$T^2 = 1, UU^\dagger = 1$ Consider the uniform ansatz (3). Time reversal symmetry can then be implemented as

$$\sum_j U_{ij}T^j = X A^i X^{-1}. \hspace{1cm} (40)$$

Note that without loss of generality we don’t need to consider a phase in this transformation because such a phase could be consistently absorbed in the MPS tensor $A^i$. Doing a second time reversal results in

$$A^i = \overline{X} X A^i X^{-1} \overline{X}^{-1}. \hspace{1cm} (41)$$

By virtue of the fundamental theorem we have that $\overline{X} X = \pm 1$. It can be shown that $X$ is unitary if the MPS is in the left canonical form, such that $X = \pm X^\top$. 


If $X$ is symmetric, writing $X = V^TV$, where $V$ is unitary because $X$ is, allows us to bring the MPS in a canonical form by means of the gauge transformation $A^i \mapsto \tilde{A}^i = VA^iV^\dagger$ which transforms according to

$$\sum_j U_{ij} \tilde{A}^j = \tilde{A}^i.$$  \hspace{1cm} (42)

For a skew-symmetric $X$ we write $X = V^\dagger V$, $V$ again being unitary, from which it follows that $\tilde{A}^i = VA^iV^\dagger$ transforms according to a quaternionic representation under $T$, up to multiplication by $U_{ij}$ \cite{22}:

$$\sum_j U_{ij} \tilde{A}^j = \Gamma \tilde{A}^i \Gamma^{-1}.$$  \hspace{1cm} (43)

The cohomological classification corresponds to $H^2_T\{Z^2, U_1\} \times H^3_T\{Z^2, U_1\} = \{e\} \times Z_2$, as follows from the Smith normal form (Appendix B). The $Z_2$ is understood as $X$ being (skew-)symmetric.

We can now also show that the entanglement spectrum in case of the non-trivial SPT phase for which $X = -X^T$ is at least doubly degenerate \cite{2}. Consider therefore the unique eigenvalue 1 right eigenvector $\rho$ of the transfer matrix $X$. In that case $\rho$ interpreted as a $D \times D$ matrix is (Hermitian) positive semidefinite by virtue of the quantum Perron-Frobenius theorem \cite{23, 24}. Consider some eigenvector $x$ of $\rho$ with positive eigenvalue $\lambda$, then by virtue of $XX^\dagger = \rho$ (proven in Appendix C), $x^\dagger X^\dagger$ is a left eigenvector of $\rho$ with the same eigenvalue $\lambda$. However, using $X^\dagger = -X$ it follows that $\text{Tr} \left( X^\dagger (x \otimes x) \right) = 0$, or in other words that $x^\dagger X^\dagger$ and $x$ are orthogonal eigenvectors belonging to the same eigenvalue $\lambda$.

$T^2 = -I$, $U \overline{U} = -I$ This case is relevant for eg. $U = Y$, $Y$ denoting the usual Pauli Y matrix, which is used for the implementation of time-reversal symmetry on spin 1/2 particles. \cite{18} Let us not restrict to this particular example and consider a general unitary $U$ satisfying the aforementioned property $U \overline{U} = -I$. Starting again from the uniform ansatz (3), considering a projective implementation of time reversal and applying it twice leads to:

$$A^i \rightarrow \sum_j U_{ij} \overline{A}^j \rightarrow -A^i = A^i,$$  \hspace{1cm} (44)

from which we conclude that translational invariant injective MPS cannot transform projectively under time-reversal symmetry. This can be understood as a tensor network interpretation of the celebrated Lieb-Schultz-Mattis theorem \cite{21} that dictates that the ground state of a system of half-integer spins - in which case time-reversal acts projectively - should be either symmetry broken (in contradiction with the assumption that the MPS is symmetric under time-reversal) or gapless (in which case the matrix product ansatz does not provide a good description).

### B. Time reversal combined with a one site shift

We can now break translational invariance by considering following ansatz and imposing time-reversal symmetry up to a shift by one site:

$$\cdots \to \begin{array}{c} A \to B \to A \to B \to \cdots \end{array}.$$  \hspace{1cm} (45)

We shall consider both the linear and projective case $U \overline{U} = \pm I$ simultaneously. The transformation of the tensors then reads

$$\begin{align*}
\sum_j U_{ij} \overline{A}^j &= e^{i(\theta_A + i\kappa)} X^B W^A X^{-1}\overline{W} \\
\sum_j U_{ij} \overline{B}^j &= e^{i(\theta_B - i\kappa)} W A^i X^{-1}.
\end{align*}$$  \hspace{1cm} (46)

We introduced a phase $\exp(\pm i\kappa)$ that will be chosen later. A second transformation results in

$$\begin{align*}
\pm A^i &= e^{-i(\theta_A + i\kappa)} XW^A X^{-1}\overline{W} \\
\pm B^i &= e^{i(\theta_B - i\kappa)} W X B^i X^{-1}\overline{W}.
\end{align*}$$  \hspace{1cm} (47)

Blocking two tensors reveals that there are no constraints on $\theta_A$, $\theta_B$ and $\kappa$ in both cases, and we also conclude that $XW = e^{i\chi}$. We are now free to choose $\kappa = \chi$, $\theta_A = \theta_B = 0$ in the linear case and $\theta_A = 0$, $\theta_B = \pi$ in the projective case and define

$$\begin{align*}
\tilde{X} &= e^{i\frac{\chi}{2}} X \\
\tilde{W} &= e^{-i\frac{\chi}{2}} W,
\end{align*}$$  \hspace{1cm} (48)

satisfying $\tilde{X} \tilde{W} = 1$, from which it follows that

$$\begin{align*}
\sum_j U_{ij} \overline{A}^j &= \tilde{X} B^i \overline{W}^{-1} \\
\sum_j U_{ij} \overline{B}^j &= \pm \overline{W} A^i \tilde{X}^{-1}.
\end{align*}$$  \hspace{1cm} (49)

Hence, there is no non-trivial SPT phase and a canonical form is obtained by writing

$$B^i = \sum_j U_{ij} \overline{W} \overline{A}^j \tilde{W}$$  \hspace{1cm} (50)

and defining $C^i = \tilde{W} A^i$:

$$\cdots \to \begin{array}{cc}
\smile & C \\
U & C
\end{array}$$  \hspace{1cm} (51)
VI. CONCLUSIONS AND OUTLOOK

In this work we showed that quasi-one-dimensional spatial symmetries can protect non-trivial SPT phases in quantum spin chains represented by matrix product states. We identified each of these phases by invoking these symmetries on injective MPS and identifying the topologically distinct ways in which these symmetries can be represented on the local tensors. For most of these phases we constructed canonical MPS ansätze that are manifestly invariant under the considered symmetries. Finally, we revisited the SPT classification in case of time-reversal symmetry and showed that time-reversal combined with a translation over one lattice site does not give rise to non-trivial phases.

A natural extension of this work would be to classify the SPT phases in two dimensions that are protected by space group symmetries. The two-dimensional space groups are known as the wallpaper groups, of which there are seventeen. We expect that imposing these symmetries on two-dimensional projected entangled-pair states (PEPS), which form the natural two-dimensional generalization of the MPS considered here, will also reveal topological obstructions on the level of the local tensors. For each of these phases, canonical ansätze could be constructed that might prove very useful in numerical simulations of physical systems for which these spatial symmetries are a relevant feature.

In particular, it would be interesting to investigate whether some of the symmetry transformations in 2D admit an implementation on the virtual level as string-like matrix product operators (MPOs). The physical application of the symmetry is then ‘gauged away’ by pulling these MPOs through the lattice. Similarly, it might be interesting to demonstrate that also time-reversal, which is because of the complex conjugation it contains a priori a very non-local symmetry, can be implemented using an MPO of non-trivial bond dimension.

ACKNOWLEDGMENTS

We would like to thank Robijn Vanhove for insightful comments regarding the extension to two dimensions, as well as Rui-Zhen Huang for many fruitful discussions on the topic of this work. B.V.-D.C. is supported by a Ph.D. fellowship from Bijzonder Onderzoeksfonds (BOF). This work has received funding from the European Research Council (ERC) under the European Unions Horizon 2020 research and innovation programme (grant agreements No 715861 (ERQUAF) and 647905 (QUTE)), and from Research Foundation Flanders (FWO) via grant GOE1520N.

[1] Z.-C. Gu and X.-G. Wen, Phys. Rev. B 80, 155131 (2009).
[2] F. Pollmann, A. M. Turner, E. Berg, and M. Oshikawa, Phys. Rev. B 81, 064439 (2010).
[3] F. Pollmann, E. Berg, A. M. Turner, and M. Oshikawa, Phys. Rev. B 85, 075125 (2012).
[4] X. Chen, Z.-C. Gu, and X.-G. Wen, Phys. Rev. B 82, 155138 (2010).
[5] X. Chen, Z.-C. Gu, and X.-G. Wen, Phys. Rev. B 83, 035107 (2011).
[6] X. Chen, Z.-C. Gu, and X.-G. Wen, Phys. Rev. B 84, 235128 (2011).
[7] X. Chen, Z.-C. Gu, Z.-X. Liu, and X.-G. Wen, Phys. Rev. B 87, 155114 (2013).
[8] N. Schuch, D. Pérez-García, and I. Cirac, Phys. Rev. B 84, 165139 (2011).
[9] B. Zeng, X. Chen, D.-L. Zhou, and X.-G. Wen, “Quantum information meets quantum matter – from quantum entanglement to topological phase in many-body systems,” (2018), arXiv:1508.02595 [cond-mat.str-el].
[10] F. Verstraete, J. I. Cirac, J. I. Latorre, E. Rico, and M. M. Wolf, Phys. Rev. Lett. 94, 140601 (2005).
[11] F. Verstraete and J. I. Cirac, Phys. Rev. B 73, 094423 (2006).
[12] D. Pérez-García, F. Verstraete, M. M. Wolf, and J. I. Cirac, “Matrix product state representations,” (2007), arXiv:quant-ph/0608197 [quant-ph].
[13] F. Haldane, Physics Letters A 93, 464 (1983).
[14] F. D. M. Haldane, Phys. Rev. Lett. 50, 1153 (1983).
[15] H. S. M. Coxeter, Introduction to geometry (New York, London, 1961).
[16] S. Jiang and Y. Ran, Phys. Rev. B 92, 104414 (2015).
[17] M. A. Nielsen and I. Chuang, “Quantum computation and quantum information.” (2002).
[18] E. Wigner, Group theory: and its application to the quantum mechanics of atomic spectra, Vol. 5 (Elsevier, 2012).
[19] D. Youla, Canadian Journal of Mathematics 13, 694 (1961).
[20] Since the group action is trivial, we find \( H^1 (Z_2 \times Z_2^p, U_1) = H^1 (Z_2 \times Z_2, U_1) \). Using the fact that \( H^k (G, U_1) = H^{k+1} (G, Z) \) and the general result \( H^p (Z_2 \times Z_2, Z) = \mathbb{Z}_2^{(p+1)/2} \) for even \( p \), we find \( H^1 (Z_2 \times Z_2^p, U_1) = \mathbb{Z}_2^p \). From the observation that \( H^2_{BR} (Z_2 \times Z_2^p, U_1) = H^2_{BR} (Z_2 \times Z_2^p, U_1) \) it follows that we can use (J30) from [7] to conclude that \( H^2_{BR} (Z_2 \times Z_2^p, U_1) = Z_2^2 \).
[21] E. Lieb, T. Schultz, and D. Mattis, Annals of Physics 16, 407 (1961).
[22] Consider a transformation in a quaternionic representation according to \( \mathbf{Q} = XAX^{-1} \), where \( X \) is skew-symmetric and unitary. \( X \) can be brought in a skew-symmetric tridiagonal form \( W \) by an orthogonal matrix \( Q \). \( W = Q^T X Q \). Unitarity of \( W \) implies that \( X \) can be written as \( X = Q^T \Gamma Q \) for an orthogonal \( Q \), showing that \( QAQ^T \) transforms as \( QAQ^T \Gamma \).
Appendix A: Group cohomology & projective representations

In this appendix we give a brief review of projective representations of finite groups and the relation to group cohomology. We first focus on the case where the group action is trivial, which is relevant in the absence of time-reversal and parity symmetry, and then turn to the more general case where non-trivial group actions are taken into account. A more complete treatment can be found in e.g. [7].

1. Trivial group action

A projective representation of a finite group $G$ can be understood as a representation of $G$ up to a phase:

$$X_g X_h = e^{i\omega(g,h)} X_{gh}. \quad (A1)$$

In case all the phases are trivial $\omega(g,h) \equiv 0$, the $X_g$ form a linear representation of $G$.

Associativity of the projective representation heavily constrains the phases and eventually leads to a classification of projective representations in terms of group cohomology. Imposing associativity $X_g (X_h X_k) = (X_g X_h) X_k$ results in following 2-cocycle condition (with trivial group action) that the $\omega(g,h)$ need to satisfy:

$$\omega(g,h) + \omega(h,k) + \omega(h,k) \equiv 0 \mod 2\pi. \quad (A2)$$

Solutions of the 2-cocycle condition are called 2-cocycles. Since in the SPT framework $G$ is interpreted as a symmetry group and its projective representations arise as the gauge matrices acting on the virtual level, $X_g$ that are related by a transformation of the form $X_g \mapsto e^{i\gamma(g)} X_g$ should be identified. Under such a redefinition the cocycles transform according to

$$\omega(g,h) \mapsto \omega(g,h) + \gamma(g) + \gamma(h) - \gamma(gh). \quad (A3)$$

Cocycles of the form $\gamma(g) + \gamma(h) - \gamma(gh)$ are called coboundaries. The solutions of the 2-cocycle condition (A2) modulo the coboundaries, $[\omega] \sim [\omega'] \iff \omega(g,h) = \omega'(g,h) + \gamma(g) + \gamma(h) - \gamma(gh)$, are classified by the second cohomology group of $G$ with respect to $U_1$, $H^2(G, U_1)$.

For a finite group it can be shown, for example by using the Smith normal form (Appendix B), that the second cohomology group is always a direct product of finite cyclic groups. This demonstrates in particular that the number of projective representations of a finite group modulo transformations $X_g \mapsto e^{i\gamma(g)} X_g$ is always finite.

Given some representative $\omega$ of a cohomology class $[\omega] \in H^2(G, U_1)$, one can always construct a $|G|$-dimensional projective representation corresponding to this cocycle $\omega$, the projective regular representation. This representation is defined by:

$$(X_g)_{g_1, g_2} = \delta_{g_2, g_1} g e^{i\omega(g_1, g)}. \quad (A4)$$

That these matrices form a projective representation follows immediately from the 2-cocycle equation $\omega(g,h) = \omega'(g,h) + \gamma(g) + \gamma(h) - \gamma(gh)$.

This representation arises when an explicit MPS representation of a given SPT phase in the RG fixed point is constructed (Section III).

2. Time-reversal and parity

As discussed in Sec. V, time-reversal is implemented as an anti-unitary action on the physical level and thus involves complex conjugation of the MPS tensors. For a general symmetry group containing a $\mathbb{Z}_2$ time-reversal symmetry subgroup, $G = H \rtimes \mathbb{Z}_2$, the action of an element $g \in G$ on the MPS tensors reads

$$\sum_j U_{ij}(g) C_g (A^j) = e^{i\varphi(g)} X_g A^j X_g^{-1}, \quad (A5)$$

where the action of $C_g$ on $A^j$ is a complex conjugation if $g$ contains time-reversal and is the identity otherwise. From subsequently acting with two group elements $g$ and $h$ on $A^j$, it follows that the $X_g$ form a generalized projective representation

$$X_g C_g (X_h) = e^{i\omega(g,h)} X_{gh}, \quad (A6)$$

which should be interpreted as the generalization of (A1) to the case of time-reversal, i.e. non-trivial group action $\varphi$ obeys the 1-cocycle equation with non-trivial group action $\alpha^T$:

$$\varphi(g) + \alpha^T(g) (\varphi(h)) = \varphi(gh) \mod 2\pi. \quad (A7)$$

The action of $\alpha_g^T$ is simply multiplication with $\pm 1$ depending on whether the group element $g \in G$ contains the generator of time-reversal or not.
As before, imposing associativity on the matrices $X_g$ results in following 2-cocycle condition:

$$\omega(g, h) + \omega(gh, k) = \omega(g, hk) + \beta^T_g (\omega(h, k)) \mod 2\pi,$$

where $\beta^T_g$ again denotes a controlled multiplication with $\pm 1$ depending on whether $g$ contains time-reversal or not. The second cohomology group $H^2_{\beta^T} (G, U_1)$ classifies the 2-cocycles that satisfy $(A8)$ modulo coboundaries of the form $\gamma(g) + \alpha^T_g (\gamma(h)) - \gamma(gh)$. The action $\beta^T_g$ is thus a linear representation of $G$, and the parity transformation is defined as $\phi(g) = \beta^T_g (c) - c$ for an arbitrary constant $c \in [0, 2\pi)$.

In case of a parity symmetry generator, the symmetry group can be written as $G = H \times \mathbb{Z}_2$, where $\mathbb{Z}_2$ denotes the parity group. The action of a symmetry $g \in G$ on the MPS tensors reads

$$\sum_j (U_g)_{ij} T_g (A^j) = X_g A^i X_g^{-1}, \quad (A9)$$

where $T_g$ amounts to taking the transpose if $g$ contains the parity transformation. A similar computation as before leads to

$$X_g P_g (X_h) = e^{i\omega(g, h)} X_{gh}, \quad (A10)$$

where $P_g$ amounts to taking the inverse transpose if $g$ contains the non-trivial element of $\mathbb{Z}_2^P$, and following 2-cocycle condition

$$\omega(g, h) + \omega(gh, k) = \omega(g, hk) + \beta^P_g (\omega(h, k)) \mod 2\pi. \quad (A11)$$

The action $\beta^P_g$ is a multiplication with $-1$ whenever $g$ contains a parity transformation.

The $\varphi(g)$ form a linear representation of $G$, i.e. they obey the 1-cocycle condition with trivial action:

$$\varphi(g) + \varphi(h) = \varphi(gh), \quad (A12)$$

classified by $H^1 (G, U_1)$. The second cohomology group $H^2_{\beta^P} (G, U_1)$ classifies the 2-cocycles obeying $(A2)$ up to equivalence $[\omega] \sim [\omega'] \iff \omega(g, h) = \omega'(g, h) + \gamma(h) - \gamma(gh)$.

In the simplest case where $H = \{e\}$, the second cohomology group is readily computed to be $H^2_{\beta^P} (\mathbb{Z}_2, U_1) = \mathbb{Z}_2$. There are thus two inequivalent generalized projective representations of $\mathbb{Z}_2^P$, these are the ones we found in $(27)$.

Finally, the formalism can be generalized to the case the symmetry group contains both time-reversal - and parity symmetry. In that case, the cohomology groups $H^2_{\beta^T} (G, U_1)$ and $H^2_{\alpha^P} (G, U_1)$ are defined by the cocycle conditions

$$\varphi(g) + \alpha^P_{\beta^T} (\varphi(h)) = \varphi(gh) \mod 2\pi, \quad (A13)$$

$$\omega(g, h) + \omega(gh, k) = \omega(g, hk) + \beta^P_{\beta^T} (\omega(h, k)) \mod 2\pi. \quad (A14)$$

Here, $\alpha^P_{\beta^T} = \alpha^T_\beta$ and $\beta^P_{\beta^T} = \beta^P \circ \beta^T$.

It was observed above that adding a coboundary to a given 2-cocycle is immaterial from the MPS point-of-view. Hence, we refer to choosing a particular representative of a cohomology class as choosing a gauge for the 2-cocycles. It is for example straightforward to show that there is a gauge in which $\omega(g, e) = 0$, $\forall g \in G$.

### Appendix B: Computing group cohomology using the Smith normal form

The problem of finding all (generalized) projective representations of a given finite symmetry group $G$ or - equivalently - computing its second cohomology group $H^2_{\beta^T} (G, U_1)$ can be reduced to a problem in linear algebra. In this section we illustrate how the second cohomology group can be computed by making use of the Smith normal form [25]. Our approach works for both trivial and non-trivial group actions $\beta$.

To make use of the full power of the Smith normal form, note that the 2-cocycle equation $(A2)$ or its generalizations with non-trivial group actions $(A8, A11)$ can be written as the linear system

$$\sum_j \Omega_{ij} \omega_j = 0, \mod 2\pi, \quad (B1)$$

which has to be solved modulo $2\pi$. Herein $\Omega_{ij}$ is a $|G|^3 \times |G|^2$ matrix containing only $\pm 1$’s. In case of a trivial group action every row contains exactly two $+1$‘s and two $-1$‘s, in case of a non-trivial group action some of these signs are switched appropriately. Every solution $\omega$ to this linear system of equations constitutes a valid 2-cocycle.

Since $\Omega$ only has entries in $\mathbb{Z}$, which constitutes a principal ideal domain, $\Omega$ can be written in Smith normal form as follows [26]:

$$PAR = \Omega. \quad (B2)$$

In this decomposition $P$ and $R$ are respectively $|G|^2 \times |G|^3$ and $|G|^2 \times |G|^2$ matrices that only contain integers and have determinant one. $\Lambda$ also only contains integers, is $|G|^3 \times |G|^2$-dimensional and is of the form
\[ \Lambda = \begin{pmatrix} \text{diag} (d_1, d_2, \ldots, d_r) & 0 \\ 0 & 0 \end{pmatrix}, \quad \text{(B3)} \]

in which the non-zero elements \( d_1, \ldots, d_r \) along the diagonal, some of which might be one, are in increasing order, \( d_1 \leq d_2 \leq \ldots \), and every element is a divisor of the next, \( d_i | d_{i+1} \). The Smith normal form \( \Lambda \) is unique. Inserting this decomposition in the system of equations \( (B1) \) gives rise to the solution

\[ \bar{\omega} = 2\pi R^{-1} \Lambda^+ \bar{\nu}. \quad \text{(B4)} \]

\( \Lambda^+ \) denotes the (unique) Moore-Penrose pseudoinverse of \( \Lambda \) that satisfies \( \Lambda \Lambda^+ \Lambda = \ Lambda \) and which is found to be

\[ \Lambda^+ = \begin{pmatrix} \text{diag} (d_1^{-1}, d_2^{-1}, \ldots, d_r^{-1}) & 0 \\ 0 & 0 \end{pmatrix}. \quad \text{(B5)} \]

\( \bar{\nu} \) is an arbitrary vector that only contains integers. Writing the solution \( (B4) \) in components yields

\[ \omega_i = \sum_{j=1}^r 2\pi \left( R^{-1} \right)_{ij} \frac{\nu_j}{d_j}. \quad \text{(B6)} \]

Because \( \bar{\nu} \) can be chosen freely, one can choose subsequently \( \nu_1 = \delta_{1,i}, \delta_{2,i}, \ldots, \delta_{r,i} \) to obtain a basis of the solution space that can be written as

\[ \omega_i = \frac{2\pi}{d_j} \left( R^{-1} \right)_{ij}, \quad \forall j \in \{1, \ldots, r\}. \quad \text{(B7)} \]

Hence, the 2-cocycles \( \bar{\omega} \) are found to be the columns of \( R^{-1} \). Since \( R \) is full rank, all the solutions \( \bar{\omega} \) are linearly independent. To classify all possible solutions, we now consider the diagonal entries of \( \Lambda \).

From \( \Lambda R \bar{\omega} = 0 \mod 2\pi \) it follows that the \( |G|^2 - r \) vanishing diagonal elements of \( \Lambda \) correspond to \( \omega_i \) that are unconstrained and can be chosen freely. These exactly correspond to 2-cocycles which are coboundaries: \( \omega (g_1, g_2) = \varphi (g_1) + \alpha g_1 (\varphi (g_2)) - \varphi (g_1 g_2) \).

From \( (B7) \) and the fact that \( R^{-1} \) contains only integers, it follows that for every diagonal entry \( d_i = 1 \), a trivial solution \( \omega_i = 0 \mod 2\pi \) is obtained.

The non-trivial solutions are those that correspond to entries \( d_i > 1 \). From \( (B7) \) and the observation that linear combinations of cocycles are also cocycles, it follows that the cocycle \( \bar{\omega} \) corresponding to some \( d_j \) generates a cyclic group. Now note that not all elements of \( \bar{\omega} \) can be divisible by \( d_j \) as this would be in contradiction with the fact that \( R^{-1} \) has determinant one. Hence, the cyclic group generated by \( \bar{\omega} \) is \( \mathbb{Z}_{d_j} \).

In conclusion following picture arises. Given some group \( G \) one can write down \( \Omega_{ij} \) that can be brought in Smith normal form \( PAR \). The diagonal entries of \( \Lambda \), \( d_1, d_2, \ldots, d_r \), determine the second cohomology group which is then of the form \( \mathbb{Z}_{d_1} \times \mathbb{Z}_{d_2} \times \ldots \times \mathbb{Z}_{d_r} \), with the understanding that \( Z_1 = \{ e \} \) denotes the trivial group. The non-trivial 2-cocycles in some arbitrary gauge correspond then to the columns of \( R^{-1} \).

### Appendix C: Proof of \( X \bar{\gamma} X^\dagger = \rho \)

In this appendix we prove the identity \( X \bar{\gamma} X^\dagger = \rho \) which was used in section VA. Hereto we start from the fact that \( \rho \) was defined as the unique right eigenvector of the transfer matrix \( E \) \( (6) \) corresponding to the eigenvalue one. Taking the complex conjugate of the eigenvalue equation and exploiting unitarity of \( U \), we can show that \( X^\dagger \bar{\gamma} X \) is also a right eigenvector with eigenvalue one which because of injectivity and thus non-degeneracy of this eigenvalue has to be equal to \( \rho \): \( X \bar{\gamma} X^\dagger = \rho \). Pictorially:

\[ (C1) \]

\[ (C2) \]

\[ (C3) \]

\[ (C4) \]

\[ (C5) \]