Matrix product operators for symmetry-protected topological phases

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Projected entangled pair states (PEPS) provide a natural description of the ground states of gapped, local Hamiltonians in which global characteristics of a quantum state are encoded in properties of local tensors. We show that on-site symmetries, as occurring in systems exhibiting symmetry-protected topological (SPT) quantum order, can be captured by a virtual symmetry of the tensors expressed as a set of matrix product operators labelled by the different group elements. A classification of SPT phases can hence be obtained by studying the topological obstructions to continuously deforming one set of matrix product operators into another. This leads to the classification of bosonic SPT states in terms of group cohomology, as originally derived by Chen et al. [1]. Our formalism accommodates perturbations away from fixed point models, and hence opens up the possibility of studying phase transitions between different SPT phases. We furthermore show how the global symmetries of SPT PEPS can be promoted into a set of local gauge constraints by introducing bosonic degrees of freedom on the links of the PEPS lattice, thereby providing a natural and general mapping between PEPS in SPT phases and topologically ordered phases.

I. INTRODUCTION

The phase diagrams of quantum many-body systems become much richer when global symmetries are imposed. In recent years it has become clear that there exist distinct phases which do not exhibit spontaneous symmetry breaking and cannot be distinguished via local order parameters. These phases are referred to as symmetry-protected topological (SPT) phases [1]. In contrast to topologically ordered systems [2], all SPT phases become equivalent once the symmetry is allowed to be explicitly broken. While this implies the corresponding SPT ground states possess only short-range entanglement, they cannot be adiabatically connected to a trivial product state without breaking the symmetry. Furthermore, they exhibit interesting edge properties when defined on a finite system with nontrivial boundary.

In recent years there has been an increasing interplay between the theory of quantum many-body systems and quantum information theory. This has led to the development of tensor network descriptions of the ground states of local, gapped Hamiltonians [3–6]. Tensor network methods have proven particularly useful in understanding the emergence of topological phenomena in quantum many-body ground states. In one dimension, Matrix Product States were used to completely classify SPT phases via the second cohomology group of their symmetry group [7–9]. In two dimensions, Projected-Entangled Pair States (PEPS) have been used to characterize systems with intrinsic topological order [10] and chiral topological insulators [15,17].

The goal of this work is to provide a complete characterization of bosonic SPT order for on-site symmetries within the PEPS formalism by formulating sufficient conditions to be satisfied by the individual tensors. Previously some powerful results for renormalization group (RG) fixed-point states with SPT order were presented by Chen et al. [13]. The present work also applies to systems with a finite correlation length. In addition, the framework presented here together with the quantum state gauging procedure of [19] yields a clear understanding of the connection between SPT phases and topologically ordered phases for all PEPS, providing a complementary description to the Hamiltonian gauging construction of Levin and Gu [20]. It also sets up a natural framework for the study of symmetry-enriched topological phases with PEPS.

We first discuss the formalism for characterizing gapped phases in PEPS with matrix product operators (MPO). Then it is shown that PEPS with global symmetries correspond to a special subclass of this general prescription. Next, we identify the short-range entangled PEPS and explain how SPT order manifests itself in these models via their unconventional edge properties. We continue by showing how gauging these SPT states yields a long-range entangled PEPS with topological order in the case of discrete groups. These concepts are then illustrated with a family of SPT PEPS that satisfy our criteria and it is shown explicitly that gauging these states leads to the ground states of the twisted quantum double models [21,22], which correspond to the Dijkgraaf-Witten discrete gauge theories [23,24]. In the supplementary material we review the relevant properties of MPO-injective PEPS, single block MPO group representations and the quantum state gauging formalism. There we also demonstrate that the PEPS gauging procedure is equivalent to the standard minimal coupling scheme for gauging Hamiltonians.
II. CHARACTERIZATION OF TOPOLOGICAL PHASES WITH MATRIX PRODUCT OPERATORS

In this section we present a general formalism to describe gapped phases with PEPS. The idea is to look for universal and discrete properties associated with the tensor network. These discrete labels are provided by the set of MPOs expressing the symmetry structure of the PEPS and form obstructions for continuously deforming two sets of MPOs into each other.

We take a simply connected region $\mathcal{R}$ of $N_h \times N_v$ sites on the square lattice $\mathcal{L} = \mathcal{R} \cup \mathcal{R}$. We focus on translation invariant systems, in which case we associate to every lattice the same rank five tensor $A = \sum_{i=1}^d \sum_{u,l,d,r=1}^D A_{uldr|i}\langle uldr \rangle$. Here $i$ is the physical index corresponding to the local physical Hilbert space $\mathbb{C}^d$ and $u,l,d,r$ are virtual indices, each of virtual dimension $D$, directed along the neighbouring edges of the lattice. Note that the arguments in this section can be made for any lattice type and apply equally well in the non-translation invariant case.

We now take all the tensors inside $\mathcal{R}$ and contract the virtual indices along any edges that connect tensors within $\mathcal{R}$. Virtual indices that connect a tensor in $\mathcal{R}$ with a tensor in $\mathcal{R}$ remain uncontracted. This procedure yields a tensor $R^I_{u,l,d,r}$ associated to $\mathcal{R}$, where $I$ is the physical index of dimension $d^N_{\alpha}N_h$ and $u(l,d,r)$ is a vector of dimension $N_h$ ($N_v, N_h, N_v$) containing the upper (left, bottom, right) virtual indices of $\mathcal{R}$. Finally we go to the double layer picture by constructing the tensor $E^R$

$$E^R_{\langle uld\rangle,\langle rrr \rangle} = \sum_{i=1}^{d_{\alpha}N_h} R^I_{u,l,d,r} \otimes R^I_{u,l',d',r'},$$

where unprimed indices correspond to the ket layer and primed indices correspond to the bra layer. Topological phases now manifest themselves via MPO symmetry properties of tensor $E^R$.

More specifically, we need to find a complete finite set $\mathcal{S}$ of linearly independent single block MPOs $O^R_\alpha$ with bond dimension $\chi_\alpha$:

$$O^R_\alpha = \sum_{u,u',l,l',d,d',r,r'} \text{tr}(B_{u,l,d,r}^{u',l',d',r'} A_{v}^{u'N_h,vN_h} A_{r}^{uN_h,v})$$

$$= B_{u,l,d,r}^{u',l',d',r'} A_{v}^{u'N_h,vN_h} A_{r}^{uN_h,v},$$

where $B_{ij}^R$ for fixed $i$ and $j$ is a $\chi_\alpha \times \chi_\alpha$ dimensional matrix, such that for every region $\mathcal{R}$

$$(O^R_\alpha \otimes I)E^R = (I \otimes O^R_\beta)E^R,$$

where $O^R_\alpha$ acts on the ket indices and $O^R_\beta$ acts on the bra indices. With single block MPOs we mean that they contain only one non-zero block when brought into canonical form [23]. There is a subtlety in defining a linearly independent set of MPOs satisfying Eq. (3). It is possible to find two linearly independent MPOs satisfying (3) that are identical on the support of $E^R$. To remove this redundancy we construct $\mathcal{S}$ by finding all solutions of (3), projecting them onto the support of $E^R$ and collecting all the linearly independent blocks in the projected MPOs. This of course requires the projector on the support of $E^R$ to be a MPO, which is the starting point of the MPO-injectivity formalism [13].

Eq. (3) together with the multiplication of MPOs provides $\mathcal{S}$ with an algebra structure. This algebra structure and the number of elements in $\mathcal{S}$ is not allowed to depend on $\mathcal{R}$. Note that the matrices $B_{ij}^R$ also do not depend on $\mathcal{R}$, i.e. for every region the MPOs $O^R_\alpha$ are constructed from the same tensors. Symmetry relations (3), the algebra structure of $\mathcal{S}$ and any possible additional discrete properties of the collection of MPOs provide universal labels of the quantum phase, independent of the details of tensors $A$.

All PEPS with intrinsic topological order are known [10,14] to satisfy (3) with the additional property that there is no relation between labels $\alpha$ and $\beta$, i.e. if $\mathcal{S}$ contains $N$ MPOs then $E^R$ satisfies $N^2$ symmetry relations. This was formalized in the framework of MPO-injectivity in [12,13], which was shown to capture all string-net models. The independence of the MPO tensors on $\mathcal{R}$ was guaranteed in the single layer picture via the intuitive pulling through property and the more technical generalized inverse property.

In the next section we explain how global symmetries are captured by another special case of (3).

III. GLOBAL SYMMETRY IN PEPS

Consider again a PEPS on the square lattice built from rank five tensors $A$, which we now interpret as linear maps from $(\mathbb{C}^D)^{\otimes 4}$ to $\mathbb{C}^d$. Firstly, we require that the tensors $A$ satisfy the axioms of MPO-injectivity [13], a framework describing general gapped phases without symmetry. Thus, the tensor $A$ (potentially after some blocking steps) becomes injective onto a subspace of the virtual space which is determined by the projector $P = A^+A$, where $A^+$ is the pseudo-inverse of $A$, that can be written as a matrix product operator

$$P = A^+A = \begin{array}{cc} A & \end{array}$$

Here, the MPO tensors are denoted as black squares and satisfy the axioms listed in [13], reviewed in the supplementary material. These axioms ensure that the same
MPO is obtained independent of the order in which the pseudo-inverses are applied and the corresponding closed MPO loop is a projector independent of its length.

We now want to describe a class of PEPS which are invariant under the on-site action $U(g)$ of a global symmetry group $G$. Hereto, we introduce another set of closed MPO loops $\{V(g), g \in G\}$, formed by rank 4 tensors which depend on the elements $g$ and are denoted by dots. These tensors satisfy property (5) and (6).

$$V(g) = V(g) \quad (g\in G)$$

Here $U(g)$ is a unitary representation of $G$. A property similar to Eq. (6) should also hold where the MPO gets pulled through the tensor from three virtual indices to one. The orientation of the MPO tensors is important because pulling the MPO through the tensor in the same direction as the arrows gives a unitary action $U(g)$ on the physical index while pulling through in the direction opposite to the arrows results in a physical action $U(g)$. With these two properties, it is clear that the MPO-injective PEPS constructed from tensors $A$ is invariant under the global symmetry action $U(g)^{\otimes N}$ for closed systems of arbitrary size, i.e. for any number of concatenated $A$ tensors. A particularly trivial case is given by injective PEPS [3], where the MPO $P$ is simply the identity $P = \mathbb{1}$ (i.e. an MPO with bond dimension 1) and the symmetry MPO $V(g)$ can always be factorized into a tensor product of local gauge transformations [25].

From Eq. (5) and (6), it immediately follows that the tensors $A : (\mathbb{C}^d)^{\otimes 4} \rightarrow \mathbb{C}^d$ are intertwiners in the following sense $U(g) A = AV(g)$ (here $V(g)$ denotes a closed MPO acting on the four virtual indices). Without loss of generality, we impose that the MPOs $V(g)$ act within the space on which $A$ is injective, such that $P V(g) P = V(g)$, i.e.

$$V(g) = V(g) \quad (g\in G)$$

and in particular $V(\mathbb{1}) = P$, with $\mathbb{1}$ the identity group element. This implies that the MPOs labeled with $g$ form a representation of $G$, since we then have $A V(g_1 g_2) = U(g_1) U(g_2) A = U(g_1) V(g_2)$, and thus $(A^* A)V(g_1 g_2) = (A^* A)V(g_1) V(g_2)$ with $A^* A = P$. A similar line of reasoning also shows that on the injectivity subspace the symmetry MPO $V(g)$ with reversed orientation (i.e. reversed arrows) equals $V(g^{-1})$.

With these properties it is now clear that the class of symmetric PEPS presented here is a special case of the general framework described in section II. If we denote the MPO corresponding to group element $g$ around a region $R$ by $V^R(g)$ then we have

$$(V^R(g) \otimes \mathbb{1}) \mathbb{E}^R = (\mathbb{1} \otimes \tilde{V}^R(g^{-1})) \mathbb{E}^R.$$ (8)

Note that in the general case we might need to split up $V^R(g)$ into multiple single block MPOs to be consistent with section II. So in contrast to the intrinsic topological case, where $\alpha$ and $\beta$ in [9] were completely uncorrelated, in the symmetry case $\alpha = g$ uniquely determines $\beta = g^{-1}$. As the formalism of section II accommodates a description of both symmetries and topological order it thus also captures symmetry-enriched topological phases within the PEPS framework.

IV. SYMMETRY-PROTECTED TOPOLOGICAL PEPS

Having discussed the general framework for gapped phases in PEPS we now focus on the subclass corresponding to symmetry-protected topological order. In the first subsection we identify the characterizing properties of short-range entangled SPT PEPS. We proceed in the second subsection with an analysis of the edge properties of non-trivial SPT PEPS.

A. Identifying SPT PEPS

As shown in [13] and argued in the previous sections, MPO-injective PEPS can describe topological phases with long-range entanglement. To single out the short-range entangled PEPS we require that the projection MPO $P$ has a single block when brought into its canonical form. If we denote the MPO tensors as matrices $B^i_j$ for external indices $i$ and $j$, this property corresponds to the fact that the transfer matrix $E_P$ constructed from contracting both external indices, i.e. $E_P = \sum_{ij} B^i_j \otimes B^j_i$ has a unique eigenvalue of largest magnitude. For RG fixed-point PEPS with injectivity subspace determined by $P$ this property implies the topological entanglement entropy is zero [27, 28]. To see this, note that the rank of the reduced density matrix of a finite region from a MPO-injective PEPS equals the rank of the projector MPO surrounding that region. Because the MPO $P$ is a projector,
we have \( \text{rank}(P) = \text{tr}(P) = \text{tr}(P^2) = \text{tr}(E_P^2) \), where \( L \) is the number of virtual bonds along the boundary of the region under consideration. We can then use the uniqueness of the largest eigenvalue \( \lambda_{\text{max}} \) of \( E_P \) to conclude that, for large regions, the rank of the reduced density matrix scales as \( \lambda_{\text{max}}^L \). This implies the zero Rényi entropy has no topological correction which for fixed points then implies that there is no topological entanglement entropy. This property should then hold throughout the gapped phase containing the fixed point.

To have a unique ground state the transfer matrix of the PEPS must have a unique fixed point. This excludes both symmetry-breaking and topological degeneracy \cite{11,29}. By taking a PEPS close enough to its isometric form we can avoid symmetry-breaking phases (and assure the gap condition \cite{7}). In the supplementary material we present a generic class of single block projector MPOs determining the injectivity subspace of PEPS that do not lead to topological degeneracy.

For SPT PEPS the symmetry MPOs are also single blocked. To see this, assume \( V(g) \) contains two different blocks, \( V(g) = PV(g)P = V_1(g) + V_2(g) \). Because \( P \) is single blocked each block of \( V(g) \) acts within the injectivity subspace of the PEPS. Looking at a single tensor this implies \( AV_1(g) = Q_1(g)A \) and \( AV_2(g) = Q_1(g)A \), with \( Q_1(g) \) and \( Q_2(g) \), satisfying \( Q_1(g) + Q_2(g) = U(g) \), necessarily being different non-unitary operators if the blocks of \( V(g) \) are different. Now one block of the MPO, say \( V_1(g) \), acting on the virtual boundary of a finite region of \( N_k \times N_v \) contracted PEPS tensors can also be mapped to an operator on the physical indices. Using Eq. \( 5 \) and \( AV_1(g) = Q_1(g)A \) we can identify this operator to be of the form \( U(g)^{\otimes N_k N_v - 1} \otimes Q_1(g) \), where the spatial position of \( Q_1(g) \) is arbitrary, i.e. it can be on any of the \( N_k \times N_v \) tensors in the region. For this equality to hold it should thus not be possible to detect the position of \( Q_1(g) \). Now take two of these states with the positions of \( Q_1(g) \) on each of them separated by a distance much larger then the correlation length. In this case the environment determining the local reduced density matrix of the site containing \( Q_1(g) \) in the first state will be the same for both states. Since \( Q_1(g) \) and \( U(g) = Q_1(g) + Q_2(g) \) act different on the support of \( A \) the local reduced density matrices are certainly different when the environment also has full support on this space. If this is not the case we can extend the argument by saying that the local reduced density matrices should be equal for every region \( R \), so for every environment. This leads us to conclude that \( V(g) \) must be single blocked.

### B. Edge properties

Because the symmetry MPOs \( V(g) \) are single blocked we can define the third cohomology class \( [\alpha] \in H^3(G, U(1)) \) associated with the MPO group representation \cite{18,30}. The third cohomology class is an example of a discrete label associated to a set of MPOs (and a quantum phase) as mentioned in section I. The short-range entangled PEPS constructed from tensors satisfying Eq. \( 5 \) and Eq. \( 6 \) has non-trivial SPT order if \( [\alpha] \) is non-trivial. The existence of non-trivial SPT order follows from the analysis of the edge properties when such a PEPS is defined on a finite lattice with a physical edge. This PEPS has open, dangling virtual indices along the boundary. For the PEPS parent Hamiltonian, derived such that the bulk is in the correct state, any virtual boundary condition gives rise to an exact ground state and the degeneracy thus scales exponentially in the length of the boundary. However, this is a generic property of all PEPS (bulk-) parent Hamiltonians. The physically relevant question is whether the Hamiltonian can be perturbed by additional terms which are invariant under \( G \) in order to gap out these edge modes and to give rise to a unique symmetric ground state. In \cite{29} an isometry was derived that maps any operator acting on the physical indices of the PEPS to an effective operator acting on the virtual indices on the boundary. Away from the RG fixed point, however, it has not been proven that this isometry preserves locality. But for a PEPS with exponential decay of correlations we conjecture that a local operator acting on the physical indices near the boundary is mapped to a (quasi-) local operator acting on the virtual degrees of freedom along the boundary, as was numerically illustrated for a particular non-topological PEPS in \cite{31}. From properties \( 5 \) and \( 6 \) it is clear that acting with \( U(g) \) on every physical site is equivalent to acting with the MPO \( V(g) \) on these dangling boundary indices of the PEPS, so that a \( G \)-symmetric local perturbation to the Hamiltonian at the physical level will give rise to an effective (quasi-) local Hamiltonian on the virtual boundary that is invariant under \( V(g) \). Ground states of the perturbed Hamiltonian are now given by closing the PEPS network with ground states of this effective edge Hamiltonian, which should be well represented by an injective MPS if it has a unique gapped ground state invariant under \( V(g) \). This is, however, a contradiction as explained by the powerful result of Chen et al. \cite{18} which states that an injective MPS cannot be invariant under the action of a family of MPOs \( V(g) \) with non-trivial third cohomology.

This implies that the effective edge Hamiltonian is either gapless, such that its ground state cannot be well represented as an MPS, or has spontaneous symmetry breaking. In the latter case, the physical state obtained by closing the PEPS network with one of the virtual symmetry breaking ground states of the effective Hamiltonian will also exhibit symmetry breaking and hence does not qualify as a symmetric state. The former case, on the other hand, implies that a local symmetric perturbation to the physical Hamiltonian is unable to gap
out the gapless edge modes, which is indeed one of the hallmarks of non-trivial SPT order. Here, we again use the fact that a PEPS with exponential decay of correlations has a gapped transfer matrix such that the gapless modes on the virtual boundary of the PEPS network can indeed be associated with physical degrees of freedom localized within a distance of the correlation length from the boundary. This possibility of explicitly identifying the degrees of freedom corresponding to the gapless edge modes is one of the benefits of the PEPS framework \[31\]. If we tune the PEPS to criticality, these edge modes will extend further into the bulk, consistent with the results of \[32\] about phase transitions between symmetry-protected and trivial phases.

V. GAUGING SPT PEPS

In this section we discuss how gauging a SPT PEPS results in a PEPS that has topological order. We then proceed by showing that there is always a way to gauge the SPT PEPS such that the gap of the parent Hamiltonian remains open. Finally, symmetry twists and monodromy defects are argued to have a natural description in the tensor network formalism.

A. Gauging SPT PEPS to topologically ordered PEPS

As the SPT PEPS satisfying Eq. (5) and (6) are invariant under the global action of a symmetry group $G$, we can now apply the quantum state gauging procedure of \[19\] to these states. It was shown in \[19\] that the virtual representation of the symmetry in the original state becomes a purely virtual symmetry of the gauged tensors, without any physical effect. More precisely, it was shown how an injective PEPS with virtual bonds in $C^D$ and a virtual symmetry representation that factorizes as $V^R(\gamma) = v(\gamma)^{\otimes L}$ (with $v(\gamma) : C^D \to C^D$) is transformed by the gauging procedure into a PEPS with virtual bonds in $C^D \otimes C[G]$ that is $G$-injective, i.e. that is injective on a subspace with projector $\sum_{g \in G} (v(\gamma) \otimes R^g(\gamma))^{\otimes L}$. Here, $L = 2(N_h + N_v)$ is the length of the boundary of the region $\mathcal{R}$ under consideration (containing $N_h \times N_v$ sites) and $R^g(\gamma)$ is the right group multiplication, which is a representation of $G$ on the new component $C[G]$ of the virtual bonds. In the language of section II this means that with $O^g_{\mathcal{R}} := (v(\gamma) \otimes R^g(\gamma))^{\otimes L}$, the double layer $E^\mathcal{R}_{\text{gauged}}$ of the gauged PEPS satisfies

\[
(O^g_{\mathcal{R}} \otimes \mathbbm{1})E^\mathcal{R}_{\text{gauged}} = E^\mathcal{R}_{\text{gauged}} = (\mathbbm{1} \otimes O^g_{\mathcal{R}})E^\mathcal{R}_{\text{gauged}}.
\]

These symmetry properties of $E^\mathcal{R}_{\text{gauged}}$ imply the PEPS has topological order in the same universality class as that of the quantum double model constructed from $G$ \[10\] \[33\].

We can easily extend this proof to the general case of section IV \[34\], where the PEPS in region $\mathcal{R}$ has a non-factorizable virtual symmetry representation given by the MPOs $V^\mathcal{R}(\gamma) : (C^D)^{\otimes L} \to (C^D)^{\otimes L}$ and is only injective on the support subspace of the projection MPO $P^\mathcal{R} = V^\mathcal{R}(\mathbbm{1})$. The resulting gauged PEPS with virtual bonds in $C^D \otimes C[G]$ still satisfies the axioms of MPO-injectivity \[13\], but is now injective onto the subspace defined by the projection MPO $P^\mathcal{R} = \sum_{g \in G} V^\mathcal{R}(\gamma) \otimes R^g(\gamma)^{\otimes L}$. Every single term is now one of the original MPO representations $V^\mathcal{R}(\gamma)$ tensored with the product representation on the new part $C[G]$ of the virtual space. The MPO representation of $P^\mathcal{R}$ will thus have a canonical form with several blocks labeled by the elements $g \in G$ and corresponding to the original MPO tensors of $V^\mathcal{R}(\gamma)$ (tensored with $R(g)^r$ on the extra part of the virtual space, but this doesn’t change the bond dimension of these blocks, nor their third cohomology class). This implies that $E^\mathcal{R}_{\text{SPT}}$ of the gauged SPT PEPS also satisfies (9), but now with $O^\mathcal{R} = V^\mathcal{R}(\gamma) \otimes R^g(\gamma)^{\otimes L}$. The topological order of the gauged SPT PEPS lies in the universality class of the Dijkgraaf-Witten gauge theories, as we show explicitly in the example in section VI.C. We emphasize that, up to the irrelevant operators $R^g(\gamma)^{\otimes L}$, the same MPO determines both the gapless edge modes of the SPT phase and, as argued in \[12\] \[13\], all the topological properties of the gauged model. This makes the gauging connection between finite group symmetry-protected topological order and intrinsic topological order —as explored at the Hamiltonian level by Levin and Gu \[20\]— explicit for all PEPS.

We note that the PEPS gauging map can equally well be used to gauge a normal subgroup $N$ of the SPT symmetry group $G$. This will give rise to a state with symmetry-enriched topological order, where the topological part corresponds to a gauge theory with gauge group $N$ and the global symmetry is given by the quotient group $G/N$ \[34\].

B. Gauging preserves the gap

We now show that two SPT PEPS are in different phases when the corresponding gauged PEPS have different topological order. Take the gapped symmetric parent Hamiltonian of the SPT PEPS $H_m = \sum_i h_i$, which is a sum over local terms $h_i$, and gauge it using the formalism of \[19\] to obtain $\tilde{G}[H_m]$ as defined in \[53\]. We have that $\tilde{G}[O] = GO$ for any symmetric operator $O$, where $G$ is the quantum state gauging map \[52\]. To see this, take the concrete situation where $O$ is a two-site operator acting on neighbouring vertices $v_1$ and $v_2$, which are connected by edge $e$ pointing from $v_1$ to $v_2$. The generalization to arbitrary operators is straightforward. The gauged operator is then $\tilde{G}[O] = \sum_{g,h \in G} |h g^{-1}\rangle_\epsilon (U_{v_1}(g) \otimes U_{v_2}(h)) O(U_{v_1}(g) \otimes \ldots$
Acting with \((U_{\alpha_3}(g) \otimes U_{\alpha_1}(h))\) on \(G\) will keep only those terms that act on sites \(v_1\) and \(v_2\) with the same group element. Using the symmetry of \(O\) we can then commute \(O\) through \((U_{\alpha_1}(g) \otimes U_{\alpha_2}(h))\) after commuting \(O\) restores \(G\). Now we can easily see that any eigenstate \(|\psi_\lambda\rangle\) of \(H_m\) with eigenvalue \(\lambda\) will give rise to an eigenstate \(G|\psi_\lambda\rangle\) of \(G[H_m]\) with the same eigenvalue. Here we of course implicitly assumed that \(|\psi_\lambda\rangle\) is not annihilated by \(G\), which will be the case when the representation under which \(|\psi_\lambda\rangle\) transforms contains the trivial representation.

The Hamiltonian of the gauged system also has a second term \(H_g\), which gives dynamics to the gauge fields by requiring the flux through every plaquette to be the identity group element. The gauging map \(G\) has the convenient property that \(H_g G = \mu G\), where \(\mu\) is the lowest eigenvalue of \(H_g\). So \(G|\psi_\lambda\rangle\) is an eigenstate of the total gauge and matter Hamiltonian \(H_g,m = G[H_m] + H_g\) with eigenvalue \(\mu + \lambda\) (in the supplementary material we show that \(H_{g,m}\) corresponds to the Hamiltonian obtained via the standard minimal coupling gauging procedure). Since \(\mu\) is just a constant shift of (a part of) the spectrum of \(H_m\), we can make the flux excitations of \(H_g\) sufficiently gapped, the gauging map does not close the gap of the SPT Hamiltonian \(H_m\) if its ground state is symmetric. So if we can connect two SPT PEPS (parent) Hamiltonians with a gapped, continuous and symmetric path we can also connect the gauged models with a gapped and continuous path.

C. Symmetry twists

If we consider SPT PEPS on a torus, then wrapping the symmetry MPO around a non-contractable loop corresponds to adding a symmetry twist. For finite groups these states have been used to identify non-trivial SPT order via their overlap matrices after applying modular transformations \([6]\). The gauging connection in the PEPS picture elucidates why this corresponds to calculating the \(S\)-matrix of the gauged topologically ordered states \([13, 36, 37]\). First of all, to have well-defined symmetry twist states we require the group elements \(\{g_x, g_y\}\) which label the twist in the \(x\)- and \(y\)-direction along the torus to commute. Acting with \(U(g)\) on every site will result in conjugation of the symmetry twists \(\{g_x, g_y\} \rightarrow \{g g_x g^{-1}, g g_y g^{-1}\}\). In the Abelian case it is thus clear that the states with symmetry twists will be symmetric. In the non-Abelian case we can construct symmetric states by adding commuting symmetry twists \(\{g_x, g_y\}\) and subsequently acting with \(\sum_{g \in G} U(g)^{\otimes N}\), where \(N\) is the number of sites. This allows to construct a number of different symmetric short-range entangled states that is equal to the number of irreducible representations of the quantum double \(D(G)\) \([10]\). Using that \(G^1 G\) is equal to the projector on the trivial representation it is clear that the overlap matrices of these states will not change after gauging. We also note that in recent work tensor networks were used to provide a notion of symmetry twists for time reversal symmetry \([35]\).

In \([39, 40]\), invariants for SPT phases were obtained by studying defects created by introducing symmetry twists with open endpoints in the ground state. The PEPS formalism allows to construct these monodromy defects in general symmetric ground states by putting an open MPO labeled by group element \(g\) on the virtual level of the tensor network. We show in the example below how one can study the symmetry properties of these defects. The PEPS gauging procedure also explicitly clarifies that these monodromy defects in the SPT state correspond to the actual fluxes of the gauged theory \([10]\).

VI. EXAMPLE: FIXED-POINT SPT STATES

Based on the instructive examples in \([11, 18]\) we now present a family of SPT PEPS with symmetry group \(G\) and 3-cocycle \(\alpha\) satisfying \([5]\) and \([6]\), study their symmetry defects and explicitly demonstrate that gauging these states yields MPO-injective PEPS that are the ground states of twisted quantum double Hamiltonians \([22]\).

A. Fixed-point SPT PEPS

The short-range entangled PEPS are defined on any trivalent lattice embedded in an oriented 2-manifold (dual to a triangular graph). They realize states equivalent to a standard SPT fixed point construction on the triangular graph \([11, 41]\). To this end we must specify an ordering on the vertices of the triangular graph which induces a direction on each edge, pointing from larger to smaller vertex. With this information we assign the following PEPS tensor \(A_\Delta \in C(G)^{\otimes 9}\) to each vertex of the trivalent lattice

\[
\int \prod_{v \in \Delta} dg_v \hat{\alpha}_e \bigotimes_{v' \in \Delta} |g_{v'}\rangle_{\Delta,v'} \bigotimes_{e' \in \Delta} |g_{v'^{-}}\rangle_{\Delta,e,v'^{-}} (g_{v'^{+}} |_{\Delta,e,v'^{+}})
\]

where edge \(e\) is oriented from \(v'^{-}\) to \(v'^{+}\) (hence \(v'^{-} < v'^{+}\)). The phase \(\hat{\alpha}_e\) for the vertex of the trivalent PEPS lattice, corresponding to a plaquette \(\Delta\) on the triangular lattice whose vertices are given counterclockwise relative to the orientation of the 2-manifold by \(v, v', v''\) (note the choice of starting vertex is irrelevant), is defined by a 3-cocycle \(\alpha\) as follows \(\alpha_\Delta := \alpha^{\sigma_x}(g_1 g_2^{-1}, g_2 g_3^{-1}, g_3)\).

\((g_1, g_2, g_3) := \pi(g_v, g_{v'}, g_{v''})\) with \(\pi\) the permutation that sorts the group elements into ascending vertex order and \(\sigma_x = \pm 1\) is the parity of the permutation (equivalently
The orientation of $\triangle$ relative to the 2-manifold. For the following example the tensor is given by

$$
\begin{align*}
= \alpha(g_1 g_2^{-1}, g_2 g_3^{-1}, g_3).
\end{align*}
$$

Note the tensor diagrams in this section use the convention that physical vertex indices are written within the body of the tensor. We also only represent the virtual and physical index combinations which correspond to non-zero values of (10). This gives a MPO constructed from the following tensors

Note that for fixed $h$ these MPOs possess a single block. We introduce the isometry $W(h_1, h_2)$

$$
W(h_1, h_2) = \alpha(g, h_1, h_2),
$$

to describe the multiplication of two MPO tensors. With this isometry we have the following relation

$$
\begin{align*}
\left[ I_{h_1} \otimes W(h_2, h_3) \right] W(h_1, h_2 h_3) &= \alpha(h_1, h_2, h_3) [W(h_1, h_2) \otimes I_{h_3}] W(h_1 h_2, h_3),
\end{align*}
$$

which is again the 3-cocycle condition Eq. (48). From Eq. (17) we thus conclude that the short-range entangled states described by the tensors of Eq. (10) lie in a symmetry-protected topological phase labeled by the cohomology class $[\alpha] \in H^3(G, U(1))$.

We would like to note that one layer of strictly local unitaries (equivalent to the circuit $D_\alpha$) acting on the vertices of the states built from the tensors in Eqs. (10) can remove the 3-cocycles, thus mapping it to a trivial product state. This is however not in contradiction with the fact that SPT states cannot be connected to the trivial product state by a low-depth quantum circuit that preserves the symmetry, as this definition requires every individual gate of the circuit to preserve the symmetry [13]. This is not the case for the circuit just described.

**B. Projective transformation of monodromy defects**

The simplest way to study symmetry defects in SPT PEPS is by treating the system on a finite cylinder
with open boundaries. We then place the MPO representing group element $g$ along the longitudinal direction of the cylinder, extending from one boundary to the other. Note that now both boundaries contain open virtual MPO indices. If we would define this PEPS on a torus it is clear that the resulting state is symmetric under $C_g$, the centralizer of $g$. The global action of an element $h_1 \in C_g$ on the physical indices of the PEPS can be rewritten as a tensor product of matrices $X_g(h_1) \otimes X^{-1}_g(h_1)$ acting on the virtual indices along the two boundaries of the cylinder. Note that $X_g(h_1)$ acts both on the virtual PEPS and MPO indices. For the fixed-point SPT PEPS we can easily find exact expressions for $X_g(h_1)$, which in this case turn out to be unitaries. We find that $X_g(h_1)$ form a projective representation, i.e.

$$X_g(h_1)X_g(h_2) = \omega_g(h_1h_2)X_g(h_1h_2),$$

where the factor set is given by the expression

$$\omega_g(h_1, h_2) = \frac{\alpha(g,h_1,h_2)\alpha(h_1,h_2,g)}{\alpha(h_1, g, h_2)}.$$  

$\omega_g(h_1, h_2)$ can be checked to satisfy the 2-cocycle condition for $h_1, h_2 \in C_g$ by repeated application of the 3-cocycle condition. For each type of symmetry defect $g$ the virtual boundary of the cylinder transforms projectively under $C_g$ with a 2-cocycle in the second cohomology class $[\omega_g] \in H^2(C_g, U(1))$. This agrees with the results of [10].

### C. Gauging the fixed-point SPT PEPS

We now apply the quantum state gauging procedure of [19] to gauge the global symmetry of the fixed-point SPT PEPS defined in the previous sections. For this we construct a gauging tensor network operator (matching that of [19] on the dual triangular graph) that maps matter states to gauge and matter states. The gauging map is defined by the following local tensors

$$\int \prod_{v \in \Delta} dh_v \bigotimes_{v \in \Delta} R_{\Delta, v}(h_v) \bigotimes_{e \in \Delta} \left| h_{v^-} h_{v^+}^{-1} \right\rangle_{\Delta, e},$$

where gauge degrees of freedom have been introduced on the edges. For our example the gauging tensor is

$$\int \prod_{v \in \Delta} dg_v \otimes \left| g_v \right\rangle_{\Delta} \langle g_v \rangle_{\Delta} L_e(g_{v^-}^-) R_e(g_{v^+}^+) \otimes \left| h_{v^-} h_{v^+}^{-1} \right\rangle_{\Delta, e}.$$  

We can apply the gauging tensors locally to the SPT PEPS to form tensors for a gauge and matter PEPS

$$\tilde{A}_\Delta := \int \prod_{v \in \Delta} dh_v \otimes \tilde{\alpha}_\Delta \bigotimes_{v \in \Delta} \left| g_v h_{v^-}^{-1} \right\rangle_{\Delta, v},$$

in our example these are

$$\tilde{A}_\Delta \bigotimes_{v \in \Delta} \left| Z_{\varepsilon \Delta, v}(h) R(h) \right\rangle \otimes \left| g_v \right\rangle_{\Delta, v} \bigotimes_{e \in \Delta} \left| h_{v^-} h_{v^+}^{-1} \right\rangle_{\Delta, e, v},$$

where

$$\tilde{A}_\Delta \bigotimes_{v \in \Delta} \left| g_v \right\rangle \langle g_v \rangle_{\Delta} L_e(g_{v^-}^-) R_e(g_{v^+}^+) \otimes \left| h_{v^-} h_{v^+}^{-1} \right\rangle_{\Delta, e, v}.$$  

The gauge constraints satisfied by the gauged PEPS $|\psi_g\rangle$ are $\tilde{P}_v |\psi_g\rangle = |\psi_g\rangle$ for every vertex $v$, where

$$\tilde{P}_v := \int \prod_{v \in \Delta} dg_v \otimes \left| R_{\Delta, v}(h) \bigotimes_{e \in \Delta} \left| g_v \right\rangle \langle g_v \rangle_{\Delta, v} \bigotimes_{e \in \Delta} \left| h_{v^-} h_{v^+}^{-1} \right\rangle_{\Delta, e, v} \right\rangle_{\Delta, v}.$$  

The gauge and matter tensor $\tilde{A}_\Delta$ is MPO-injective with respect to a purely virtual symmetry inherited from the symmetry transformation of the SPT tensor $A_\Delta$ and it also intertwines a physical symmetry to a virtual symmetry due to the transformation of the gauging tensors

$$\tilde{A}_\Delta \bigotimes_{e \in \Delta} \left| Z_{\varepsilon \Delta, v}(h) R(h) \right\rangle \otimes \left| g_v \right\rangle_{\Delta, v} \bigotimes_{e \in \Delta} \left| h_{v^-} h_{v^+}^{-1} \right\rangle_{\Delta, e, v}.$$  

We next apply a local circuit $\tilde{C}_\Lambda$ to explicitly map the gauge and matter model to a twisted quantum double ground state on the gauge degrees of freedom alone. This circuit is given by the tensor product of the following local unitary on each site

$$\tilde{C}_\Delta := \int \prod_{v \in \Delta} dg_v \otimes \left| g_v \right\rangle \langle g_v \rangle_{\Delta} L_e(g_{v^-}^-) R_e(g_{v^+}^+) \otimes \left| h_{v^-} h_{v^+}^{-1} \right\rangle_{\Delta, e, v},$$

which maps the gauge constraints to local rank one projectors on the matter degrees of freedom at each vertex $C_\Lambda \tilde{P}_v \tilde{C}_\Lambda = \int \prod_{v \in \Delta} \left| g_v \right\rangle \langle g_v \rangle_{\Delta} L_e(g_{v^-}^-) R_e(g_{v^+}^+).$ From this we infer that the gauged PEPS will have its gauge and matter degrees of freedom disentangled under the circuit $\tilde{C}_\Lambda$. To see this explicitly we apply the circuit locally to each PEPS tensor, along with a unitary change of basis on the virtual
level (leaving the physical state invariant) to form the tensor $\tilde{A}_\Delta$ which is defined to be

$$
\tilde{C}_\Delta \tilde{A}_\Delta \bigotimes_{e \in \Delta} U_{\Delta, e, v_2^e} \otimes U_{\Delta, e, v_3^e} = \int \prod_{v \in \Delta} d_{v_2} d_{v_3} \tilde{\alpha}_\Delta \\
\bigotimes_{v \in \Delta} |k_{v_2}^e, g_{v_3}^{-1} \rangle_{\Delta, e, v_2^e}, (g_{v_2}^{-1}, k_{v_3}^e) |g_{v_3}^{-1}, k_{v_2}^e \rangle_{\Delta, e, v_3^e}, \quad (26)
$$

where $U := \int d_g |g \rangle \otimes SL^1(g)$, with $S |g \rangle := |g^{-1} \rangle$, satisfies $(g, h)U = (g, gh^{-1})$. For our example this tensor is given by

$$
\begin{align*}
\tilde{\alpha}(g_1 g_2^{-1}, g_2 g_3^{-1}, g_3)
\end{align*}
\quad (27)
$$

This disentangled PEPS tensor $\tilde{A}_\Delta$ is now MPO-injective on the subspace projected on with the sum of the symmetry MPOs of the SPT PEPS, and the intertwining condition of the physical vertex symmetry takes it to a trivial action on the virtual space

$$
\tilde{A}_\Delta \bigotimes_{e \in \Delta} [Z^e_{\Delta, e} (h) R(h)^{\otimes 2}] \otimes 1^{\otimes 2} = \tilde{A}_\Delta \quad (28)
$$

$$
\bigotimes_{v \in \Delta} R_{\Delta, v}(h) \tilde{A}_\Delta = \tilde{A}_\Delta \bigotimes_{e \in \Delta} 1^{\otimes 2} \otimes R(h)^{\otimes 2}. \quad (29)
$$

From this we see that $\tilde{A}_\Delta$ separates into a trivial local component on the matter degrees of freedom yielding the state $\bigotimes_e \int d_{g_2} \otimes_{\Delta_3 e} \langle g_{v_3} \rangle_{\Delta, e, v_3^e}$, and the following tensors on the gauge degrees of freedom

$$
\int \prod_{v \in \Delta} d_{g_2} \tilde{\alpha}_\Delta \bigotimes_{e \in \Delta} |g_{v_2}^{-1} \rangle_{\Delta, e, v_2^e}, (g_{v_2}^{-1}, k_{v_3}^e) |g_{v_3}^{-1}, k_{v_2}^e \rangle_{\Delta, e, v_3^e}. \quad (30)
$$

These tensors corresponding to the gauge degrees of freedom yields a PEPS representation of the ground state of a 2D twisted quantum double with 3-cocycle $\alpha$, which is equal to the standard representation on the subspace obtained by mapping $\otimes_{\Delta_3 e} |g \rangle_{\Delta, e, v} \mapsto |g \rangle_{v}$ and $\otimes_{\Delta_3 e} |g \rangle_{\Delta, e, v} \mapsto |g \rangle_{v}$ for our example this tensor is

$$
\begin{align*}
\tilde{\alpha}(g_1 g_2^{-1}, g_2 g_3^{-1}, g_3)
\end{align*}
\quad (31)
$$

Note that in the Abelian case the tensors in (31) reduce to the string-net tensors [44, 45] after a suitable mapping between 3-cocycles and $F$-symbols [16] (in the non-Abelian case one has to change to the basis of irreducible representations to make the identification).

**VII. CONCLUSIONS**

We have presented a unified picture of characterizing all gapped phases in PEPS, with or without symmetries, via MPOs. For this we have generalized the characterization of a global symmetry in injective PEPS to the framework of MPO-injectivity [12, 13]. Unlike in the injective case [20], where the symmetry representation on the virtual indices factorizes, the PEPS tensors can have a virtual symmetry representation which is given by non-factorizable MPOs. We subsequently identified the short-range entangled PEPS as those having a single block in the projection MPO onto the injectivity subspace. If the corresponding single block MPO virtual symmetry representation has a non-trivial third cohomology class it gives rise to unconventional edge properties and thus to symmetry-protected topological PEPS. This identification of the virtual PEPS structure corresponding to SPT order opens new routes to study transitions between these phases, as was done in [17, 18] for the condensation transitions between topological and trivial phases.

We find that applying the quantum state gauging procedure of [19] to a SPT PEPS transforms its MPO representation of $\mathcal{G}$ into a purely virtual symmetry of the gauged tensors. Put differently, the resulting gauge-invariant PEPS also satisfies the axioms of MPO-injectivity, but with the projection MPO onto the injectivity subspace having a block structure labeled by the group elements $g$. This block structure in the projection MPO characterizes the phases of the twisted quantum double models, which are known to have intrinsic topological order. It was shown in [13] that this projection MPO determines all the topological properties of the gauged PEPS. This relation explains the mechanism behind the braiding statistics approach to SPT phases [20] at the level of the corresponding quantum states. We have illustrated these concepts for a family of RG fixed-point states, which contain all the bosonic SPT phases with a finite on-site symmetry group.

The general formalism presented in this paper describes both symmetries and topological order in PEPS. So, in principle, it also captures symmetry-enriched topological phases. The quantum state gauging procedure can be adapted to gauge only a normal subgroup of the global symmetry group of a SPT PEPS, which allows one to explicitly construct special classes of SET PEPS. An open question is how the corresponding MPOs encode the discrete, universal labels of the SET phase and how to extract them. We further expect that a better un-
standing of excitations in MPO-injective PEPS will yield insights into the physical properties of SET phases such as symmetry fractionalization. We plan to study these matters in future work.[34].

Another question which presents itself is how to generalize these constructions to fermionic systems. It would be interesting to see if applying the same principles to the formalism of fermionic PEPS naturally gives rise to the (partial) classification of fermionic SPT phases based on supercohomology theory.[50]. The quantum state gauging procedure works equally well for fermionic systems however the gauge degrees of freedom are always bosonic. It would thus be interesting to see if there is an alternative way of obtaining fermionic systems with intrinsic topological order from the fermionic SPT phases.

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Supplementary Material

A. Axioms for MPO-injectivity

This section reviews the axioms of MPO-injectivity as presented in [13].

We interpret the tensors $A$ of an MPO-injective PEPS as linear maps from the virtual to the physical space and apply the pseudo-inverse $A^+$, which gives rise to a projector that can be written as a MPO:

\begin{align}
A A^+ A &= (32)
\end{align}

We further require this MPO to satisfy the pulling through property as shown in Eq. (33).

\begin{align}
A A &= (33)
\end{align}

The same property should also hold where the MPO gets pulled from three virtual indices to one or vice versa. This makes the presence of this MPO locally undetectable in the PEPS. Using the pulling through property, it is easy to check that the requirement for the MPO to be a projector is equivalent to the property shown in Eq. (34)

\begin{align}
&= (34)
\end{align}

We also need a technical requirement such that the properties of the PEPS grow in a controlled way with the number of sites. For example, we want two concatenated tensors to be injective on the space projected on by the MPO surrounding these two tensors. For this we need that there exists a tensor $X$, depicted in (35),

\begin{align}
X :=  (35)
\end{align}

such that we have the generalized inverse property (36).

\begin{align}
&= (36)
\end{align}

The generalized inverse property allows one to prove many useful things like the intersection property or an explicit expression for the ground state manifold on a torus [13].

B. General class of MPOs for SPT PEPS

In the main text it was explained that the projector MPO $A^+ A$, where $A$ is the tensor of a SPT PEPS, should be single blocked. In this appendix we give a sufficient minimal condition on this MPO such that it gives rise to a state without topological degeneracy.

Because the MPO is injective and a projector for every length we know that the MPO acting on itself gives a new injective representation of the original MPO. So there exists a matrix $X$, which we call the reduction tensor, acting on the virtual level of the MPO that brings both representations in the same form [25] and satisfies $XX^* = X^* X = 1_D$, where $1_D$ is the projector on a $D$-dimensional space. This is shown graphically in (37).

\begin{align}
&= (37)
\end{align}

We now consider the class of injective projector MPOs where the reduction tensor is rotationally invariant and property (38) holds. Note that (38) does not follow from (37).

\begin{align}
&= (38)
\end{align}

Using these two conditions it is easy to show that this MPO satisfies the pulling through property as shown in (39).

\begin{align}
&= (39)
\end{align}

If we now multiply three MPOs the resulting tensor can be reduced to the original MPO tensor in two possible ways. By acting with the reduction tensor only on the right virtual indices these two ways should be equivalent up to a complex number $\alpha$ as depicted in (40).

\begin{align}
&= \alpha (40)
\end{align}

Because the reduction tensors are rotationally invariant (40) is equivalent to (41), after ignoring the factor $\alpha$ which is irrelevant for this discussion.
In [13] it was shown that all the ground states of MPO-injective PEPS parent Hamiltonians on a torus take the form of (42), where periodic boundary conditions are assumed and $Q$ is a general tensor called the ground state tensor that is undetectable via the physical indices.

It is clear that generic solutions of $Q$ can be obtained by concatenating reduction tensors. Equation (41) can then be used to show that all the resulting ground states are equivalent. By using the reduction tensor one can also take together the MPOs in the neighbourhood of $Q$. The resulting ground state will contain a MPO with a matrix on its virtual indices given by (43).

Because this matrix should be locally undetectable it cannot break the translation symmetry. If the MPO would not be embedded in the PEPS this would imply that the matrix has to commute with all the MPO tensors. But because the MPO is injective these tensors span the space of all $\chi \times \chi$ matrices, with $\chi$ the virtual bond dimension of the MPO. Therefore the matrix in (43) can only be the identity matrix times a constant. It is however not a priori clear that the same reasoning still holds when the MPO is embedded in the PEPS. But because we consider PEPS that is MPO-injective we have sufficient access to the MPO containing matrix (43) to conclude that it can only have a trivial physical effect. This shows that there is no topological degeneracy for MPO-injective PEPS where the projector MPO is injective and its reduction tensor is rotationally invariant.

As a technical comment we would also like to mention that no further requirements on the single block projector MPOs that can satisfy the axioms of MPO-injectivity. This would imply that MPO-injective PEPS which have no topological entanglement entropy also do not give rise to a topological degeneracy.

C. Third cohomology class of a single block MPO group representation

In this appendix we repeat the definition of the third cohomology class of an injective MPO representation of a finite group $G$ as introduced in [18]. For details about group cohomology theory we refer to [1].

Multiplying two MPOs labeled by group elements $g_1$ and $g_2$ should be equal to the MPO labeled by $g_2g_1$ for every length. Because the MPOs are injective we again know there exists a gauge transformation on the virtual indices of the MPO that brings both representations in the same form [25]. This means there exists a matrix $X(g_1, g_2)$ such that figure (44) holds.

If we now multiply three MPOs labeled by $g_1$, $g_2$ and $g_3$ there are two ways to reduce the multiplied MPOs to the MPO labeled by $g_3g_2g_1$. When only acting on the right virtual indices these two ways should be the same up to a complex number labeled by $g_1$, $g_2$ and $g_3$. This is shown in figure (45).

By multiplying four MPOs one sees that $\alpha$ has to satisfy a consistency condition. This is because the two different paths between the same reduction procedures as shown in (46) and (47) should give rise to the same complex number.
Using (45) it is easy to check that this consistency condition is
\[ \frac{\alpha(g_3, g_2, g_1)\alpha(g_3, g_2g_1, g_0)\alpha(g_2, g_1, g_0)}{\alpha(g_3, g_2, g_1, g_0)\alpha(g_3, g_2, g_1, g_0)} = 1. \] (48)

Since this is exactly the cocycle condition it implies that \( \alpha \) is a 3-cocycle. Note that \( X(g_1, g_2) \) is defined up to a complex number \( \beta(g_1, g_2) \). This freedom can only change the 3-cocycle in (45) by
\[ \alpha'(g_3, g_2, g_1) = \alpha(g_3, g_2, g_1)\frac{\beta(g_2, g_3)\beta(g_1, g_3g_2)}{\beta(g_1, g_2)\beta(g_2g_1, g_3)}. \] (49)

Thus we see that \( \alpha \) is defined up to a coboundary. For this reason we label the single block MPO group representation with an element of the third cohomology group \( H^3(G, \mathbb{C}) \). Using the fact that \( H^3(G, \mathbb{R}) = \mathbb{Z}_4 \) (and that \( \mathbb{R} \) as an additive group is isomorphic to \( \mathbb{R}^+ \) as a multiplicative group), we thus obtain that the non-trivial third cohomology class of the MPO is an element of \( H^3(G, U(1)) \).

D. Gauging SPT PEPS yields topological PEPS

We generalize the proof presented in \([19]\) to show that gauging a SPT PEPS results in a MPO-injective PEPS with the projector MPO having multiple blocks in its canonical form labeled by the group elements.

Let us first recount the definition of the projector onto the gauge invariant subspace. For this we require a directed graph \( \Lambda \) in which the vertices are enumerated and the edges are directed from larger to smaller vertex. To each vertex \( v \in \Lambda \) we associate a Hilbert space \( \mathbb{H}_v \) together with a representation \( U_v(g) \) of the group \( G \) and to each edge \( e \in \Lambda \) we associate a Hilbert space isomorphic to the group algebra \( \mathbb{H}_e \cong \mathbb{C}[G] \). We define a matter Hilbert space \( \mathbb{H}_m := \bigotimes_{e \in \Lambda} \mathbb{H}_v \) and a gauge Hilbert space \( \mathbb{H}_g := \bigotimes_{e \in \Lambda} \mathbb{H}_e \), which together form the full Hilbert space \( \mathbb{H}_{g,m} := \mathbb{H}_g \otimes \mathbb{H}_m \). The relevant states in \( \mathbb{H}_{g,m} \) satisfy a local gauge invariance condition for each vertex, i.e. they lie in the simultaneous +1 eigenspace of the following operators
\[ P_v := \int \text{d}g_v U_v(g_v) \bigotimes_{e \in \mathcal{E}^+_v} R_e(g_e) \bigotimes_{e \in \mathcal{E}^-_v} L_e(g_e) \] (50)

where \( \mathcal{E}^+_v \) (\( \mathcal{E}^-_v \)) is the set of adjacent edges directed away from (towards) vertex \( v \). We then define the projector onto the subspace of gauge invariant states as \( P_\Lambda := \prod_v P_v \) and the analogous projection \( P_\Gamma \) for any operator \( O \) supported on a subset \( \Gamma \subseteq \Lambda \) (which contains the bounding vertices of all its edges) given by
\[ P_\Gamma[O] := \int \prod_{v \in \Gamma} \text{d}g_v \bigotimes_{e \in \mathcal{E}^+_v} U_v(g_e) \bigotimes_{e \in \mathcal{E}^-_v} L_e(g_e) R_e(g_e) R_e(g_e) ]^\dagger \] (51)

where the edge \( e \) points from \( v_e^+ \) to \( v_e^- \).

We proceed to describe a gauging procedure for models defined purely on matter degrees of freedom \( \mathbb{H}_m \). To apply \( P_\Lambda \) and \( P_\Gamma \) we first require a notion of embedding states and operators from \( \mathbb{H}_m \) into \( \mathbb{H}_{g,m} \). For this we define the gauging map for matter states \( |\psi\rangle \in \mathbb{H}_m \) as
\[ G[|\psi\rangle] := \bigotimes_{e \in \Gamma} P(|\psi\rangle \bigotimes_{e \in \Gamma} |1\rangle_e), \] (52)

and for matter operators \( O \in \mathbb{L}(\mathbb{H}_m) \) as
\[ G_\Gamma[O] := \bigotimes_{e \in \Gamma} P_e[O \bigotimes_{e \in \Gamma} |1\rangle_e]. \] (53)

Now consider a region \( R \) in the SPT PEPS, which defines a state in \( \mathbb{H}_m \), such that the tensors act as an injective map on the space \( \mathbb{V}_R = P^R(\mathbb{V}) \otimes L P^R \), where \( \mathbb{V}_v \) denotes the Hilbert space associated with a virtual index, \( P^R = \mathcal{V}^R(1) \) is a single-block projector MPO of length \( L \) and \( L \) is the number of open virtual indices along the boundary \( \partial R \). We denote the range of this map as \( \mathbb{R} \), with \( \dim \mathbb{R} = \dim \mathbb{V}_R \). Let \( \{ |\phi_i\rangle, i = 1, \ldots, \dim \mathbb{R} \} \) be
the vertices which have one or more edges

and set vertices for which all edges and neighbouring vertices

adapted to the case where the edge degrees of freedom

are doubled with controlled group multiplications and

absorbed in neighbouring vertices. We denote by $\mathcal{R}^c$ the

set vertices for which all edges and neighbouring vertices

are also contained in $\mathcal{R}$. The set $\Delta \mathcal{R} = \mathcal{R} \setminus \mathcal{R}^c$ contains

the vertices which have one or more edges $e \in \partial \mathcal{R}$.

The physical state $|\Phi_i, \{g_e\}_i\rangle$ corresponding to the state $|\Phi_i\rangle$ in the virtual boundary space $\mathcal{W}_{\partial \mathcal{R}} = \mathcal{V}_\mathcal{R}^R \otimes \mathcal{V}_e^L$, where $\mathcal{V}_e = \mathbb{C}[G]$ is the Hilbert space associated with the extra virtual index after gauging, is given by

$$|\Phi_i, \{g_e\}_i\rangle = \prod_{v \in \Delta \mathcal{R}} U_v(g_v) \bigotimes_{e' \in E_v \cap \mathcal{R}} R_{e'}(g_{e'}) \bigotimes_{e \in E_v \cap \mathcal{R}} L_e(g_e) \prod_{v' \in \mathcal{R}^c} P_{v'} \left(|\phi_i\rangle \bigotimes_{e \in \mathcal{R}} |1\rangle_e\right).$$

It now follows that $\langle \Phi_i, \{g_e\}_i | \Phi_i', \{g_e\}_i'\rangle = 0$ if there is no

g $\in G$ such that $\{g_e\}_i = \{g_e, g\}$. To see this, note that the physical states of the edge degrees of freedom between two vertices in $\Delta \mathcal{R}$ allow to determine the elements $\{g_e\}_i$ up to a global transformation $\{g_e\}_i \rightarrow \{g_e, g\}_i$. Having resolved $\{g_e\}_i$ up to a global factor $g$, the inner product of all edge degrees of freedom will force the interior gauge transformations in ket and bra to be equal up to the global transformation $g$.

So we have

$$\langle \Phi_i, \{g_e\}_i | \Phi_i', \{g_e\}_i'\rangle = \langle \phi_i | U^R(g) | \phi_i' \rangle,$$

where $U^R(g)$ is the tensor product of $U(g)$ over the sites in $\mathcal{R}$. Using the symmetry properties of SPT PEPS as presented in section III of the main text we also have

$$\langle \phi_i | U^R(g) | \phi_i' \rangle = \langle \tilde{\phi}_i | V^R(g) | \tilde{\phi}_i' \rangle,$$

where $V^R(g)$ is the symmetry MPO of length $L$ acting on the virtual boundary space $\mathcal{V}_\mathcal{R}^R$. So we find that the preimage of every bulk state $|\Phi_i, \{g_e\}_i\rangle$ is the set of states

$$\{V^R(g) \otimes R'_e(g_e)^{\otimes L} | \Phi_i, \{g_e\}_i\rangle, \forall g \in G\}.$$ This establishes the topological MPO-injectivity of the gauged PEPS as explained in the main text.

E. Gauging symmetric Hamiltonians and ground states

In this appendix we apply the gauging procedure of [19] to trivial and SPT Hamiltonians with symmetric perturbations and find that they are mapped to Hamiltonians in the phase of quantum double and twisted quantum double models respectively. We then go on to describe

the gauging of the fixed point ground states (with no perturbation).

First we apply the gauging procedure to a symmetric Hamiltonian defined on the matter degrees of freedom, each with Hilbert space $\mathcal{H}_e \cong \mathbb{C}[G]$ and symmetry action $U_e(g) = R_e(g)$, associated to the vertices of a graph $\Lambda$ embedded in a closed oriented 2-manifold. The Hamiltonian is given by

$$H_m = \alpha \sum_{v \in \Lambda} h_v^0 + \sum_{e \in \Lambda} \beta_m \sum_{v \in \Lambda} \mathcal{E}_m^e + \sum_{m \in \mathcal{C}(G)} \varepsilon_m \sum_{\rho} B_m^\rho.$$
Note that each term commutes with all local gauge constraints \( \{ P_v \} \) and the physics takes place within this gauge invariant subspace. To see more clearly that this gauge theory is equivalent to an unconstrained quantum double model we will apply a local disentangling circuit to reveal a clear tensor product structure, allowing us to ‘spend’ the gauge constraints to remove the matter degrees of freedom.

We define the disentangling circuit as the product of local unitaries \( C_\Lambda := \prod_v C_v \), where \( C_v := \int dg_v \langle g_v \| \prod_{e \in \Lambda^v} R_e(g_v) \prod_{e \in E^v} L_e(g_v) \rangle \). Note the order in the product is irrelevant since \( \{ C_v, C_v' \} = 0 \).

This circuit induces the following transformation on the gauge projectors: \( C_\Lambda P_v C_\Lambda^\dagger = \int dg_v R_v(g_v) \), hence any state \( |\psi\rangle \) in the gauge invariant subspace (simultaneous +1 eigenstate of all \( P_v \)) is disentangled into a tensor product of symmetric states on all matter degrees of freedom with an unconstrained state \( |\psi\rangle' \in \mathbb{H}_g \) on the gauge degrees of freedom \( C_\Lambda |\psi\rangle = |\psi\rangle' \otimes v \int dg_v \langle g_v |. \)

Now we apply the disentangling circuit to the Hamiltonian \( H_{\text{sym}} \). First note the pure gauge terms \( F_e \) and \( B_p^m \) are invariant under conjugation by \( C_v \).

The vertex terms are mapped to \( C_v h_v^0 C_v^\dagger = \int dg_v R_v(g_v) \otimes_{e \in E^v} R_e(g_v) \otimes_{e \in E^v} L_e(g_v) \). Since the disentangled vertex degrees of freedom are invariant under \( R_v(g_v) \) we see that this Hamiltonian term acts as \( \int dg_v \otimes_{e \in E^v} R_e(g_v) \otimes_{e \in E^v} L_e(g_v) \) on the relevant gauge degrees of freedom. We recognize this as the vertex term from a quantum double model. Finally we examine the transformation of the interaction terms \( C_v G_{e} [e^m] C_v^\dagger = \frac{1}{|G|} \langle m | \langle m |_e \rangle \), which yield local fields on the gauge degrees of freedom that induce string tension. Hence we see that the gauge plus matter Hamiltonian after disentangling becomes a local Hamiltonian \( H_{\text{g}} := C_v H_{g,m} C_v^\dagger \) acting purely on the gauge degrees of freedom

\[
H_g = \alpha \sum_v \int dg_v \otimes_{e \in E^v} R_e(g_v) \otimes_{e \in E^v} L_e(g_v) + \sum_{m \in \mathbb{Z}} \beta_m \sum_{v} |m\rangle \langle m|_e + \frac{1}{|G|} \sum_{e \in \Lambda} \sum_{m \in \mathbb{G}} \bar{B}_p^m \]  

(57)

which describes a quantum double model with string tension and flux perturbations. Note that a spontaneous symmetry breaking phase transition in the ungauged model is mapped to a string tension induced anyon condensation transition by the gauging procedure.

This gauging procedure easily extends to nontrivial SPT Hamiltonians which are defined on triangular graphs embedded in closed oriented 2-manifolds. The only modification required is to replace the trivial vertex terms \( h_v^0 \) by nontrivial terms \( h_v^\alpha \) which defined to be

\[
\int \langle g_v | \otimes_{e \in E^v} \alpha_\Delta \langle g_v | \langle g_v' | \otimes_{e \in E^v} \alpha_\Delta \langle g_v' | \langle g_v' | \]  

(58)

where \( S(v) \) is the star of \( v \), \( L(v) \) is the link of \( v \) and \( \alpha_\Delta \in U(1) \) for plaquette \( \Delta \), whose vertices are given counterclockwise (relative to the orientation of the 2-manifold) by \( v, v', v'' \), is defined by the 3-cocycle \( \alpha_\Delta := \alpha^{\sigma_\gamma} (g_1 g_2^{-1}, g_2 g_3^{-1}, g_3 g_1^{-1}) \) where \( (g_1, g_2, g_3, g_4) := \pi(g_v, g_v, g_v') \) with \( \pi \) the permutation that sorts the group elements into ascending vertex label order (with the convention that \( g_v \) immediately precedes \( g_v \)) and \( \sigma_\gamma = \pm 1 \) is the parity of the permutation. The terms \( h_v^\alpha \) are clearly symmetric under global right group multiplication and flux perturbations. Note, importantly, the phase functions \( \alpha_\Delta \) now depend only on the gauge degrees of freedom. Finally we rewrite the pure gauge Hamiltonian terms without reference to the matter degrees of freedom, which become irrelevant as the matter degrees of freedom in any gauge invariant state must be in the symmetric state \( \sum_v \langle g_v | \).

\[
\int \langle g_v | \otimes_{e \in E^v} \alpha_\Delta \langle g_v | \langle g_v' | \otimes_{e \in E^v} \alpha_\Delta \langle g_v' | \langle g_v' | \]  

(59)

This can be recognized as the vertex term of a 2D twisted quantum double model (i.e. a lattice Dijkgraaf-Witten theory for the group \( \mathbb{G} \) and cocycle \( \alpha \)).

One can apply the gauging procedure directly to the ground states of the nontrivial SPT Hamiltonian defined in Eq. (58) which we define in terms of the following local
where $\tilde{\alpha}_\Delta \in U(1)$ is a function of the degrees of freedom on plaquette $\Delta$, whose vertices are given counterclockwise, relative to the orientation of the 2-manifold, by $v, v', v''$ (note the choice of starting vertex is irrelevant) and is defined by a 3-cocycle as follows

$$\alpha_\Delta := \alpha^{\sigma_\pi}(g_1, g_2, g_3) = \pi(g_v, g_{v'}, g_{v''})$$

with $\pi$ the permutation that sorts the group elements into ascending vertex label order and $\sigma_\pi = \pm 1$ is the parity of the permutation (equivalently the orientation of $\Delta$ embedded within the 2-manifold). Note $D_\alpha$ can easily be written as a product of commuting 3-local gates.

To define SPT fixed point states we start with the trivial state $|SPT(0)\rangle := \bigotimes_v \int d g_v |g_v\rangle$, which is easily seen to be symmetric under global right group multiplication. One can also check that $D_\alpha$ is symmetric under conjugation by global right group multiplication by utilizing the 3-cocycle condition satisfied by each $\tilde{\alpha}_\Delta$.

With this we define nontrivial SPT fixed point states $|SPT(\alpha)\rangle := D_\alpha |SPT(0)\rangle$, which are symmetric by construction. To see that $|SPT(\alpha)\rangle$ is the ground state of the SPT Hamiltonian $\sum_v h_v^\alpha$ we note $h_v^\alpha = D_\alpha h_v^0 D_\alpha^\dagger$ which again is proved using the 3-cocycle condition.

We will now gauge the SPT fixed point states by applying the state gauging map to $D_\alpha$, since the input variables of the circuit carry the same information as the virtual indices of the fixed point SPT PEPS this should make the correspondence between the two pictures more clear.

$$GD_\alpha = \int \prod_{v \in \Lambda} dg_v \prod_{\Delta \in \Lambda} \tilde{\alpha}_\Delta \bigotimes_{v \in \Lambda} |g_v\rangle \langle g_v|$$

Under the local disentangling circuit this transforms to

$$C_{\Delta} GD_\alpha = \int \prod_{v \in \Lambda} dg_v \prod_{\Delta \in \Lambda} \tilde{\alpha}_\Delta \bigotimes_{v \in \Lambda} |h_v^{-1} g_v\rangle \langle g_v|$$

where we can see that the matter degrees of freedom have been disentangled and the cocycles $\tilde{\alpha}_\Delta$ depend on both the group variables on the edges and the inputs on the vertices (which correspond to PEPS virtual degrees of freedom).

The explicit connection to the fixed point SPT PEPS is made by replacing the basis at each vertex $|g_v\rangle_v$ by an analogous basis of the diagonal subspace of variables at each plaquette surrounding the vertex $\bigotimes_{v \in S(v)} |g_v\rangle_{\Delta,v}$. This description lends directly to a PEPS description where a tensor is assigned to each plaquette of the original graph (i.e. the PEPS is constructed on the dual graph). This in turn is why we must apply a seemingly modified version of the gauging operator of [19] to gauge the PEPS correctly and we note that on the subspace where redundant variables are identified the PEPS gauging operator is identical to the standard gauging operator.