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# Classifying quantum phases using MPS and PEPS

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We give a classification of gapped quantum phases of one-dimensional systems in the framework of Matrix Product States (MPS) and their associated parent Hamiltonians, for systems with unique as well as degenerate ground states, and both in the absence and presence of symmetries. We find that without symmetries, all systems are in the same phase, up to accidental ground state degeneracies. If symmetries are imposed, phases without symmetry breaking (i.e., with unique ground states) are classified by the cohomology classes of the symmetry group, this is, the equivalence classes of its projective representations, a result first derived in [X. Chen, Z.-C. Gu, and X.-G. Wen, Phys. Rev. B **83**, 035107 (2011); arXiv:1008.3745]. For phases with symmetry breaking (i.e., degenerate ground states), we find that the symmetry consists of two parts, one of which acts by permuting the ground states, while the other acts on individual ground states, and phases are labelled by both the permutation action of the former and the cohomology class of the latter. Using Projected Entangled Pair States (PEPS), we subsequently extend our framework to the classification of two-dimensional phases in the neighborhood of a number of important cases, in particular systems with unique ground states, degenerate ground states with a local order parameter, and topological order. We also show that in two dimensions, imposing symmetries does not constrain the phase diagram in the same way it does in one dimension. As a central tool, we introduce the *isometric form*, a normal form for MPS and PEPS which is a renormalization fixed point. Transforming a state to its isometric form does not change the phase, and thus, we can focus on to the classification of isometric forms.

## I. INTRODUCTION

### A. Background

Understanding the phase diagram of correlated quantum many-body systems, that is, the different types of order such systems can exhibit, is one of the most important and challenging tasks on the way to a comprehensive theory of quantum many-body systems. Compared to classical statistical models, quantum systems exhibit a much more complex behavior, such as phases with topological order as in the fractional quantum Hall effect, which cannot be described using Landau's paradigm of local symmetry breaking.

In the last years, tensor network based ansatzes, such as Matrix Product States<sup>1</sup> (MPS) and Projected Entangled Pair States<sup>2</sup> (PEPS), have proven increasingly successful in describing ground states of quantum many-body systems. In particular, it has been shown that MPS and PEPS can approximate ground states of gapped quantum systems efficiently:<sup>3-5</sup> this is, not only the ground state of systems with local order, but also, for instance, the ground states of topological insulators are well represented by those states. Since MPS and PEPS provide a characterization of quantum many-body states from a local description, they are promising candidates for a generalization of Landau's theory. Moreover, they can be used to construct exactly solvable models, as every MPS and PEPS appears as the exact ground state of an associated parent Hamiltonian.<sup>1,6-8</sup>

In this paper, we apply the framework of MPS and PEPS to the classification of gapped quantum phases

by studying systems with exact MPS and PEPS ground states. Here, we define two gapped systems to be in the same phase if and only if they can be connected by a smooth path of gapped local Hamiltonians. Along such a path, all physical properties of the state will change smoothly, and as the system follows a quasi-local evolution,<sup>9</sup> global properties are preserved. A vanishing gap, on the other hand, will usually imply a discontinuous behavior of the ground state and affect global properties of the system. In addition, one can impose symmetries on the Hamiltonian along the path, which in turn leads to a more refined classification of phases.

In the presence of symmetries, the above definition of gapped quantum phases can be naturally generalized to systems with symmetry breaking, i.e., degenerate ground states, as long as they exhibit a gap above the ground state subspace. Again, ground states of such systems are well approximated by MPS and PEPS, which justifies why we study those phases by considering systems whose ground state subspace is spanned by MPS and PEPS. On the other hand, the approach will not work for gapless phases, as the MPS description typically cannot be applied to them.

### B. Results

Using our framework, we obtain the following classification of quantum phases:

For one-dimensional (1D) gapped systems with a unique ground state, we find that there is only a single phase, represented by the product state. Imposing a constrain in form of a local symmetry  $U_g$  (with symme-

try group  $G \ni g$ ) on the Hamiltonian leads to a more rich phase diagram. It can be understood from the way in which the symmetry acts on the virtual level of the MPS,  $U_g \cong V_g \otimes \bar{V}_g$ , where the  $V_g$  are projective representations of  $G$ . In particular, different phases under a symmetry are labelled by the different equivalence classes of projective representations  $V_g$  of the symmetry group  $G$ ,<sup>10</sup> which are in one-to-one correspondence to the elements of its second cohomology group  $H^2(G, U(1))$  (this has been previously studied in Ref. 11).

For one-dimensional gapped systems with degenerate ground states, we find that in the absence of symmetries, all systems with the same ground state degeneracy can be transformed into another along a gapped adiabatic path. In order to make these degeneracies stable against perturbations, symmetries need to be imposed on the Hamiltonian. We find that any such symmetry decomposes into two parts,  $P_g$  and  $W_h$ . Here,  $P_g$  acts by permuting the symmetry broken ground states of the system. To describe  $W_h$ , choose a “reference” ground state, and let  $H \subset G$  be the subgroup for which  $P_h$  acts trivially on the reference state: Then,  $W_h$  ( $h \in H$ ) is a unitary symmetry of the reference state, which again acts on the virtual level as  $W_h \cong V_h \otimes \bar{V}_h$ , with  $V_h$  a projective representation of  $H$ . Together,  $P_g$  and  $W_h$  form an induced representation. The different phases of the system are then labelled both by the permutation action  $P_g$  of  $U_g$  on the symmetry broken ground states (or alternatively by the subgroup  $H \subset G$  for which  $P_h$  leaves the reference state invariant), and by the equivalence classes of projective representations  $V_h$  of  $H$ .

Our classification of phases is robust with respect to the definition of the gap: Two systems which are within the same phase can be connected by a path of Hamiltonians which is gapped even in the thermodynamic limit; conversely, along any path interpolating between systems in different phases the gap closes already for any (large enough) finite chain. On the other hand, we demonstrate that the classification of phases is very sensitive to the way in which the symmetry constraints are imposed, and we present various alternative definitions, some of which yield more fine-grained classifications, while others result in the same classification as without symmetries. In particular, we also find that phases under symmetries are not stable under taking multiple copies, and thus should not be regarded a resource in the quantum information sense.

Parts of our results can be generalized to two dimensions (2D), with the limitation that we can only prove gaps of parent Hamiltonians associated with PEPS in restricted regions. These regions include systems with unique ground states and with local symmetry breaking as well as topological models. We show that within those regions, these models label different quantum phases, with the product state, Ising Hamiltonians, and Kitaev’s double models<sup>12</sup> as their representatives. We also find that in these regions, imposing symmetries on the Hamiltonian does not alter the phase diagram, and, more gen-

erally, that symmetry constraints on two- and higher-dimensional systems must arise from a different mechanism than in one dimension.

As a main tool for our proofs, we introduce a new standard form for MPS and PEPS which we call the *isometric form*. Isometric forms are renormalization fixed points which capture the relevant features of the quantum state under consideration, both for MPS and for the relevant classes of PEPS. Parent Hamiltonians of MPS can be transformed into their isometric form along a gapped path, which provides a way to renormalize the system without actually blocking sites. This reduces the classification of quantum phases to the classification of phases for isometric MPS/PEPS and their parent Hamiltonians, which is considerably easier to carry out due to its additional structure.

### C. Structure of the paper

The paper is structured as follows: In Section II, we prove the results for the one-dimensional case: We start by introducing MPS (Sec. II A) and parent Hamiltonians (Sec. II B), and define phases without and with symmetries (Sec. II C). We then introduce the isometric form and show that the problem of classifying phases can be reduced to classifying isometric forms (Sec. II D). Subsequently, we first classify 1D phases without symmetries (Sec. II E), then phases of systems with unique ground states under symmetries (Sec. II F), and finally phases of symmetry broken systems under symmetries (Sec. II G).

In Section III, we discuss the 2D scenario. We start by introducing PEPS (Sec. III A) and characterize the region in which we can prove a gap (Sec. III B). We then classify PEPS without symmetries (Sec. III C) and show that symmetries don’t have an effect comparable to one dimension (Sec. III D).

Section IV contains discussions of various topics which have been omitted from the preceding sections. Most importantly, in Sec. IV B and C, we discuss various ways in which phases, in particular in the presence of symmetries, can be defined, and the way in which this affects the classification of phases, and in Sec. IV D we provide examples illustrating our classification.

## II. RESULTS IN ONE DIMENSION

In this section, we will derive the classification of phases for one-dimensional systems both with unique and with degenerate ground states, and both in the absence and the presence of symmetries. We will start by giving the necessary definitions—we will introduce Matrix Product States and their parent Hamiltonians, and define what we mean by phases both without and with symmetries. Then, we will state and prove the classification

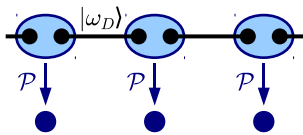


FIG. 1. MPS are constructed by applying a linear map  $\mathcal{P}$  to maximally entangled pairs  $|\omega_D\rangle := \sum_{i=1}^D |i, i\rangle$  of bond dimension  $D$ .

of phases for the various scenarios (with some technical parts placed in appendices).

Note that for clarity, we will keep discussions in this section to a minimum. Extensive discussion of various aspects (motivation of the definitions, alternative definitions, etc.) can be found in Sec. IV.

### A. Matrix Product States

In the following, we will study translational invariant systems on a finite chain of length  $N$  with periodic boundary conditions. While we do not consider the thermodynamic limit, we require relevant properties such as spectral gaps to be uniform in  $N$ .

#### 1. Definition of MPS

Consider a spin chain  $(\mathbb{C}^d)^{\otimes N}$ . A (translational invariant) Matrix Product State (MPS)  $|\mu[\mathcal{P}]\rangle$  of bond dimension  $D$  on  $(\mathbb{C}^d)^{\otimes N}$  is constructed by placing maximally entangled pairs

$$|\omega_D\rangle := \sum_{i=1}^D |i, i\rangle$$

between adjacent sites and applying a linear map  $\mathcal{P} : \mathbb{C}^D \otimes \mathbb{C}^D \rightarrow \mathbb{C}^d$ , as depicted in Fig. 1;<sup>13</sup> this is,  $|\mu[\mathcal{P}]\rangle = \mathcal{P}^{\otimes N} |\omega_D\rangle^{\otimes N}$ . The map  $\mathcal{P}$  is sometimes called the *MPS projector* (though it need not be a projector).

#### 2. Standard form

The definition of MPS is robust under blocking sites: Blocking  $k$  sites into one super-site of dimension  $d^k$  gives a new MPS with the same bond dimension, with projector  $\mathcal{P}' = \mathcal{P}^{\otimes k} |\omega_D\rangle^{\otimes(k-1)}$ , where the maximally entangled pairs are again placed as in Fig. 1.

By blocking and using gauge degrees of freedom (including changing  $D$ ), any MPS which is well-defined in the thermodynamic limit can be brought into its *standard form*, where  $\mathcal{P}$  is supported on a “block-diagonal” space,  $(\ker \mathcal{P})^\perp = \mathcal{H}_1 \oplus \dots \oplus \mathcal{H}_A$ , with

$$\mathcal{H}_\alpha = \text{span}\{|i, j\rangle : \zeta_{\alpha-1} < i, j \leq \zeta_\alpha\}. \quad (1)$$

Here,  $0 = \zeta_0 < \zeta_1 < \dots < \zeta_A = D$  gives a partitioning of  $1, \dots, D$ ; we define  $D_i := \zeta_i - \zeta_{i-1}$ . The case where  $A = 1$  (i.e.  $\mathcal{P}$  is injective) is called the *injective* case, whereas the case with  $A > 1$  is called *non-injective*.

In the following, we will assume w.l.o.g. that all MPS are in their standard form—note that this might involve the blocking of sites of the original model. Moreover, we will impose that  $\mathcal{P}$  is surjective, this can be achieved by restricting  $\mathbb{C}^d$  to the image of  $\mathcal{P}$ .

### B. Parent Hamiltonians

For any MPS (in its standard form) one can construct local *parent Hamiltonians* which have this MPS as their ground state. A (translational invariant) parent Hamiltonian

$$H = \sum_{i=1}^N h(i, i+1)$$

consists of local terms  $h(i, i+1) \equiv h \geq 0$  acting on two adjacent sites  $(i, i+1)$  whose kernels exactly support the two-site reduced density operator of the corresponding MPS, i.e.,

$$\ker h = (\mathcal{P} \otimes \mathcal{P})(\mathbb{C}^D \otimes |\omega_D\rangle \otimes \mathbb{C}^D). \quad (2)$$

By construction,  $H \geq 0$  and  $H|\mu[\mathcal{P}]\rangle = 0$ , i.e.,  $|\mu[\mathcal{P}]\rangle$  is a ground state of  $H$ . It can be shown that the ground state space of  $H$  is  $A$ -fold degenerate, and spanned by the states  $|\mu[\mathcal{P}|_{\mathcal{H}_\alpha}]\rangle$ , where  $\mathcal{P}|_{\mathcal{H}_\alpha}$  is the restriction of  $\mathcal{P}$  to  $\mathcal{H}_\alpha$ .<sup>1,6,7</sup> This associates a family of parent Hamiltonians to every MPS, and by choosing  $h$  a projector, the mapping between MPS and Hamiltonians becomes one-to-one.

Given this duality between MPS and their parent Hamiltonians, we will use the notion of MPS and parent Hamiltonians interchangeably whenever appropriate.

### C. Definition of quantum phases

Vaguely speaking, we will define two systems to be in the same phase if they can be connected along a continuous path of gapped local Hamiltonians, possibly preserving certain symmetries; here, *gapped* means that the Hamiltonian keeps its spectral gap even in the thermodynamic limit. The intuition is that along any gapped path, the expectation value of any local observable will change smoothly, and the converse is widely assumed to also hold.<sup>14</sup>

The rigorous definitions are as follows.

#### 1. Phases without symmetries

Let  $H_0$  and  $H_1$  be a family of translational invariant gapped local Hamiltonians on a ring (with periodic

boundary conditions). Then, we say that  $H_0$  and  $H_1$  are in the same phase if and only if there exists a finite  $k$  such that after blocking  $k$  sites,  $H_0$  and  $H_1$  are two-local,

$$H_p = \sum_{i=1}^N h_p(i, i+1), \quad p = 0, 1,$$

and there exists a translational invariant path

$$H_\gamma = \sum_{i=1}^N h_\gamma(i, i+1), \quad 0 \leq \gamma \leq 1,$$

with two-local  $h_\gamma$  such that

- i)  $h_0 = h_{\gamma=0}$ ,  $h_1 = h_{\gamma=1}$
- ii)  $\|h_\gamma\|_{\text{op}} \leq 1$
- iii)  $h_\gamma$  is a continuous function of  $\gamma$
- iv)  $H_\gamma$  has a spectral gap above the ground state manifold which is bounded below by some constant  $\Delta > 0$  which is independent of  $N$  and  $\gamma$ .

In other words, two Hamiltonians are in the same phase if they can be connected by a local, bounded-strength, continuous, and gapped path.

Note that this definition applies both to Hamiltonians with unique and with degenerate ground states.

## 2. Phases with symmetries

Let  $H_p$  ( $p = 0, 1$ ) be a Hamiltonian acting on  $\mathcal{H}_p^{\otimes N}$ ,  $\mathcal{H}_p = \mathbb{C}^{d_p}$ , and let  $U_g^p$  be a linear unitary representation of some group  $G \ni g$  on  $\mathcal{H}_p$ . We then say that  $U_g$  is a symmetry of  $H_p$  if  $[H_p, (U_g^p)^{\otimes N}] = 0$  for all  $g \in G$ ; note that  $U_g^p$  is only defined up to a one-dimensional representation of  $G$ ,  $U_g^p \leftrightarrow e^{i\phi_g^p} U_g^p$ . Then, we say that  $H_0$  and  $H_1$  are in the same phase under the symmetry  $G$  if there exists a phase gauge for  $U_g^0$  and  $U_g^1$  and a representation  $U = U_g^0 \oplus U_g^1 \oplus U_g^{\text{path}}$  of  $G$  on a Hilbert space  $\mathcal{H} = \mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \mathcal{H}_{\text{path}}$ , and an interpolating path  $H_\gamma$  on  $\mathcal{H}$  with the properties given in the preceding section, such that  $[H_\gamma, U_g^{\otimes N}] = 0$ , and where  $H_0$  and  $H_1$  are supported on  $\mathcal{H}_0$  and  $\mathcal{H}_1$ , respectively.

There are a few points to note about this definition: First, we allow for an arbitrary representation of the symmetry group along the path; we will discuss in Sec. IV C why this is not a restriction. Second, we impose that  $H_0$  and  $H_1$  are supported on orthogonal Hilbert spaces: This allows us to compare e.g. the spin-1 AKLT state with the spin-0 state under  $\text{SO}(3)$  symmetry, but we will impose this even if the two representations are the same; we will discuss how to circumvent this in Sec. IV C. Note that, just as without symmetries, this definition should be understood after an appropriate blocking of sites.

## 3. Robust definition of phases

In addition to the properties listed in the definition of phases in Sec. II C 1 above, one usually requires a phase

to be robust, i.e., an open set in the space of allowed Hamiltonians: For every Hamiltonian

$$H = \sum_{i=1}^N h(i, i+1)$$

there should be an  $\epsilon > 0$  such that

$$H = \sum_{i=1}^N \left[ h(i, i+1) + \epsilon k(i, i+1) \right]$$

is in the same phase for any bounded-strength  $k(i, i+1)$  which obeys the required symmetries.

We are not going to rigorously address robustness of phases in the present paper; however, it should be pointed out that, in the absence of symmetries, Hamiltonians with degenerate MPS ground states do not satisfy this property: In its standard form, the different ground states of a non-injective MPS are *locally* supported on linearly independent subspaces, and we can use a translational invariant local perturbation  $\epsilon k(i)$  to change the energy of any of the ground states proportionally to  $\epsilon N$ , thereby closing the gap for a  $N \propto 1/\epsilon$ . On the other hand, in the presence of a symmetry which permutes the different ground states (such a symmetry always exists), those perturbations are forbidden, and the phase becomes stable. (A rigorous stability proof for MPS phases would make use of the stability condition for frustration-free Hamiltonians proven in Ref. 15 and its generalization to symmetry-broken phases analogous to the one discussed in Ref. 16: The condition is trivially satisfied by the renormalization fixed points of MPS,<sup>17</sup> and using the exponential convergence of MPS to their fixed point,<sup>17</sup> the validity of the stability condition, and thus the stability of MPS phases, follows.)

Therefore, when classifying phases of systems with degenerate ground states, one should keep in mind that in order to make this a robust definition, a symmetry which protects the degeneracy is required.

## 4. Restriction to parent Hamiltonians

We want to classify the quantum phases of gapped Hamiltonians which have exact MPS ground states (or, in the case of degeneracies, the same ground state subspace as the corresponding parent Hamiltonian). Fortunately, with our definition of phases it is sufficient to classify the phases for parent Hamiltonians themselves: Given any two gapped Hamiltonians  $H$  and  $H'$  which have the same ground state subspace, the interpolating path  $\gamma H + (1 - \gamma)H'$  has all desired properties, and in particular it is gapped. Note that this also shows that all parent Hamiltonians for a given MPS are interchangeable.

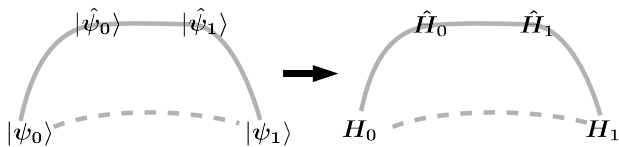


FIG. 2. Construction of the interpolating path for MPS and parent Hamiltonians. Instead of interpolating between the MPS  $|\psi_0\rangle$  and  $|\psi_1\rangle$  directly (dotted line), we first show how to interpolate each of the two states towards a standard form  $|\hat{\psi}_p\rangle$ , the *isometric form*, and then construct an interpolating path between the isometric forms. Note that using the parent Hamiltonian formalism, any such path in the space of MPS yields a path in the space of Hamiltonians right away.

## D. The isometric form

### 1. Reduction to a standard form

Given two MPS  $|\mu[\mathcal{P}_p]\rangle$ ,  $p = 0, 1$ , together with their nearest-neighbor parent Hamiltonians  $H_p$ , we want to see whether  $H_0$  and  $H_1$  are in the same phase, i.e., whether we can construct a gapped interpolating path. We will do so by interpolating between  $\mathcal{P}_0$  and  $\mathcal{P}_1$  along a path  $\mathcal{P}_\gamma$ , in such a way that it yields a path  $H_\gamma$  in the space of parent Hamiltonians which satisfies the necessary continuity and gappedness requirements.

In order to facilitate this task, we will proceed in two steps, as illustrated in Fig. 2: In a first step, we will introduce a standard form for each MPS—the *isometric form*—which is always in the same phase as the MPS itself. This will reduce the task of classifying phases to the classification of phases for isometric MPS, which we will pursue subsequently.

### 2. The isometric form

Let us now introduce the *isometric form* of an MPS. The isometric form captures the essential entanglement and long-range properties of the state and forms a fixed point of a renormalization procedure,<sup>17</sup> and every MPS can be brought into its isometric form by stochastic local operations.<sup>18</sup> Most importantly, as we will show there exists a gapped path in the space of parent Hamiltonians which interpolates between any MPS and its isometric form.

Given an MPS  $|\mu[\mathcal{P}]\rangle$ , decompose

$$\mathcal{P} = QW, \quad (3)$$

with  $W$  an isometry  $WW^\dagger = \mathbb{1}$  and  $Q > 0$ , by virtue of a polar decomposition of  $\mathcal{P}|_{(\ker \mathcal{P})^\perp}$ ; w.l.o.g., we can assume  $0 < Q \leq \mathbb{1}$  by rescaling  $\mathcal{P}$ . The *isometric form* of  $|\mu[\mathcal{P}]\rangle$  is now defined to be  $|\mu[W]\rangle$ , the MPS described by  $W$ , the isometric part of the tensor  $\mathcal{P}$ .

To see that  $|\mu[\mathcal{P}]\rangle$  and  $|\mu[W]\rangle$  are in the same phase,

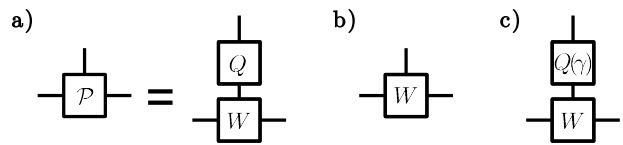


FIG. 3. Isometric form of an MPS. **a)** The MPS projector  $\mathcal{P}$  can be decomposed into a positive map  $Q$  and an isometric map  $W$ . **b)** By removing  $Q$ , one obtains the isometric form  $W$  of the MPS. **c)** Interpolation to the isometric form is possible by letting  $Q_\gamma = \gamma Q + (1 - \gamma)\mathbb{1}$ .

define an interpolating path  $|\mu[\mathcal{P}_\gamma]\rangle$ ,  $\mathcal{P}_\gamma = Q_\gamma W$ , with

$$Q_\gamma = \gamma Q + (1 - \gamma)\mathbb{1}, \quad 1 \geq \gamma \geq 0;$$

note that the path can be seen as a stochastic deformation  $|\mu[\mathcal{P}_\gamma]\rangle = Q_\gamma^{\otimes N} |\mu[\mathcal{P}_0]\rangle$ , cf. Fig. 3. Throughout the path, the MPS stays in standard form, and in the non-injective case, the blocking pattern which is encoded in the structure of  $\ker \mathcal{P}$  stays unchanged.

Let us now see that  $|\mu[\mathcal{P}]\rangle \equiv |\mu[\mathcal{P}_1]\rangle$  and its isometric form  $|\mu[W]\rangle \equiv |\mu[\mathcal{P}_0]\rangle$  are in the same phase. To this end, consider the parent Hamiltonian  $H_0 = \sum h_0(i, i+1)$  of the isometric MPS  $|\mu[\mathcal{P}_0]\rangle$ , with  $h_0$  a projector. Let

$$\Lambda_\gamma = (Q_\gamma^{-1})^{\otimes 2},$$

and define the  $\gamma$ -deformed Hamiltonian

$$H_\gamma := \sum h_\gamma(i, i+1), \quad \text{with } h_\gamma := \Lambda_\gamma h_0 \Lambda_\gamma \geq 0.$$

Since  $h_0 |\mu[\mathcal{P}_0]\rangle = 0$ , it follows that  $h_\gamma |\mu[\mathcal{P}_\gamma]\rangle = 0$  (and in fact, the kernel of  $h$  is always equal to the support of the two-site reduced state), i.e.,  $H_\gamma$  is a parent Hamiltonian of  $|\mu[\mathcal{P}_\gamma]\rangle$ . Note that the family  $H_\gamma$  of Hamiltonians is continuous in  $\gamma$  by construction.

It remains to show that the path  $H_\gamma$  is uniformly gapped, i.e., there is a  $\Delta > 0$  which lower bounds the gap of  $H_\gamma$  uniformly in  $\gamma$  and the systems size  $N$ : This establishes that the  $|\mu[\mathcal{P}_\gamma]\rangle$  are all in the same phase. The derivation is based on a result of Nachtergaele<sup>6</sup> (extending the results of Ref. 1 for the injective case), where a lower bound (uniform in  $N$ ) on the gap of parent Hamiltonians is derived, and can be found in Appendix A. The central point is that the bound on the gap depends on the correlation length  $\xi$  and the gap of  $H_\gamma$  restricted to  $\xi$  sites, and since both depend smoothly on  $\gamma$ , and  $\xi \rightarrow 0$  as  $\gamma \rightarrow 0$ , a uniform lower bound on the gap follows; for the non-injective case, one additionally needs that the overlap of different ground states goes to zero as  $\gamma \rightarrow 0$ .

### 3. Isometric form and symmetries

An important point about the isometric form  $|\mu[\mathcal{P}_0]\rangle$  of an MPS  $|\mu[\mathcal{P}_1]\rangle$  is that both remain in the same phase even if symmetries are imposed. The reason is that using gauge transformations

$$\mathcal{P} \longleftrightarrow \mathcal{P}(Y \otimes (Y^{-1})^T)$$

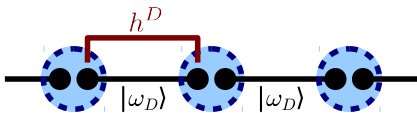


FIG. 4. The isometric form of an injective MPS consists of maximally entangled states  $|\omega_D\rangle$  with bond dimension  $D$  between adjacent sites, where each site is a  $D^2$ -level system. The local Hamiltonian terms  $h^D$ , Eq. (4), acts only on the degrees of freedom corresponding to the central entangled pair.

—such transformations do not change  $|\mu[\mathcal{P}]\rangle$ —any  $\mathcal{P}$  can be brought into a standard form where  $\text{tr}_{\text{left}}[\mathcal{P}^\dagger\mathcal{P}] = \mathbb{1}_{\text{right}}$  [cf. Refs. 1 and 7]; in this standard form, any symmetry  $U_g^{\otimes N}$  of the MPS  $|\mu[\mathcal{P}]\rangle$  can be understood as some unitary  $X_g$  acting on the virtual level,<sup>19</sup>

$$U_g\mathcal{P} = \mathcal{P}X_g.$$

In the polar decomposition  $\mathcal{P} = QW$ , Eq. (3), we have that  $Q = \sqrt{\mathcal{P}\mathcal{P}^\dagger}$ , and thus

$$\begin{aligned} Q^2 &= \mathcal{P}\mathcal{P}^\dagger = U_g^\dagger \mathcal{P} X_g X_g^\dagger \mathcal{P}^\dagger U_g \\ &= U_g^\dagger \mathcal{P}\mathcal{P}^\dagger U_g = U_g^\dagger Q^2 U_g. \end{aligned}$$

This is, for any  $g \in G$  the matrices  $Q^2$  and  $U_g$  are diagonal in a joint basis, and therefore  $[Q, U_g] = 0$ , and it follows that both the interpolating path  $|\mu[\mathcal{P}_\gamma]\rangle = Q_\gamma^{\otimes N} |\mu[\mathcal{P}_0]\rangle$  and its parent Hamiltonian  $H_\gamma$  are invariant under  $U_g$ .

### E. Phase diagram without symmetries

The preceding discussion show that in order to classify quantum phases (both without and with symmetries), it is sufficient to consider isometric MPS and their parent Hamiltonians. In the following, we will carry out this classification for the scenario where no symmetries are imposed. We will find that without symmetries, the phase of the system only depends on the ground state degeneracy, as any two systems with the same ground state degeneracy are in the same phase (and clearly the ground state degeneracy cannot be changed without closing the gap).

#### 1. Unique ground state

Let us start with the injective case where the Hamiltonian has a unique ground state. In that case, the isometry  $W$  is a unitary. We can now continuously undo the rotation  $W$ —this clearly is a smooth gapped path and does not change the phase. This yields the state  $|\mu[\mathcal{P} = \mathbb{1}]\rangle = |\omega_D\rangle^{\otimes N}$ , consisting of maximally entangled pairs of dimension  $D$  between adjacent sites which can only differ in their bond dimension  $D$ , cf. Fig. 4. The

parent Hamiltonian is a sum of commuting projectors of the form

$$h^D = \mathbb{1} - |\omega_D\rangle\langle\omega_D| \quad (4)$$

and thus gapped. (Here,  $h^D$  should be understood as acting trivially on the leftmost and rightmost ancillary particle, and non-trivially on the middle two, cf. Fig. 4.) Moreover, for different  $D$  and  $D'$  one can interpolate between these states via a path of commuting Hamiltonian with local terms

$$h^\theta = \mathbb{1} - |\omega(\theta)\rangle\langle\omega(\theta)|, \quad (5)$$

where  $|\omega(\theta)\rangle = \sqrt{\theta}|\omega_D\rangle + \sqrt{1-\theta}|\omega_{D'}\rangle$ . It follows that any two isometric injective MPS, and thus any two injective MPS, are in the same phase. In particular, this phase contains the product state as its canonical representant.

Note that in the previous derivation, the dimensions of the local Hilbert spaces differ. One can resolve this by thinking of both systems as being embedded in a larger Hilbert space, or by adding ancillas; we discuss this further in Sec. IV.

#### 2. Degenerate ground states

Let us now consider the case of non-injective MPS, i.e., systems with degenerate ground states? First, consider the case with block sizes  $D_\alpha := \dim \mathcal{H}_\alpha = 1$ , i.e.,  $\mathcal{P} \equiv \mathcal{P}_{\text{GHZ}} = \sum_\alpha |\alpha\rangle\langle\alpha, \alpha|$  (up to a rotation of the physical system): This describes an  $\mathcal{A}$ -fold degenerate GHZ state with commuting Hamiltonian terms

$$h = \mathbb{1} - \sum_\alpha |\alpha\rangle\langle\alpha, \alpha|. \quad (6)$$

For  $D_\alpha \neq 1$ , we have that (again up to local rotations)

$$\mathcal{P} = \sum_\alpha |\alpha\rangle\langle\alpha, \alpha| \otimes \mathbb{1}_{D_\alpha^2},$$

where  $\mathbb{1}_{D_\alpha^2}$  acts on  $\mathcal{H}_\alpha$  in (1). This describes a state

$$\sum_\alpha |\alpha, \dots, \alpha\rangle \otimes |\omega_{D_\alpha}\rangle^{\otimes N} \quad (7)$$

(cf. Fig. 5), i.e., a GHZ state with additional local entanglement between adjacent sites, where the amount of local entanglement  $D_\alpha$  can depend on the value  $\alpha$  of the GHZ state. [Since the  $D_\alpha$  can be different, the correct interpretation of (7) is  $|\omega_{D_1}\rangle^{\otimes N} \oplus \dots \oplus |\omega_{D_\mathcal{A}}\rangle^{\otimes N}$ , with the  $|\alpha\rangle$  labelling the direct sum components locally.] The corresponding Hamiltonian is a sum of the GHZ Hamiltonian (6) and terms

$$\sum_\alpha |\alpha\rangle\langle\alpha| \otimes (\mathbb{1} - |\omega_{D_\alpha}\rangle\langle\omega_{D_\alpha}|),$$

which are responsible for the local entanglement. This Hamiltonian commutes with the GHZ part (this can be

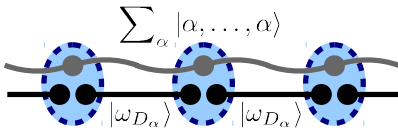


FIG. 5. Structure of the isometric form for non-injective MPS: The state consists of a GHZ state  $\sum_{\alpha} |\alpha, \dots, \alpha\rangle$  (gray) and maximally entangled pairs between adjacent sites  $|\omega_{D_{\alpha}}\rangle$ , where the bond dimension  $D_{\alpha}$  can couple to the value  $\alpha$  of the GHZ state.

understood by the fact that the GHZ state breaks the local symmetry, i.e., there is a preferred local basis), and one can again interpolate to the pure GHZ state with  $D'_{\alpha} = 1$  analogously to the injective case, Eq. (5).

### 3. Summary: Classification of phases

Together, we obtain the following result on the classification of 1D phases in the absence of symmetries: Any two systems with MPS ground states with the same ground state degeneracy are in the same phase; the canonical representative of these phases are the product and the GHZ-type states, respectively. Since the ground state degeneracy cannot be smoothly changed without closing the gap, this completes the classification.

## F. Phase under symmetries: unique ground state

Let us now discuss the classification of phases in the presence of symmetries, as defined in Sec. II C 2. We will in the following first discuss the case of injective MPS, i.e., systems with unique ground states. Note that we will consider the symmetry of the blocked MPS, but as we have argued when defining phases under symmetries, this does not affect the classification.

An important prerequisite for the subsequent discussion is the observation that any MPS has a gauge degree of freedom

$$e^{i\theta} |\mu[\mathcal{P}]\rangle = |\mu[e^{i\phi} \mathcal{P}(Y \otimes Y^*)]\rangle, \quad (8)$$

where  $Y$  is right-invertible (i.e., there exists  $Y^{-1}$  s.th.  $YY^{-1} = \mathbb{1}_D$ , but  $Y$  need not be square), and  $Y^* = (Y^{-1})^T$ . Conversely, it turns out that any two  $\mathcal{P}$  representing the same state are related by a gauge transformation (8).

#### 1. Projective representations and the classification of phases

Let  $U_g$  be a linear unitary representation of a symmetry group  $G$ . We start from the fact that for any  $U_g$ -invariant MPS  $|\mu[\mathcal{P}]\rangle$  and parent Hamiltonian, there

is a standard form for  $\mathcal{P}$  and a phase gauge for  $U_g$  such that

$$U_g \mathcal{P} = \mathcal{P} (V_g \otimes \bar{V}_g), \quad (9)$$

where the bar denotes the complex conjugate.<sup>19</sup> Here, the  $V_g$  form a projective unitary representation of group  $G$ , i.e.,  $V_g V_h = e^{i\omega(g,h)} V_{gh}$ ; cf. Appendix B for details. As  $V_g$  appears together with its complex conjugate in (9), it is only defined up to a phase,  $V_g \leftrightarrow e^{i\chi_g} V_g$ , and thus,  $\omega(g, h)$  is only determined up to the equivalence relation

$$\omega(g, h) \sim \omega(g, h) + \chi_{gh} - \chi_g - \chi_h \pmod{2\pi}.$$

The equivalence classes induced by this relation form a group under addition (this is, tensor products of representations), which is isomorphic to the second cohomology group  $H^2(G, U(1))$  of  $G$  over  $U(1)$ ; thus, we will also call them *cohomology classes*.

In the following, we will show that in the presence of symmetries, the different phases are exactly labelled by the cohomology class of the virtual realization  $V_g$  of the symmetry  $U_g$  determined by Eq. (9); this result was previously found in Ref. 11.

#### 2. Equality of phases

Let us first show that MPS with the same cohomology class for  $V_g$  in (9) can be connected by a gapped path. We will do so by considering the isometric point, where  $\mathcal{P}$  is unitary; recall that the transformation to the isometric point commutes with the symmetry, so that (9) still holds. Then, (9) can be rephrased as

$$\hat{U}_g = \mathcal{P}^\dagger U_g \mathcal{P} = V_g \otimes \bar{V}_g,$$

this is, the action of the symmetry can be understood as  $\hat{U}_g = V_g \otimes \bar{V}_g$  acting on the virtual system, in a basis characterized by  $\mathcal{P}$ .

Now consider two MPS with isometric forms  $\mathcal{P}_0$  and  $\mathcal{P}_1$ , and symmetries

$$\begin{aligned} \hat{U}_g^0 &= \mathcal{P}_0^\dagger U_g^0 \mathcal{P}_0 = V_g^0 \otimes \bar{V}_g^0, \\ \hat{U}_g^1 &= \mathcal{P}_1^\dagger U_g^1 \mathcal{P}_1 = V_g^1 \otimes \bar{V}_g^1, \end{aligned}$$

where  $V_g^0$  and  $V_g^1$  are in the same cohomology class. We can now interpolate between the two MPS with bond dimensions  $D_0$  and  $D_1$  (in the ‘‘convenient basis’’ corresponding to  $\hat{U}_g^0$  and  $\hat{U}_g^1$ ) along the path  $|\omega(\gamma)\rangle^{\otimes N}$ , where

$$|\omega(\gamma)\rangle = (1 - \gamma) \sum_{i=1}^{D_0} |i, i\rangle + \gamma \sum_{i=D_0+1}^{D_1} |i, i\rangle, \quad (10)$$

which is an MPS with bond dimension  $D_0 + D_1$ . Again, the parent Hamiltonian along this path is commuting and thus gapped, and changes smoothly with  $\gamma$ . This path can be understood as a path with symmetry

$$(V_g^0 \oplus V_g^1) \otimes (\bar{V}_g^0 \oplus \bar{V}_g^1) = \hat{U}_g^0 \oplus \hat{U}_g^1 \oplus \hat{U}_g^{\text{path}}, \quad (11)$$



(cf. Ref. 11), with

$$\hat{U}_g^{\text{path}} = (V_g^0 \otimes \bar{V}_g^1) \oplus (V_g^1 \otimes \bar{V}_g^0)$$

(this is where equality of the cohomology classes is required, since only then  $\hat{U}_g^{\text{path}}$  forms a linear representation).

### 3. Separation of phases

As we have seen, MPS for which  $V_g$  in Eq. (9) is in the same cohomology class fall into the same phase. Let us now show that conversely, states with different cohomology classes fall into different phases. We will prove this again in the framework of MPS, i.e., we will show that there cannot be a smooth MPS path connecting two such states. Note that it is clear that the interpolation given above cannot work, as now  $V_g^0 \oplus V_g^1$  does not form a representation any more.

The idea of the impossibility proof is to consider a chain of arbitrary length  $N$  and show that along any well-behaved path  $H_\gamma, \mathcal{P}_\gamma$  needs to change continuously, which results in a continuous change in the way the symmetry acts on the virtual system. In turn, such a continuous change cannot change the cohomology class. While this argument is based on the fact that the chain is finite (as the continuity bounds depend on  $N$ ), it works for arbitrary system size  $N$ ; also, our argument implies that in order to interpolate between two systems with different cohomology classes, i.e., in different phases, the gap of the Hamiltonian will have to close for a *finite* chain, and not only in the thermodynamic limit. (This can be understood from the fact that along an MPS path, the virtual representation of the symmetry is well defined even for finite chains, so that it cannot change without closing the gap. While we believe that cohomology classes label gapped phases beyond MPS, this will likely not hold exactly for finite chains, thus leaving the possibility of a higher order phase transition when interpolating beyond MPS.) We will now proceed by fixing some  $\gamma$  along the path and show the continuity in an environment  $\gamma + d\gamma$ .

Fix some  $\gamma$ , with corresponding ground state  $|\mu[\mathcal{P}_\gamma]\rangle$  of  $H_\gamma$ , where  $\mathcal{P}_\gamma$  is w.l.o.g. in its standard form where  $U_g \mathcal{P}_\gamma = \mathcal{P}_\gamma (V_g \otimes \bar{V}_g)$  with  $V_g$  unitary. Now consider  $H_{\gamma+d\gamma}$  with  $d\gamma \ll 1$  small, and expand its ground state as

$$|\mu[\mathcal{P}_{\gamma+d\gamma}]\rangle = \sqrt{1 - \lambda^2} |\mu[\mathcal{P}_\gamma]\rangle + \lambda |\chi_\gamma\rangle$$

with  $\langle \chi_\gamma | \mu[\mathcal{P}_\gamma] \rangle = 0$ . With  $H_{\gamma+d\gamma} = H_\gamma + dH$ ,

$$\begin{aligned} 0 &= \langle \mu[\mathcal{P}_{\gamma+d\gamma}] | H_{\gamma+d\gamma} | \mu[\mathcal{P}_{\gamma+d\gamma}] \rangle \\ &= \lambda^2 \langle \chi_\gamma | H_\gamma | \chi_\gamma \rangle + \langle \mu[\mathcal{P}_{\gamma+d\gamma}] | dH | \mu[\mathcal{P}_{\gamma+d\gamma}] \rangle \quad (12) \\ &\geq \lambda^2 \Delta - \|dH\|, \end{aligned}$$

where  $\Delta$  is the spectral gap of  $H_\gamma$ . Since  $\lambda = \left| \langle \mu[\mathcal{P}_\gamma] | \mu[\mathcal{P}_{\gamma+d\gamma}] \rangle \right|$  and  $dH \rightarrow 0$  as  $d\gamma \rightarrow 0$ , this shows that

$|\mu[\mathcal{P}_\gamma]\rangle$  is continuous in  $\gamma$ , and since  $|\mu[\mathcal{P}_\gamma]\rangle$  is a polynomial in  $\mathcal{P}_\gamma$ , it follows that  $\mathcal{P}_\gamma$  can be chosen to be a continuous function of  $\gamma$  as well.

Let us now study how the virtual representation of the symmetry is affected by a continuous change  $\mathcal{P}_{\gamma+d\gamma} = \mathcal{P}_\gamma + d\mathcal{P}$ . Let us first consider the case where  $\mathcal{P}_\gamma$  and  $d\mathcal{P}$  are supported on the same virtual space, i.e., the bond dimension does not change, and let us restrict the discussion to the relevant space. The representation of the symmetry on the virtual level becomes<sup>19</sup>

$$Z_g \otimes Z_g^* = \mathcal{P}_{\gamma+d\gamma}^{-1} U_g \mathcal{P}_{\gamma+d\gamma},$$

where  $Z_g \equiv Z_g(\lambda)$  is invertible, and  $Z_g^* = (Z_g^{-1})^T$ , cf. Eq. (8). Since both  $\mathcal{P}_{\gamma+d\gamma}$  and its inverse change continuously, one can find a gauge such that this also holds for  $Z_g$ .

It remains to see that a continuous change of the representation  $Z_g$  does not change its cohomology class; note that the choice of gauge for  $\mathcal{P}_{\gamma+d\gamma}$ , Eq. (8), leads to a transformation  $Z_g \leftrightarrow Y Z_g Y^{-1}$  which does not affect the cohomology class. Let us first assume that  $Z_g \equiv Z_g(\lambda)$  is differentiable, and let

$$Z_g = U_g + U'_g d\gamma, \quad (13)$$

and  $U_g U_h = e^{i\omega(g,h)} U_{gh}$ . Then, we can start from

$$Z_g Z_h = e^{i[\omega(g,h) + \omega'(g,h)d\gamma]} Z_{gh}$$

(note that smoothness of  $Z_g$  implies smoothness of  $\exp[i\omega(g,h)] = \text{tr}[Z_g Z_h] / \text{tr}[Z_{gh}]$ ) and substitute (13). Collecting all first-order terms in  $d\gamma$ , we find that

$$U_g U'_h + U'_g U_h = e^{i\omega(g,h)} U'_{gh} + i\omega'(g,h) e^{i\omega(g,h)} U_{gh}.$$

Left multiplication with  $U_h^{-1} U_g^{-1} = e^{-i\omega(g,h)} U_{gh}^{-1}$  yields

$$U_h^{-1} U'_h + U_h^{-1} U_g^{-1} U'_g U_h = U_{gh}^{-1} U'_{gh} + i\omega'(g,h) \mathbb{1},$$

and by taking the trace and using its cyclicity in the second term, we obtain

$$\omega'(g,h) = -i(\phi_g + \phi_h - \phi_{gh}) \quad (14)$$

with  $\phi_g = \text{tr}[U_g^{-1} U'_g]$ : This proves that differentiable changes of  $Z_g$  can never change the cohomology class of  $\omega$ .

In case  $Z_g \equiv Z_g(\lambda)$  is continuous but not differentiable, we can use a smoothing argument: For any  $\epsilon$ , we can find a differentiable  $\hat{Z}_g(\lambda, \epsilon)$  such that  $\|\hat{Z}_g(\lambda, \epsilon) - Z_g(\lambda)\| \leq \epsilon$ , and define  $\omega_{\lambda, \epsilon}(g, h)$  via

$$e^{i\omega_{\lambda, \epsilon}(g, h)} = \text{tr}[Z_g(\lambda, \epsilon) Z_h(\lambda, \epsilon) Z_{gh}^{-1}(\lambda, \epsilon)].$$

This  $\omega_{\lambda, \epsilon}(g, h)$  (and in particular its real part) varies again according to (14) for any  $\epsilon$  and thus does not change its cohomology class, and since it is  $O(\epsilon)$ -close to  $\omega_\lambda(g, h)$ , the same holds for the cohomology class of  $Z_g(\lambda)$ .

In order to complete our proof, we also need to consider the case where  $\mathcal{P}_{\gamma+d\gamma}$  is supported on a larger space than  $\mathcal{P}_\gamma$ . (The converse can be excluded by choosing  $d\gamma$  sufficiently small.) This can be done by considering the symmetry on the smaller space, and is done in Appendix C. Together, this continuity argument shows that we cannot change the cohomology class of the symmetry  $U_g$  on the virtual level along a smooth gapped path  $H_\gamma$  and thus completes the classification of phases with unique ground states in the presence of symmetries.

### G. Phases under symmetries: Systems with symmetry breaking

Having discussed systems with unique ground states, we will now turn our attention to systems with symmetry breaking, i.e., degenerate ground states, corresponding to non-injective MPS. Recall that in that case, the MPS projector  $\mathcal{P}$  is supported on a “block-diagonal” space

$$\mathcal{H} = \bigoplus_{\alpha=1}^A \underbrace{\mathbb{C}^{D_\alpha} \otimes \mathbb{C}^{D_\alpha}}_{=: \mathcal{H}_\alpha}. \quad (15)$$

Before starting, let us note that different from the injective case, symmetry broken systems can be invariant under non-trivial projective representations as well. However, we can always find a blocking  $k$  such that the symmetry of the symmetry on the blocked system is represented linearly (see Sec. IV C), and we will consider that scenario in the following.

#### 1. Induced representations and the structure of systems with symmetry breaking

Let us first explain how the physical symmetry is realized on the virtual level—we will see that it has the form of a so-called *induced representation* of a projective representation (the proof can be found in Appendix D). Consider an non-injective MPS  $|\mu[\mathcal{P}]\rangle$  and its parent Hamiltonian. Then, any invariance of the Hamiltonian under a linear unitary representation of a group  $G$  can be understood as invariance under an equivalent linear representation  $U_g$  which—with the correct gauge for  $\mathcal{P}$ , and in the correct basis—acts on the virtual system as

$$\hat{U}_g = P_g \bigoplus_{\mathbf{a}} \left( \bigoplus_{\alpha \in \mathbf{a}} V_h^\alpha \otimes \bar{V}_h^\alpha \right). \quad (16)$$

Here,  $P_g$  is a permutation representation of  $G$  permuting blocks with different  $\alpha$ 's in (15).  $P_g$  leads to a natural partitioning of  $\{1, \dots, A\}$  into minimal subsets  $\mathbf{a}$  invariant under the action of all  $P_g$  which we call *irreducible*; the first direct sum in (16) runs over those irreducible sets  $\mathbf{a}$ . The  $V_h^\alpha$  are unitaries, where  $h \equiv h(g, \alpha)$  is a function of  $g$  and  $\alpha$ . Before explaining their algebraic structure,

note that  $P_g$  can be thought of as composed of permutations  $P_g^\alpha$  acting on irreducible subsets, and (16) can be rewritten as a direct sum over irreducible subsets,

$$\hat{U}_g = \bigoplus_{\mathbf{a}} P_g^\alpha \left( \bigoplus_{\alpha \in \mathbf{a}} V_h^\alpha \otimes \bar{V}_h^\alpha \right). \quad (17)$$

In the following, we will describe the structure of the symmetry for one irreducible subset  $\mathbf{a}$ ; in fact, degeneracies corresponding to different subsets  $\mathbf{a}$  are not of particular interest, as they are not protected by the symmetry (which acts trivially between them) and are thus not stable under perturbations of the Hamiltonian. For a single irreducible subset  $\mathbf{a}$ , the symmetry

$$P_g^\alpha \left( \bigoplus_{\alpha \in \mathbf{a}} V_h^\alpha \otimes \bar{V}_h^\alpha \right) \quad (18)$$

has the following structure (which is known as an *induced representation*): Fix the permutation representation  $P_g^\alpha$ , pick an element  $\alpha_0 \in \mathbf{a}$ , and define a subgroup  $H \subset G$  as

$$H = \{g : \pi_g(\alpha_0) = \alpha_0\}$$

where  $\pi_g$  is the action of  $P_g$  on the sectors,  $\mathcal{H}_{\pi_g(\alpha)} = P_g \mathcal{H}_\alpha$ . Further, fix a projective representation  $V_h^\alpha$  of the subgroup  $H$ . Then, the action of  $V_h^\alpha$  can be boosted to the full group  $G$  in (18) by picking representatives  $k_\beta$  of the disjoint cosets  $k_\beta H$ , and labelling them such that  $\pi_{k_\beta}(\alpha_0) = \beta$ . Then, for every  $g$  and  $\alpha$ , there exist unique  $h$  and  $\beta$  such that

$$gk_\alpha = k_\beta h, \quad (19)$$

and this is how  $h \equiv h(g, \alpha)$  in (18) is determined. Note that the action of the permutation is to map  $\alpha$  to  $\beta$ , so that (19) carries the full information of how to boost the representation  $V_h^\alpha$  of the subset  $H$  to the full group; this is known as an *induced representation*. (It is straightforward to check that this is well-defined.)

Before classifying the phases, let us briefly comment on the structure of (17). The sectors  $\alpha$  correspond to different symmetry broken ground states. The splitting into different irreducible blocks  $\mathbf{a}$  corresponds to the breaking of symmetries *not* contained in  $U_g$ , and it is thus not stable under perturbations. Within each block,  $U_g$  has subsymmetries which can be broken by the ground states—the  $\alpha \in \mathbf{a}$ —and subsymmetries which are not broken by the ground states—corresponding to the symmetry action  $V_h^\alpha \otimes \bar{V}_h^\alpha$  defined on subspaces  $H$ , where the symmetry acts as in the injective case.

#### 2. Structure of symmetry broken phases

In the following, we will prove that two Hamiltonians with symmetry breaking are in the same phase iff *i*) the permutation representations  $P_g$  are the same (up to relabelling of blocks), and *ii*) for each irreducible subset  $\mathbf{a}$ ,

the projective representation  $V_h^a$  has the same cohomology class. (In different words, we claim that two systems are in the same phase if  $U_g$  permutes the symmetry broken ground states in the same way, and if the effective action of the symmetry on each symmetry broken ground state satisfies the same condition as in the injective case.) Note that having the same  $P_g$  allows us to even meaningfully compare the  $V_h^a$  as the subgroups  $H$  can be chosen equal. Also note that since the permutation is effectively encoded in the subgroup  $H$ , we can rephrase the above classification by saying that a phase is characterized by the choice of a subgroup  $H$  together with one of its cohomology classes.

As a simple example, the Ising Hamiltonians  $H_x = \sum \sigma_i^x \sigma_{i+1}^x$  and  $H_z = \sum \sigma_i^z \sigma_{i+1}^z$  are in different phases if the  $\mathbb{Z}_2$  symmetry  $(\sigma^x)^{\otimes N}$  is imposed: While  $H_z$  can break the symmetry,  $H_x$  can not and thus belongs to a different phase.

### 3. Equality of phases

The proof of equality requires again to devise an interpolating path in the space of MPS which is sufficiently well-behaved (i.e., it yields a smooth and gapped path in the set of parent Hamiltonians). It turns out that we can use essentially the same construction as in the injective case: We interpolate along a path

$$|\omega_1(\gamma)\rangle^{\otimes N} \oplus \cdots \oplus |\omega_{\mathcal{A}}(\gamma)\rangle^{\otimes N} \equiv \sum_{\alpha} |\alpha, \dots, \alpha\rangle |\omega_{\alpha}(\gamma)\rangle^{\otimes N}$$

in a space with local dimensions  $\sum_{\alpha} (D_{\alpha}^0 + D_{\alpha}^1)^2$ , where

$$|\omega_{\alpha}(\gamma)\rangle = (1 - \gamma) \sum_{i=1}^{D_{\alpha}^0} |i, i\rangle + (1 - \gamma) \sum_{i=D_{\alpha}^0+1}^{D_{\alpha}^0+D_{\alpha}^1} |i, i\rangle ;$$

the joint symmetry is given by

$$\bigoplus_a P_g^a \left( \bigoplus_{\alpha \in a} (V_h^a \oplus W_h^a) \otimes (\bar{V}_h^a \oplus \bar{W}_h^a) \right) ,$$

where  $V_h^a$  and  $W_h^a$  denote the projective representations for the two systems (as in the injective case, it can be thought of being embedded in the physical symmetry by blocking two sites). Again, the Hamiltonian along the path is the sum of the GHZ Hamiltonian and projectors of the form  $\mathbb{1} - |\omega_{\alpha}(\gamma)\rangle \langle \omega_{\alpha}(\gamma)|$  which couple to the GHZ degree of freedom; the resulting Hamiltonian is commuting and therefore gapped throughout the path.

### 4. Separation of phases

Let us now show that two phases which differ in either the permutation representation  $P_g$  or the cohomology classes of the  $V_h^a$  cannot be transformed into each other along a gapped path. As in the injective case, we

will make use of a continuity argument. The argument will go in two parts: On the one hand, continuity implies that each of the symmetry broken ground states changes continuously, and thus the permutation action  $P_g$  of  $U_g$  stays the same. The effective action  $V_h^a \otimes \bar{V}_h^a$  (modulo permutation) of the symmetry on each of the symmetry broken ground states, on the other hand, can be classified by reducing the problem to the injective case.

Let us first show that the symmetry broken ground states change continuously. Let  $|\psi_{\gamma}^{\alpha}\rangle := |\mu[\mathcal{P}_{\gamma}^{\alpha}]\rangle$  be the (orthogonal) symmetry broken ground states of  $H_{\gamma}$ , with  $\mathcal{P}_{\gamma}^{\alpha} := \mathcal{P}_{\gamma}|_{\mathcal{H}_{\alpha}}$  the restriction of  $\mathcal{P}_{\gamma}$  to  $\mathcal{H}_{\alpha}$  (this describes an injective MPS). For small changes  $d\gamma$ , we can again (as in Sec. II F 3) use continuity and gappedness of  $H_{\gamma}$  to show that the ground state subspaces of  $H_{\gamma}$  and  $H_{\gamma+d\gamma} = H_{\gamma} + dH$  are close to each other, i.e., there exist ground states  $|\chi_{\gamma+d\gamma}^{\alpha}\rangle$  of  $H_{\gamma+d\gamma}$  such that

$$|\psi_{\gamma}^{\alpha}\rangle - |\chi_{\gamma+d\gamma}^{\alpha}\rangle \leq O^*(dH) ,$$

where  $O^*(dH)$  goes to zero as  $dH$  goes to zero. Since the  $|\chi_{\gamma+d\gamma}^{\alpha}\rangle$  can be expanded in terms of the  $|\psi_{\gamma+d\gamma}^{\alpha}\rangle$ , they are MPS,  $|\chi_{\gamma+d\gamma}^{\alpha}\rangle = |\mu[\mathcal{Q}_{\gamma+d\gamma}^{\alpha}]\rangle$ . Using continuity of the roots of polynomials, we infer that we can choose  $|\mathcal{Q}_{\gamma+d\gamma}^{\alpha} - \mathcal{P}_{\gamma}^{\alpha}| \leq O^*(dH)$ . On the other hand, this implies that the  $\mathcal{Q}_{\gamma+d\gamma}^{\alpha}$  are almost supported on  $\mathcal{H}_{\alpha}$ , and thus  $|\mathcal{Q}_{\gamma+d\gamma}^{\alpha} - \mathcal{P}_{\gamma+d\gamma}^{\alpha}| \leq O^*(dH)$ . Together, this shows that

$$|\mathcal{P}_{\gamma}^{\alpha} - \mathcal{P}_{\gamma+d\gamma}^{\alpha}| \leq O^*(dH) ,$$

i.e., the  $\mathcal{P}_{\gamma}^{\alpha}$ , and thus the symmetry broken ground states  $|\psi_{\gamma}^{\alpha}\rangle$ , change continuously. Since  $P_g$  describes the permutation action of the physical symmetry  $U_g$  on the symmetry broken ground states, which is a discrete representation, it follows that  $P_g$  is independent of  $\gamma$ , i.e., it cannot be changed along a gapped path  $H_{\gamma}$ .

In a second step, we can now break the problem down to the injective scenario. To this end, do the following for each irreducible block of  $P_g$ : Fix the  $\alpha_0$  used to define the subgroup  $H$  and its representation  $V_h^a$ , restrict the physical symmetry  $U_g$  to  $g \in H$ , and consider the injective ground state  $|\mu[\mathcal{P}_{\gamma}^{\alpha_0}]\rangle$  and the correspondingly restricted parent Hamiltonian (this can be done by adding local projectors restricting the system to the subspace given by  $\alpha_0$ ). Since  $U_g$ ,  $g \in H$ , leaves  $|\mu[\mathcal{P}_{\gamma}^{\alpha_0}]\rangle$  invariant up to a phase, it is a symmetry of the restricted parent Hamiltonian; it acts on the virtual level as  $V_h^a \otimes \bar{V}_h^a$ . The results for the injective case now imply that it is impossible to change the cohomology class of  $V_h^a$ , thus completing the proof.

### III. TWO DIMENSIONS

#### A. Projected Entangled Pair States

##### 1. Definition

Projected Entangled Pair States (PEPS) form the natural generalization of Matrix Product States to two dimensions:<sup>2</sup> For  $\mathcal{P} : (\mathbb{C}^D)^{\otimes 4} \rightarrow \mathbb{C}^d$ , the PEPS  $|\mu[\mathcal{P}]\rangle$  is obtained by placing maximally entangled pairs  $|\omega_D\rangle$  on the links of a 2D lattice and applying  $\mathcal{P}$  as in Fig. 6. As with MPS, PEPS can be redefined by blocking, which allows to obtain standard forms for  $\mathcal{P}$ , discussed later on. Parent Hamiltonians for PEPS are constructed (as in 1D) as sums of local terms which have the space supporting the  $2 \times 2$  site reduced state as their kernel.

##### 2. Cases of interest

As in 1D, each PEPS has an isometric form to which it can be continuously deformed, yielding a continuous path of  $\gamma$ -deformed Hamiltonians along which the ground state degeneracy is preserved. There are three classes of PEPS which are of special interest.

First, the *injective case*, where  $\mathcal{P}$  is injective, and  $|\mu[\mathcal{P}]\rangle$  is the unique ground state of its parent Hamiltonian.<sup>8</sup>

Second, the block-diagonal case, where  $(\ker \mathcal{P})^\perp = \bigoplus_{\alpha=1}^A \mathcal{H}_\alpha$ , with  $\mathcal{H}_\alpha = \text{span}\{|i, j, k, l\rangle : \zeta_{\alpha-1} < i, j, k, l \leq \zeta_\alpha\}$ ; this corresponds again to GHZ-type states and Hamiltonians with  $A$ -fold degenerate ground states. These systems are closely related to the 1D non-injective case—they exhibit breaking of some local symmetry, and the ground state subspace is spanned by  $|\mu[\mathcal{P}|_{\mathcal{H}_\alpha}]\rangle$ .

Third, the case where the isometric form of  $\mathcal{P}$  is

$$\mathcal{P} = \sum_g V_g \otimes \bar{V}_g \otimes W_g \otimes \bar{W}_g \quad (20)$$

(the ordering of the systems is top–down–left–right), with  $V_g$  and  $W_g$  unitary representations of a finite group  $G$  containing all irreps of  $G$  at least once; this scenario corresponds to systems where the ground state degeneracy depends on the topology of the system, and which

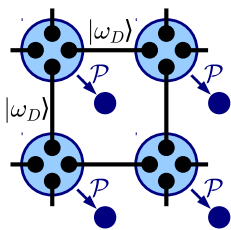


FIG. 6. PEPS are constructed analogously to MPS by applying linear maps  $\mathcal{P}$  to a 2D grid of maximally entangled states  $|\omega_D\rangle$ .

thus exhibit some form of topological order;<sup>20</sup> in particular, for  $V_g$  and  $W_g$  the regular representation of  $G$ , the isometric form of these PEPS describes Kitaev’s double model of the underlying group.<sup>12</sup> All these three classes have parent Hamiltonians at the isometric point which are commuting and thus gapped.

#### B. Gap in two dimensions

##### 1. Gap in the thermodynamic limit

The major difference to the case of 1D systems is that it is much more difficult to assess whether the parent Hamiltonian is gapped in the thermodynamic limit, and examples which become gapless at some finite deformation  $0 < \gamma_{\text{crit}} < 1$  of the isometric form exist. For instance, the coherent state corresponding to the classical Ising model<sup>21</sup> on a hexagonal lattice at the critical temperature has critical correlations and is thus gapless,<sup>22</sup> while it is injective and therefore its isometric form is gapped. In fact, this example illustrates that a smooth change in  $\mathcal{P}$  can even lead to a non-local change in the PEPS  $|\mu[\mathcal{P}]\rangle$ .

Fortunately, it turns out that in some environment of commuting Hamiltonians (and in particular in some environment of the three classes introduced above), a spectral gap can be proven. To this end, let  $\tilde{H} = \sum \tilde{h}_i$ ,  $\tilde{h}_i \geq \mathbb{1}$  with ground state energy  $\lambda_{\min}(\tilde{H}) = 0$ , where the condition

$$\tilde{h}_i \tilde{h}_j + \tilde{h}_j \tilde{h}_i \geq -\frac{1}{8}(1 - \Delta)(\tilde{h}_i + \tilde{h}_j) \quad (21)$$

holds for some  $\Delta > 0$  (here, each  $h_i$  acts on  $2 \times 2$  plaquettes on a square lattice); in particular, this is the case for commuting Hamiltonians. Then,

$$\tilde{H}^2 = \sum_i \underbrace{\tilde{h}_i^2}_{\geq h_i} + \sum_{\langle ij \rangle} \tilde{h}_i \tilde{h}_j + \sum'_{\substack{\langle ij \rangle \\ \geq 0}} \tilde{h}_i \tilde{h}_j \geq \Delta \tilde{H} \quad (22)$$

(where the second and third sum run over overlapping and non-overlapping  $\tilde{h}_i$ ,  $\tilde{h}_j$ , respectively), which implies that  $\tilde{H}$  has a spectral gap between 0 and  $\Delta$ , cf. Ref. 1.

As we show in detail in Appendix E, condition (21) is robust with respect to  $\gamma$ -deformations of the Hamiltonian. In particular, for any PEPS  $|\mu[\mathcal{P}]\rangle$  with commuting parent Hamiltonian (such as the three cases presented above), it still holds for the parent of  $Q^{\otimes N}|\mu[\mathcal{P}]\rangle$  as long as  $\lambda_{\min}(Q)/\lambda_{\max}(Q) \gtrsim 0.967$ . Thus, while considering the isometric cases does not allow us to classify all Hamiltonians as in 1D, we can still do so for a non-trivial subset in the space of Hamiltonians.

#### C. Classification of isometric PEPS without symmetries

Let us now classify the three types of isometric PEPS introduced previously in the absence of symmetries; to-

gether with the results of the previous subsection, this will provide us with a classification of quantum phases in some environment of these cases.

### 1. Systems with unique or GHZ-type ground state

As in one dimension, any injective isometric  $\mathcal{P}$  can be locally rotated to the scenario where  $\mathcal{P} = \mathbb{1}$ , this is, it consists of maximally entangled pairs between adjacent sites. This entanglement can again be removed along a commuting path  $h^\theta$ , Eq. (5), as in one dimension. This implies that any injective PEPS and its parent Hamiltonian which is sufficiently close to being isometric is in the same phase as the product state.

The case with block-diagonal  $\mathcal{P}$ , such as for GHZ-like states, is also in complete analogy to one dimension: Up to a rotation, it is equivalent to the  $\mathcal{A}$ -fold degenerate GHZ state with additional maximally entangled pairs between adjacent sites, whose bond dimension  $D_\alpha$  can again couple to the (classical) value of the GHZ state. This local entanglement can again be removed along a commuting path, as in one dimension, and we find that all block-diagonal PEPS which are close enough to being isometric can be transformed into the  $\mathcal{A}$ -fold degenerate GHZ state along a gapped adiabatic path.

### 2. Systems with topological order

What about the topological case of Eq. (20)? Of course, additional local entanglement  $|\omega_D\rangle$  can be present independently of the topological part of the state, which corresponds to replacing  $V_g$  by  $V_g \otimes \mathbb{1}$  (and correspondingly for  $W_g$ ), and this entanglement can be manipulated and removed along a commuting path.

However, it turns out that the bond dimension  $D$  of the local entanglement can couple to the topological part of the state even though there is no local symmetry breaking. In particular, the bond dimension  $D_\alpha$  can couple to the irreps  $R^\alpha(g)$  of  $V_g$  and  $W_g$ , i.e., we can change the multiplicity  $D_\alpha$  of individual irreps  $R^\alpha(g)$ ,

$$\bigoplus_{\alpha} R^\alpha(g) \longleftrightarrow \bigoplus_{\alpha} R^\alpha(g) \otimes \mathbb{1}_{D_\alpha} .$$

The interpolation between different multiplicities  $D_\alpha$  can be done within the set of commuting Hamiltonians, by observing that the Hamiltonian consists of two commuting parts:<sup>20</sup> One ensures that the product of each irrep around a plaquette is the identity, and the other controls the relative weight of the different subspaces and thus allows to change multiplicities. The underlying idea can be understood most easily by considering a two-qubit toy model consisting of the two commuting terms

$$h_z = \frac{1}{2}(\mathbb{1} - Z \otimes Z) , \\ h_x(\theta) = \Lambda_\theta^{\otimes 2} \frac{1}{2}(\mathbb{1} - X \otimes X) \Lambda_\theta^{\otimes 2} ,$$

where  $\Lambda_\theta = \begin{pmatrix} \theta & 0 \\ 0 & 1 \end{pmatrix}$ : The term  $h_z$  enforces the even-parity subspace  $\alpha|00\rangle + \beta|11\rangle$ , while  $h_x(\theta)$  takes care that the relative weight within this subspace is  $|00\rangle + \theta^2|11\rangle$ , which allows to smoothly interpolate between  $|00\rangle$  and  $|00\rangle + |11\rangle$  within the set of commuting Hamiltonians.

Together, this proves that for a given group  $G$ , all PEPS of the form (20), with representations  $V_g$  and  $W_g$  which contain all irreducible representations of  $G$ , yield PEPS which are in the same phase. On the other hand, it is not clear whether the converse holds: Given two finite groups  $G, H$  with corresponding representations  $V_g, W_g$  and  $V'_h, W'_h$ , for which Eq. (20) yields the same (or a locally equivalent) map  $\mathcal{P}$ —which means that the two models are in the same phase—is it true that the two groups are equal? While we cannot answer this question, let us remark that since both models can be connected by a gapped path, one can use quasi-adiabatic continuation<sup>9,23</sup> to show that their excitations need to have the same braiding statistics; this is, the representations of their doubles need to be isomorphic as braided tensor categories. Note that in Ref. 24, the map  $\mathcal{P}$  is used to map doubles to equivalent string-net models.

### 3. More types of local entanglement

Let us remark that while we have characterized the equivalence classes of isometric PEPS for the three aforementioned classes, this characterization is not complete, even beyond the difficulty of proving a gap: There are PEPS which can be transformed to those cases by local unitaries or low-depth local circuits, yet  $\mathcal{P}$  has a different structure. The reason is that unlike in 1D, local entanglement need not be bipartite. E.g., one could add four-partite GHZ states around plaquettes: while this is certainly locally equivalent to the original state, it will change the kernel of  $\mathcal{P}$ , since only bipartite maximally entangled states can be described by a mapping  $\mathcal{P} \rightarrow \mathcal{P} \otimes \mathbb{1}$ . Thus, the previous classification can be extended to a much larger class of isometric tensors, by including all symmetries of  $\ker \mathcal{P}$  which can arise due to adding local entanglement.

## D. Symmetries in two dimensions

How does the situation change when we impose symmetries on the system and require the Hamiltonian path to commute with some unitary representation  $U_g$ ? Surprisingly, imposing symmetries in two dimensions has a much weaker effect than in one dimension, as we will show in the following. In particular, we will demonstrate how to interpolate along a symmetry-preserving path between arbitrary injective PEPS, and between any two GHZ-type PEPS given that the permutation action of the symmetry on the symmetry broken ground states is the same; note that the symmetry can in particular stabilize the degeneracy of GHZ-type states. Recall, however,

that in the following we only show how to construct continuous paths of PEPS; in order to turn this into a classification of phases under symmetries, we need to restrict to the regions characterized in Sec. III B where we can prove a gap. Yet, the following arguments show that the reasoning used for one-dimensional systems with symmetries will not apply in two dimensions, and a more refined framework might be needed.

### 1. Systems with unique ground states

Let us start by studying the injective case. There, it has been shown<sup>25</sup> that any two maps  $\mathcal{P}$  and  $\mathcal{P}'$  which describe the same PEPS are related via a gauge transformation

$$\mathcal{P}' = \mathcal{P}(e^{i\phi} Y \otimes Y^* \otimes Z \otimes Z^*), \quad (23)$$

with  $Y^* = (Y^{-1})^T$ . This implies that any unitary invariance of  $|\mu[\mathcal{P}]\rangle$  can be understood as a symmetry

$$\hat{U}_g = \mathcal{P}^{-1} U_g \mathcal{P} = V_g \otimes \bar{V}_g \otimes W_g \otimes \bar{W}_g$$

acting on the on the virtual system, with  $V_g$  and  $W_g$  projective unitary representations.

While this is in complete analogy to the one-dimensional case, there is an essential difference: The representation of the symmetry on the virtual level is not invariant under blocking sites. By blocking  $k \times \ell$  sites, we obtain a new PEPS projector with symmetries  $V'_g = V_g^{\otimes k}$  and  $W'_g = W_g^{\otimes \ell}$ , respectively. However, taking tensor products changes the cohomology class, and in particular, for any finite-dimensional representation  $V_g$  there exists a finite  $k$  such that  $V_g^{\otimes k}$  is in the trivial cohomology class. This is, by blocking a *finite* number of sites, any two PEPS  $|\mu[\mathcal{P}_0]\rangle$  and  $|\mu[\mathcal{P}_1]\rangle$  can be brought into a form where the symmetry on the virtual level is represented by  $V_g^0, W_g^0$ , and  $V_g^1, W_g^1$  which are all in the trivial cohomology class.

At this point, we can proceed as in the 1D case and construct an interpolating path which preserves the symmetry using non-maximally entangled states  $|\omega(\gamma)\rangle$  [Eq. (10)], now with joint symmetry

$$(V_g^0 \oplus V_g^1) \otimes (\bar{V}_g^0 \oplus \bar{V}_g^1) \otimes (W_g^0 \oplus W_g^1) \otimes (\bar{W}_g^0 \oplus \bar{W}_g^1).$$

Note that the whole construction can be understood as the sequential application of two one-dimensional interpolations (since at the isometric point the horizontal and vertical directions decouple) and thus, all arguments concerning technical points such as the embedding in the physical space can be directly transferred.

### 2. Systems with local symmetry breaking

The results of Ref. 25 for the relation of two maps  $\mathcal{P}$  and  $\mathcal{P}'$ , Eq. (23), can be readily generalized to relate

different representations of a PEPS with local symmetry breaking, i.e., GHZ-type states. It follows that for any such PEPS, a symmetry can be understood at the virtual level as

$$\hat{U}_g = P_g \bigoplus_{\mathbf{a}} \left( \bigoplus_{\alpha \in \mathbf{a}} V_h^\alpha \otimes \bar{V}_h^\alpha \otimes W_h^\alpha \otimes \bar{W}_h^\alpha \right).$$

where again the  $P_g$  permutes the sectors, the  $\mathbf{a}$  are minimal subsets invariant under  $P_g$ , and the  $V_h^\alpha$  and  $W_h^\alpha$ , together with  $P_g$ , form an induced projective representation.

The permutation action  $P_g$  of the symmetry is invariant under blocking. Thus, we can apply the same type of continuity argument as in 1D to show that different permutations  $P_g$  label different phases. (Since this argument proves that there cannot be a gapped path of Hamiltonians on any finite chain connecting systems with different  $P_g$ , it holds independently of whether we can prove a gap on the Hamiltonian along the path, as long as the initial and final systems are gapped.) On the other hand, the projective representations behave under blocking just as in the injective case: They map to tensor products of themselves, and thus, we can choose a blocking such that the  $V_h^\alpha$  and  $W_h^\alpha$  are all in the trivial cohomology class. If moreover the  $P_g$  are equal, we can construct an interpolating path of PEPS just as in one dimension.

## IV. DISCUSSION

In this section, we discuss various aspects which have been omitted in the previous sections.

### A. Matrix Product States

#### 1. Injectivity and translational invariance

In order to obtain injectivity, it is necessary to block sites (say,  $k$  sites per block). Thus, the notion of locality changes: For instance, a two-local path of parent Hamiltonians is  $2k$ -local on the unblocked system. Also, along such a path we can maintain translational invariance only under translations by  $k$  sites, i.e., on the blocked system.

However, the number of sites which need to be blocked to obtain injectivity is fairly small, namely  $O(\log D)$  for typical cases<sup>26</sup> and  $O(D^4)$  in the worst case.<sup>27</sup> In particular, this is much more favorable than what is obtained using renormalization methods,<sup>11</sup> where in addition to injectivity one has to go to block sizes beyond the correlation length.

It should be noted that several of our arguments apply without blocking, thus strictly preserving translational invariance. In particular, the way in which symmetries act on the virtual level is the same without blocking, and the impossibility proofs for interpolating paths also apply equally. On the other hand, it is not clear whether

we can construct interpolating paths without reaching injectivity of  $\mathcal{P}$ : While we can move to isometric  $\mathcal{P}$  along gapped paths, the structure of those isometric points is now much more rich; for instance, the AKLT projector is of that form. Also, certain alternative definitions of phases under symmetries (cf. Sec. IV B) behave differently under translational invariance. Finally, in the case of symmetry broken systems, imposing translational invariance can result in *projective* representations as physical symmetries (this is discussed in Sec. IV C), which leads to a much more involved structure of the 1D induced representation in Eq. (D9).

## 2. Different MPS definition

Typically, MPS are defined using a set of matrices  $A^i$  as

$$\sum_{i_1, \dots, i_N} \text{tr}[A^{i_1} \dots A^{i_N}] |i_1, \dots, i_N\rangle .$$

This definition can be easily related to our definition in terms of MPS projectors via

$$\mathcal{P} = \sum_{i, \alpha, \beta} A_{\alpha\beta}^i |i\rangle \langle \alpha, \beta| .$$

Injectivity of  $\mathcal{P}$  translates to the fact that the  $\{A^i\}_i$  span the whole space of matrices, and the “block-diagonal” support space in the non-injective case corresponds to restricting the  $A^i$ ’s to be block-diagonal and spanning the space of block-diagonal matrices.

The effect of symmetries in this language can be written as follows: Eq. (9) becomes

$$\sum_j (U_g)_{ij} A^j = V_g^T A^i \bar{V}_g ,$$

and Eq. (16)

$$\sum_j (\hat{U}_g)_{ij} A^j = P_g^\dagger V_g^T A^i \bar{V}_g P_g ,$$

where the  $P_g$  now permute the blocks of the  $A^i$ ’s, and together with  $V_g$  form an induced representation.

While the matrix formalism using the  $A^i$ ’s is more common, we choose the projector formulation since we believe it is more suitable for the purposes of this paper (with the exception of describing the block structure in the non-injective case): the  $\mathcal{P}$ , or parts of it, are the maps which we use to conjugate the Hamiltonian with to get to the isometric form, and which we conjugate the  $U_g$  with to obtain the effective action of the symmetry on the bonds. Also, in this formulation the isometric point is characterized simply by maximally entangled pairs with  $U \otimes \bar{U}$  symmetry, rather than by an MPS with Kronecker delta tensors, and is thus more intuitive to deal with.

## B. Definition of phases

### 1. Different definitions of phases

There are other definitions of quantum phases: For instance, instead of gappedness one can ask for a path of Hamiltonians along which the ground states do not change abruptly. One can also right away consider the ground states instead of the Hamiltonian and ask whether two states can be transformed into each other using (approximately) local transformations.<sup>11</sup> Both these definitions are implied by ours: The existence of a gapped path implies that the ground states change smoothly, cf. Eq. (12), and using quasi-adiabatic continuation,<sup>9</sup> any gapped path of Hamiltonians yields a quasi-local transformation between the ground states.<sup>23</sup>

### 2. Local dimension and ancillas

In our definition of phases, we allowed to compare systems with different local Hilbert space dimension. One way to think of this is to consider the smaller system as being embedded in the larger system. A more flexible way is to allow for the use of ancillas to extend the local Hilbert space. In fact, these ancillas are automatically obtained when blocking: Recall that we restricted our attention to the subspace actually used by  $\mathcal{P}$ ; the remaining degrees of freedom (if sufficiently many to allow for a tensor product structure) can be used to construct ancillas. An explicit way to do so is to block two isometric tensors together: The state now contains a maximally entangled pair  $|\omega_D\rangle$  (correlated to the GHZ in the non-injective case) which can be considered as a  $D^2$ -dimensional ancilla system.

Note that we can, in the same way, obtain ancillas for systems with symmetries: After blocking three isometric sites, the maximally entangled states in the middle are invariant under  $\bar{V}_g \otimes V_g \otimes \bar{V}_g \otimes V_g$ . Since also two maximally entangled states between sites (1, 4) and (2, 3) are invariant under that symmetry, the symmetry acts trivially on this two-dimensional subspace which thus constitutes an ancilla qubit not subject to the symmetry action.

## C. Symmetries

### 1. Definition with restricted symmetry representations

When defining phases under symmetries, we have allowed for arbitrary representations of the symmetry group along the path. What if we want to restrict to only the representation of the initial and final symmetry,  $U_g^0$  and  $U_g^1$ , respectively? It turns out that does not pose a restriction for compact groups, as long as at least one of the effective representations  $U_g^0$  or  $U_g^1$  after blocking to the normal form is faithful. Namely,

given such a faithful representation  $U_g$ , we have that  $\chi_U(g) = \text{tr} U_g = |\text{tr}[V_g]|^2 \geq 0$  (with  $V_g \otimes \bar{V}_g$  the virtual realization of  $U_g$ ), which implies that any representation  $W_g$  is contained as a subrepresentation in  $U_g^{\otimes N}$  for  $N$  large enough. (For finite groups, this follows as the multiplicity  $\frac{1}{|G|} \sum_g \chi_U(g)^N \bar{\chi}_W(g)$  is dominated by  $\chi_W(1)$  since  $|\chi_U(g)|$  is maximal for  $g = 1$ , cf. Ref. 28; for Lie groups, this argument needs to be combined with a continuity argument, cf. Ref. 29). Thus, starting from the symmetry representation  $U_g^0$  or  $U_g^1$ , we can effectively obtain any representation needed for the interpolating path by blocking  $N$  sites, proving equivalence of the two definitions.

### 2. Definition with only one symmetry representation

If the two systems to be compared are invariant under the same symmetry  $U_g^0 = U_g^1$ , we might want to build a path invariant under that symmetry, instead of considering the symmetry  $U_g = U_g^0 \oplus U_g^1$  as in our definition. In fact, these two definitions turn out to be equivalent, since we can easily map a path with symmetry  $U_g$  to one with symmetry  $U_g^0 = U_g^1$ , and vice versa. Given a path  $|\psi(\lambda)\rangle$  (with corresponding Hamiltonian) with symmetry  $U_g^0$ , we can add an unconstrained ancilla qubit (cf. Sec. IV B 2) at each site and consider the path  $|\psi(\lambda)\rangle \otimes (\sqrt{1-\lambda}|0\rangle + \sqrt{\lambda}|1\rangle)^{\otimes N}$ , thus embedding the system in a space with symmetry  $U_g$ .

Conversely, we can map any path with symmetry  $U_g$  to a path with symmetry  $U_g^0 = U_g^1$ . To this end, we can use  $U_g = U_g^0 \otimes \mathbb{1}_2$  to interpret the path as a path involving one system with  $U_g$ -symmetry and one unconstrained ancilla qubit per site, which again can be understood as being part of a  $(U_g^0)^{\otimes 2}$ -invariant subspace, cf. Sec. IV B 2. Note that the factorization  $U_g = U_g^0 \otimes \mathbb{1}_2$  requires  $U_g^0$  and  $U_g^1$  to have the same phase, which motivates why we chose to lock the phase between  $U_g^0$  and  $U_g^1$  in such a scenario.

### 3. Definitions with different classifications

Defining phases in the presence of symmetries is subtle, as different definitions can yield very different classifications. In the following, we discuss some alternative definitions and their consequences.

One possibility would be not to allow for an arbitrary gauge of the phases of the symmetries in  $U_g^0$  and  $U_g^1$ , but to keep the gauge fixed. In that case, the 1D representations in (B1) and (D1) can enter the classification: While finite representations can be still removed by blocking sites, continuous representations remain different even after blocking and cannot be changed into each other continuously, and thus, phases are additionally labelled by the continuous 1D representations of the symmetry.

This classification changes once more if one allows to compare blocks of different lengths for the two systems:

E.g., for  $U(1)$  any two continuous representations  $e^{in_0\vartheta}$  and  $e^{in_1\vartheta}$  of  $\vartheta \in U(1)$  can be made equal by blocking  $|n_1|$  and  $|n_0|$  sites, respectively, as long as the signs of  $n_0$  and  $n_1$  are equal. Therefore, in that case the phases are additionally labelled by the signs of the 1D representations; this case has been considered in Ref. 11.

To give an example where one might want to fix the phase relation between  $U_g^0$  and  $U_g^1$ , consider the two product states  $|0000\dots\rangle$  and  $|0101\dots\rangle$  under  $U(1)$  symmetry: Both  $U_g^0$  and  $U_g^1$  arise as subblocks of  $R_\phi \otimes R_\phi$  [with  $R_\phi = \exp(i\phi Z/2)$  the original  $U(1)$  representation], which suggests to fix the phase relation and in turn separates the two phases; note that this can be seen as a way to reinforce translational invariance.

### 4. A definition with only one phase

We are now going to present an alternative definition of phases under symmetries which yields a significantly different classification, namely that all systems with the same ground state degeneracy are in the same phase, just as without symmetries. The aim of this discussion is to point out that it is important to fix the representation of the symmetry group, and not only the symmetry group itself, in order to obtain a meaningful classification of phases in the presence of symmetries.

We impose that along the path, the system is invariant under some (say, faithful) representation of the symmetry group, which may however change along the path. Then, however, it is possible to transform any state to pairs of maximally entangled states between adjacent sites in the *same* basis, and therefore to the same parent Hamiltonian, by rotating the isometric form. Thus, all injective systems can be transformed to the same Hamiltonian preserving symmetries, and similarly for symmetry broken systems. It follows that even with symmetries, all systems are in the same phase as long as they have the same ground state degeneracy.

Note that while in our approach, we also use rotations to bring the system into a simple form, these “rotations” should just be thought of as choosing a convenient basis, and not as actual rotations. In particular, due to our way of imposing the two symmetry representations on orthogonal subspaces,  $U_g = U_g^1 \oplus U_g^2$ , we never need to fix two different bases for the same subspace.

### 5. Projective symmetries

While our definition of phases under symmetries can be applied to both linear and projective representations, we found that in the injective case, symmetries are in fact always linear (cf. Appendix B). In the non-injective case, however, there exist systems having projective symmetries, such as the Majumdar-Ghosh model, which has the ground states  $(|01\rangle - |10\rangle)^{\otimes N}$  and the same state translated by one lattice site. This model is invariant



under  $SU(2)/\mathbb{Z}_2$  [which can be understood as a projective representation of  $SO(3)$ ] and under the Pauli matrices (a projective representation of  $D_2 = \mathbb{Z}_2 \times \mathbb{Z}_2$ ). On the other hand, any  $d$ -dimensional projective representation becomes linear (up to trivial phases) after taking its  $d$ 'th power; thus, classifying phases under linear symmetries as we did is in fact sufficient. Alternatively, any projective representation can be lifted to a linear representation, which is still a symmetry of the Hamiltonian: E.g., any  $U_g$ -invariant Hamiltonian,  $[H, U_g^{\otimes N}] = 0$ , is also invariant under  $e^{i\phi}U_g$ , and thus under the representation  $V_k \equiv k$  of the group  $K = \langle U_g \rangle$  generated by the  $U_g$  by itself.

On the other hand, in case we want to build a joint symmetry representation  $U_g = U_g^0 \oplus U_g^1$  before blocking, and do not want to lift the joint representation to a larger group, we get constraints on  $U_g^0$  and  $U_g^1$ : Firstly, both of them need to be in the same cohomology class—while the cohomology class can be changed by blocking, one might want to compare systems with a particular notion of locality. Also note that even if both symmetries are in the same cohomology class, one needs to adjust the trivial phases such that  $\omega(g, h)$  is actually equal up to a one-dimensional representation of the group, since otherwise  $U_g$  does not form a representation; note however that this is actually a consequence of our requirement that  $U_g$  forms a representation and does not follow from an underlying symmetry.

## 6. Multiple copies and phases as a resource

An interesting observation is that the classification of 1D phases under symmetries is not stable if one takes multiple copies. For instance, one can construct a path of smooth gapped Hamiltonians which interpolates from two copies of the AKLT state to the trivial state while preserving  $SO(3)$  symmetry. More generally, for any two states  $|\mu[\mathcal{P}_0]\rangle$  and  $|\mu[\mathcal{P}_1]\rangle$  there exist  $k_0$  and  $k_1$  such that  $|\mu[\mathcal{P}_0]\rangle^{\otimes k_0}$  can be converted to  $|\mu[\mathcal{P}_1]\rangle^{\otimes k_1}$ . This follows from the observation made in Sec. III D for two-dimensional systems: Taking tensor products changes the projective representation on the bond, and it is always possible to obtain a linear representation by taking a finite number of copies.

From a quantum information perspective, this shows that MPS which belong to different phases should not be regarded as a resource such as entanglement, but rather as characterized by conserved quantities such as parity (i.e., described by a finite group). The minimum requirement for a resource should be that it cannot be created “for free” (e.g., by the quasi-local evolution created by a gapped path<sup>9</sup>). However, an arbitrary even number of copies of the AKLT state can be created from one trivial state, which demonstrates that phases under symmetries should not be considered resources.

## 7. Other symmetries

While we have discussed the classification of phases for local symmetries  $U_g^{\otimes N}$ , very similar ideas can be used to classify phases under global symmetries such as inversion or time reversal symmetry.<sup>10,11,30</sup> The fundamental concept—that two  $\mathcal{P}$  representing the same MPS or PEPS are related by a gauge transformation—equally applies in the case of global symmetries. However, it should be noted that there is an essential difference, in that the representation structure of the global symmetry need not lead to a representation structure on the virtual level, which in turn leads to classification criteria beyond cohomology classes. Let us illustrate this for reflection symmetry: Reflection is realized by applying a flip (swap) operator  $\mathbb{F}$  to the *virtual* system, together with an operation  $\pi$  on the physical system reversing the ordering of the blocked sites. Thus, for an injective MPS  $|\mu[\mathcal{P}]\rangle$  with reflection symmetry, we have that

$$\pi \mathcal{P} \mathbb{F} = \mathcal{P}(V_{-1} \otimes \bar{V}_{-1}) ,$$

where  $V_{-1}$  is the virtual representation of the non-trivial element of  $\mathbb{Z}_2 \equiv \{+1, -1\}$ . (Note that if  $\mathcal{P}$  is injective,  $\pi$  cannot be trivial, since otherwise  $\mathbb{F} = V_{-1} \otimes \bar{V}_{-1}$  which is impossible; this shows that an injective MPS cannot have reflection symmetry unless it contains more than one site per block.) Applying a second reflection, we find that

$$\begin{aligned} \mathcal{P} &= \pi(\pi \mathcal{P} \mathbb{F}) \mathbb{F} = \pi \mathcal{P}(V_{-1} \otimes \bar{V}_{-1}) \mathbb{F} \\ &= (\pi \mathcal{P} \mathbb{F})(\bar{V}_{-1} \otimes V_{-1}) = \mathcal{P}(V_{-1} \bar{V}_{-1} \otimes \bar{V}_{-1} V_{-1}) \end{aligned}$$

i.e., the  $\mathbb{Z}_2$  group structure of the symmetry is represented on the virtual level as  $V_{-1} \bar{V}_{-1} = e^{i\phi} \mathbb{1}$ —similar to a projective representation, but with an additional complex conjugation. This relation allows for phases  $e^{i\phi} = \pm 1$ , corresponding to symmetric and antisymmetric unitaries  $V_{-1}$ , which cannot be connected continuously and thus label different phases; this observation has been used in Refs. 10 and 30 to prove the separation of the AKLT phase from the trivial phase under either time reversal or inversion symmetry.

## D. Examples

### 1. The six phases with $D_2$ symmetry

As an example for the classification of one-dimensional phases in the presence of symmetries, let us discuss the different phases under  $D_2 = \mathbb{Z}_2 \times \mathbb{Z}_2$  symmetry, which appears e.g. as a subsymmetry of  $SO(3)$  invariant models; we will see that there is a total of six different phases under  $D_2$  symmetry.

Let us label the elements of  $D_2 = \mathbb{Z}_2 \times \mathbb{Z}_2$  by  $e \equiv (0, 0)$ ,  $x \equiv (1, 0)$ ,  $z \equiv (0, 1)$ , and  $y \equiv (1, 1)$ , with componentwise addition modulo 2.  $D_2 = \{e, x, y, z\}$  forms a subgroup of  $SO(3)$  by identifying  $(1, 0)$  with an  $x$ -rotation by  $\pi$

and  $(0, 1)$  with a  $z$ -rotation by  $\pi$ . There are two equivalence classes of projective representations, corresponding to the integer and half-integer representations of  $\text{SO}(3)$ . In particular, the one-dimensional spin-0 representation  $\rho_e^1 = \rho_x^1 = \rho_y^1 = \rho_z^1 = 1$  belongs to the trivial class, and the two-dimensional spin- $\frac{1}{2}$  representation  $\rho_x^2 = X$ ,  $\rho_y^2 = Y$ , and  $\rho_z^2 = Z$  (with  $X, Y, Z$  the Pauli matrices) belongs to the non-trivial class. For the following examples, we will always consider systems with physical spin  $S = 1$ ; we label the basis elements by their  $S_z$  spin component,  $|-1\rangle$ ,  $|0\rangle$ , and  $|1\rangle$ , and denote the physical representation of the symmetry group by

$$\begin{aligned} R_x &= \exp[i\pi S_x] = -|-1\rangle\langle +1| - |0\rangle\langle 0| - |1\rangle\langle -1|, \\ R_z &= \exp[i\pi S_z] = -|-1\rangle\langle -1| + |0\rangle\langle 0| - |1\rangle\langle +1|, \\ R_y &= \exp[i\pi S_y] = +|-1\rangle\langle +1| - |0\rangle\langle 0| + |1\rangle\langle -1|. \end{aligned}$$

For systems with unique ground states, there are two possible phases. One contains the trivial state  $|0, \dots, 0\rangle$ , which can be trivially written as an MPS with bond dimension  $D = 1$ , and

$$\mathcal{P}_{\text{triv}} = |0\rangle;$$

clearly, applying any physical transformation  $R_w$  ( $w = x, y, z$ ) to the physical spin translates to applying the one-dimensional representation  $1 \otimes 1$  on the virtual system. The corresponding Hamiltonian is

$$H_{\text{triv}} = -\sum_i |0\rangle\langle 0| + \text{const}. \quad (24)$$

The second phase with unique ground state is illustrated by the AKLT state,<sup>31</sup> which can be written as an MPS with  $D = 2$ , and a projector

$$\mathcal{P}_{\text{AKLT}} = \Pi_{S=1}(\mathbb{1} \otimes iY),$$

with  $\Pi_{S=1}$  the projector onto the  $S = 1$  subspace, and  $iY = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$ . Since we have that  $R_x = \Pi_{S=1} X \otimes X \Pi_{S=1}$ , and correspondingly for  $y$  and  $z$ , it follows that the symmetry operations are represented on the virtual level as  $R_x \mathcal{P} = \mathcal{P}(X \otimes \bar{X})$ ,  $R_y \mathcal{P} = \mathcal{P}(Y \otimes \bar{Y})$ , and  $R_z \mathcal{P} = \mathcal{P}(Z \otimes \bar{Z})$ , which is a non-trivial projective representation of  $\text{SO}(3)$ . The corresponding Hamiltonian is the AKLT Hamiltonian

$$H_{\text{AKLT}} = \sum_i [\vec{S}_i \cdot \vec{S}_{i+1} + \frac{1}{3}(\vec{S}_i \cdot \vec{S}_{i+1})^2 + \text{const}].$$

In order to classify all phases with symmetry breaking, we need to consider all proper subgroups of  $D_2$ . There are four of them:

$$\begin{aligned} H_x &= \{e, x\} \\ H_z &= \{e, z\} \\ H_y &= \{e, y\} \text{ and} \\ H_{\text{triv}} &= \{e\} \end{aligned}$$

The first three are isomorphic to  $\mathbb{Z}_2$ , which has only trivial projective representations, and thus, each of them labels one phase; since  $H_{\text{triv}}$  also has only trivial representations, it corresponds to a fourth phase with symmetry breaking. The number of symmetry broken ground states is  $|D_2/H|$ , i.e., the first three cases have two-fold degenerate ground states, and the last case a four-fold degenerate one.

Let us start with  $H_z$ . A representant of that phase is a GHZ-type state of the form

$$|\text{GHZ}_z\rangle = | +1, \dots, +1\rangle + | -1, \dots, -1\rangle,$$

which can be written as an MPS with  $D = 2$  and

$$\mathcal{P}_{\text{GHZ}_z} = | +1\rangle\langle 0, 0| + | -1\rangle\langle 1, 1|,$$

where the basis elements  $|0\rangle$  and  $|1\rangle$  correspond to two symmetry broken sectors. The action of the symmetry on the virtual level is

$$\begin{aligned} R_x \mathcal{P}_{\text{GHZ}_z} &= -\mathcal{P}_{\text{GHZ}_z} [|0, 0\rangle\langle 1, 1| + |1, 1\rangle\langle 0, 0|] \\ R_z \mathcal{P}_{\text{GHZ}_z} &= -\mathcal{P}_{\text{GHZ}_z} [|0, 0\rangle\langle 0, 0| + |1, 1\rangle\langle 1, 1|] \end{aligned}$$

and correspondingly for  $R_y$ ; i.e., while  $R_z$  acts within the symmetry broken sectors,  $R_x$  (and  $R_y$ ) acts by permuting the different sectors. The corresponding Hamiltonian is the GHZ Hamiltonian

$$H_{\text{GHZ}_z} = -\sum_i [|+1, +1\rangle\langle +1, +1| + |-1, -1\rangle\langle -1, -1|]_{i, i+1}.$$

The same type of ground state and Hamiltonian is found for the subgroups  $H_x$  and  $H_y$  with correspondingly interchanged roles (i.e.,  $R_x$  and  $R_y$ , respectively, do not permute the ground states). Note that these three phases are indeed distinct in the presence of  $D_2$  symmetry, as there is no way how to smoothly change the element of the symmetry group which does not permute the symmetry broken sectors. (This is related to the fact that  $D_2/H$  is discrete, i.e., we are breaking a discrete symmetry; note that breaking of continuous symmetries does not fit the MPS framework since this would correspond to an infinite number of blocks in the MPS and would require gapless Hamiltonians.)

Finally, choosing  $H_{\text{triv}} = \{e\}$  gives a phase which fully breaks the  $D_2$  symmetry. A representative of this phase can be constructed by blocking two sites, with the four basis states

$$\begin{aligned} |\hat{1}\rangle &= | +1\rangle | +x\rangle, & |\hat{2}\rangle &= | +1\rangle | -x\rangle, \\ |\hat{3}\rangle &= | -1\rangle | +x\rangle, & |\hat{4}\rangle &= | -1\rangle | -x\rangle, \end{aligned}$$

where  $|\pm x\rangle$  are the  $S_x$  eigenstates with eigenvalues  $\pm 1$ ,

$$|\pm x\rangle \propto | -1\rangle \pm \sqrt{2}|0\rangle + | +1\rangle.$$

We have that

$$\begin{aligned} R_x | \pm x\rangle &= -| \pm x\rangle, & R_z | \pm 1\rangle &= -| \pm 1\rangle, \\ R_x | \pm 1\rangle &= -| \mp 1\rangle, & R_z | \pm x\rangle &= -| \mp x\rangle. \end{aligned}$$

It follows that all  $R_w \otimes R_w$  ( $w = x, y, z$ ) act as permutations on the basis  $\{|\hat{1}\rangle, |\hat{2}\rangle, |\hat{3}\rangle, |\hat{4}\rangle\}$ :

$$\begin{aligned} (R_x \otimes R_x) &: |\hat{1}\rangle \leftrightarrow |\hat{3}\rangle; |\hat{2}\rangle \leftrightarrow |\hat{4}\rangle; \\ (R_z \otimes R_z) &: |\hat{1}\rangle \leftrightarrow |\hat{2}\rangle; |\hat{3}\rangle \leftrightarrow |\hat{4}\rangle; \\ (R_y \otimes R_y) &: |\hat{1}\rangle \leftrightarrow |\hat{4}\rangle; |\hat{2}\rangle \leftrightarrow |\hat{3}\rangle. \end{aligned}$$

Thus, the GHZ type state

$$|\text{GHZ}_4\rangle = \sum_{k=1}^4 |\hat{k}, \dots, \hat{k}\rangle,$$

which is an MPS with  $D = 4$  and

$$\mathcal{P}_{\text{GHZ}_4} = \sum_{k=1}^4 |\hat{k}\rangle \langle k, k|,$$

breaks all symmetries of  $D_2$ , and represents yet another distinct phase with symmetry  $D_2 = \mathbb{Z}_2 \times \mathbb{Z}_2$ ; the corresponding Hamiltonian is

$$H_{\text{GHZ}_4} = - \sum_j \left[ \sum_{k=1}^4 |\hat{k}, \hat{k}\rangle \langle \hat{k}, \hat{k}|_{j,j+1} \right],$$

where the label  $j$  refers to the blocked sites.

## 2. Phases under $\text{SO}(3)$ and $\text{SU}(2)$ symmetry

Let us now consider symmetry under rotational invariance, imposed either as  $\text{SO}(3)$  or as  $\text{SU}(2)$  symmetry. We will find that under  $\text{SO}(3)$  symmetry, there are two possible phases, represented by the spin-1 AKLT state and the trivial spin-0 state, respectively; on the other hand, we will show that if we impose  $\text{SU}(2)$  symmetry, there is only a single phase, as the AKLT state can be transformed into the trivial state keeping  $\text{SU}(2)$  symmetry.

Let us start with  $\text{SO}(3)$  symmetry. In order to compare the AKLT state to the trivial spin-0 state, we need a representation of  $\text{SO}(3)$  which contains both the spin-1 and spin-0 representation; we will denote the representation as

$$R_{\hat{n}}(\theta) = \exp[i\theta \hat{n} \cdot \mathbf{S}] \oplus 1.$$

While we could start with such a symmetry representation right away, let us discuss how to obtain the same setting from a spin-1 chain by blocking: Blocking two spin-1 sites gives a system with total spin  $1 \otimes 1 = 2 \oplus 1 \oplus 0$ , containing both a spin-1 and spin-0 subspace. It is straightforward to check that after blocking two sites and applying a rotation  $1 \otimes iY$ , the isometric form of the AKLT state is

$$\hat{\mathcal{P}}_{\text{AKLT}} = \mathbb{1}, \quad (25)$$

where the identity is on the two virtual spins with representation  $\frac{1}{2} \otimes \frac{1}{2} = 1 \oplus 0$ . The physical rotation  $R_{\hat{n}}$  acts

on the virtual indices with the projective spin- $\frac{1}{2}$  representation of the rotation group; it follows that the AKLT state is in the non-trivial equivalence class under  $\text{SO}(3)$  symmetry. The trivial spin-1 state, on the other hand, is obtained by placing singlets between pairs of spin-1 sites [i.e., between sites (1, 2), (3, 4), etc.]. After blocking these pairs, we obtain a product state with the spin-0 state at each site, which is an MPS with  $D = 1$  and the trivial projector

$$\hat{\mathcal{P}}_{\text{triv}} = |S = 0\rangle. \quad (26)$$

Thus, the rotation group  $R_{\hat{n}}(\theta)$  acts with the trivial representation on the virtual indices, and the trivial state is thus in a different phase than the AKLT chain.

It should be noted that while  $D_2$  is a subgroup of  $\text{SO}(3)$ , this does not imply that  $\text{SO}(3)$  exhibits all phases of  $D_2$ —indeed, the symmetry broken phases are missing. The reason is that while for any subgroup  $H \subset D_2$ ,  $D_2/H$  is finite, this is not true for  $\text{SO}(3)$ . Since however  $\text{SO}(3)/H$  labels the symmetry broken ground states, this corresponds to breaking a continuous symmetry, which leads to gapless phases and cannot be described in the framework of Matrix Product States.

Let us now turn our attention towards  $\text{SU}(2)$  symmetry, and explicitly construct an interpolating path between the isometric projectors for the AKLT state, Eq. (25), and the trivial state, Eq. (26). Note that the difference is that now for both  $\hat{\mathcal{P}}_{\text{AKLT}}$  and  $\hat{\mathcal{P}}_{\text{triv}}$ , the symmetry action on the virtual level is a linear representation of  $\text{SU}(2)$  (namely the spin- $\frac{1}{2}$  and the spin-0 representation, respectively). We can now provide an interpolating path  $|\Psi_\gamma\rangle = |\omega(\gamma)\rangle^{\otimes N}$ , with

$$|\omega(\gamma)\rangle = \gamma|0, 0\rangle + (1 - \gamma)(|1, 1\rangle + |2, 2\rangle),$$

where  $|\Psi_0\rangle$  corresponds to the isometric form (25) of the AKLT state, and  $|\Psi_1\rangle$  to the isometric form (26) of the trivial state. Furthermore, for  $U \in \text{SU}(2)$ , the whole path is invariant under the on-site symmetry

$$(1 \oplus U) \otimes (1 \oplus \bar{U}) = 1 \oplus (U \oplus \bar{U}) \oplus (U \otimes \bar{U}) \quad (27)$$

which contains the symmetries  $1$  and  $U \otimes \bar{U}$  of the trivial and the AKLT state as subsymmetries; this proves that under  $\text{SU}(2)$  symmetry, the AKLT state and the trivial state are in the same phase. Note that the symmetry (27) is only a representation of  $\text{SU}(2)$ , but not of  $\text{SO}(3)$ , as integer and half-integer spin representations belong to inequivalent classes of projective representations of  $\text{SO}(3)$ ; also, we cannot obtain this symmetry by starting only from the spin-0 and spin-1 representation of  $\text{SU}(2)$ , as they are not faithful representations. Note that this interpolating path can already be ruled out by imposing a parity constraint on the total number of half-integer representations, by e.g. associating them to fermions.

## V. CONCLUSION AND OUTLOOK

In this paper, we have classified the possible phases of one-dimensional, and to a certain extent two-dimensional, systems in the framework of Matrix Product States and PEPS. We have done so by studying Hamiltonians with exact MPS and PEPS ground states, and classifying under which conditions it is possible or impossible to connect two such Hamiltonians along a smooth and gapped path of local Hamiltonians.

We have found that in the absence of symmetries, all systems are in the same phase, up to accidental ground state degeneracies. Imposing local symmetries leads to a more refined classification: For systems with unique ground states, different phases are labelled by equivalence classes of projective representations, this is, cohomology classes of the group; for systems with degenerate ground states, we found that the symmetry action can be understood as composed of a permutation (permuting the symmetry broken ground states) and a representation of a subgroup (acting on the individual ground states), which together form an induced representation, and different phases are labelled by the permutation action (this is, the subgroup) and the cohomology classes of the subgroup. In this classification, systems in the same phase can be connected along a path which is gapped even in the thermodynamic limit, while for systems in different phases, the gap along any interpolating path will close even for a finite chain.

We have subsequently studied two-dimensional systems and considered three classes of phases, namely product states, GHZ states, and topological models based on quantum doubles. We have shown that all of these phases are stable in some region, and demonstrated that within that region, and more generally within the framework used for MPS, imposing symmetries does not further constrain the phase diagram.

We have also compared different definitions of phases under symmetries and found that very different classifications can be obtained depending on the definition chosen, ranging from scenarios where symmetries don't affect the classification at all, to scenarios where the classification is more fine-grained and e.g. the one-dimensional representations of the group partly or fully enter the classification. In this context, it is interesting to note that there is a hierarchy in the classification of phases as the spatial dimension increases: Zero-dimensional phases are labelled by 1D representations of the symmetry group (this is, its first cohomology group). This label vanishes in one dimension, and phases are now classified by the second cohomology group. This label, in turn, vanishes in three dimensions, and although we have demonstrated that we can't infer symmetry constraints from the continuity of the PEPS projectors  $\mathcal{P}$  alone, it is expected that phases under symmetries in two and more dimensions are still classified by higher order cohomology groups.<sup>32,33</sup>

A central tool in our proofs has been the *isometric form* of an MPS or PEPS. Isometric MPS and PEPS are fixed

points of renormalization transformations, and any MPS can be transformed into its isometric form along a gapped path in Hamiltonian space; this result allows us to restrict our classification of one-dimensional quantum phases to the case of isometric RG fixed points. Moreover, it gives us a tool to carry out renormalization transformations in a local fashion, this is, without actually having to block and renormalize the system; it thus provides a rigorous justification for the application of RG flows towards the classification of quantum phases. Let us add that the possibility to define an isometric form, as well as the possibility to interpolate towards it along a continuous path of parent Hamiltonians, still holds for not translational invariant systems; however, without translational invariance we are lacking tools to assess the gappedness of the Hamiltonian.

Let us note that MPS have been previously applied to the classification of phases of one-dimensional quantum systems:<sup>11,30,34</sup> In particular, in Ref. 30, MPS have been used to demonstrate the symmetry protection of the AKLT phase, and in Ref. 11, renormalization transformations<sup>17</sup> and their fixed points on MPS have been applied to the classification of quantum phases for one dimensional systems with unique ground states both with and without symmetries, giving a classification based on cohomology classes and 1D representations. Beyond that, RG fixed points of PEPS have also been used towards the classification of phases for two-dimensional systems.<sup>14,35</sup>

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### Appendix A: Gap proof for the 1D path

In the following, we show that the family of  $\gamma$ -deformed parent Hamiltonians which arise from the MPS path  $|\mu[\mathcal{P}_\gamma]\rangle$  interpolating between an MPS and its isometric form is gapped. Recall that this family was defined as  $H_\gamma := \sum h_\gamma(i, i+1)$ , with  $h_\gamma := \Lambda_\gamma h_0 \Lambda_\gamma > 0$ .

We want to show that the path  $H_\gamma$  is uniformly gapped, i.e., there is a  $\Delta > 0$  which lower bounds the gap of  $H_\gamma$  uniformly in  $\gamma$  and the systems size  $N$ : This establishes that the  $|\mu[\mathcal{P}_\gamma]\rangle$ , and the corresponding  $H_\gamma$ , are all in the same phase. To this end, we use a result of Nachtergaele<sup>6</sup> (extending the result of Ref. 1 for the

injective case), where it is shown that any parent Hamiltonian is gapped, and a lower bound on the gap (uniform in  $N$ ) is given.

In the following, we will use the results of Ref. 6 to derive a uniform lower bound on the gap for all  $H_\gamma$ ,  $1 \geq \gamma \geq 0$ . Let the MPS matrices  $[A_i(\gamma)]_{kl} := \sum_{k,l} \langle i | \mathcal{P}_\gamma | k, l \rangle | k \rangle \langle l |$  (cf. Sec. IV A 2); in the normal form, the  $A_i(\gamma)$  have a block structure  $A_i(\gamma) = \bigoplus A_i^\alpha(\gamma)$ . Let  $\mathbb{E}^\alpha(\gamma) := \sum_i A_i^\alpha(\gamma) \otimes \overline{A_i^\alpha(\gamma)}$ , and let  $|\text{spec } \mathbb{E}^\alpha(\gamma)| = \{\lambda_1^\alpha(\gamma) > \lambda_2^\alpha(\gamma) > \dots \geq 0\}$  be the ordered absolute value of the spectrum of  $\mathbb{E}^\alpha(\gamma)$  (not counting duplicates). Then,  $\lambda_2(\gamma)/\lambda_1(\gamma) < 1$ , and since the spectrum is continuous in  $\gamma \in [0, 1]$ , and the degeneracy of  $\lambda_1$  is  $\mathcal{A}$ ,<sup>6</sup> the existence of a uniform upper bound  $1 > \tau_\alpha > \lambda_2^\alpha(\gamma)/\lambda_1^\alpha(\gamma)$  follows. For  $\alpha \neq \beta$ , let

$$\Omega_{\alpha,\beta}^p(\gamma) = \sup_{X,Y} \frac{\langle \Phi[A^\alpha(\gamma); X] | \Phi[A^\beta(\gamma); Y] \rangle}{\| \Phi[A^\alpha(\gamma); X] \| \| \Phi[A^\beta(\gamma); Y] \|},$$

where  $|\Phi[C; X]\rangle := \sum_{i_1, \dots, i_p} \text{tr}[C_{i_1} \dots C_{i_p} X] |i_1, \dots, i_p\rangle$ ; i.e.,  $\Omega_{\alpha,\beta}^p(\gamma)$  is the maximal overlap of the  $p$ -site reduced states of the MPS described by the blocks  $A^\alpha(\gamma)$  and  $A^\beta(\gamma)$ . With  $\mathcal{S}_\alpha(\gamma) := \{\sum_i \text{tr}[A_i^\alpha(\gamma) X] |i\rangle |X\rangle\}$ , and  $\mathcal{O}(\mathcal{X}, \mathcal{Y})$  the maximal overlap between normalized vectors in the subspaces  $\mathcal{X}$  and  $\mathcal{Y}$ , we have that  $\Omega_{\alpha,\beta}^p(\gamma) \leq \mathcal{O}(\mathcal{S}_\alpha(\gamma)^{\otimes p}, \mathcal{S}_\beta(\gamma)^{\otimes p}) \leq \mathcal{O}(\mathcal{S}_\alpha(\gamma), \mathcal{S}_\beta(\gamma))^p$ . Moreover, since  $\mathcal{S}_\alpha(0) \perp \mathcal{S}_\beta(0)$ , and  $\mathcal{S}_\bullet(\gamma) = Q_\gamma \mathcal{S}_\bullet(0)$ , we have that

$$\begin{aligned} \mathcal{O}(\mathcal{S}_\alpha(\gamma), \mathcal{S}_\beta(\gamma)) &\leq \sup_{\langle v|w\rangle=0} \frac{|\langle v | Q_\gamma^2 | w \rangle|}{\|Q_\gamma |v\rangle\| \|Q_\gamma |w\rangle\|} \\ &= \sup_{\langle v|w\rangle=0} \sqrt{\frac{|M_{12}|^2}{M_{11}M_{22}}}, \end{aligned}$$

where  $M = \pi Q_\gamma^2 \pi^\dagger$ ,  $\pi = |0\rangle\langle v| + |1\rangle\langle w|$ , is some  $2 \times 2$  submatrix of  $Q_\gamma^2$ . For  $M > 0$ ,

$$\begin{aligned} \frac{|M_{12}|^2}{M_{11}M_{22}} &\leq 1 - \frac{\lambda_{\min}(M)}{\lambda_{\max}(M)} \leq 1 - \frac{\lambda_{\min}(Q_\gamma^2)}{\lambda_{\max}(Q_\gamma^2)} \\ &\leq 1 - \lambda_{\min}(Q^2) =: \kappa < 1, \end{aligned}$$

and we find that  $\Omega_{\alpha,\beta}^p(\gamma) \leq \kappa^p$ . Thus, there exists a  $p$  s.th.

$$K^p(\gamma) := \frac{4(\mathcal{A}-1)\kappa^p}{1-2(\mathcal{A}-1)\kappa^p} + \sum_\alpha D^2 \tau_\alpha^p \frac{1+D^2 \tau_\alpha^p}{1-D^2 \tau_\alpha^p} < 1/\sqrt{2},$$

and as Nachtergaele shows,<sup>6</sup>  $\frac{1}{2} \Delta_{2p}(\gamma) (1 - \sqrt{2} K^p(\gamma))^2$  is a lower bound on the spectral gap of  $H_\gamma$ . Here,  $\Delta_{2p}(\gamma)$  is the gap of  $H_\gamma$ , restricted to  $2p$  sites, which has a uniform lower bound as the restricted Hamiltonian is continuous in  $\gamma$ . This proves that  $H_\gamma$  has a uniform spectral gap for  $0 \leq \gamma \leq 1$ .

## Appendix B: Standard form for injective MPS under symmetries

In this section, we discuss how  $U_g$ -symmetry of an injective MPS is represented on the virtual level. To start with, it has been shown<sup>19</sup> that any two tensors  $\mathcal{P}$  and  $\mathcal{P}'$  which (up to a phase) represent the same MPS can be related by a gauge transformation

$$\mathcal{P}' = \mathcal{P}(e^{i\phi} V \otimes \bar{V}).$$

Given an MPS  $|\mu[P]\rangle$  with  $U_g$ -invariant parent Hamiltonian (where  $U_g$  is a linear or projective representation), it follows that  $|\mu[P]\rangle$  is invariant under  $U_g$  up to a phase and thus, the action of  $U_g$  on  $|\mu[P]\rangle$  can be understood on the virtual level as

$$U_g \mathcal{P} = \mathcal{P}(e^{i\phi_g} V_g \otimes \bar{V}_g), \quad (\text{B1})$$

or

$$\hat{U}_g := \mathcal{P}^{-1} U_g \mathcal{P} = (e^{i\phi_g} V_g \otimes \bar{V}_g);$$

note that  $\hat{U}_g$  forms again a representation. From this, it follows that the  $V_g$  form a projective representation, and in turn that  $\phi_g$  forms a 1D representation of  $G$ . This shows that  $\hat{U}_g$ , and thus  $U_g$ , is a *linear* representation of  $G$ —systems with MPS ground states without symmetry breaking cannot be invariant under projective representations. (Strictly speaking, we only find that  $\phi_g$  is in the same cohomology class as a linear representation, but in order to compare two systems, we need the same gauge for  $\phi_g^0$  and  $\phi_g^1$ , so we choose them to be linear representations.)

Under blocking, the physical symmetry  $U_g$  in (B1) is mapped to  $U_g^{\otimes k}$ , restricted to the range of the blocked map  $\mathcal{P}^{\otimes k} |\omega_D\rangle^{\otimes (k-1)}$ .  $V_g$  remains unchanged under blocking; this suggests that it is suitable as a characteristic of a quantum phase (which we expect to be stable under blocking). The 1D representation  $e^{i\phi_g}$ , on the other hand, changes under blocking to  $e^{ik\phi_g}$ . In particular, if the 1D representation is finite, it can be removed by blocking, while this is not possible for continuous representations such as of  $U(1)$ .

However, our definition of quantum phases allows us to fully remove the 1D representation  $e^{i\phi_g}$  in (B1) even if it is continuous, using the phase degree of freedom which we included in our definition. Consider first the scenario where we are free to choose the phase degree of freedom for the initial and final system independently. Then, we can choose to replace  $U_g$  by  $e^{i\phi_g} U_g$ , which will make the phase in (B1) vanish. Second, consider the case where the two physical symmetries are equal,  $U_g^0 = U_g^1 =: U_g$ . Then, we can choose the phase gauge such that the 1D representation for one system vanishes,

$$U_g^0 = V_g^0 \otimes \bar{V}_g^0.$$

On the other hand, since  $U_g^0 = U_g^1$ , we have that

$$e^{i\phi_g^1} V_g^1 \otimes \bar{V}_g^1 = V_g^0 \otimes \bar{V}_g^0$$

which also implies that  $e^{i\phi_g^1} = 1$  [e.g., by looking at any non-zero matrix element  $(i, i) \times (j, j)$ ]. Finally, if  $U_g^0$  and  $U_g^1$  only share a subblock, this means that  $V_g^0 = X_g^0 \oplus Y_g^0$  s.th.  $X_g^0 \otimes \bar{X}_g^0$  yields that subblock, and similiary for  $V_g^1$ , which again shows that  $e^{i\phi_g^1} = 1$ .

### Appendix C: Continuity of cohomology class where subspace changes

This appendix contains the proof omitted at the end of Sec. II F 3 (all the notation is the same as introduced there): That the cohomology class obtained from  $\mathcal{P}_\gamma$  and  $\mathcal{P}_{\gamma+d\gamma}$  is the same even if  $\mathcal{P}_{\gamma+d\gamma}$  is supported on a larger space than  $\mathcal{P}_\gamma$ . We will again show this for differentiable  $\mathcal{P}_\gamma$ , it extends to continous  $\mathcal{P}_\gamma$  by approximating them by a sequence of differentiable functions. Let  $\mathcal{P}_{\gamma+d\gamma} = \mathcal{P}_\gamma + \mathcal{P}'_\gamma d\gamma$ , with

$$\mathcal{P}_\gamma = \begin{bmatrix} P & 0 \\ 0 & 0 \end{bmatrix}$$

and

$$\mathcal{P}'_\gamma = \begin{bmatrix} A & B \\ C & D \end{bmatrix},$$

and note that the same block structure has to hold for the physical symmetry (as it is a symmetry for the whole path),

$$U_g = \begin{bmatrix} Q_g & 0 \\ 0 & R_g \end{bmatrix},$$

with  $R_g, S_g$  unitary. To first order in  $d\gamma$ , the action of the symmetry on the virtual space is

$$\tilde{U}_g = \mathcal{P}_{\gamma+d\gamma}^{-1} U_g \mathcal{P}_{\gamma+d\gamma} = T^{-1} K_g T + O(d\gamma^2),$$

with

$$K_g = \begin{bmatrix} (\mathbb{1} + X)\bar{Q}_g - X\bar{R}_g & \bar{Q}_g X - X\bar{R}_g \\ (\mathbb{1} + X)(\bar{R} - \bar{Q}) & (\mathbb{1} + X)\bar{R}_g - \bar{Q}_g X \end{bmatrix},$$

$$T = \begin{bmatrix} \mathbb{1} & 0 \\ 0 & C^{-1}D \end{bmatrix},$$

$X = (P + A d\gamma)^{-1} B D^{-1} C d\gamma$ , and the ‘‘dressed representations’’

$$\begin{aligned} \bar{Q}_g &= (P + A d\gamma)^{-1} Q_g (P + A d\gamma), \\ \bar{R}_g &= C^{-1} R_g C. \end{aligned}$$

(This can be derived using the Schur complement to express  $\mathcal{P}_{\gamma+d\gamma}^{-1}$  and can be readily checked by left multiplication with  $\mathcal{P}_{\gamma+d\gamma}$ .) It follows that the upper left block of  $K_g K_h$  is

$$(\mathbb{1} + X)\bar{Q}_g \bar{Q}_h - X\bar{R}_g \bar{R}_h + O(d\gamma^2),$$

i.e., the upper left block of  $U_g$  (which corresponds to the virtual subspace used by  $\mathcal{P}_\gamma$ ) forms a representation to first order in  $d\gamma$ . The part corresponding to each of the two bonds thus forms a projective representation which changes smoothly in  $\gamma$ , and which therefore cannot change its cohomology class. Since the cohomology class has to be the same for all subblocks, this completes the proof.

### Appendix D: Standard form for non-injective MPS under symmetries

In the following, we will show that for any non-injective MPS  $|\mu[\mathcal{P}]\rangle$  with a parent Hamiltonian which is invariant under some local symmetry  $U_g$ , the symmetry can be represented as the symmetry (16) of  $\mathcal{P}$ . It is clear from (2) that any  $\mathcal{P}$  with this symmetry will result in a Hamiltonian with the same symmetry. In the following, we will prove the converse.

Using the same arguments as in Ref. 36, one can show that any  $U_g$ -invariance of a parent Hamiltonian (at the moment, we are talking of a *single* unitary  $U_g$  and only carry the subscript  $g$  for ‘‘future use’’) can be understood as resulting from an effective action

$$\hat{U}_g := \mathcal{P}^{-1} U_g \mathcal{P} = P_g \left[ \bigoplus_{\alpha} e^{i\phi_g^{\alpha}} V_g^{\alpha} \otimes \bar{V}_g^{\alpha} \right] \quad (D1)$$

of the symmetry operation on the virtual system, using the correct gauge for  $\mathcal{P}$ . Here,  $V_g^{\alpha}$  is unitary, the direct sum runs over the Hilbert spaces  $\mathcal{H}_{\alpha}$  in (15), and  $P_g$  permutes those Hilbert spaces. (Proof sketch, cf. Ref. 36:  $U_g$ -invariance of the Hamiltonian means that  $U_g$  maps ground states to ground states. The different sectors  $\mathcal{H}_{\alpha}$ , corresponding to different symmetry broken sectors, must be treated independently, since they don’t interfere on any OBC interval. Thus,  $U_g$  can on the one hand permute sectors and change their phase—this gives the  $P_g$  and  $\exp[i\phi_g^{\alpha}]$ —and it can on the other hand act non-trivially on each sector—since each of the sectors behaves like an injective MPS, this gives the  $V_g^{\alpha} \otimes \bar{V}_g^{\alpha}$ .)

In the following, we will assume that  $P_g$  acts irreducibly on the system in the sense that there are no subsets of  $\{1, \dots, \mathcal{A}\}$  invariant under all  $P_g$ . We can always achieve this situation by splitting (D1) into a direct sum over such irreducible cases.

Let us now study what a linear representation structure

$$\hat{U}_g \hat{U}_h = \hat{U}_{gh} \quad (D2)$$

( $g, h \in G$ ) implies for the algebraic structure of  $P_g, V_g^{\alpha}$ , and  $e^{i\phi_g^{\alpha}}$ . (We can always achieve a linear representation by blocking; also note that the following argument can be generalized to projective representations.) First, since  $P_g$  is the only part of (D1) which is not block diagonal, it follows that the  $P_g$  form a linear representation of  $G$ .

(Linearity follows since the entries of  $P_g$  are 0 and 1). Let us define

$$W_g^\alpha := e^{i\phi_g^\alpha} V_g^\alpha \otimes \bar{V}_g^\alpha. \quad (\text{D3})$$

Then, using (D1) the representation structure (D2) is equivalent to the relation

$$W_g^{\pi_h(\alpha)} W_h^\alpha = W_{gh}^\alpha \quad (\text{D4})$$

for the  $W_g^\alpha$ , where the permutations  $\pi_h$  are defined via  $\mathcal{H}_{\pi_h(\alpha)} = P_h(\mathcal{H}_\alpha)$  and thus form a representation,  $\pi_g \pi_h = \pi_{gh}$ .

Let us now show that (D4) implies that the  $\hat{U}_g$  can be understood as an induced representation; the following proof is due to S. Beigi.<sup>37</sup> Fix some  $\alpha_0$ , and let

$$H := \{h : h \in G, \pi_h(\alpha_0) = \alpha_0\}.$$

Then, (D4) implies that  $W_h^{\alpha_0}$  is a linear representation of  $H$ . We know we can write  $G$  as the disjoint union over cosets  $k_\beta H$  labelled by the blocks  $\beta = 1, \dots, \mathcal{A}$ , for a (non-unique) choice of  $k_\beta \in G$  chosen such that  $\pi_{k_\beta}(\alpha_0) = \beta$ . (This is where we need irreducibility.) We now have that

$$W_g^\beta \stackrel{(D4)}{=} W_{gk_\beta}^{\pi_{k_\beta^{-1}(\beta)}} W_{k_\beta^{-1}}^\beta = W_{gk_\beta}^{\alpha_0} W_{k_\beta^{-1}}^\beta \quad (\text{D5})$$

where we have used that  $\pi_{k_\beta^{-1}(\beta)} = \pi_{k_\beta^{-1}}(\beta) = \alpha_0$ . Using the decomposition of  $G$  in cosets, we have that  $g$  and  $\beta$  uniquely determine  $\gamma$  and  $h \in H$  by virtue of

$$gk_\beta = k_\gamma h \quad (\text{D6})$$

and thus, continuing (D5),

$$W_g^\beta \stackrel{(D4)}{=} W_{k_\gamma}^{\pi_h(\alpha_0)} W_h^{\alpha_0} W_{k_\beta^{-1}}^\beta = W_{k_\gamma}^{\alpha_0} W_h^{\alpha_0} W_{k_\beta^{-1}}^\beta,$$

using that  $\pi_h(\alpha_0) = \alpha_0$ . We can now replace  $W_{k_\beta^{-1}}^\beta$  using that

$$\mathbb{1} = W_{k_\beta k_\beta^{-1}}^\beta \stackrel{(D4)}{=} W_{k_\beta}^{\pi_{k_\beta^{-1}(\beta)}} W_{k_\beta^{-1}}^\beta = W_{k_\beta}^{\alpha_0} W_{k_\beta^{-1}}^\beta.$$

Substituting this above, we finally obtain that

$$W_g^\beta = W_{k_\gamma}^{\alpha_0} W_h^{\alpha_0} (W_{k_\beta}^{\alpha_0})^{-1}, \quad (\text{D7})$$

i.e.,  $W_g^\beta$  is fully determined by the representation  $W_h^{\alpha_0}$  on  $H$ , together with the (arbitrary) unitaries  $W_{k_\beta}^{\alpha_0}$  for all coset representatives  $k_\beta$ .

We now define a rotation

$$K = \bigoplus_{\delta} W_{k_\delta}^{\alpha_0};$$

then, in the rotated basis,  $\hat{U}_g$  reads

$$K^\dagger \hat{U}_g K = P_g \left[ \bigoplus_{\beta} W_h^{\alpha_0} \right],$$

using that  $\pi_g(\beta) = \pi_{k_\gamma}(\pi_h(\pi_{k_\beta^{-1}}(\beta))) = \pi_{k_\gamma}(\pi_h(\alpha_0)) = \gamma$ . If we now substitute back

$$W_h^{\alpha_0} = e^{i\phi_h^{\alpha_0}} V_h^{\alpha_0} \otimes \bar{V}_h^{\alpha_0}$$

[Eq. (D3)] in

$$W_g^{\alpha_0} W_h^{\alpha_0} = W_{gh}^{\alpha_0}, \quad g, h \in H$$

[Eq. (D4)], we find that  $V_h^{\alpha_0}$  forms a projective representation of  $H$ , and  $e^{i\phi_h^{\alpha_0}}$  a linear representation of  $H$ .

Thus, we can write

$$K^\dagger \hat{U}_g K = \tilde{U}_g D_g$$

with

$$\tilde{U}_g = P_g \left[ \bigoplus_{\beta} V_h^{\alpha_0} \otimes \bar{V}_h^{\alpha_0} \right] \quad (\text{D8})$$

and

$$D_g = \bigoplus_{\beta} e^{i\phi_h^{\alpha_0}}, \quad (\text{D9})$$

where  $h \equiv h(g, \beta)$  is determined by (D6). The diagonal operator  $D_g$  acts independently on the different symmetry broken ground states of the system and thus commutes with the Hamiltonian; therefore, we can remove it by choosing the proper gauge for the physical symmetry according to our definition of phases under symmetries. If the symmetry of the initial and the final state overlap on a subsector of the ground state space, this implies (as for the injective case, Appendix B) that the 1D representations for this sector in  $D_g$  are the same and thus can be removed by a joint gauge transformation. Together, this shows that for the classification of phases under symmetries in the non-injective case, any symmetry can be understood as a direct sum over independent sectors, where on each sector the action of the symmetry is given by (D8), where  $h \equiv h(g, \beta)$  is determined by (D6).

## Appendix E: Robustness of the 2D gap

Here, we prove the robustness of a gap based on a condition of the form

$$\tilde{h}_i \tilde{h}_j + \tilde{h}_i \tilde{h}_j \geq -\frac{1}{8}(1 - \Delta_{ij})(\tilde{h}_i + \tilde{h}_j); \quad (\text{E1})$$

where we consider a square lattice with  $\tilde{h}_i \geq \mathbb{1}$  acting on  $2 \times 2$  plaquettes,  $\Delta_{ij} = \Delta_a$  for directly adjacent plaquettes  $i, j$  sharing two spins, and  $\Delta_{ij} = \Delta_d$  for diagonally adjacent plaquettes  $i, j$  having one spin in common. (In Section III B, we have given the simplified version where  $\Delta_a = \Delta_d = \Delta$ .) Then,

$$\tilde{H}^2 = \sum_i \underbrace{\tilde{h}_i^2}_{\geq h_i} + \sum_{\langle ij \rangle} \tilde{h}_i \tilde{h}_j + \sum'_{\substack{\langle ij \rangle \\ \geq 0}} \underbrace{\tilde{h}_i \tilde{h}_j}_{\geq 0} \geq \frac{\Delta_a + \Delta_d}{2} \tilde{H},$$

which implies a gap in the spectrum of  $\tilde{H}$  between 0 and  $\Delta = (\Delta_a + \Delta_d)/2 > 0$ , and thus a lower bound  $\Delta$  on the gap of  $\tilde{H}$ , cf. Ref. 1.

Let us now study the robustness of (E1) under  $\gamma$ -deformation of the Hamiltonian. Let  $h_i, h_j$  be projectors which satisfy  $h_i h_j + h_j h_i \geq -\frac{1}{8}(1 - \Delta_{ij})(h_i + h_j)$ . (The proof can be modified for the  $h_i$  not being projectors.) Let  $h_i$  be supported on systems  $AB$ , and  $h_j$  on systems  $BC$ , where the number of sites in systems  $A, B$ , and  $C$  is  $a, b$ , and  $c = a$ , respectively. (For the square lattice,  $a = b = c = 2$  for directly neighboring terms, and  $a = c = 3, b = 1$  for diagonally adjacent terms.) With  $Q_\gamma = (1 - \gamma)\mathbb{1} + \gamma Q \leq \mathbb{1}$  as in the one-dimensional case,

let  $\Lambda_{\gamma,X} = (Q_\gamma^{-1})^{\otimes x}$ , with  $X = A, B, C$  and  $x = a, b, c$ . Then, the  $\gamma$ -deformed Hamiltonians are

$$\begin{aligned} h_i(\gamma) &= (\Lambda_{\gamma,A} \otimes \Lambda_{\gamma,B}) h_i (\Lambda_{\gamma,A} \otimes \Lambda_{\gamma,B}), \\ h_j(\gamma) &= (\Lambda_{\gamma,B} \otimes \Lambda_{\gamma,C}) h_j (\Lambda_{\gamma,B} \otimes \Lambda_{\gamma,C}). \end{aligned}$$

Let us define

$$\begin{aligned} \Theta_\gamma &:= \Lambda_{\gamma,B}^2 - \mathbb{1} \geq 0, \\ q &:= \lambda_{\min}(Q) < 1, \\ \mu_\gamma &:= ((1 - \gamma) + \gamma \lambda_{\min}(Q))^{-2} \geq 1, \end{aligned}$$

such that  $Q_\gamma^{2a} \geq \frac{1}{\mu_\gamma^a} \mathbb{1}$ , and  $(\mu_\gamma^b - 1)\mathbb{1} \geq \Theta_\gamma$ . Then, we find that

$$\begin{aligned} &h_i \Lambda_{\gamma,B}^2 h_j + h_j \Lambda_{\gamma,B}^2 h_i + \frac{1}{8} \mu_\gamma^a [1 - \Delta_{ij} + 8(\mu_\gamma^b - 1)] (h_i \otimes \Lambda_{\gamma,C}^{-2} + \Lambda_{\gamma,A}^{-2} \otimes h_j) \\ &\geq h_i \Lambda_{\gamma,B}^2 h_j + h_j \Lambda_{\gamma,B}^2 h_i + \frac{1}{8} [1 - \Delta_{ij} + 8(\mu_\gamma^b - 1)] (h_i \otimes \mathbb{1}_C + \mathbb{1}_A \otimes h_j) \\ &= h_i \Theta_\gamma h_j + h_j \Theta_\gamma h_i + h_i [(\mu_\gamma^b - 1)\mathbb{1}] h_i + h_j [(\mu_\gamma^b - 1)\mathbb{1}] h_j + h_i h_j + h_j h_i + \frac{1}{8}(1 - \Delta_{ij})(h_i + h_j) \\ &\geq (h_i + h_j) \Theta_\gamma (h_i + h_j) \geq 0. \end{aligned}$$

By multiplying this with  $\Lambda_{\gamma,A} \otimes \Lambda_{\gamma,B} \otimes \Lambda_{\gamma,C}$  from both sides, we obtain a lower bound of type (E1) for the  $\gamma$ -deformed Hamiltonian,

$$h_i(\gamma) h_j(\gamma) + h_j(\gamma) h_i(\gamma) \geq -\frac{1}{8} [1 - \Delta_{ij}(\gamma)] [h_i(\gamma) + h_j(\gamma)], \quad (\text{E2})$$

with  $\Delta_{ij}(\gamma) = \mu_\gamma^a \Delta_{ij} + (1 + 7\mu_\gamma^a - 8\mu_\gamma^{a+b})$ . This can be used to find an environment of any point in which the system is still gapped. In particular, in the case where the isometric parent Hamiltonian is commuting, and as-

suming a square lattice, the lower bound on the spectral gap provided by (E2) is

$$\Delta(\gamma) = \frac{\Delta_a(\gamma) + \Delta_d(\gamma)}{2} = 1 + 4\mu_\gamma^2(1 + \mu_\gamma - 2\mu_\gamma^2).$$

This gap vanishes at  $\mu_\gamma \approx 1.07$ , limiting the maximal deformation of the isometric tensor to  $\lambda_{\min}(Q)/\lambda_{\max}(Q) \approx 0.967$ .

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