Classifying quantum phases using matrix product states and projected entangled pair states

Norbert Schuch,[1] David Pérez-García,[2] and Ignacio Cirac[3]
[1]*Institute for Quantum Information, California Institute of Technology, MC 305-16, Pasadena, California 91125, USA*
[2]*Departamento Analisis Matematico and IMI, Universidad Complutense de Madrid, E-28040 Madrid, Spain*
[3]*Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Strasse 1, D-85748 Garching, Germany*
(Received 15 March 2011; published 31 October 2011)

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 in both the absence and the 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, that is, the equivalence classes of its projective representations, a result first derived by Chen, Gu, and Wen [Phys. Rev. B **83**, 035107 (2011)]. 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 labeled 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.

DOI: 10.1103/PhysRevB.84.165139 PACS number(s): 71.10.Hf, 03.65.Ud

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[1] (MPS) and projected entangled pair states[2] (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:[3–5] That 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.[1,6–8]

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 quasilocal evolution,[9] 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, that is, 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 constraint in form of a local symmetry U_g (with symmetry 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 labeled by the different equivalence classes of projective representations V_g of the symmetry group

G,[10] which are in one-to-one correspondence to the elements of its second cohomology group $\mathrm{H}^2(G,\mathrm{U}(1))$ (this has been previously studied in Ref. 11).

For 1D 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 labeled 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[12] as their representatives. We also find that in these regions, imposing symmetries on the Hamiltonian does not alter the phase diagram, and, more generally, 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 Sec. II, we prove the results for the 1D case: We start by introducing MPS (Sec. II A) and parent Hamiltonians (Sec. II B) and defining 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 Sec. 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 do not 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 Secs. IV B and IV 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 derive the classification of phases for 1D systems both with unique and with degenerate ground states and in both the absence and the presence of symmetries. We start by giving the necessary definitions; we introduce MPS and their parent Hamiltonians and define what we mean by phases both without and with symmetries. Then we state and prove the classification of phases for the various scenarios (with some technical parts placed in Appendixes).

Note that, for clarity, we 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 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) MPS $|\boldsymbol{\mu}[\mathcal{P}]\rangle$ 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 $\mathcal{P} : \mathbb{C}^D \otimes \mathbb{C}^D \to \mathbb{C}^d$, as depicted in Fig. 1 (Ref. 13); that is,

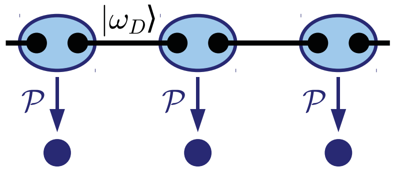

FIG. 1. (Color online) MPS are constructed by applying a linear map $\mathcal{P}$ to maximally entangled pairs $|\omega_D\rangle := \sum_{i=1}^{D}|i,i\rangle$ of *bond dimension* D.

$|\boldsymbol{\mu}[\mathcal{P}]\rangle = \mathcal{P}^{\otimes N}|\omega_D\rangle^{\otimes N}$. 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, $(\ker\mathcal{P})^{\perp} = \mathcal{H}_1 \oplus \cdots \oplus H_{\mathcal{A}}$, with

$$\mathcal{H}_\alpha = \mathrm{span}\{|i,j\rangle : \zeta_{\alpha-1} < i,j \leqslant \zeta_\alpha\}. \tag{1}$$

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

In the following, we assume, without loss of generality, that all MPS are in their standard form; note that this might involve the blocking of sites of the original model. Moreover, we 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 $h(i,i+1) \equiv h \geqslant 0$ acting on two adjacent sites $(i,i+1)$ whose kernels exactly support the two-site reduced density operator of the corresponding MPS, that is,

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

By construction, $H \geqslant 0$ and $H|\boldsymbol{\mu}[\mathcal{P}]\rangle = 0$, that is, $|\boldsymbol{\mu}[\mathcal{P}]\rangle$ is a ground state of H. It can be shown that the ground-state space of H is $\mathcal{A}$-fold degenerate and spanned by the states $|\boldsymbol{\mu}[\mathcal{P}|_{\mathcal{H}_\alpha}]\rangle$, where $\mathcal{P}|_{\mathcal{H}_\alpha}$ is the restriction of $\mathcal{P}$ to $\mathcal{H}_\alpha$.[1,6,7] 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 use the notion of MPS and parent Hamiltonians interchangeably whenever appropriate.

C. Definition of quantum phases

Vaguely speaking, we 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.[14]

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

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

with two-local h_γ such that

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

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 to Hamiltonians both 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 1D 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 $U = U_g^0 \oplus U_g^1 \oplus U_g^{\mathrm{path}}$ of G on a Hilbert space $\mathcal{H} = \mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \mathcal{H}_{\mathrm{path}}$ and an interpolating path H_γ 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 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, for example, the spin-1 AKLT state with the spin-0 state under SO(3) symmetry, but we impose this even if the two representations are the same; we 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, that is, 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

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

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 noninjective 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 ϵN, 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,[17] and using the exponential convergence of MPS to their fixed point,[17] 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.

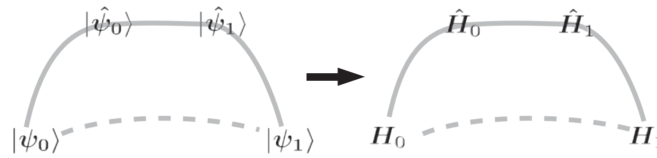

FIG. 2. Construction of the interpolating path for MPS and parent Hamiltonians. Instead of interpolating between the MPS $|\psi_0\rangle$ and $|\psi_1\rangle$ directly (dotted line), we first show how to interpolate each of the two states toward a standard from $|\hat\psi_p\rangle$, the *isometric form*, 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 $|\boldsymbol{\mu}[\mathcal{P}_p]\rangle$, $p=0,1$, together with their nearest-neighbor parent Hamiltonians H_p, we want to see whether H_0 and H_1 are in the same phase, that is, whether we can construct a gapped interpolating path. We 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_γ in the space of parent Hamiltonians which satisfies the necessary continuity and gappedness requirements.

In order to facilitate this task, we proceed in two steps, as illustrated in Fig. 2: In a first step, we 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 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,[17] and every MPS can be brought into its isometric form by stochastic local operations.[18] Most importantly, as we show, there exists a gapped path in the space of parent Hamiltonians which interpolates between any MPS and its isometric form.

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

$$\mathcal{P} = Q\, W, \tag{3}$$

with W an isometry $WW^\dagger = \mathbb{1}$ and $Q > 0$, by virtue of a polar decomposition of $\mathcal{P}|_{(\ker\mathcal{P})^\perp}$; without loss of generality, we can assume $0 < Q \leqslant \mathbb{1}$ by rescaling $\mathcal{P}$. The *isometric form* of $|\boldsymbol{\mu}[\mathcal{P}]\rangle$ is now defined to be $|\boldsymbol{\mu}[W]\rangle$, the MPS described by W, the isometric part of the tensor $\mathcal{P}$.

To see that $|\boldsymbol{\mu}[\mathcal{P}]\rangle$ and $|\boldsymbol{\mu}[W]\rangle$ are in the same phase, define an interpolating path $|\boldsymbol{\mu}[\mathcal{P}_\gamma]\rangle$, $\mathcal{P}_\gamma = Q_\gamma W$, with

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

note that the path can be seen as a stochastic deformation $|\boldsymbol{\mu}[\mathcal{P}_\gamma]\rangle = Q_\gamma^{\otimes N}|\boldsymbol{\mu}[\mathcal{P}_0]\rangle$ (cf. Fig. 3). Throughout the path, the MPS stays in standard form, and in the noninjective case, the

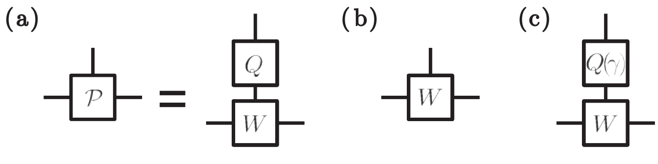

FIG. 3. Isometric form of an MPS. (a) The MPS projector $\mathcal{P}$ can be decomposed into a positive map Q and an isometric map W. (b) By removing Q, one obtains the isometric form W of the MPS. (c) Interpolation to the isometric form is possible by letting $Q_\gamma = \gamma Q + (1-\gamma)\mathbb{1}$.

blocking pattern which is encoded in the structure of $\ker\mathcal{P}$ stays unchanged.

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

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

and define the γ-deformed Hamiltonian

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

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

It remains to show that the path H_γ is uniformly gapped; that is, there is a $\Delta > 0$ which lower bounds the gap of H_γ uniformly in γ and the systems size N: This establishes that the $|\boldsymbol{\mu}[\mathcal{P}_\gamma]\rangle$ are all in the same phase. The derivation is based on a result of Nachtergaele[6] (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 ξ and the gap of H_γ restricted to ξ sites, and since both depend smoothly on γ, and $\xi \to 0$ as $\gamma \to 0$, a uniform lower bound on the gap follows; for the noninjective case, one additionally needs that the overlap of different ground states goes to zero as $\gamma \to 0$.

3. *Isometric form and symmetries*

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

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

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

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

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

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

That 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 $|\boldsymbol{\mu}[\mathcal{P}_\gamma]\rangle = Q_\gamma^{\otimes N}|\boldsymbol{\mu}[\mathcal{P}_0]\rangle$ and its parent Hamiltonian H_γ are invariant under U_g.

E. Phase diagram without symmetries

The preceding discussion show thats 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 carry out this classification for the scenario where no symmetries are imposed. We 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 $|\boldsymbol{\mu}[\mathcal{P} = \mathbb{1}]\rangle = |\omega_D\rangle^{\otimes N}$, 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

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

and thus gapped. [Here h^D should be understood as acting trivially on the leftmost and rightmost ancillary particle, and nontrivially 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

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

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.

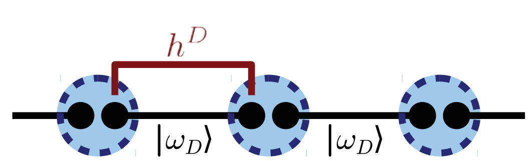

FIG. 4. (Color online) The isometric form of an injective MPS consists of maximally entangled states $|\omega_D\rangle$ with bond dimension D between adjacent sites, where each site is a D^2-level system. The local Hamiltonian terms h^D [Eq. (4)] acts only on the degrees of freedom corresponding to the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

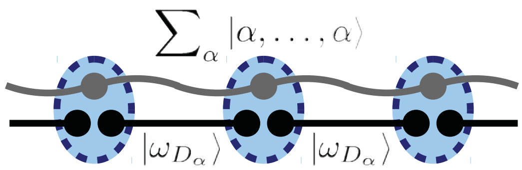

FIG. 5. (Color online) Structure of the isometric form for noninjective MPS. The state consists of a GHZ state $\sum_\alpha |\alpha,\ldots,\alpha\rangle$ (gray) and maximally entangled pairs between adjacent sites $|\omega_{D_\alpha}\rangle$, where the bond dimension D_α can couple to the value α of the GHZ state.

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 is Sec. IV.

2. *Degenerate ground states*

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

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

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 Eq. (1). This describes a state

$$\sum_\alpha |\alpha,\ldots,\alpha\rangle \otimes |\omega_{D_\alpha}\rangle^{\otimes N} \tag{7}$$

(cf. Fig. 5), that is, a GHZ state with additional local entanglement between adjacent sites, where the amount of local entanglement D_α can depend on the value α of the GHZ state. (Since the D_α can be different, the correct interpretation of Eq. (7) is $|\omega_{D_1}\rangle^{\otimes N} \oplus \cdots \oplus |\omega_{D_\mathcal{A}}\rangle^{\otimes N}$, with the $|\alpha\rangle$ labeling 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 understood by the fact that the GHZ state breaks the local symmetry; that is, 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 representant 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. In the following we first discuss the case of injective MPS, that is, systems with unique ground states. Note that we 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

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

where Y is right-invertible (i.e., there exists Y^{-1} such that $YY^{-1} = \mathbb{1}_D$, 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 $|\boldsymbol{\mu}[\mathcal{P}]\rangle$ and parent Hamiltonian, there is a standard form for $\mathcal{P}$ and a phase gauge for U_g such that

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

where the bar denotes the complex conjugate.[19] Here the V_g form a projective unitary representation of group G, that is, $V_gV_h = e^{i\omega(g,h)}V_{gh}$ (cf. Appendix B for details). As V_g appears together with its complex conjugate in Eq. (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

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

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

In the following, we show that in the presence of symmetries, the different phases are exactly labeled 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 Eq. (9) can be connected by a gapped path. We 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

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

that 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

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

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

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

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 γ. This path can be understood as a path with symmetry

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

(cf. Ref. 11), with

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

(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 prove this again in the framework of MPS; that is, we 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_γ, $\mathcal{P}_\gamma$ 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, that is, 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 γ along the path and show the continuity in an environment $\gamma + d\gamma$.

Fix some γ, with corresponding ground state $|\boldsymbol{\mu}[\mathcal{P}_\gamma]\rangle$ of H_γ, where $\mathcal{P}_\gamma$ is, without loss of generality, 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

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

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

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

where Δ is the spectral gap of H_γ. Since $\lambda = \||\boldsymbol{\mu}[\mathcal{P}_\gamma]\rangle - |\boldsymbol{\mu}[\mathcal{P}_{\gamma+d\gamma}]\rangle|$ and $dH \to 0$ as $d\gamma \to 0$, this shows that $|\boldsymbol{\mu}[\mathcal{P}_\gamma]\rangle$ is continuous in γ, and since $|\boldsymbol{\mu}[\mathcal{P}_\gamma]\rangle$ is a polynomial in $\mathcal{P}_\gamma$, it follows that $\mathcal{P}_\gamma$ can be chosen to be a continuous function of γ 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, that is, 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[19]

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

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 $Z_g \leftrightarrow YZ_gY^{-1}$, which does not affect the cohomology class. Let us first assume that $Z_g \equiv Z_g(\lambda)$ is differentiable, and let

$$Z_g = U_g + U_g'\,d\gamma, \tag{13}$$

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

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

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

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

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

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

with $\phi_g = \mathrm{Tr}[U_g^{-1}U_g']$: This proves that differentiable changes of Z_g can never change the cohomology class of ω.

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

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

This $\omega_{\lambda,\epsilon}(g,h)$ (and in particular its real part) varies again according to (14) for any ϵ 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_γ 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 now turn our attention to systems with symmetry breaking, that is, degenerate ground states, corresponding to noninjective MPS. Recall that in that case, the MPS projector $\mathcal{P}$ is supported on a "block-diagonal" space,

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

Before starting, let us note that different from the injective case, symmetry-broken systems can be invariant under nontrivial 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 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 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 noninjective MPS $|\boldsymbol{\mu}[\mathcal{P}]\rangle$ 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

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

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

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

In the following, we describe the structure of the symmetry for one irreducible subset a; in fact, degeneracies corresponding to different subsets 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 a, the symmetry

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

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

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

where π_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^a of the subgroup H. Then the action of V_h^a can be boosted to the full group G in Eq. (18) by picking representatives k_β of the disjoint cosets $k_\beta H$, and labeling them such that $\pi_{k_\beta}(\alpha_0) = \beta$. Then, for every g and α, there exist unique h and β such that

$$g k_\alpha = k_\beta h, \qquad (19)$$

and this is how $h \equiv h(g,\alpha)$ in (18) is determined. Note that the action of the permutation is to map α to β, so that (19) carries the full information of how to boost the representation V_h^a 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 α correspond to different symmetry-broken ground states. The splitting into different irreducible blocks 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 $\alpha \in a$—and subsymmetries which are not broken by the ground states—corresponding to the symmetry action $V_h^a \otimes \bar{V}_h^a$ defined on subspaces H, where the symmetry acts as in the injective case.

2. Structure of symmetry-broken phases

In the following, we prove that two Hamiltonians with symmetry breaking are in the same phase if and only if (i) the permutation representations P_g are the same (up to relabeling of blocks) and (ii) for each irreducible subset 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 cannot 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

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

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

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

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 make use of a continuity argument. The argument goes in two parts: On 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 $|\psi_\gamma^\alpha\rangle := |\boldsymbol{\mu}[\mathcal{P}_\gamma^\alpha]\rangle$ be the (orthogonal) symmetry-broken ground states of H_γ, 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_γ to show that the ground-state subspaces of H_γ and $H_{\gamma+d\gamma} = H_\gamma + dH$ are close to each other; that is, there exist ground states $|\chi_{\gamma+d\gamma}^\alpha\rangle$ of $H_{\gamma+d\gamma}$ such that

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

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, $|\chi_{\gamma+d\gamma}^\alpha\rangle = |\boldsymbol{\mu}[\mathcal{Q}_{\gamma+d\gamma}^\alpha]\rangle$. Using continuity of the roots of polynomials, we infer that we can choose $|\mathcal{Q}_{\gamma+d\gamma}^\alpha - \mathcal{P}_\gamma^\alpha| \leqslant O^*(dH)$. On the other hand, this implies that the $\mathcal{Q}_{\gamma+d\gamma}^\alpha$ are almost supported on $\mathcal{H}_\alpha$, and thus $|\mathcal{Q}_{\gamma+d\gamma}^\alpha - \mathcal{P}_{\gamma+d\gamma}^\alpha| \leqslant O^*(dH)$. Together, this shows that

$$\left|\mathcal{P}_\gamma^\alpha - \mathcal{P}_{\gamma+d\gamma}^\alpha\right| \leqslant O^*(dH);$$

that is, 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 γ; that is, it cannot be changed along a gapped path H_γ.

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 α_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 $|\boldsymbol{\mu}[\mathcal{P}_\gamma^{\alpha_0}]\rangle$ and the correspondingly restricted parent Hamiltonian (this can be done by adding local projectors restricting the system to the subspace given by α_0). Since U_g, $g \in H$, leaves $|\boldsymbol{\mu}[\mathcal{P}_\gamma^\alpha]\rangle$ 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 form the natural generalization of MPS to two dimensions[2]: For $\mathcal{P} : (\mathbb{C}^D)^{\otimes 4} \to \mathbb{C}^d$, the PEPS $|\boldsymbol{\mu}[\mathcal{P}]\rangle$ 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 2×2 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

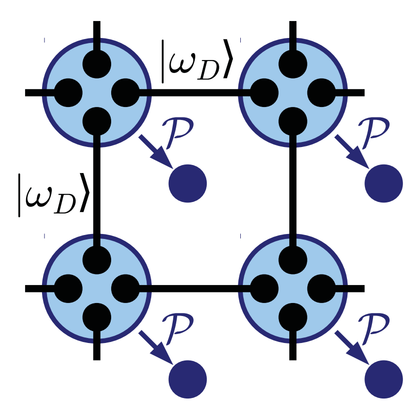

FIG. 6. (Color online) PEPS are constructed analogously to MPS by applying linear maps $\mathcal{P}$ to a 2D grid of maximally entangled states $|\omega_D\rangle$.

of γ-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 $|\boldsymbol{\mu}[\mathcal{P}]\rangle$ is the unique ground state of its parent Hamiltonian.[8]

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

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

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

(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 thus exhibit some form of topological order[20]; 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.[12] 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 $0 < \gamma_{\mathrm{crit}} < 1$ of the isometric form exist. For instance, the coherent state corresponding to the classical Ising model[21] on a hexagonal lattice at the critical temperature has critical correlations and is thus gapless,[22] 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 nonlocal change in the PEPS $|\boldsymbol{\mu}[P]\rangle$.

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 $\tilde{H} = \sum \tilde{h}_i$, $\tilde{h}_i \geqslant \mathbb{1}$ with ground-state energy $\lambda_{\min}(\tilde{H}) = 0$, where the condition

$$\tilde{h}_i\tilde{h}_j + \tilde{h}_j\tilde{h}_i \geqslant -\tfrac{1}{8}(1-\Delta)(\tilde{h}_i + \tilde{h}_j) \tag{21}$$

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

$$\tilde{H}^2 = \sum_i \underbrace{\tilde{h}_i^2}_{\geqslant h_i} + \sum_{\langle ij\rangle} \tilde{h}_i\tilde{h}_j + \sum{}' \underbrace{\tilde{h}_i\tilde{h}_j}_{\geqslant 0} \geqslant \Delta\tilde{H} \tag{22}$$

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

As we show in detail in Appendix E, condition (21) is robust with respect to γ-deformations of the Hamiltonian. In particular, for any PEPS $|\boldsymbol{\mu}[\mathcal{P}]\rangle$ with commuting parent Hamiltonian (such as the three cases presented above), it still holds for the parent of $Q^{\otimes N}|\boldsymbol{\mu}[\mathcal{P}]\rangle$ 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 nontrivial 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; together with the results of the previous section, this provides 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 $\mathcal{P} = \mathbb{1}$; that is, it consists of maximally entangled pairs between adjacent sites. This entanglement can again be removed along a commuting path h^θ [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_α 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 with $V_g \otimes \mathbb{1}$ (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_α can couple to the irreps $R^\alpha(g)$ of V_g and W_g; that is, we can change the multiplicity D_α 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_α can be done within the set of commuting Hamiltonians by observing that the Hamiltonian consists of two commuting parts:[20] 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 makes it possible to change multiplicities. The underlying idea can be understood most easily by considering a two-qubit toy model consisting of the two commuting terms,

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

where $\Lambda_\theta = \left(\begin{smallmatrix} \theta & 0 \\ 0 & 1 \end{smallmatrix}\right)$: 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 makes it possible 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 quasiadiabatic continuation[9,23] to show that their excitations need to have the same braiding statistics; that 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. For example, 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 $\mathcal{P} \to \mathcal{P} \otimes \mathbb{1}$. 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 show in the following. In particular, we 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 1D 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 be shown[25] that any two maps $\mathcal{P}$ and $\mathcal{P}'$ which describe the same PEPS are related via a gauge transformation

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

with $Y^* = (Y^{-1})^T$. This implies that any unitary invariance of $|\boldsymbol{\mu}[\mathcal{P}]\rangle$ 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 1D 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. That is, by blocking a *finite* number of sites, any two PEPS $|\boldsymbol{\mu}[\mathcal{P}_0]\rangle$ and $|\boldsymbol{\mu}[\mathcal{P}_1]\rangle$ 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 nonmaximally entangled states $|\omega(\gamma)\rangle$ [Eq. (10)], now with joint symmetry

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

Note that the whole construction can be understood as the sequential application of two 1D 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, that is, GHZ-type states. It follows that for any such PEPS, a symmetry can be understood at the virtual level as

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

where again the P_g permutes the sectors, the a are minimal subsets invariant under P_g, and the V_h^a and W_h^a, 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^a and W_h^a 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, that is, 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[26] and $O(D^4)$ in the worst case.[27] In particular, this is much more favorable than what is obtained using renormalization methods,[11] 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 Affleck-Kennedy-Lieb-Tasaki (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

$$\sum_{i_1,\ldots,i_N} \mathrm{Tr}[A^{i_1}\cdots A^{i_N}]|i_1,\ldots,i_N\rangle.$$

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

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

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 noninjective 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: Equation (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 noninjective 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 δ 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.[11] 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 quasiadiabatic continuation,[9] any gapped path of Hamiltonians yields a quasilocal transformation between the ground states.[23]

2. Local dimension and ancillas

In our definition of phases, we made it possible 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 noninjective 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 2D 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 $\chi_U(g) = \mathrm{Tr}\,U_g = |\mathrm{Tr}[V_g]|^2 \geqslant 0$ (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 the 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 labeled 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: For example, for U(1) any two continuous representations $e^{in_0\vartheta}$ and $e^{in_1\vartheta}$ of $\vartheta \in \mathrm{U}(1)$ 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 labeled 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 $|0000\cdots\rangle$ and $|0101\cdots\rangle$ 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 noninjective 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 $\mathrm{SU}(2)/\mathbb{Z}_2$ [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 dth 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: For example, 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. First, 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 1D 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 $|\boldsymbol{\mu}[\mathcal{P}_0]\rangle$ and $|\boldsymbol{\mu}[\mathcal{P}_1]\rangle$ there exist k_0 and k_1 such that $|\boldsymbol{\mu}[\mathcal{P}_0]\rangle^{\otimes k_0}$ can be converted to $|\boldsymbol{\mu}[\mathcal{P}_1]\rangle^{\otimes k_1}$. This follows from the observation made in Sec. III D for 2D 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 quasilocal evolution created by a gapped path[9]). 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.[10,11,30] 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 π on the physical system reversing the ordering of the blocked sites. Thus, for an injective MPS $|\boldsymbol{\mu}[\mathcal{P}]\rangle$ 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 nontrivial element of $\mathbb{Z}_2 \equiv \{+1, -1\}$. (Note that if $\mathcal{P}$ is injective, π 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

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

that is, 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. 10,30 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 1D 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, for example, as a subsymmetry of SO(3) invariant models; we 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 π and (0,1) with a z rotation by π. There are two equivalence classes of projective representations, corresponding to the integer and half-integer representations of SO(3). In particular, the 1D spin-0 representation $\rho_e^1 = \rho_x^1 = \rho_y^1 = \rho_z^1 = 1$ belongs to the trivial class, and the 2D 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 nontrivial class. For the following examples, we 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 $|0,\ldots,0\rangle$, which can be trivially written as an MPS with bond dimension $D=1$, and

$$\mathcal{P}_{\mathrm{Triv}} = |0\rangle;$$

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

$$H_{\mathrm{Triv}} = -\sum_i |0\rangle\langle 0| + \mathrm{const.} \tag{24}$$

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

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

with $\Pi_{S=1}$ the projector onto the $S=1$ subspace and $iY=\left(\begin{smallmatrix}0&1\\-1&0\end{smallmatrix}\right)$. 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 nontrivial projective representation of SO(3). The corresponding Hamiltonian is the AKLT Hamiltonian

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

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

$$H_x=\{e,x\},\quad H_z=\{e,z\},$$
$$H_y=\{e,y\},\quad \text{and}\quad H_{\mathrm{Triv}}=\{e\}.$$

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_{Triv} also has only trivial representations, it corresponds to a fourth phase with symmetry breaking. The number of symmetry-broken ground states is $|D_2/H|$; that is, the first three cases have twofold degenerate ground states and the last case a fourfold degenerate one.

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

$$|\mathrm{GHZ}_z\rangle = |+1,\ldots,+1\rangle + |-1,\ldots,-1\rangle,$$

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

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

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

$$R_x\mathcal{P}_{\mathrm{GHZ}_z} = -\mathcal{P}_{\mathrm{GHZ}_z}\left[|0,0\rangle\langle 1,1| + |1,1\rangle\langle 0,0|\right],$$
$$R_z\mathcal{P}_{\mathrm{GHZ}_z} = -\mathcal{P}_{\mathrm{GHZ}_z}\left[|0,0\rangle\langle 0,0| + |1,1\rangle\langle 1,1|\right],$$

and correspondingly for R_y; that is, 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

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

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 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, that is, 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 $H_{\mathrm{Triv}}=\{e\}$ 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,

$$|\hat{1}\rangle = |+1\rangle|+x\rangle,\quad |\hat{2}\rangle = |+1\rangle|-x\rangle,$$
$$|\hat{3}\rangle = |-1\rangle|+x\rangle,\quad |\hat{4}\rangle = |-1\rangle|-x\rangle,$$

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

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

We have that

$$R_x|\pm x\rangle = -|\pm x\rangle,\quad R_z|\pm 1\rangle = -|\pm 1\rangle,$$
$$R_x|\pm 1\rangle = -|\mp 1\rangle,\quad R_z|\pm x\rangle = -|\mp x\rangle.$$

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

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

Thus, the GHZ-type state

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

which is an MPS with $D=4$ and

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

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

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

where the label j refers to the blocked sites.

2. *Phases under* SO(3) *and* SU(2) *symmetry*

Let us now consider symmetry under rotational invariance, imposed either as SO(3) or as SU(2) symmetry. We find that under 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 show that if we impose SU(2) symmetry, there is only a single phase, as the AKLT state can be transformed into the trivial state keeping SU(2) symmetry.

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

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

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

$$\hat{\mathcal{P}}_{\mathrm{AKLT}} = \mathbb{1}, \tag{25}$$

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

$$\hat{\mathcal{P}}_{\mathrm{Triv}} = |S = 0\rangle. \tag{26}$$

Thus, the rotation group $R_{\hat{\boldsymbol{n}}}(\theta)$ 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 SO(3), this does not imply that 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 SO(3). Since, however, 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 MPS.

Let us now turn our attention toward 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 $\hat{P}_{\mathrm{AKLT}}$ and $\hat{P}_{\mathrm{Triv}}$, the symmetry action on the virtual level is a linear representation of 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 from (26) of the trivial state. Furthermore, for $U \in$ SU(2), the whole path is invariant under the on-site symmetry

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

which contains the symmetries 1 and $U \otimes \bar{U}$ of the trivial and the AKLT state as subsymmetries; this proves that under 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 SU(2), but not of SO(3), as integer and half-integer spin representations belong to inequivalent classes of projective representations of SO(3); also, we cannot obtain this symmetry by starting only from the spin-0 and spin-1 representation of 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, for example, associating them to fermions.

V. CONCLUSION AND OUTLOOK

In this paper, we have classified the possible phases of 1D, and to a certain extent 2D, systems in the framework of MPS 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 labeled by equivalence classes of projective representations, that 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 labeled by the permutation action (that 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 2D 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 do not affect the classification at all, to scenarios where the classification is more fine-grained and, for example, the 1D 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 labeled by 1D representations of the symmetry group (that 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 cannot 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.[32,33]

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 1D 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, that is, without actually having to block and renormalize the system; it thus provides a rigorous justification for the application of RG flows toward the classification of quantum phases. Let us add that the possibility to define an isometric form, as well as the possibility to interpolate toward 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 1D quantum systems:[11,30,34] In particular, in Ref. 30, MPS have been used to demonstrate the symmetry protection of the AKLT phase, and in Ref. 11, renormalization transformations[17] and their fixed points on MPS have been applied to the classification of quantum phases for 1D 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 toward the classification of phases for 2D systems.[14,35]

ACKNOWLEDGMENTS

We acknowledge helpful discussions with Salman Beigi, Oliver Buerschaper, Steve Flammia, Stephen Jordan, Alexei Kitaev, Robert König, Spiros Michalakis, John Preskill, Volkher Scholz, Frank Verstraete, and Michael Wolf. This work has been supported by the Gordon and Betty Moore Foundation through Caltech's Center for the Physics of Information, NSF Grant No. PHY-0803371, ARO Grant No. W911NF-09-1-0442, Spanish Grants No. I-MATH, No. MTM2008-01366, and No. S2009/ESP-1594, the European project QUEVADIS, and the DFG (Forschergruppe 635).

APPENDIX A: GAP PROOF FOR THE 1D PATH

In the following, we show that the family of γ-deformed parent Hamiltonians which arise from the MPS path $|\boldsymbol{\mu}[\mathcal{P}_\gamma]\rangle$ 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_γ is uniformly gapped; that is, there is a $\Delta > 0$ which lower bounds the gap of H_γ uniformly in γ and the systems size N: This establishes that the $|\boldsymbol{\mu}[\mathcal{P}_\gamma]\rangle$, and the corresponding H_γ, are all in the same phase. To this end, we use a result of Nachtergaele[6] (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 use the results of Ref. 6 to derive a uniform lower bound on the gap for all H_γ, $1 \geqslant \gamma \geqslant 0$. 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 $|\mathrm{spec}\,\mathbb{E}^\alpha(\gamma)| = \{\lambda_1^\alpha(\gamma) > \lambda_2^\alpha(\gamma) > \cdots \geqslant 0\}$ 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 λ_1 is $\mathcal{A}$,[6] the existence of a uniform upper bound $1 > \tau_\alpha > \lambda_2^\alpha(\gamma)/\lambda_1^\alpha(\gamma)$ follows. For $\alpha \neq \beta$, let

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

where $|\Phi[C;X]\rangle := \sum_{i_1,\dots,i_p}\mathrm{Tr}[C_{i_1},\dots,C_{i_p}X]|i_1,\dots,i_p\rangle$; that is, $\Omega^p_{\alpha,\beta}(\gamma)$ 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 $\mathcal{S}_\alpha(\gamma) := \{\sum_i \mathrm{Tr}[A_i^\alpha(\gamma)X]|i\rangle|X\}$, and $\mathcal{O}(\mathcal{X},\mathcal{Y})$ the maximal overlap between normalized vectors in the subspaces $\mathcal{X}$ and $\mathcal{Y}$, we have that $\Omega^p_{\alpha,\beta}(\gamma) \leqslant \mathcal{O}(\mathcal{S}_\alpha(\gamma)^{\otimes p},\mathcal{S}_\beta(\gamma)^{\otimes p}) \leqslant \mathcal{O}(\mathcal{S}_\alpha(\gamma),\mathcal{S}_\beta(\gamma))^p$. 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

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

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

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

and we find that $\Omega^p_{\alpha,\beta}(\gamma) \leqslant \kappa^p$. Thus, there exists a p such that

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

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

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

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

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 ϕ_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 ϕ_g is in the same cohomology class as a linear representation, but in order to compare two systems, we need the same gauge for ϕ_g^0 and ϕ_g^1, so we choose them to be linear representations.)

Under blocking, the physical symmetry U_g in Eq. (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 Eq. (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 with $e^{i\phi_g}U_g$, which will make the phase in Eq. (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 nonzero matrix element $(i,i) \times (j,j)$]. Finally, if U_g^0 and U_g^1 only share a subblock, this means that $V_g^0 = X_g^0 \oplus Y_g^0$ such that $X_g^0 \otimes \bar{X}_g^0$ yields that subblock, and similary 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 again show this for differentiable $\mathcal{P}_\gamma$; it extends to continuous $\mathcal{P}_\gamma$ 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"

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

(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

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

that is, 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 γ, 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 NONINJECTIVE MPS UNDER SYMMETRIES

In the following, we show that for any noninjective MPS $|\boldsymbol{\mu}[\mathcal{P}]\rangle$ 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 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

$$\hat{U}_g := \mathcal{P}^{-1}\, U_g\, \mathcal{P} = P_g\Big[\bigoplus_\alpha e^{i\phi_g^\alpha} V_g^\alpha \otimes \bar{V}_g^\alpha\Big] \tag{D1}$$

of the symmetry operation on the virtual system, using the correct gauge for $\mathcal{P}$. Here V_g^α is unitary, the direct sum runs over the Hilbert spaces $\mathcal{H}_\alpha$ in Eq. (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 do not interfere on any open boundary conditions (OBC) interval. Thus, U_g can, on 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 nontrivially 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 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

$$\hat{U}_g \hat{U}_h = \hat{U}_{gh} \tag{D2}$$

($g,h \in G$) implies for the algebraic structure of P_g, V_g^α, 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

$$W_g^\alpha := e^{i\phi_g^\alpha} V_g^\alpha \otimes \bar{V}_g^\alpha. \tag{D3}$$

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

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

for the W_g^α, where the permutations π_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.[37] Fix some α_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 $k_\beta H$ labeled by the blocks $\beta = 1,\dots,\mathcal{A}$, for a (nonunique) 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

$$W_g^\beta \overset{(D4)}{=} W_{gk_\beta}^{\pi_{k_\beta^{-1}}(\beta)} W_{k_\beta^{-1}}^\beta = W_{gk_\beta}^{\alpha_0} W_{k_\beta^{-1}}^\beta, \tag{D5}$$

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 β uniquely determine γ and $h \in H$ by virtue of

$$g k_\beta = k_\gamma h \tag{D6}$$

and thus, continuing (D5),

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

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

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

Substituting this above, we finally obtain that

$$W_g^\beta = W_{k_\gamma}^{\alpha_0}\, W_h^{\alpha_0}\, \big(W_{k_\beta}^{\alpha_0}\big)^{-1}; \tag{D7}$$

that is, W_g^β 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_β.

We now define a rotation

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

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

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

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 $e^{i\phi_h^{\alpha_0}}$ forms a linear representation of H.

Thus, we can write

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

with

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

and

$$D_g = \bigoplus_\beta e^{i\phi_h^{\alpha_0}}, \tag{D9}$$

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 noninjective 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

$$\tilde{h}_i\tilde{h}_j + \tilde{h}_i\tilde{h}_j \geqslant -\tfrac{1}{8}(1-\Delta_{ij})(\tilde{h}_i + \tilde{h}_j); \tag{E1}$$

where we consider a square lattice with $\tilde{h}_i \geqslant \mathbb{1}$ acting on 2×2 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 Sec. III B, we have given the simplified version where $\Delta_a = \Delta_d = \Delta$.) Then,

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

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 Δ on the gap of $\tilde{H}$ (cf. Ref. 1).

Let us now study the robustness of (E1) under γ deformation of the Hamiltonian. Let h_i, h_j be projectors which satisfy $h_ih_j + h_jh_i \geqslant -\frac{1}{8}(1-\Delta_{ij})(h_i + h_j)$. (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 $Q_\gamma = (1-\gamma)\mathbb{1} + \gamma Q \leqslant \mathbb{1}$ as in the 1D case, let $\Lambda_{\gamma,X} = (Q_\gamma^{-1})^{\otimes x}$, with $X = A,B,C$ and $x = a,b,c$. Then the γ-deformed Hamiltonians are

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

Let us define

$$\Theta_\gamma := \Lambda_{\gamma,B}^2 - \mathbb{1} \geqslant 0,$$
$$q := \lambda_{\min}(Q) < 1,$$
$$\mu_\gamma := [(1-\gamma) + \gamma\lambda_{\min}(Q)]^{-2} \geqslant 1,$$

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

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

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 γ-deformed Hamiltonian,

$$h_i(\gamma)h_j(\gamma) + h_j(\gamma)h_i(\gamma) \geqslant -\tfrac{1}{8}[1-\Delta_{ij}(\gamma)][h_i(\gamma) + h_j(\gamma)], \tag{E2}$$

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

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

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

[1] M. Fannes, B. Nachtergaele, and R. F. Werner, Commun. Math. Phys. **144**, 443 (1992).

[2] F. Verstraete and J. I. Cirac, e-print arXiv:cond-mat/0407066 (to be published).

[3] F. Verstraete and J. I. Cirac, Phys. Rev. B **73**, 094423 (2006).

[4] M. Hastings, J. Stat. Mech. (2007) P08024.

[5] M. B. Hastings, Phys. Rev. B **76**, 035114 (2007).

[6] B. Nachtergaele, Commun. Math. Phys. **175**, 565 (1996).

[7] D. Pérez-García, F. Verstraete, M. M. Wolf, and J. I. Cirac, Quantum Inf. Comput. **7**, 401 (2007).

[8] D. Pérez-García, F. Verstraete, J. I. Cirac, and M. M. Wolf, Quantum Inf. Comput. **8**, 0650 (2008).

[9] M. B. Hastings and X. G. Wen, Phys. Rev. B **72**, 045141 (2005).

[10] F. Pollmann, A. M. Turner, E. Berg, and M. Oshikawa, Phys. Rev. B **81**, 064439 (2010).

[11] X. Chen, Z. C. Gu, and X. G. Wen, Phys. Rev. B **83**, 035107 (2011).

[12] A. Kitaev, Ann. Phys. **303**, 2 (2003), e-print arXiv:quant-ph/9707021.

[13] F. Verstraete, D. Porras, and J. I. Cirac, Phys. Rev. Lett. **93**, 227205 (2004).

[14] X. Chen, Z. Gu, and X. Wen, Phys. Rev. B **82**, 155138 (2010).

[15]S. Michalakis and J. Pytel, e-print arXiv:1109.1588 (to be published).
[16]S. Bravyi and M. B. Hastings, e-print arXiv:1001.4363 (to be published).
[17]F. Verstraete, J. I. Cirac, J. I. Latorre, E. Rico, and M. M. Wolf, Phys. Rev. Lett. **94**, 140601 (2005).
[18]C. H. Bennett, S. Popescu, D. Rohrlich, J. A. Smolin, and A. V. Thapliyal, Phys. Rev. A **63**, 012307 (2000).
[19]D. Pérez-García, M. M. Wolf, M. Sanz, F. Verstraete, and J. I. Cirac, Phys. Rev. Lett. **100**, 167202 (2008).
[20]N. Schuch, I. Cirac, and D. Pérez-García, Ann. Phys. **325**, 2153 (2010).
[21]F. Verstraete, M. M. Wolf, D. Pérez-García, and J. I. Cirac, Phys. Rev. Lett. **96**, 220601 (2006).
[22]M. B. Hastings and T. Koma, Commun. Math. Phys. **265**, 781 (2006).
[23]S. Bachmann, S. Michalakis, B. Nachtergaele, and R. Sims, e-print arXiv:1102.0842 (to be published).
[24]O. Buerschaper and M. Aguado, Phys. Rev. B **80**, 155136 (2009).
[25]D. Pérez-García, M. Sanz, C. E. Gonzalez-Guillen, M. M. Wolf, and J. I. Cirac, New J. Phys. **12**, 025010 (2010).
[26]D. Pérez-García, M. Sanz, A. Cadarso, M. Wolf, and J. Cirac (unpublished).
[27]M. Sanz, D. Pérez-García, M. M. Wolf, and J. I. Cirac, IEEE Trans. Inf. Theory **56**, 4668 (2010).
[28]W. Fulton and J. Harris, *Representation Theory: A First Course* (Springer, Berlin, 1991).
[29][http://mathoverflow.net/questions/58633].
[30]F. Pollmann, E. Berg, A. M. Turner, and M. Oshikawa, e-print arXiv:0909.4059 (to be published).
[31]A. Affleck, T. Kennedy, E. H. Lieb, and H. Tasaki, Commun. Math. Phys. **115**, 477 (1988).
[32]R. Dijkgraaf and E. Witten, Commun. Math. Phys. **129**, 393 (1990).
[33]A. Kitaev (private communication).
[34]L. Fidkowski and A. Kitaev, Phys. Rev. B **83**, 075103 (2011).
[35]Z. Gu, Z. Wang, and X. Wen, e-print arXiv:1010.1517 (to be published).
[36]M. Sanz, M. M. Wolf, D. Perez-Garcia, and J. I. Cirac, Phys. Rev. A **79**, 042308 (2009).
[37]S. Beigi (private communication).