Classifying quantum phases using MPS and PEPS

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We apply the framework of Matrix Product States (MPS) and Projected Entangled Pair States (PEPS) and their associated parent Hamiltonians to the classification of quantum phases in one and higher dimensions, where we define two systems to be in the same phase if they can be connected via a path of gapped Hamiltonians. In one dimension, we prove that any two Hamiltonians with MPS ground states are in the same phase if and only if they have the same ground state degeneracy. Subsequently, we extend our framework to the classification of two-dimensional quantum phases in the neighborhood of a number of important cases, such as systems with unique ground states, local symmetry breaking, and topological order. As a central tool in our derivation, we introduce the *isometric form* of MPS and PEPS. Isometric forms are renormalization fixed points both for MPS and for relevant classes of PEPS, and are connected to the original MPS via a gapped path in Hamiltonian space. Our construction thus yields a way to implement renormalization flows locally, this is, without actual renormalization.

I. INTRODUCTION

When are two quantum mechanical systems in the same quantum phase? The answer to this question depends on how being in the same phase is defined. One approach is to characterize phases by the structure of their ground states, measured by an order parameter such as the magnetization: Two systems are said to be in the same phase if certain order parameters behave the same way. However, this definition depends on the class of order parameters considered, and for instance topological phases are not covered by Landau theory which characterizes phases by local order parameters, and require the use of non-local string order operators.

Alternatively, instead of comparing ground states by looking at order parameters, one can classify quantum phases by asking whether it is possible to interpolate between two systems in a smooth way, i.e., without crossing a phase transition, along a continous path in the space of Hamiltonians. Again, the classification of phases depends on the definition of "smooth": For instance, one can require smoothness only for local observables, for a specific set of non-local observables, or even for the ground state itself. An even stronger criterion is obtained by requiring that along the whole path, the Hamiltonian of the system has to remain gapped, as this implies that any observable changes smoothly as well[1] (see Ref. 2 for the converse). Interestingly, this "dynamic" classification can give very different results from the "static" one obtained by comparing the initial and final state only: In particular, it is possible to interpolate between system which exhibit different types of order without crossing a phase transition by choosing an appropriate path.[3] (Note however that such paths can be ruled out by imposing symmetry constraints.[4,5])

In this paper, we apply the framework of Matrix Product States (MPS)[6] and Projected Entangled Pair States (PEPS)[7] to the classification of quantum phases of lattice system in one an higher dimensions. MPS and PEPS form a hierachy of states which allows to efficiently approximate ground states of gapped quantum lattice systems in one and higher dimensions,[8–10] and are thus well suited to characterize phases of quantum systems. Equally importantly for our aims, MPS and PEPS naturally appear as ground states of associated "parent Hamiltonians",[6,11–13] which will allow us to construct gapped paths in the space of Hamiltonians based on paths in the space of MPS and PEPS.

More precisely, in this work we consider gapped Hamiltonians which have exact MPS and PEPS ground states, and study when two such Hamiltonians are in the same phase; here, we define two Hamiltonians to be in the same phase if and only if there exists a continuous path of local and gapped Hamiltonians which connects the two systems. In one dimension, we prove that all Hamiltonians are in the same phase as long as they have the same ground state degeneracy; canonical representants of those phases are product and GHZ states and their Hamiltonians, respectively. For two-dimensional systems, where proving gaps is considerably more involved than in one dimension, we give conditions under which in some environment of a given system, all PEPS and their associated Hamiltonians can be proven to be in the same phase; systems satisfying this condition include product states, GHZ states, and states with topological order.

In order to simplify the construction of gapped paths between different Hamiltonians, we will introduce a 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. We show how to transform an MPS/PEPS parent Hamiltonian into its isometric form along a gapped path; this can be understood as a renormalization transformation without blocking sites, i.e., without actual renormalization. This reduces the problem of classifying quantum phases to the problem of classifying quantum phases for isometric MPS/PEPS and their parent Hamiltonians, which is considerably easier to carry out due to its additional structure.

II. ONE DIMENSION

A. Matrix Product States

A (translational invariant) Matrix Product State (MPS) $|\boldsymbol{\mu}[\mathcal{P}]\rangle$ of *bond dimension* D on a spin chain $(\mathbb{C}^d)^{\otimes N}$ 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;[14] this is, $|\boldsymbol{\mu}[\mathcal{P}]\rangle = \mathcal{P}^{\otimes N} |\omega_D\rangle^{\otimes N}$. The definition of MPS is robust under blocking k sites, by letting $\mathcal{P}' = \mathcal{P}^{\otimes k} |\omega_D\rangle^{\otimes(k-1)}$. Blocking allows to bring any MPS into its *standard form*[12] where $\mathcal{P}$ is either injective (the *injective case*), or supported on a "block-diagonal" space, $(\ker \mathcal{P})^\perp = \mathcal{H}_1 \oplus \cdots \oplus H_\mathcal{A}$, with $\mathcal{H}_\alpha = \mathrm{span}\{|i,j\rangle : \zeta_{\alpha-1} < i,j \leq \zeta_\alpha\}$. Here, $0 = \zeta_0 < \zeta_1 < \cdots < \zeta_\mathcal{A} = D$ is a partitioning of $0,\dots,D$; we define $D_i := \zeta_i - \zeta_{i-1}$, $\dim \mathcal{H}_\alpha = D_i^2$. In the following, we will w.l.o.g. assume all MPS to be in their standard form, and moreover impose that $\mathcal{P}$ is surjective (i.e. restrict to the relevant subspace of $\mathbb{C}^d$). Note that in order to have the standard form, we need to block at least until $d \geq \sum D_i^2$.

For any MPS one can construct local *parent Hamiltonians* which have this MPS as their ground state: A parent Hamiltonian $H = \sum h_k$ consists of local terms $h_k \geq 0$ acting on two adjacent sites $(k, k+1)$ whose kernels exactly support the two-site reduced density operator of the corresponding MPS, i.e., $\ker h_k = (\mathcal{P}\otimes\mathcal{P})(\mathbb{C}^D \otimes |\omega_D\rangle \otimes \mathbb{C}^D)$. By construction, $H \geq 0$ and $H|\boldsymbol{\mu}[\mathcal{P}]\rangle = 0$, i.e., $|\boldsymbol{\mu}[\mathcal{P}]\rangle$ 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 $|\boldsymbol{\mu}[\mathcal{P}|_{H_\alpha}]\rangle$.[6,11,12] This associates a class of parent Hamiltonians to every MPS, and by choosing the h_k to be projectors, the mapping between MPS and Hamiltonians becomes one-to-one. Thus, from now on we will talk of MPS and their parent Hamiltonians synonymously whenever appropriate.

B. Construction of a gapped path

Let us now delineate how we are going to tackle the classification of quantum phases for MPS. We will consider a pair of gapped local Hamiltonians $\tilde{H}_1$ and $\tilde{H}_2$ having MPS ground states $|\psi_1\rangle = |\boldsymbol{\mu}[\mathcal{P}_1]\rangle$ and $|\psi_2\rangle = |\boldsymbol{\mu}[\mathcal{P}_2]\rangle$, respectively. While the Hamiltonians $\tilde{H}_i$ need not be the parent Hamiltonians of their associated MPS $|\boldsymbol{\mu}[\mathcal{P}_i]\rangle$ (e.g., they might not be frustration free), we require that their ground state subspace equals the ground state subspace of the associated parent Hamiltonian H_i: The fact that both $\tilde{H}_i$ and H_i are local, gapped, and have the identical ground state subspace implies that we can interpolate between the initial Hamiltonians and the parent Hamiltonians of the MPS along a path $\lambda\tilde{H}_i + (1-\lambda)H_i$ of gapped and local Hamiltonians. Thus, we can restrict our attention to MPS and their associated parent Hamiltonians, and we will do so from now on.

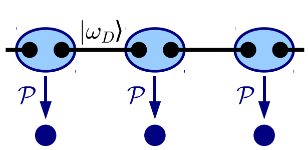

FIG. 1. MPS are constructed by applying a linear map $\mathcal{P}$ to maximally entangled pairs $|\omega_D\rangle := \sum_{i=1}^{D} |i,i\rangle$ of *bond dimension* D.

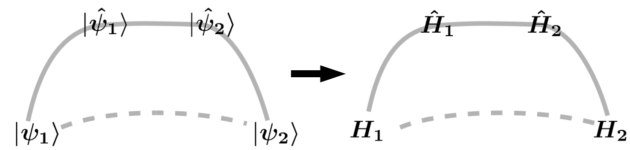

FIG. 2. Construction of the interpolating path for MPS and parent Hamiltonians. Instead of interpolating between the MPS $|\psi_1\rangle$ and $|\psi_2\rangle$ directly (dotted line), we first show how to interpolate each of the two states towards a standard from $|\hat{\psi}_i\rangle$, the *isometric 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.

The scenario we are therefore going to consider is the following: We are given two MPS $|\boldsymbol{\mu}[\mathcal{P}_i]\rangle$, $i = 1,2$ in their standard form, together with their nearest-neighbor parent Hamiltonians H_i, and we want to construct a gapped path interpolating between H_1 and H_2. We will do so by constructing a path $|\boldsymbol{\mu}[\mathcal{P}(\lambda)]\rangle$ connecting the corresponding MPS $|\boldsymbol{\mu}[\mathcal{P}_1]\rangle$ and $|\boldsymbol{\mu}[\mathcal{P}_2]\rangle$ by appropriately interpolating between $\mathcal{P}_1$ and $\mathcal{P}_2$ along $\mathcal{P}(\lambda)$. In order to facilitate this interpolation, we will split it in two parts: First, we introduce a normal form, the *isometric form*, for each of the two MPS, and show how to interpolate to the isometric form along a gapped path; and second, we show under which conditions one can interpolate in between two isometric form along a gapped path. The whole interpolation proceduce, including the intermediate isometric forms, is illustrated in Fig. 2.

C. The isometric form

In the following, we will introduce a new normal form for MPS, the *isometric form*, which captures the essential entanglement and long-range properties of the state, and which is a fixed point of a renormalization procedure:[15] Every MPS can be brought into its normal form by stochastic local operations,[16] and as we will show, there exists a gapped path in the space of parent Hamiltonians which interpolates between any MPS and its isometric form.

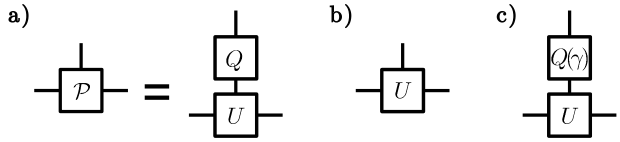

FIG. 3. Isometric form of an MPS. **a)** The MPS projector $\mathcal{P}$ can be decomposed into a positive map Q and an isometric map U. **b)** By removing Q, one obtains the isometric form U of the MPS. **c)** Interpolation to the isometric form is possible by letting $Q(\gamma) = \gamma Q + (1-\gamma)\mathbb{1}$.

For any MPS $|\boldsymbol{\mu}[\mathcal{P}]\rangle$, we can decompose $\mathcal{P} = QU$, with U an isometry $UU^\dagger = \mathbb{1}$ and $Q > 0$, by virtue of a polar decomposition of $\mathcal{P}|_{(\ker\mathcal{P})^\perp}$; w.l.o.g., we can assume $0 < Q \leq \mathbb{1}$ by rescaling $\mathcal{P}$. Now define

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

and consider the family of MPS $|\boldsymbol{\mu}[\mathcal{P}(\gamma)]\rangle$ described by $\mathcal{P}(\gamma) := Q(\gamma)U$. In particular, $\mathcal{P}(0) = U$ is an isometric map, giving rise to the *isometric form* $|\boldsymbol{\mu}[\mathcal{P}(0)]\rangle$ of the MPS $|\boldsymbol{\mu}[\mathcal{P}]\rangle = |\boldsymbol{\mu}[\mathcal{P}(1)]\rangle$, together with an interpolating path $|\boldsymbol{\mu}[\mathcal{P}(\gamma)]\rangle$; note that $|\boldsymbol{\mu}[\mathcal{P}(\gamma)]\rangle = Q(\gamma)^{\otimes N}|\boldsymbol{\mu}[\mathcal{P}(0)]\rangle$, cf. Fig. 3. Throughout the path, the MPS retains its standard form with the blocking pattern unchanged, which is encoded in the structure of $\ker\mathcal{P}$.

Let us now construct a continuous family of parent Hamiltonians for the MPS path $|\boldsymbol{\mu}[\mathcal{P}(\gamma)]\rangle$. To this end, start from the isometric case $|\boldsymbol{\mu}[\mathcal{P}(0)]\rangle$, and a corresponding parent Hamiltian $H = \sum h_k$ with the h_k projectors. Let $\Lambda_\gamma = \left(Q(\gamma)^{-1}\right)^{\otimes 2}$, and define the γ-*deformed Hamiltonian* $H(\gamma) := \sum h_k(\gamma)$ by virtue of $h_k(\gamma) := \Lambda_\gamma h_k \Lambda_\gamma \geq 0$. Since $h_k|\boldsymbol{\mu}[\mathcal{P}(0)]\rangle = 0$, it follows that $h_k(\gamma)|\boldsymbol{\mu}[\mathcal{P}(\gamma)]\rangle = 0$ (and in fact, the kernel of h_k is always equal to the support of the two-site reduced state), i.e., $H(\gamma) = \sum h_i(\gamma)$ is a parent Hamiltonian for $|\boldsymbol{\mu}[\mathcal{P}(\gamma)]\rangle$. Note that the family $H(\gamma)$ of Hamiltonians is continuous in γ by construction.

It remains to show that the path $H(\gamma)$ is uniformly gapped, i.e., there is a $\Delta > 0$ which lower bounds the gap of $H(\gamma)$ uniformly in 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[11] (extending the results of Ref. 6 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 $H(\gamma)$ 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 non-injective case, one additionally needs that the overlap of different ground states goes to zero as $\gamma \to 0$.

D. Classification of isometric MPS

As we have seen, every MPS has a corresponding isometric form which captures its essential features, and its parent Hamiltonian can be adiabatically transformed to its isometric counterpart along a gapped path. This reduces the task of understanding the phase diagram of MPS and their parent Hamiltonians to characterizing the possible phases for isometric MPS.

Let us first consider the injective isometric case. There, $\mathcal{P}$ is unitary, and thus equivalent to $\mathcal{P}' = \mathbb{1}$ up to a local unitary transformation: Thus, an isometric injective MPS is locally equivalent to maximally entangled states $|\omega_D\rangle$ between adjacent sites as in Fig. 1. The parent Hamiltonian is a sum of commuting projectors of the form $\mathbb{1} - |\omega_D\rangle\langle\omega_D|$, and thus gapped. Moreover, for different D and D' one can interpolate between these states via a path of commuting Hamiltonian with local terms $\mathbb{1} - |\omega(\theta)\rangle\langle\omega(\theta)|$, 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.

What happens in the case of non-injective MPS? First, consider the case with block sizes $D_\alpha := \dim\mathcal{H}_\alpha = 1$, i.e., $\mathcal{P} \equiv \mathcal{P}_{\mathrm{GHZ}} = \sum_\alpha |\alpha\rangle\langle\alpha,\alpha|$: This describes an $\mathcal{A}$-fold degenerate GHZ state with commuting Hamiltonian terms $h_k = \mathbb{1} - \sum_\alpha |\alpha,\alpha\rangle\langle\alpha,\alpha|$. For $D_\alpha \neq 1$, we have that (up to local unitaries) $\mathcal{P} = \sum_\alpha |\alpha\rangle\langle\alpha,\alpha|\otimes\mathbb{1}_{D_\alpha}$. This corresponds to a state $\sum_\alpha |\alpha,\dots,\alpha\rangle \otimes |\omega_{D_\alpha}\rangle^{\otimes N}$, i.e., 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. Here, the Hamiltonian is a sum of the GHZ Hamiltonian 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), and one can again interpolate to the pure GHZ state with $D'_\alpha = 1$ analogously to the injective case.

Combining this with the construction of the preceding subsection which allows to bring any MPS into its isometric form along a gapped path, we find that any two MPS and their parent Hamiltonians can be transformed into each other along a gapped path as long as the ground state degeneracy, this is, the number $\mathcal{A}$ of blocks in $\ker\mathcal{P}$, is the same. Note that this is the strongest classification of phases of Matrix Product States we can hope for, since the ground state degeneracy cannot be changed without closing the gap, i.e., states with different $\mathcal{A}$ are necessarily in different phases.

E. Quantum phases under symmetries

Can our approach to the classification of one-dimensional phases, in particular the transformation towards the isometric point, be extended to systems with symmetry constraints on the Hamiltonian, such as fermionic systems which obey parity symmetry, or SU(2)–invariant Hamiltonians? Given an MPS $|\boldsymbol{\mu}[\mathcal{P}]\rangle$, it has been shown that it is U_g–symmetric (where U_g is a unitary representation of some group G) if and only if $\mathcal{P} = e^{i\theta_g} U_g \mathcal{P} (V_g \otimes \bar{V}_g)$, where the V_g are certain unitaries.[17] As for a polar decomposition $\mathcal{P} = QU$, it holds that $Q = \sqrt{\mathcal{P}\mathcal{P}^\dagger}$, we find that

$$\begin{aligned} Q^2 = \mathcal{P}\mathcal{P}^\dagger &= e^{i\theta_g} U_g \mathcal{P} (V_g \otimes \bar{V}_g)(V_g \otimes \bar{V}_g)^\dagger \mathcal{P}^\dagger U_g^\dagger e^{-i\theta_g} \\ &= U_g \mathcal{P}\mathcal{P}^\dagger U_g^\dagger = U_g Q^2 U_g^\dagger \ , \end{aligned}$$

this is, Q^2 is invariant under conjugation by U_g and thus block diagonal with respect to the irreducible representations of U_g. This implies the same block structure for Q, and thus, $Q = U_g Q U_g^\dagger$. Therefore, it is possible to interpolate between $\mathcal{P}(1) \equiv \mathcal{P} = QU$ and its isometric form $\mathcal{P}(0) = U$ along a path which preserves the symmetry of the projector, and thus of the MPS and its parent Hamiltonian. This proves that one-dimensional quantum phases can be classified by considering isometric renormalization fixed points only; a classification of these fixed points (based on the second cohomology group of G) can be found in Ref. 5.

III. TWO DIMENSIONS

A. Projected Entangled Pair States

Projected Entangled Pair States (PEPS) form the natural generalization of Matrix Product States to two dimensions:[7] 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. 4. 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.

As in 1D, each PEPS has an isometric form to which it can be continuously deformed, yielding a continuous path of γ-deformed Hamiltonians along which the ground state degeneracy is preserved (and for a PEPS with symmetries[18] this can again be done along a symmetry-preserving path). 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.[13] Second, the block-diagonal case, where $(\ker \mathcal{P})^\perp = \bigoplus_{\alpha=1}^{\mathcal{A}} \mathcal{H}_\alpha$, with $\mathcal{H}_\alpha = \mathrm{span}\{|i,j,k,l\rangle :$ $\zeta_{\alpha-1} < i,j,k,l \le \zeta_\alpha\}$; this corresponds again to GHZ-type states and Hamiltonians with $\mathcal{A}$-fold degenerate ground states. The third case is where the isometric form of $\mathcal{P}$ is

$$\mathcal{P} = \sum_g V_g \otimes V_g \otimes \bar{V}_g \otimes \bar{V}_g \ , \tag{1}$$

with V_g a unitary representation 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;[19] in particular, for the regular representation at the isometric points, these PEPS describe Kitaev's double model of the underlying group.[20] All these three classes have parent Hamiltonians at the isometric point which are commuting and thus gapped.

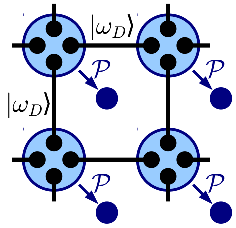

FIG. 4. PEPS are constructed analogously to MPS by applying linear maps $\mathcal{P}$ to a 2D grid of maximally entangled states $|\omega_D\rangle$.

B. Gap in two dimensions

The major difference to the case of 1D systems is that statements about the gap of the parent Hamiltonian are much more difficult to make, and examples which become gapless at some finite deformation $0 < \gamma_{\mathrm{crit}} < 1$ exist, e.g. the coherent state corresponding to the classical Ising model on an hexagonal lattice at the critical point:[21] it has critical correlations and is thus gapless,[22] while injectivity implies that its isometric form is gapped. 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 $\tilde{H} = \sum \tilde{h}_i$, $\tilde{h}_i \ge \mathbb{1}$ with ground state energy $\lambda_{\min}(\tilde{H}) = 0$, where the condition

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

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

$$\tilde{H}^2 = \sum_i \underbrace{\tilde{h}_i^2}_{\ge h_i} + \sum_{<ij>} \tilde{h}_i \tilde{h}_j + \sum{}' \underbrace{\tilde{h}_i \tilde{h}_j}_{\ge 0} \ge \Delta \tilde{H} \ , \tag{2}$$

(where the second and third sum run over overlapping and non-overlapping $\tilde{h}_i$, $\tilde{h}_j$, respectively), which implies that $\tilde{H}$ has no eigenvalues between 0 and Δ, cf. Ref. 6.

As we show in detail in Appendix B, condition (2) 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 $\lambda_{\min}(Q)/\lambda_{\max}(Q) \gtrapprox 0.967$. Thus, while considering the isometric cases does not allow us to classify all Hamiltonians as in 1D, we can still do so for a non-trivial subset in the space of Hamiltonians.

C. Classification of isometric PEPS

Let us now classify the three types of isometric PEPS introduced previously; together with the results of the previous subsection, this will provide us with a classification of quantum phases in some environment of these cases. First, the injective isometric case can again be locally rotated to the scenario where $\mathcal{P} = \mathbb{1}$, i.e., maximally entangled pairs between adjacent sites, which can again be removed along a path of commuting Hamiltonians; therefore, any PEPS/Hamiltonian which is sufficiently close to an isometric injective one is in the same phase as the product state. Correspondingly, the block-diagonal case is in complete analogy to the one-dimensional case – it is locally equivalent to the $\mathcal{A}$-fold degenerate GHZ state and Hamiltonian, as it only differs by local entanglement (which can again depend on the value of the GHZ state).

What about the topological case of Eq. (1)? Of course, additional local entanglement $|\omega_D\rangle$ can be present independently of the topological part of the state, corresponding to replacing V_g by $V_g \otimes \mathbb{1}$, and it can be manipulated and removed along a commuting path. However, it turns out that D can additionally couple to the irreps $R^\alpha(g)$ of V_g, i.e., we can change the multiplicity D_α of individual irreps $R^\alpha(g)$, $\bigoplus R^\alpha(g) \to \bigoplus R^\alpha(g) \otimes \mathbb{1}_{D_\alpha}$; this implies that for a given group G, all representations V_g which contain all irreducible representations of G yield PEPS which are in the same phase. The interpolation between different multiplicities D_α can again be done within the set of commuting Hamiltonians. This works since the Hamiltonian consists of two commuting parts: One ensures that the product of each irrep around a plaquette is the identity, and the other controls the relative weight of the different subspaces and thus allows to change multiplicities. The underlying idea can be understood most easily by considering a two-qubit toy model consisting of the two commuting terms $h_z = \frac{1}{2}(\mathbb{1} - Z \otimes Z)$ and $h_x(\theta) = \Lambda_\theta^{\otimes 2}\,\frac{1}{2}(\mathbb{1} - X \otimes X)\,\Lambda_\theta^{\otimes 2}$, 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 allows to smoothly interpolate between $|00\rangle$ and $|00\rangle + |11\rangle$ within the set of commuting Hamiltonians.

We have seen that for a given group G, all representations V_g containing all irreps yield PEPS via (1) 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_h, for which Eq. (1) yields the same map $\mathcal{P}$ – which means that the two models are in the same phase – is it true that the two groups are equal? While we cannot answer this question, let us remark that since both models can be connected by a gapped path, one can use quasi-adiabatic continuation[1] to show that their excitations need to have the same braiding statistics; this is, the representations of their doubles need to be isomorphic as braided tensor categories. Note that in Ref. 23, the map $\mathcal{P}$ is used to map doubles to equivalent string-net models.

Let us remark that while we have characterized the equivalence classes of isometric PEPS for the three aforementioned classes, this characterization is not complete: There are PEPS which are locally equivalent to those cases, yet $\mathcal{P}$ has different symmetries. The reason is that unlike in 1D, local entanglement need not be bipartite. E.g., one could add four-partite GHZ states around plaquettes: while this is certainly locally equivalent to the original state, it will change the kernel of $\mathcal{P}$, since only bipartite maximally entangled states can be described by a mapping $\mathcal{P} \to \mathcal{P} \otimes \mathbb{1}$. 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 be induced by locally adding entanglement.

IV. CONCLUSION AND OUTLOOK

In this paper, we have classified quantum phases of one- and two dimensional quantum many-body systems with Matrix Product and PEPS ground states. To this end, we have employed the framework of parent Hamiltonians to explicitly construct gapped paths which connect different Hamiltonians. For one dimension, we could prove that the phase of a system is classified exactly by the degeneracy of its ground states. Concerning two-dimensional systems, we have considered three classes of phases, namely product states, GHZ states, and topological models based on quantum doubles, and shown that all of them are stable in some environment of their fixed points.

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

Let us note that MPS have been previously applied to the classification of phases of one-dimensional quantum systems:[5,24,25] In particular, in Ref. 24, MPS have been used to demonstrate the symmetry protection of the AKLT phase, and in Ref. 5, renormalization transformations[15] and their fixed points on MPS have been used to classify quantum phases in one dimension with and without symmetries. Beyond that, RG fixed points of PEPS have been used to classify phases of two-dimensional systems.[2,26]

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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 $H(\gamma) := \sum h_i(\gamma)$, with $h_i(\gamma) := \Lambda_\gamma h_i \Lambda_\gamma > 0$.

We want to show that the path $H(\gamma)$ is uniformly gapped, i.e., there is a $\Delta > 0$ which lower bounds the gap of $H(\gamma)$ uniformly in γ and the systems size N: This establishes that the $|\boldsymbol{\mu}[\mathcal{P}(\gamma)]\rangle$, and the corresponding $H(\gamma)$, are all in the same phase. To this end, we use a result of Nachtergaele[11] (extending the result of Ref. 6 for the injective case), where it is shown that any parent Hamiltonian is gapped, and a lower bound on the gap (uniform in N) is given.

In the following, we will use the results of Ref. 11 to derive a uniform lower bound on the gap for all $H(\gamma)$, $1 \geq \gamma \geq 0$. Let the MPS matrices $[A_i(\gamma)]_{kl} := \sum_{k,l} \langle i|\,\mathcal{P}(\gamma)\,|k,l\rangle\,|k\rangle\langle l|$; 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 $|\mathrm{spec}\,\mathbb{E}^\alpha(\gamma)| = \{\lambda_1^\alpha(\gamma) > \lambda_2^\alpha(\gamma) > \cdots \geq 0\}$ be the ordered absolute value of the spectrum of $\mathbb{E}^\alpha(\gamma)$ (not counting duplicates). Then, $\lambda_2(\gamma)/\lambda_1(\gamma) < 1$, and since the spectrum is continuous in $\gamma \in [0;1]$, and the degeneracy of λ_1 is $\mathcal{A}$,[11] the existence of a uniform upper bound $1 > \tau_\alpha > \lambda_2^\alpha(\gamma)/\lambda_1^\alpha(\gamma)$ follows. For $\alpha \neq \beta$, let

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

where $|\Phi[C;X]\rangle := \sum_{i_1,\dots,i_p} \mathrm{tr}[C_{i_1}\dots C_{i_p}X]\,|i_1,\dots,i_p\rangle$; i.e., $\Omega^p_{\alpha,\beta}(\gamma)$ 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 $\Omega^p_{\alpha,\beta}(\gamma) \leq \mathcal{O}(\mathcal{S}_\alpha(\gamma)^{\otimes p}, \mathcal{S}_\beta(\gamma)^{\otimes p}) \leq \mathcal{O}(\mathcal{S}_\alpha(\gamma), \mathcal{S}_\beta(\gamma))^p$. Moreover, since $\mathcal{S}_\alpha(0) \perp \mathcal{S}_\beta(0)$, and $\mathcal{S}_\bullet(\gamma) = Q(\gamma)S_\bullet(0)$, we have that

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

where $M = \pi Q(\gamma)^2 \pi^\dagger$, $\pi = |0\rangle\langle v| + |1\rangle\langle w|$, is some 2×2

submatrix of $Q(\gamma)^2$. For $M > 0$,

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

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

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

and as Nachtergaele shows,[11] $\frac{1}{2}\Delta_{2p}(\gamma)(1-\sqrt{2}K^p(\gamma))^2$ is a lower bound on the spectral gap of H^γ. Here, $\Delta_{2p}(\gamma)$ is the gap of $H(\gamma)$, restricted to $2p$ sites, which has a uniform lower bound as the restricted Hamiltonian is continous in γ. This proves that H^γ has a uniform spectral gap for $0 \le \gamma \le 1$.

Appendix B: Robustness of the 2D gap

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

$$\tilde{h}_i\tilde{h}_j + \tilde{h}_i\tilde{h}_j \ge -\tfrac{1}{8}(1-\Delta_{ij})(\tilde{h}_i + \tilde{h}_j) \ ; \qquad \text{(B1)}$$

where we consider a square lattice with $\tilde{h}_i \ge \mathbb{1}$ 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 Section III B, we have given the simplified version where $\Delta_a = \Delta_d = \Delta$.) Then,

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

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. 6.

Let us now study the robustness of (B1) under γ-deformation of the Hamiltonian. Let h_i, h_j be projectors which satisfy $h_ih_j + h_jh_i \ge -\frac{1}{8}(1-\Delta_{ij})(h_i+h_j)$. (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 $Q(\gamma) = (1-\gamma)\mathbb{1} + \gamma Q \le \mathbb{1}$ as in the one-dimensional case, let $\Lambda_{\gamma,X} = \big(Q(\gamma)^{-1}\big)^{\otimes x}$, with $X = A, B, C$ and $x = a, b, c$. Then,

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

Let us define

$$\Theta_\gamma := \Lambda^2_{\gamma,B} - \mathbb{1} \ge 0 \ ,$$
$$q := \lambda_{\min}(Q) < 1 \ ,$$
$$\mu_\gamma := ((1-\gamma) + \gamma\lambda_{\min}(Q))^{-2} \ge 1 \ ,$$

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

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

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 (B1) for the γ-deformed Hamiltonian,

$$h_i(\gamma)h_j(\gamma) + h_j(\gamma)h_i(\gamma) \ge -\tfrac{1}{8}[1-\Delta_{ij}(\gamma)][h_i(\gamma)+h_j(\gamma)] \ , \qquad \text{(B2)}$$

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 (B2) is

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

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