Quantum many-body systems exhibit a variety of phases at zero temperature. Identifying the quantum phases that appear in a given system—determine the phase diagram of the system—is a pivotal task e.g., in condensed matter physics. A quantum phase is an equivalence class in the space of Hamiltonians. Broadly speaking, two local gapped Hamiltonians belong to the same quantum phase if one can be smoothly connected to the other by a path of local gapped Hamiltonians. All local gapped Hamiltonians on a one dimensional (1D) lattice belong to the same phase in the absence of symmetries, and can be smoothly connected to a “trivial” Hamiltonian whose ground state is a product state. However, distinct phases can appear when the Hamiltonians are required to have a symmetry. In one dimension, a local gapped Hamiltonian with a global symmetry can belong either to a symmetry broken phase, characterized by degenerate ground states that are not all symmetric, or to one of possibly several distinct symmetry protected phases, in which the ground state is unique and symmetric. An example of a non-trivial symmetry protected phase is the Haldane phase, which is protected by spatial inversion, time-reversal or a $Z_2 \times Z_2$ (rotations by $\pi$ around two orthogonal axes) symmetry. This means that Hamiltonians in the Haldane phase have a unique and symmetric ground state, and cannot be smoothly connected to a trivial Hamiltonian as long as one of these symmetries is enforced. In two or higher dimensions topological phases, characterized by ground states with non-zero topological entanglement entropy, can also appear. But such phases do not exist in 1D systems.

Symmetry breaking can be identified from the ground state expectation value of a local observable that does not commute with the symmetry (local order parameter). The choice of a local order parameter depends on the model and may not be obvious, in particular, when the ground state is symmetric under a subgroup of the symmetry. On the other hand, string or non-local order parameters have been proposed to distinguish certain symmetry protected phases. In this paper we describe a method to identify quantum phases in classical simulations of 1D quantum many-body systems, without using local or string order parameters.

The method is based on the efficient description of ground states of 1D local gapped Hamiltonians as matrix product states (MPSs). Quantum phases in 1D have also been classified using MPS description of ground states, which provides a more comprehensive framework for their identification in classical simulations. Here we describe how to identify phases by examining if various MPS descriptions of a symmetric ground state, obtained by restricting the MPS matrices to transform under different projective representations of the symmetry, satisfy a condition known as injectivity. For example, in a large class of 1D symmetry broken phases, MPS descriptions of symmetric ground states are non-injective for any choice of projective representation. The appendix contains basic examples of projective representations and details of two technical results that are employed in the main discussion of the paper.

We begin by reviewing relevant aspects of the MPS formalism for translation invariant systems. Consider a 1D lattice $L$ made of $L$ sites each described by a $d$-dimensional vector space $V$. An translation invariant matrix product state $|\Psi\rangle$ of $L$ can be expanded as

$$
|\Psi\rangle = \sum_{i_1, \ldots, i_L=1}^d \text{Tr}(\hat{A}_{i_1}\hat{A}_{i_2}\ldots\hat{A}_{i_L})|i_1, i_2, \ldots, i_L\rangle,
$$

where $\text{Tr}$ denotes matrix trace, $|i_1, i_2, \ldots, i_L\rangle = \otimes_{k\in\mathbb{L}} |i_k\rangle$, $|i_k\rangle$ is a local basis on site $k$, and $\hat{A}_{i_k}$ are site-independent, $\chi \times \chi$ matrices acting on vector space $\mathbb{W}$, $\hat{A}_{i_k} : \mathbb{W} \to \mathbb{W}$. Here $\chi$ is called the bond dimension of the MPS. We will assume that the MPS is in the canonical form in which matrices $\hat{A}$ satisfy $\hat{A}\hat{A}^\dagger = I$ [19]. In this paper we consider the thermodynamic limit, $L \to \infty$, in order to accommodate symmetry breaking.

In a translation invariant MPS $\hat{A}$, two point correla-
tions, \( C(l) \equiv \langle \partial_m \partial_n | - \langle \partial_m | \partial_n \rangle \), can be obtained as
\[
C(l) = \text{Tr}(\hat{Y}^{-1} \hat{T}^{l-1} \hat{Y}^{-1}) - \text{Tr}(\hat{Y} \hat{T}^{l-1}) \text{Tr}(\hat{Y} \hat{T}^{-1}),
\]
where \( \hat{Y} \equiv \sum_{ij} \hat{o}_{ij} A_i \otimes A_i^* \), \(|m-n| = l + 1\), and
\[
\hat{T} \equiv \sum_{i=1}^{d} A_i \otimes A_i^* \tag{3}
\]
is the transfer matrix, see Fig. 1. The range of correlations in an MPS is determined by the degeneracy of the largest modulus eigenvalue \( \lambda_{\text{max}} \) of the transfer matrix. In the canonical form \( |\lambda_{\text{max}}| = 1 \), if the largest eigenvalue is unique then \( \lambda_{\text{max}} = 1 \) \[16\]. In the latter case the MPS is said to be injective \[20\]. An injective MPS has a finite correlation length. This can be explained as follows. An injective MPS satisfies \( \lim_{l \to \infty} \text{C}(l) \approx 0 \) \[16\]. The range of correlations in an injective MPS is determined by the transfer matrix \( \hat{T} \). For instance, it describes the GHZ state: \( \frac{1}{\sqrt{2}} \sum_{i} |i, i, i, \rangle = \delta_{ii} \).

A special case of non-injectivity is when the MPS matrices decompose as \( \hat{A}_i = \hat{I}_f \otimes \hat{A}_i' \), where \( \hat{I}_f = f \times f \) identity matrix and the largest eigenvalue of the transfer matrix \( \hat{T}' \) constructed from the matrices \( \hat{A}_i' \) is unique. In this case we say that MPS \( \hat{A} \) is inflated. An inflated MPS is non-injective (the transfer matrix of MPS \( \hat{A} \) has \( f^2 \) eigenvalues with modulus 1) but has short-range correlations. It is readily checked that MPS \( \hat{A} \) describes the same quantum many-body state that is described by the injective MPS formed with the matrices \( \hat{A}_i' \). That is, expectation value and correlations, Eq. (2), of local observables obtained from the MPSs \( \hat{A} \) and \( \hat{A}' \) are equal. Let us introduce the concept of a symmetry group \( \mathcal{G} \) on the lattice \( \mathcal{L} \) by means of a unitary linear representation \( \hat{U}_g : \mathcal{V} \to \mathcal{V} \) on each site \( \forall \), \( \hat{U}_g \hat{U}_h = \hat{U}_{g,h} \) \( \forall g, h \in \mathcal{G} \). In the rest of the paper we only consider matrix product states that have a global symmetry under the action of \( \mathcal{G} \). MPS \( |\Psi\rangle \), Eq. (1), has a global symmetry \( \mathcal{G} \), or equivalently \( |\Psi\rangle \) is \( \mathcal{G} \)-symmetric, if
\[
|\Psi\rangle = \bigotimes_{s \in \mathcal{L}} \hat{U}_g |\Psi\rangle, \quad \forall g \in \mathcal{G}. \tag{4}
\]
The global symmetry implies a constraint on matrices \( \hat{A}_i \), namely, \( |\Psi\rangle \) is \( \mathcal{G} \)-symmetric iff matrices \( \hat{A}_i \) satisfy \[21, 22\]
\[
\sum_{i'} \langle \hat{U}^*_g \rangle_{i' i} \hat{A}_i = e^{i\theta_g} \hat{A}_i, \quad \forall g \in \mathcal{G}, \tag{5}
\]
where the phases \( e^{i\theta_g} \) \[22\] form a one dimensional representation of \( \mathcal{G} \) and \( \hat{V}_g : \mathcal{W} \to \mathcal{W} \) are unitary matrices (for an MPS in the canonical form) that form a \( \chi \)-dimensional projective representation of \( \mathcal{G} \)—a representation that fulfills the group product only up to a phase, \( \hat{V}_g \hat{V}_h = e^{i\omega(g,h)} \hat{V}_{g,h} \) \( \forall g, h \in \mathcal{G} \). We refer to \( \hat{V}_g \) as the bond representation of the \( \mathcal{G} \)-symmetric MPS \( \hat{A} \).

We now turn to addressing the goal of this paper. We have a local, gapped, translation invariant \[24\] and \( \mathcal{G} \)-symmetric Hamiltonian \( \hat{H} \) on the lattice \( \mathcal{L} \) i.e.,
\[
[\hat{H}, \bigotimes_{s \in \mathcal{L}} \hat{U}_g] = 0, \quad \forall g \in \mathcal{G}. \tag{6}
\]

Our goal is to identify if \( \hat{H} \) belongs to one of possibly several phases protected by symmetry \( \mathcal{G} \) or to a phase in which symmetry \( \mathcal{G} \) is broken in the ground states. **Identification of symmetry protected phases.** If the ground state of \( \hat{H} \) is unique and \( \mathcal{G} \)-symmetric then \( \hat{H} \) belongs to one of possibly several quantum phases protected by the symmetry \( \mathcal{G} \). Distinct symmetry protected phases are in one to one correspondence with the elements of the second cohomology group \( H^2(\mathcal{G}, U(1)) \), which also label different equivalence classes of projective representations of \( \mathcal{G} \). Linear representations of \( \mathcal{G} \) (the identity element of \( H^2(\mathcal{G}, U(1)) \)) correspond to the trivial symmetry protected phase. For example, the second cohomology group of \( \text{SO}(3) \) is \( \mathbb{Z}_2 \) and there are 2 distinct phases protected by \( \mathcal{G} = \text{SO}(3) \) symmetry: the trivial phase corresponding to integer spin representations (linear), and a phase corresponding to half-integer spin (projective) representations of \( \text{SO}(3) \). For brevity, we will say “a symmetry protected phase \( \omega \)” and “a representation in \( \omega \)” to respectively mean a phase protected by symme-
try \( G \) and a representation of \( G \) in the equivalence class that corresponds to the element \( \omega \in H^2(G, U(1)) \).

Symmetry protected phases have also been characterized using MPS descriptions of ground states. If the ground state of a local gapped Hamiltonian is unique then it has a finite correlation length and can be described by an injective MPS [14–16, 25]. Furthermore, if \( \hat{H} \) belongs to a symmetry protected phase \( \omega \in H^2(G, U(1)) \) then an injective MPS description of its ground state has a bond representation in \( \omega \) [28].

Consider an SO(3)-symmetric Hamiltonian on a spin 1 chain that belongs to the SO(3) protected phase corresponding to projective (half-integer spins) representations of SO(3), and whose ground state \( |\Psi^{proj}\rangle \) is described by an injective MPS \( A^{proj} \) with spin 1/2 bond representation [Fig. 2(a)] (i.e., the unitary representation \( \hat{V}_g \) in Eq. (5) is generated by the Pauli matrices). A simple example of such a ground state is the AKLT state \([6, 26]\).

State \( |\Psi^{proj}\rangle \) can also be described by an inflated MPS, for instance, comprised of matrices \( \hat{A}_k^{proj} \equiv \hat{W}^{-1}(\hat{I}_2 \otimes \hat{A}_k^{proj})\hat{W} \) where \( \hat{I}_2 \) is the identity in the spin 1/2 representation and \( \hat{W} \) is the change of basis from the tensor product of two spin 1/2 representations, \( \text{span}\{ |\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\downarrow\rangle \} \), to the direct sum of spin 0 and spin 1 representations i.e.,

\[
\frac{1}{\sqrt{2}}( |\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle) \oplus \text{span}\{ |\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\downarrow\rangle \}.
\]

Thus, \( |\Psi^{proj}\rangle \), which belongs to the non-trivial SO(3) protected phase, is also described by MPS \( A^{proj} \), which has integer spins bond representation (direct sum of spin 0 and spin 1). Note that this does not contradict the MPS based classification of symmetry protected phases because MPS \( A^{proj} \) is non-injective. The situation is reversed for a ground state in the trivial SO(3) protected phase [e.g., MPS \( B^{proj} \) depicted in Fig. 2(b)], namely, an injective MPS description of the state has integer spins bond representation while MPS descriptions of the state with half-integer spins bond representation are inflated.

More generally, if \( \hat{H} \) belongs to a symmetry protected phase \( \omega \in H^2(G, U(1)) \) its ground state \( |\Psi\rangle \) can be described by an MPS with a bond representation in any \( \omega' \) different from \( \omega \) but such an MPS description must be non-injective and obtained by inflating an injective MPS

\[
\hat{H}^{BLBQ} = \sum_{k \in \mathcal{L}} \cos \theta \left( \hat{S}_k \hat{S}_{k+1} \right) + \sin \theta \left( \hat{S}_k \hat{S}_{k+1} \right)^2, \tag{7}
\]

(see appendix Sec. II). Specifically, an MPS description of \( |\Psi\rangle \) with bond representation \( \hat{V}_g^{\omega'} \) in \( \omega' \) is comprised of matrices \( \hat{A}_k^{\omega'} \equiv \hat{W}^{-1}(\hat{I}_f \otimes \hat{A}_k^{proj})\hat{W} \), where (i) \( \hat{A}_k^{proj} \) is an injective MPS description of \( |\Psi\rangle \) with bond representation \( \hat{V}_g^{\omega} \) in \( \omega \), (ii) \( \hat{I}_f \) is the identity in a \( f \)-dimensional representation \( \hat{V}_g^{\omega} \) in \( \omega \), and (iii) \( \hat{W} \) is the change of basis from the tensor product of representations \( \hat{V}_g^{\omega} \) and \( \hat{V}_g^{\omega'} \) to the representation \( \hat{V}_g^{\omega'} \). (\( \omega' \) is chosen such that \( \omega \) and \( \omega' \) are related in this way.)

Thus, if we could obtain an MPS description of \( |\Psi\rangle \) that satisfies Eq. (5) for a given equivalence class of bond representation then we could iterate through the different equivalent classes \( \omega \in H^2(G, U(1)) \) and identify the phase of \( \hat{H} \) from the \( \omega \) that results in an injective MPS description of \( |\Psi\rangle \). In MPS simulations, this can be achieved by choosing an initial \( G \)-symmetric state with a bond representation in the given \( \omega \) and ensuring that the symmetry, Eq. (5), is protected in the simulation at all times. In practice, an MPS description of the ground state(s) of a given Hamiltonian can be obtained e.g., by means of the Density Matrix Renormalization Group [27] (DMRG) and the Time-Evolving Block Decimation [29] (TEBD) algorithms. One way to ensure that the DMRG and TEBD simulations produce a symmetric ground state is to incorporate the (necessary and sufficient) symmetry constraint Eq. (6) in the MPS ansatz.

It is well understood how to do this when the bond representation \( \hat{V}_g \). Eq. (5), is a linear representation. In this case, the MPS matrices \( \hat{A}_k \) decompose in terms of the Clebsch-Gordan (CG) coefficients of the group \( G \), which depend on the choice of the bond representation, and coefficients \( \vec{x} \) that are not fixed by the symmetry (Wigner-Eckart theorem). An initial \( G \)-symmetric MPS with a specific bond representation is constructed from the corresponding CG coefficients and randomly chosen \( \vec{x} \). The symmetry is protected in each iteration of the DMRG and TEBD algorithms by only updating the \( \vec{x} \) part of the MPS. We refer to [29, 32] for details.

When the bond representation is a projective representation, Eq. (5) can be incorporated in the MPS in the same way by exploiting the fact that projective representations of \( G \) can be lifted to linear representations of another group \( R(G) \), called the representation group of \( G \) [32]. The group \( R(G) \) is a central extension of \( G \) and in many cases of interest is also a covering group of \( G \). For example, integer (linear) and half-integer (projective) spin representations of SO(3) respectively are linear representations of SU(2)—the double cover of SO(3). Thus, when the bond representation is projective, MPS matrices decompose in terms of CG coefficients of \( R(G) \).

To demonstrate the method consider the spin 1 bilinear biquadratic Heisenberg model on an infinite chain \( \mathcal{L} \):

\[
\hat{H}^{BLBQ} = \sum_{k \in \mathcal{L}} \cos \theta \left( \hat{S}_k \hat{S}_{k+1} \right) + \sin \theta \left( \hat{S}_k \hat{S}_{k+1} \right)^2,
\]
where \( \hat{S} \equiv (\hat{S}^x, \hat{S}^y, \hat{S}^z) \) are spin 1 matrices. This model has a global SO(3) symmetry and exhibits \( \frac{11}{18}, \frac{13}{18}, \frac{14}{18} \) the two distinct SO(3)-symmetry protected phases: There is a phase transition at \( \theta = -\pi/4 \) from the trivial phase, \( \theta < -\pi/4 \), to the (Haldane) phase corresponding to half-integer spin representations of SO(3).

For a given \( \theta \), we used the SU(2)-symmetric TEBD algorithm \[31\] to obtain two MPS descriptions of the SO(3)-symmetric ground state by restricting the bond representation to integer and half-integer spin representations respectively. In the two cases we chose an initial SO(3)-symmetric MPS with integer and half-integer spins bond representations respectively, which resulted in restricting the bond representation to these equivalence classes at all times in the SU(2)-symmetric simulation \[32\]. From the plot in Fig. 3 we find that for \( \theta < -\pi/4 \) the MPS description of the ground state is injective for integer spins bond representation and non-injective—inflicted with degeneracy of \( \lambda_{max} \) equal to 4 \[33\]—for half-integer spins bond representation, and vice-versa for \( \theta > -\pi/4 \). Thus, we conclude that \( H_{\text{SO(3)}} \) belongs to the trivial phase for \( \theta < -\pi/4 \) and to the Haldane phase for \( \theta > -\pi/4 \). At the critical point \( \theta = -\pi/4 \) we find that the MPS description of the approximated ground state is injective when the bond representation is restricted to either integer or half-integer spin representations \[34\].

Identification of symmetry broken phases. If \( \hat{H} \), Eq. (6), belongs to a phase in which the global symmetry \( \mathcal{G} \) is broken then it has a degenerate ground subspace and there exist ground states that are not \( \mathcal{G} \)-symmetric.

More relevant to our purpose is that in a large class of symmetry broken phases there exist \( \mathcal{G} \)-symmetric ground states all of which are GHZ-type states dressed with local entanglement (see appendix Sec. III), and consequently their MPS descriptions are non-injective [for a bond representation in any equivalence class \( \omega \in H_2(\mathcal{G}, U(1)) \).

For example, consider the spin-1/2 transverse field quantum Ising model on an infinite chain \( \mathcal{L} \),

\[
\hat{H}_{\text{Ising}} = \sum_{k \in \mathcal{L}} \hat{\sigma}_k^x \hat{\sigma}_{k+1}^x + h \hat{\sigma}_k^z, \tag{8}
\]

where \( \hat{\sigma}_k^x \) are Pauli matrices and \( h \) is the magnetic field in the transverse direction. This model has a \( Z_2 \) symmetry generated by a global spin flip, \( \bigotimes_{k \in \mathcal{L}} \hat{\sigma}_k^x \), on all sites. It exhibits a second-order phase transition at \( h = 1 \) from the disordered phase, \( h > 1 \)—a trivial phase where the ground state is unique and \( Z_2 \)-symmetric—to the symmetry broken phase (ordered phase) where the ground state is 2-fold degenerate \[3]\. For instance, at \( h = 0 \) the ground subspace is spanned by states \(|\cdots\uparrow\uparrow\cdots\rangle\) and \(|\cdots\downarrow\downarrow\cdots\rangle\), mapped to each other by the symmetry. There also exist two \( Z_2 \)-symmetric ground states which are GHZ states: \( \frac{1}{\sqrt{2}} (|\cdots\uparrow\uparrow\cdots\rangle \pm |\cdots\downarrow\downarrow\cdots\rangle) \). In fact, as argued in Sec. III of the appendix, \( Z_2 \)-symmetric ground states throughout the symmetry broken phase contain GHZ-type correlations, and consequently their MPS descriptions are non-injective. This is illustrated by the plot in Fig. 4. We find that the MPS description of \( Z_2 \)-symmetric ground states of the Ising model is non-injective for \( h < 1 \) and injective for \( h > 1 \), from which we infer that the symmetry is broken for \( h < 1 \).

Example with \( D_2 \cong Z_2 \times Z_2 \) symmetry. Finally, consider a lattice model that exhibits both a non-trivial symmetry protected phase and a symmetry broken phase. The spin 1 Heisenberg model on an infinite chain \( \mathcal{L} \),

\[
\hat{H}_{\text{Heis}} = \sum_{k \in \mathcal{L}} \hat{S}_k^x \hat{S}_{k+1}^x + D(S_k^z)^2 \tag{9}
\]

has a global \( D_2 \) symmetry generated by rotations \( \hat{R}^x = \exp(i\pi \hat{S}^x) \) and \( \hat{R}^z = \exp(i\pi \hat{S}^z) \). Since \( H_{\text{Heis}}(D_2, U(1)) = Z_2 \) there are 2 distinct \( D_2 \) symmetry protected phases, both of which are exhibited by this model \[17, 38\]. There is a phase transition at \( D \approx 0.97 \) \[39\] from the trivial...
("large-D") phase, \( D > 0.97 \), to the Haldane phase. The model exhibits another phase transition at \( D \approx -0.3 \) to an antiferromagnetic phase in which the \( D_2 \) symmetry is broken to a \( Z_2 \) symmetry corresponding to the non-zero expectation value of \( \hat{S}^z \).

From the plot in Fig. 5 we find that in the large-D phase the MPS description of the ground state is injective if the bond representation is linear and non-injective (inflated) if it is projective, and vice-versa in the Haldane phase. In the symmetry broken phase, MPS descriptions of the \( D_2 \)-symmetric ground states are non-injective if the bond representation is either linear or projective since both cases correspond to a GHZ-type state.

Outlook. Given a 1D quantum lattice model with a global symmetry we have described how to identify both symmetry protected and symmetry broken gapped phases exhibited by the model in a simple way (by examining the injectivity condition in the ground state MPS), once the symmetry [Eq. (\ref{symmetry_condition})] is exactly incorporated in the MPS ansatz. The method can be repeated within a symmetry broken phase to identify gapped phases that are protected by or break the residual symmetry. Symmetries are commonly incorporated in MPS algorithms to obtain computational speedup in simulations (see e.g., \cite{29, 32}). The results presented here demonstrate that incorporating symmetries in MPS algorithms can also be useful to determine the gapped phase diagram of a 1D quantum many-body system.

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References

[1] Local means that the many-body Hamiltonian is a sum of terms each of which only acts non-trivially on a small number of neighbouring sites, and gapped means there is a finite energy difference between the ground subspace and the first excited state in the thermodynamic limit.

[2] By a smoothly connected path of Hamiltonians we mean that ground state properties vary smoothly as the Hamiltonian is varied along the path.

[3] F. Pollmann, A. M. Turner, Erez Berg, and Masaki Oshikawa, Phys. Rev. B 81, 064439 (2010).

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

[5] N. Schuch, D. Perez-Garcia, I. Cirac, Phys. Rev. B 84, 165139 (2011).

[6] F.D.M. Haldane, Phys. Rev. Lett. 50, 1153 (1983), Phys. Lett. 93, 464 (1983).

[7] A. Kitaev and J. Preskill, Phys. Rev. Lett. 96, 110404 (2006).

[8] M. Levin and X.-G. Wen, Phys. Rev. Lett. 96, 110405 (2006).

[9] In the 1D quantum Ising model—which has a global spin flip symmetry—the local order parameter is the ground state spin magnetization: it is zero in the disordered phase and non-zero in the ordered phase (which breaks the symmetry).

[10] M. den Nijs and K. Rommelse, Phys. Rev. B 40, 4709 (1989).

[11] J. Haegeman, D. P.-Garcia, I. Cirac and N. Schuch, Phys. Rev. Lett. 109, 050402 (2012).

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

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

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

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

[16] F. Perez-Garcia, Quantum Inf. Comput. 7, 401 (2007).

[17] F. Pollmann and A. M. Turner, Phys. Rev. B 86, 125441 (2012).

[18] W. Li, A. Weichselbaum J. von Delft, Phys. Rev. B 88, 245121 (2013).

[19] For a given bond dimension, the canonical form of the MPS is unique up to unitary transformations \( V : \mathcal{W} \rightarrow \mathcal{W} \), i.e., state \( |\Psi\rangle \) can be equivalently described by a canonical MPS comprised of matrices \( V^\dagger A_i V \). Other equivalent (canonical) MPS descriptions of \( |\Psi\rangle \) are obtained by inflating the bond dimension as described in the paper.

[20] There exists a such that the map \( \Gamma_n(\hat{X}) = \sum_{i_1,\ldots,i_n} \text{Tr}(\hat{A}_{i_1} \cdots \hat{A}_{i_n}) |i_1,\ldots,i_n\rangle \) is injective. For a comprehensive discussion on injectivity of MPS descriptions see [10].

[21] D. Perez-Garcia, M.M. Wolf, M. Sanz, F. Verstraete, and J.I. Cirac, Phys. Rev. Lett. 100, 167202 (2008).

[22] M. Sanz, M. M. Wolf, D. Prez-Garcia, and J. I. Cirac, Phys. Rev. A 79, 042308 (2009).

[23] In certain cases the factor \( e^{i\theta} \) that appears in Eq. (\ref{symmetry_condition}) leads to a further classification of symmetry protected phases \( \Phi \). In this paper we do not consider these cases and ignore \( e^{i\theta} \) in Eq. (\ref{symmetry_condition}).

[24] In this paper we consider translationally invariant Hamiltonians.

FIG. 5. (Color online) Degeneracy of the largest (modulus 1) eigenvalue \( \lambda_{\max} \) of the transfer matrix \( \hat{T} \), Eq. (\ref{transfer_matrix}), for two MPS descriptions of the \( D_2 \)-symmetric ground states of \( H_{\text{HEIS}} \), Eq. (\ref{heis}), obtained by restricting the bond representation to linear (\( \times \)) and projective (\( \circ \)) representations respectively. Ground states were obtained using the \( R(D_2) \)-symmetric TEBD algorithm (appendix Sec. IV) with \( \chi \leq 100 \). (The depicted phase boundaries are approximate.)
tonians for concreteness. But we expect that our results also apply to non-translationally invariant systems. In the latter, the transfer matrix becomes site dependent and injectivity of MPS descriptions is diagnosed by examining the eigenvalues of the transfer matrix for each site of the lattice.

[25] The unique ground state of a local gapped Hamiltonian can also be described by an inflated (non-injective) MPS. However, MPS simulations do not usually produce inflated descriptions. This is also not desired in practice since an inflated MPS approximates the ground state with a lower accuracy as compared to an injective MPS with the same bond dimension. One can try to detect artificially inflated MPS descriptions by checking if the simulation continues to produce an inflated MPS after decreasing the bond dimension. On the other hand, in this paper we describe how MPS simulations can be constrained—by enforcing suitable symmetry constraints on the MPS—to produce inflated MPS descriptions which are robust to changing the bond dimension.

[26] I. Affleck et al., Phys. Rev. Lett. 59, 799 (1987).
[27] S.R. White, Phys. Rev. Lett. 69, 2863 (1992).
[28] G. Vidal, Phys. Rev. Lett. 91, 147902 (2003); Phys. Rev. Lett. 98, 070201 (2007).
[29] I. P. McCulloch and M. Gulacsi, Europhys. Lett. 57, 852 (2002).
[30] S. Singh, H.-Q. Zhou, and G. Vidal, New J. Phys. 12, 033029 (2010).
[31] S. Singh, R.N.C. Pfeifer and G. Vidal, Phys. Rev. A 82, 050301 (2010); S. Singh, R.N.C. Pfeifer, G. Vidal and G. Brennen, Phys. Rev. B 89, 075112 (2014).
[32] A. Weichselbaum, Annals of Physics 327, 2972-3047 (2012).
[33] L. L. Boyle and Kerrie F. Green, Mathematical and Physical Sciences A 288, 1351, pp. 237-269 (1978).
[34] A. Luchli, G. Schmid, and S. Trebst, Phys. Rev. B 74, 144426 (2006); Z.-X. Liu et. al., Phys. Rev. B 85, 195144 (2012).
[35] If each site $V$ of a lattice transforms as an integer spin representation of SO(3) then the bond representation (on space $W$) of an SO(3)-symmetric MPS belonging to the lattice may be restricted to either only integer or only half-integer spin representations because both cases correspond to a non-vanishing intertwiner (Clebsch-Gordan coefficients) between the spaces $V \otimes W$ and $W$.
[36] The symmetric TEBD simulation resulted in a minimal inflation of the MPS when the bond representation was appropriately constrained. For example, when the bond representation was restricted to integer spin representations in the Haldane phase [Fig. 3] the simulation produced an inflated MPS with a bond dimension that was $f = 2$ times the injective MPS bond dimension, which corresponds to inflating the injective MPS by taking tensor product with identity in the spin $\frac{1}{2}$ representation. As a result, we find that the degeneracy of the largest eigenvalue of the transfer matrix of the inflated MPS is equal to $f^2 = 4$.
[37] At a critical point the ground state has a divergent correlation length which cannot be captured by an MPS with a finite bond dimension, and an MPS simulation only produces an approximation to the ground state—a “nearby” state lying in either gapped phase around the critical point. Here, in addition to a finite bond dimension, restricting the bond representation to integer or half-integer spin representations constrains the simulation to produce a nearby (injective) MPS lying in the Haldane or the trivial phase respectively.
[38] Z.-C. Gu and X.-G. Wen, Phys. Rev. B 80, 155131 (2009).
[39] S. Hu, B. Normand, X. Wang, and L. Yu, Phys. Rev. B 84, 220402 (2011).
APPENDIX

I. Projective representations

A (unitary) projective representation \( \hat{V}_g \) of a group \( \mathcal{G} \) fulfills the group product only up to a phase factor, \( \hat{V}_g \hat{V}_h = e^{i\omega(g,h)} \hat{V}_{g,h}, \forall g, h \in \mathcal{G} \).

Example 1: Consider the group \( D_2 \cong \mathbb{Z}_2 \times \mathbb{Z}_2 \) generated by rotations \( R^z = \exp(i\pi S^z) \) and \( R^z = \exp(i\pi S^x) \). The group product is

\[
g_{ij} g_{mn} = g_{mod(i+m,2),mod(j+n,2)}, \quad i, j, m, n \in \{0,1\}.
\]

The representation \( \hat{V}_{ij} \) of \( D_2 \) given by the Pauli matrices,

\[
\hat{V}_{00} = \left( \begin{array}{cc} 1 & 0 \\ 0 & 1 \end{array} \right), \quad \hat{V}_{01} = \left( \begin{array}{cc} 1 & 0 \\ 0 & -1 \end{array} \right), \quad \hat{V}_{10} = \left( \begin{array}{cc} 1 & 0 \\ 0 & 1 \end{array} \right), \quad \hat{V}_{11} = \left( \begin{array}{cc} 0 & -i \\ 0 & 0 \end{array} \right),
\]

is a projective representation since it fulfills the group product only up to a phase factor,

\[
\hat{V}_{00} \hat{V}_{mn} = \hat{V}_{mn}, \quad \hat{V}_{01} \hat{V}_{10} = \hat{V}_{10} \hat{V}_{01} = i \hat{V}_{11},
\]

\[
\hat{V}_{01} \hat{V}_{11} = i \hat{V}_{10}, \quad \hat{V}_{11} \hat{V}_{01} = -i \hat{V}_{10},
\]

which cannot be removed by scaling the representation matrices.

Example 2: Half-integer spin representations are projective representations of \( \text{SO}(3) \). For example, in the spin \( \frac{1}{2} \) representation, generated by \( \hat{S}_z = \hat{S}_x/2 \) (\( \sigma_z \) are the Pauli matrices), the composition of two \( \pi \) rotations, say, around the \( z \)-axis is \( e^{-i 2 \pi \hat{S}_z} = -I \). Thus, the spin \( \frac{1}{2} \) representation is a projective representation of \( \text{SO}(3) \) owing to the appearance of the factor \(-1\).

Example 3: The group \( \mathbb{Z}_n \) has no non-trivial projective representations.

A projective representation \( \hat{V}_g \) of a group \( \mathcal{G} \) is defined only up to a phase, \( \hat{V}_g \leftrightarrow e^{i\phi_g} \hat{V}_g \), which results in equivalence classes of projective representations under the relation \( \omega(g,h) \sim \omega(g,h) + \phi_g + \phi_h - \phi_{g,h} \mod 2\pi \). The equivalence classes form a group that is isomorphic to the second cohomology group \( H^2(\mathcal{G},U(1)) \). A linear representation simply corresponds to \( \omega(g,h) = 0 \) for all \( g, h \) in \( \mathcal{G} \) and to the identity element of \( H^2(\mathcal{G},U(1)) \).

II. Symmetric matrix product states in a symmetry protected phase

Consider a local, gapped and \( \mathcal{G} \)-symmetric Hamiltonian \( \hat{H} \) on a one dimensional lattice that belongs to the symmetry protected phase corresponding to \( \omega \in H_2(\mathcal{G},U(1)) \). Any MPS description of the (unique) ground state \( |\Psi\rangle \) of \( \hat{H} \) is possibly (i) injective, (ii) GHZ-type non-injective, or (iii) inflated type non-injective. In this section we argue that an MPS description of \( |\Psi\rangle \) that has a bond representation in an equivalence class \( \omega' \in H_2(\mathcal{G},U(1)) \), \( \omega' \neq \omega \), must be inflated [i.e. we will argue to rule out options (i) and (ii)]. This result was used in the paper to identify symmetry protected phases.

First, clearly \( |\Psi\rangle \) cannot be described by a GHZ-type non-injective MPS with a bond representation in \( \omega' \) since a GHZ-type non-injective MPS has long-range correlations while \( |\Psi\rangle \) has short-range correlations.

Next, since \( |\Psi\rangle \) is the unique ground state of a 1D local gapped Hamiltonian it can be described by an injective MPS \( |\psi\rangle \). According to the MPS based characterization of symmetry protected phases, an injective MPS description of \( |\Psi\rangle \) has a bond representation in the equivalence class \( \omega \in H_2(\mathcal{G},U(1)) \) \( \not\equiv \omega' \). Let \( |\Psi\rangle \) be described by an injective MPS \( \hat{A} \). One may hope that the equivalence class \( (\omega) \) of the bond representation of MPS \( \hat{A} \) may be changed by applying a unitary transformation \( \hat{W} \) to the MPS matrices, \( \hat{W}^\dagger \hat{A} \hat{W} \), thus defeating the MPS based characterization of symmetry protected phases. However, we show below that if MPS \( \hat{A} \) and MPS \( \hat{A}' = \hat{W}^\dagger \hat{A} \hat{W} \) describe the same \( \mathcal{G} \)-symmetric state then \( \hat{W} \) must commute with \( \mathcal{G} \),

\[
\hat{W} \hat{V}_g = \hat{V}_g \hat{W}, \quad \forall g \in \mathcal{G}.
\]

[Consequently, \( \hat{W} \) acts as a scalar matrix in the bond representation (Schrödinger’s lemma), and cannot e.g., map a projective representation in one equivalence class to a projective representation in another equivalence class.] This can be derived as follows. Matrices \( \hat{A}' = \hat{W}^\dagger \hat{A} \hat{W} \) must also satisfy Eq. (5).

\[
\sum_i (\hat{U}_g)_{ii'} \hat{A}'_{ii'} = (\hat{V}_g \hat{A}' \hat{V}_g^\dagger), \quad \forall g \in \mathcal{G}.
\]

Substituting \( \hat{A}' = \hat{W}^\dagger \hat{A} \hat{W} \) in Eq. (11),

\[
\hat{W}^\dagger \sum_i (\hat{U}_g)_{ii'} \hat{A}_i \hat{W} = \hat{V}_g \hat{W}^\dagger \hat{A} \hat{W} \hat{V}_g, \quad \forall g \in \mathcal{G}.
\]

By multiplying \( \hat{W}^\dagger \hat{W} \) on both sides of Eq. (11) we obtain

\[
\hat{W}^\dagger \sum_i (\hat{U}_g)_{ii'} \hat{A}_i \hat{W} = \hat{V}_g \hat{W}^\dagger \hat{A} \hat{W} \hat{V}_g, \quad \forall g \in \mathcal{G}.
\]

From Eq. (12) and Eq. (13) we obtain Eq. (10).

Thus, an MPS description of \( |\Psi\rangle \) with a bond representation in \( \omega' \neq \omega \) cannot be injective or GHZ-type non-injective. The only option left to obtain an MPS description with a bond representation in \( \omega' \) is to inflate an injective MPS description of \( |\Psi\rangle \) as described in the paper.

III. Symmetric matrix product states in a symmetry broken phase

Consider an infinite lattice \( \mathcal{L} \) where each site transforms as a \( d \)-dimensional unitary representation \( \hat{U}_g \) of
FIG. 6. (Color online) (a) State $|\Psi_g\rangle$, Eq. 14, as obtained by acting the symmetry on state $|\Psi_{\alpha}\rangle$ described by an injective MPS $\hat{A}$. (b) Reduced density matrix $\hat{\rho}_g$ for $r$ sites in state $|\Psi_g\rangle$; $|L\rangle, |R\rangle$ are the dominant right and left eigenvectors of the transfer matrix $\hat{T} = \sum_{i,j=1}^{d} A_i \otimes A_j^*$ respectively. Shown is the simplification of the expression for $\hat{\rho}_g$ by using $U^\dagger_g U_g = \hat{I}$ and $\lim_{t \to \infty} \hat{T}^t = |L\rangle \langle R|$. (c) Tr($\hat{\rho}_g \hat{\rho}_h$), Eq. 16.

a discrete group $\mathcal{G}$. Also consider a local, gapped, translation invariant and $\mathcal{G}$-symmetric Hamiltonian $\hat{H}$ on the lattice that belongs to a quantum phase in which the symmetry $\mathcal{G}$ is spontaneously broken in the ground states. That is, $\hat{H}$ has a degenerate ground subspace and there exist ground states that are not $\mathcal{G}$-symmetric. In this section we argue that, for a large class of symmetry broken phases, MPS descriptions of the $\mathcal{G}$-symmetric ground states are non-injective. This result was used in the paper to identify symmetry breaking phases. In one dimension, continuous global symmetries cannot be spontaneously broken in local gapped Hamiltonians in accordance with the Mermin-Wagner theorem, so we do not consider this case here. Also see e.g., \cite{12} for a related discussion.

Lemma 1. Consider a translation invariant state $|\Psi\rangle$ of the lattice $\mathcal{L}$ that is described by an injective (canonical) MPS $\hat{A}$. Let $\lambda$ denote the largest modulus eigenvalue of the matrix

$$
\hat{Y}_g \equiv \sum_{i,j=1}^{d} (U_g)_{ij} \hat{A}_i \otimes \hat{A}_j^*,
$$

Then $|\lambda| \leq 1$ for any $g \in \mathcal{G}$ with equality iff $|\Psi\rangle$ is $\mathcal{G}$-symmetric.

This result is proved in \cite{21} as Lemma 1. $\square$

Lemma 2. Assume that there exists a ground state $|\Psi_{\alpha}\rangle$ of $\hat{H}$ that is invariant only under the action of the identity element $e$ of $\mathcal{G}$ and that is described by an injective MPS $\hat{A}$. The state [Fig. 6(a)]

$$
|\Psi_g\rangle \equiv \bigotimes_{k \in \mathcal{L}} \hat{U}_g |\Psi_e\rangle, \quad g \neq e,
$$

is also a ground state of $\hat{H}$ (since $\hat{H}$ is $\mathcal{G}$-symmetric). Denote by $\hat{\rho}_g$ and $\hat{\rho}_h$ the reduced density matrices for $r$ sites in the states $|\Psi_g\rangle$ and $|\Psi_h\rangle$ respectively ($g, h \in \mathcal{G}, g \neq h$) [Fig. 6(b)]. Then for sufficiently large $r$, the overlap of $\hat{\rho}_g$ and $\hat{\rho}_h$, $\text{Tr}(\hat{\rho}_g \hat{\rho}_h)$, is exponentially small (i.e., loosely speaking, ground states $|\Psi_g\rangle$ and $|\Psi_h\rangle$ become “locally” orthogonal after blocking $r$ sites of $\mathcal{L}$).

Proof: The overlap of $\hat{\rho}_g$ and $\hat{\rho}_h$ is [Fig. 6(c)]

$$
\text{Tr}(\hat{\rho}_g \hat{\rho}_h) \approx \langle L \rangle^{\otimes 2} \langle \hat{X}_{hr}^r \hat{Y}_{rh}^r \rangle |R\rangle^{\otimes 2},
$$

where $|L\rangle, |R\rangle$ are the dominant left and right eigenvectors of the transfer matrix $\hat{T} = \sum_{i,j=1}^{d} A_i \otimes A_j^*$ respectively, $\hat{X}_{hr} \equiv \sum_{i,j=1}^{d} (U_h)_{ij} A_i \otimes A_j$, and $\hat{Y}_{gh}^r$ is defined according to Eq. (14). Denote by $\lambda_x$ and $\lambda_y$ the largest modulus eigenvalue of matrices $\hat{X}_{hr}^r$ and $\hat{Y}_{gh}^r$ respectively. From lemma 1 it follows that $\lambda_x < 1, \lambda_y < 1$. This implies that for sufficiently large $r$ we have

$$
\text{Tr}(\hat{\rho}_g \hat{\rho}_h) \approx O(\exp(-r \xi_x)\exp(-r \xi_y)),
$$

where $\xi_x = -\frac{1}{\ln \lambda_x}$ and $\xi_y = -\frac{1}{\ln \lambda_y}$. $\square$

Lemma 3. (Existence of $\mathcal{G}$-symmetric ground states.)

(a) If the group $\mathcal{G}$ is Abelian then $\hat{H}$ always has ground states that are $\mathcal{G}$-symmetric. (b) If $\mathcal{G}$ is non-Abelian $\hat{H}$ may not have any $\mathcal{G}$-symmetric ground states.

Proof (a). Let lattice $\mathcal{L}$ be described by a (infinite dimensional) vector space $\mathcal{V}(\mathcal{L})$. Under the action of the global symmetry $\mathcal{G}$, $\mathcal{V}(\mathcal{L})$ decomposes as $\mathcal{V}(\mathcal{L}) \cong \bigoplus_{\alpha} \mathcal{V}_\alpha$ where $\alpha$ labels irreducible representations of $\mathcal{G}$. According to Schur’s lemma the $\mathcal{G}$-symmetric Hamiltonian $\hat{H} : \mathcal{V}(\mathcal{L}) \to \mathcal{V}(\mathcal{L})$ is block diagonal as

$$
\hat{H} = \bigoplus_{\alpha} \hat{H}_\alpha, \quad \hat{H}_\alpha : \mathcal{V}_\alpha \to \mathcal{V}_\alpha.
$$

We can obtain eigenvectors of $\hat{H}$ in each symmetry sector $\alpha$ by diagonalizing each block $\hat{H}_\alpha$ separately. If $\mathcal{G}$ is Abelian then all irreps $\alpha$ are one dimensional. Clearly, all eigenvectors of $\hat{H}$ transform as a one dimensional irrep of $\mathcal{G}$ i.e., all eigenvectors are symmetric up to an overall phase. In particular, if the ground state is $n$-fold degenerate then there exist exactly $n \mathcal{G}$-symmetric ground states $\{|\Psi_{\alpha}^{\text{sym}}\rangle\}$,

$$
\hat{U}_g |\Psi_{\alpha}^{\text{sym}}\rangle = f_\alpha |\Psi_{\alpha}^{\text{sym}}\rangle, \quad \forall g \in \mathcal{G}, f_\alpha \in \mathbb{C}, \quad |f_\alpha| = 1.
$$

If the symmetry is broken then there must exist at least two ground states that transform as different one dimensional irreps of $\mathcal{G}$. This ensures that there exist superpositions of the two ground states, $a|\Psi_{\alpha}^{\text{sym}}\rangle + b|\Psi_{\alpha'}^{\text{sym}}\rangle$, that
are non-symmetric since the two terms in the superposition pick up different phase factors \( f_\alpha \) and \( f_\alpha' \) under the action of the symmetry. \( \square \)

**Proof (b).** If \( \mathcal{G} \) is non-Abelian then the ground subspace can transform as an irrep \( \alpha \) with dimension larger than one. In this case, and if no other ground states are present, clearly none of the ground states are \( \mathcal{G} \)-symmetric. \( \square \)

Finally, we argue that if the ground subspace of \( \tilde{H} \) is spanned by the states \( \{ |\Psi_g\rangle, \forall g \in \mathcal{G} \} \) of lemma 2 then \( \mathcal{G} \)-symmetric ground states \( \{ |\Psi^{\text{sym}}\rangle \} \) of \( \tilde{H} \) (lemma 3) are GHZ-type states, namely, equal probability superpositions of locally orthogonal states, generally after blocking the lattice. This implies that in this case \( \mathcal{G} \)-symmetric ground states of \( \tilde{H} \) have long range correlations and consequently their MPS descriptions are non-injective.

Let us block the lattice \( \mathcal{L} \) such that states \( \{ |\Psi_g\rangle, \forall g \in \mathcal{G} \} \) become locally orthogonal (lemma 2). Since states \( \{ |\Psi_g\rangle, \forall g \in \mathcal{G} \} \) span the ground subspace, a generic ground state \( |\Psi\rangle \) of \( \tilde{H} \) can be expanded as

\[
|\Psi\rangle = \sum_{h \in \mathcal{G}} c_h |\Psi_h\rangle, \quad c_h \in \mathbb{C}. \tag{20}
\]

If state \( |\Psi\rangle \) is \( \mathcal{G} \)-symmetric then \( |\Psi\rangle = \tilde{U}_g |\Psi\rangle \forall g \in \mathcal{G} \), that is,

\[
\sum_{m \in \mathcal{G}} c_m |\Psi_m\rangle = \sum_{h \in \mathcal{G}} c_h \tilde{U}_g |\Psi_h\rangle. \tag{21}
\]

Changing the dummy summation variable \( m = g.h \) and using \( |\Psi_{g,h}\rangle = \tilde{U}_g |\Psi_h\rangle \) we obtain

\[
\sum_{g,h \in \mathcal{G}} c_{g,h} |\Psi_{g,h}\rangle = \sum_{h \in \mathcal{G}} c_h |\Psi_{g,h}\rangle. \tag{22}
\]

It follows that \( c_{g,h} = c_h, \forall g, h \in \mathcal{G} \) which implies \( c_g = c_e, \forall g \in \mathcal{G} \). Thus, any \( \mathcal{G} \)-symmetric ground state \( |\Psi^{\text{sym}}\rangle \) of \( H \) can be written as

\[
|\Psi^{\text{sym}}\rangle = \sum_{g \in \mathcal{G}} c_e |\Psi_g\rangle, \tag{23}
\]

where \( c_e = \pm \frac{1}{\sqrt{|\mathcal{G}|}} \) (normalization). Thus, a \( \mathcal{G} \)-symmetric ground state \( |\Psi^{\text{sym}}\rangle \) of \( \tilde{H} \) is a GHZ-type state. \( \square \)

We interpret the plots in Fig. 4 and Fig. 5 to indeed indicate symmetry breaking resulting from the mechanism discussed above, namely, the symmetric ground states belonging to the symmetry broken phase exhibited in those models contain GHZ-type broken phase exhibited in those models contain GHZ-type correlations and can be expanded according to Eq. 23.

**IV. \( R(D_2) \)-symmetric TEBD algorithm**

The \( D_2 \)-symmetric ground states used for the plot in Fig. 5 were obtained by means of the \( R(D_2) \)-symmetric version of the TEBD algorithm; \( R(D_2) \) denotes the representation group \( \mathcal{R} \) of \( D_2 = Z_2 \times Z_2 \). The \( R(D_2) \)-symmetric TEBD algorithm was implemented by following \( [30] \) but replacing the irreps and Clebsch-Gordan coefficients of SU(2) with those of \( R(D_2) \). In this section we summarize this data for \( R(D_2) \).

\( R(D_2) \) is a finite non-Abelian group. It has four one-dimensional irreps and one two-dimensional irrep, which we simply label as \( \{ 0, 1, 2, 3 \} \) and \( 4 \) respectively. The 1-d irreps correspond to linear irreps of \( D_2 \) and the 2-d irrep corresponds to a projective representation of \( D_2 \) (see Sec. 1). The Clebsch-Gordan (CG) rules for the direct decomposition of the tensor product of the various pairs of irreps of \( R(D_2) \), symbolically

\[
p \otimes q \cong \bigoplus r, \quad p, q, r \in \{ 0, 1, 2, 3, 4 \},
\]

and the CG coefficients that describe the corresponding change of basis are summarized in Table 1.

| \( p \otimes q \) | \( \otimes r \) | \( \text{CG coeffs} \) |
|----------------|----------------|----------------|
| \( 0 \otimes q \) | \( q \) | \( I_q \) |
| \( q \otimes q, q \neq 4 \) | \( 0 \) | \( 1 \) |
| \( 4 \otimes 1 \) | \( 4 \) | \( \sigma_z \) |
| \( 4 \otimes 2 \) | \( 4 \) | \( \sigma_x \) |
| \( 4 \otimes 3 \) | \( 4 \) | \( \sigma_y \) |
| \( 4 \otimes 4 \) | \( 0 \otimes 1 \oplus 2 \oplus 3 \) | \( 0 \rightarrow \gamma \sigma_y \) |
| | | \( 1 \rightarrow \gamma \sigma_z \) |
| | | \( 2 \rightarrow i \gamma I \) |
| | | \( 3 \rightarrow - \gamma \sigma_z \) |

TABLE I. Clebsch-Gordan coefficients for the group \( R(D_2) \). \( \{ \sigma_x, \sigma_y, \sigma_z, I \} \): Pauli matrices; \( I_q \): identity in irrep \( q \); \( \gamma = \frac{1}{\sqrt{2}} \).