Detection of symmetry-protected topological phases in one dimension

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A topological phase is a phase of matter which cannot be characterized by a local order parameter. It has been shown that gapped symmetric phases in one-dimensional (1D) systems can be completely characterized using tools related to projective representations of the symmetry groups. We explain two ways to detect these symmetry protected topological phases in 1D. First, we give a numerical approach for directly extracting the projective representations from a matrix-product state representation. Second, we derive nonlocal order parameters for time-reversal and inversion symmetry, and discuss a generalized string order for local symmetries for which the regular string-order parameter cannot be applied. We furthermore point out that the nonlocal order parameter for these topological phases is actually related to topological surfaces.

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I. INTRODUCTION

Most phases of matter can be identified by measuring a local order parameter. These order parameters reveal spontaneous symmetry breaking.[1] In the Z_2-symmetric Ising model we find, for example, an ordered and a disordered phase which can be distinguished by an order parameter that measures the magnetization. Over recent decades, it has been discovered that distinct quantum phases (separated by quantum phase transitions) can occur even when there is no local order parameter or spontaneous breaking of a global symmetry. These phases are usually referred to as "nontrivial topological phases".[2] One of the simplest examples of a topological phase is the Haldane phase in quantum spin chains with odd integer spin.[3,4] By tuning various parameters, such as anisotropy terms, this state can be driven through a critical point. Yet on both sides of the critical point, there is no spontaneous symmetry breaking. A mystery then is to find some nonlocal order parameter or another property that changes at the critical point. Such a property was first found by considering the ground state of an exactly solvable model (the "AKLT state" introduced by Affleck, Kennedy, Lieb, and Tasaki[5,6]). This state was found to exhibit several unexpected properties, such as a nonlocal "string order" and edge states. Both extend also to states within the same phase.[7]

It turns out that the topological phases in the spin-1 chain can be understood in terms of "fractionalization" of symmetry operations at the edges, and that these are reflected in the bulk as well, by nontrivial degeneracies in the entanglement.[8] In other words, different phases correspond to inequivalent projective representation of the symmetries present. These topological phases can be protected by any of the following symmetries: spatial-inversion symmetry, time-reversal symmetry, or the $Z_2 \times Z_2$ symmetry (rotations by π about a pair of orthogonal axes).[8,9] The same approach can be applied to phases with other symmetry groups—the phases can simply be classified by enumerating the possible types of projective representation of the appropriate group. This approach was furthermore shown to give a complete classification of phases in one dimension, and elaborated in various directions.[9–11]

As the symmetry-protected phases (by definition) cannot be characterized by any symmetry breaking, there exist no local properties in the bulk which can be measured to distinguish the phases. On the other hand, for certain cases, nonlocal order parameters have been derived to distinguish different symmetry-protected phases. For example, the string order mentioned above can be applied whenever the phases are stabilized by a $Z_2 \times Z_2$ symmetry,[7] and some aspects of it have recently been generalized to other local symmetries.[12,13] Furthermore, it has been found recently that string order can actually be observed experimentally: Endres *et al.*, using high-resolution imaging, observed string order in low-dimensional quantum gases in an optical lattice.[14]

In this paper, we show how to convert the mathematical description of topological phases into concrete characterizations (such as were found for the AKLT state). First, we introduce a practical numerical procedure for calculating the projective representation of the symmetries of a given state, starting from a matrix-product state (MPS). The projective representations can then be used to identify *any* symmetry-protected phase. However, this procedure is practical only when one has a matrix-product representation of the state (or at least has a way of determining its entanglement spectrum). Second, we therefore also discuss other nonlocal order parameters, generalizations of string order, which can be calculated from *any* representation of the wave function using, e.g., Monte Carlo simulations, or possibly even measured experimentally. In particular, we reconsider and generalize the den Nijs and Rommelse string order for local symmetries[7] and show that it works because of a selection rule that changes at the critical point. We conclude with an alternative order parameter for local symmetries (introduced in Ref. 13). The former type of order parameter is an easier way to identify phases for many symmetry groups. However, we point out that there are some groups to which it does not apply, while Haegeman *et al.*'s[13] order parameter always works. This order parameter also has a conceptual interpretation: it can be represented as partition functions on surfaces such as tori, which gives an actual topological interpretation to topological phases.

This paper is organized as follows: We first briefly review properties of MPS's and their transformation under symmetry operations in Sec. II. In Sec. III, we show how to distinguish MPS representations of different symmetry-protected topological phases and present numerical results for a spin-1 Heisenberg chain. In Sec. IV, we analyze nonlocal order parameters which can be calculated from any representation of the wave function. (The Appendix gives an example of a phase that cannot be identified using the den Nijs–Rommelse string order, but can be identified with the more general order of Ref. 13.) In Sec. V we show how the nonlocal order parameter can be interpreted as a topological quantity. We conclude the paper by summarizing our results in Sec. VI.

II. SYMMETRIES IN MATRIX-PRODUCT STATES

A. Matrix-product states

We use a matrix-product-state representation[15] to understand and to define nonlocal order parameters for topological phases in one dimension (1D). We consider translationally invariant MPS's, using the framework contained in Ref. 16. A translationally invariant quantum state on a chain of length L can be written in the following MPS form:

$$|\psi\rangle = \sum_{j_1,\ldots,j_L} B^T A_{j_1} \cdots A_{j_L} B |j_1,\ldots,j_L\rangle, \tag{1}$$

where A_j are $\chi \times \chi$ matrices, and $|j_k\rangle$ represents local states at site k. The $\chi \times 1$ matrix B determines the boundary conditions. In this paper we consider the case of infinite chains and the boundary matrices can be ignored. Ground states of one-dimensional, gapped systems can be efficiently approximated by an MPS representation,[17–19] in the sense that the value of χ needed to approximate the ground-state wave function to a given accuracy converges to a finite value as $L \to \infty$. We follow Ref. 16 and use infinite matrix-product states (iMPS's) for translationally invariant, infinite chains. In the iMPS representation, we write the matrices A_j as a product of $\chi \times \chi$ complex matrices Γ_j and positive, real, diagonal matrices Λ [see Fig. 1(a) for a diagrammatic representation]. The matrices Γ_j and Λ can be chosen to be in a canonical form; that is, the transfer matrix

$$T_{\alpha\alpha';\beta\beta'} = \sum_j \Gamma_{j,\alpha\beta} (\Gamma_{j,\alpha'\beta'})^* \Lambda_\beta \Lambda_{\beta'} \tag{2}$$

should have a right eigenvector $\delta_{\beta\beta'} (= \mathbb{1})$ with eigenvalue $\eta = 1$ (* denotes complex conjugation). Similarly,

$$\tilde{T}_{\alpha\alpha';\beta\beta'} = \sum_j \Lambda_\alpha \Lambda_{\alpha'} (\Gamma_{j,\alpha'\beta'})^* \Gamma_{j,\alpha\beta} \tag{3}$$

has a left eigenvector $\delta_{\alpha\alpha'}$ with $\eta = 1$ [see Fig. 1(b) for a diagrammatic representation]. In this case, the diagonal matrix Λ contains the Schmidt values λ_α for a decomposition into two half-infinite chains,

$$|\psi\rangle = \sum_\alpha \lambda_\alpha |\alpha L\rangle |\alpha R\rangle, \tag{4}$$

where $|\alpha L\rangle$ and $|\alpha R\rangle$ ($\alpha = 1,\ldots,\chi$) are orthonormal basis vectors of the left and right partitions, respectively. The states $|\alpha L\rangle$ and $|\alpha R\rangle$ can be obtained by multiplying together all the matrices to the left and right of the bond, i.e., if the broken bond is between sites 0 and 1, then the right Schmidt states are given by

$$|\alpha R\rangle = \sum_{\{j_k\},k>0} \left[\prod_{l>0} \Gamma_{j_l} \Lambda \right]_{\alpha\gamma} |j_1, j_2, \ldots\rangle. \tag{5}$$

Here, γ is the index of the row of the matrix; when the chain is infinitely long, the value of γ affects only an overall factor in the wave function. Reviews of MPS's as well as the canonical form can be found in Refs. 16, 20, and 21.

Furthermore, we must require that our state is not a cat state. The condition turns out to be that $\mathbb{1}$ is the *only* eigenvector with eigenvalue $|\eta| = 1$.[12] The second largest (in terms of absolute value) eigenvalue ϵ_2 determines the largest correlation length

$$\xi = -\frac{1}{\ln|\epsilon_2|}. \tag{6}$$

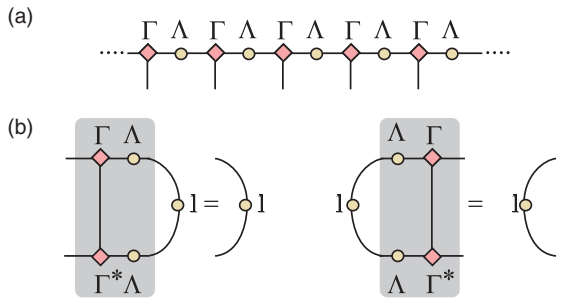

FIG. 1. (Color online) (a) Diagrammatic representation of an iMPS formed by the tensors Γ and Λ. The horizontal line represents the bond indices $1,\ldots,\chi$ and the vertical lines the physical indices $1,\ldots,d$. (b) Condition for the MPS to be in the canonical form [i.e., the transfer matrices Eqs. (2) and (3) have the identity as eigenvectors with eigenvalue 1].

B. Symmetry protected topological phases

If a state $|\psi\rangle$ is invariant under an *internal symmetry*, which is represented in the spin basis as a unitary matrix $\Sigma_{jj'}$, then the Γ_j matrices must transform under $\Sigma_{jj'}$ in such a way that the product in Eq. (1) does not change (up to a phase). Thus the transformed matrices can be shown to satisfy[8,12]

$$\sum_{j'} \Sigma_{jj'} \Gamma_{j'} = e^{i\theta} U^\dagger \Gamma_j U, \tag{7}$$

where U is a unitary matrix which commutes with the Λ matrices, and $e^{i\theta}$ is a phase factor [see Fig. 2(a) for a diagrammatic representation]. As the symmetry element g is varied over the whole group, a set of phases and matrices $e^{i\theta_g}$ and U_g results. The phases form a 1D representation (i.e., a character) of the symmetry group. The matrices U_g form a χ-dimensional (projective) representation of the symmetry group. A projective representation is like an ordinary regular representation up to phase factors; i.e., if $\Sigma^g \Sigma^h = \Sigma^{gh}$, then

$$U_g U_h = e^{i\rho(g,h)} U_{gh}. \tag{8}$$

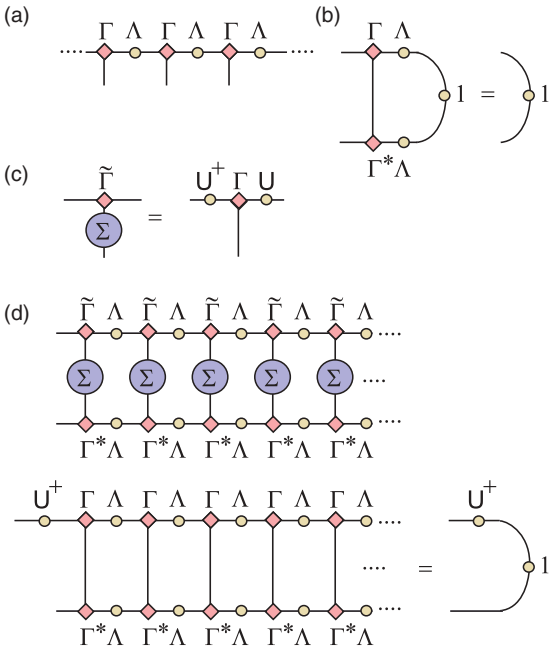

FIG. 2. (Color online) (a) Transformation of an iMPS which is invariant under an internal symmetry operation Σ. Here $\tilde{\Gamma}$ can be Γ, Γ^*, or Γ^T. (b) Eigenvalue equation $T^\Sigma X = \eta X$ for the generalized transfer matrix. The upper part corresponds to the transformed wave function and the lower part to the original one. We find $|\eta| = 1$ if and only if the state is symmetric under this transformation. (c) Overlap of Schmidt states $|\alpha R\rangle$ with their symmetry-transformed partners. If the chain is assumed to be very long, the overlap can be expressed in terms of the eigenvector X corresponding to the largest-magnitude eigenvector $|\eta| = 1$ of the generalized transfer matrix (filled gray circles). The right boundary yields an overall phase factor which we ignore here (see text for details).

The phases $\rho(g,h)$, called the "factor set" of the representation, can be used to classify different topological phases.[8,9,11,22] Consider for example a model which is invariant under a $Z_2 \times Z_2$ symmetry of rotations $\mathcal{R}_x = \exp(i\pi S^x)$ and $\mathcal{R}_z = \exp(i\pi S^z)$. The phases for each spin rotation individually (e.g., $U_x^2 = e^{i\alpha}\mathbb{1}$) can be removed by redefining the phase of the corresponding U matrix. However, the representations of $\mathcal{R}_x\mathcal{R}_z$ and $\mathcal{R}_z\mathcal{R}_x$ can also differ by a phase, which it turns out must be ± 1:

$$U_x U_z = \pm U_z U_x. \tag{9}$$

That is, the matrices either commute or anticommute. This resulting phase cannot be gauged away because the phases of U_x and U_z enter both sides of the equation in the same way. Thus we have two different classes of projective representations.

We can derive a similar relation to Eq. (7) for time-reversal and inversion symmetry.[8] For a time-reversal transformation $\Gamma_{j'}$ is replaced by $\Gamma^*_{j'}$ (complex conjugate) on the left-hand side. In the case of inversion symmetry $\Gamma_{j'}$ is replaced by $\Gamma^T_{j'}$ (transpose) on the left-hand side of Eq. (7). In both cases we can distinguish two different phases depending on whether $U_{\mathcal{I}} U^*_{\mathcal{I}} = \pm\mathbb{1}$ and $U_{\mathrm{TR}} U^*_{\mathrm{TR}} = \pm\mathbb{1}$. Details on the classification of topological phases can be found in, e.g., Refs. 8–11 and 22.

III. DETECTING SYMMETRY-PROTECTED TOPOLOGICAL PHASES IN MPS REPRESENTATIONS

The definitions in the previous section tell us exactly what kind of topological phases exist in 1D and how to classify them. This does not, however, give us a direct method to detect different phases. In Ref. 8 it is pointed out that topologically nontrivial phases must have degeneracies in the entanglement spectrum. However, this does not distinguish among various nontrivial topological states (when there is more than one). Furthermore, density matrix renormalization group (DMRG) calculations sometimes produce states which have a degenerate entanglement spectrum for another reason (such as cat states for a phase with broken symmetry).

In this section we show how to directly obtain the projective representations U, for a state that is respresented in the form of an iMPS; i.e., we have access to the Γ_j and Λ matrices. These matrices can be conveniently obtained using various numerical methods, e.g., the infinite time-evolving block decimation (iTEBD) method.[16] The iTEBD method is a descendant of the density matrix renormalization group method.[23] Once the algorithm has converged to the ground state, the matrices are already in the desired canonical form.

We will now explain how the U matrices may be obtained by diagonalizing transfer matrices.[12] First of all, we determine the implications of the fact that the iMPS is invariant under certain symmetry operations, i.e., we require that $|\langle\psi|\tilde{\psi}\rangle| = 1$ with $|\tilde{\psi}\rangle$ being the transformed state. This implies that a "generalized" transfer matrix

$$T^\Sigma_{\alpha\alpha';\beta\beta'} = \sum_j \left(\sum_{j'} \Sigma_{jj'} \tilde{\Gamma}_{j',\alpha\beta} \right) (\Gamma_{j,\alpha'\beta'})^* \Lambda_\beta \Lambda_{\beta'} \tag{10}$$

must have a largest eigenvalue $|\eta| = 1$,

$$T^\Sigma_{\alpha\alpha';\beta\beta'} X_{\beta\beta'} = \eta X_{\alpha\alpha'}; \tag{11}$$

see also the diagrammatic representation in Fig. 1(b). Here Σ is an internal symmetry operation and $\tilde{\Gamma}_j$ is equal to Γ_j, Γ^*_j, or Γ^T_j, depending on the symmetry of the system (the complex conjugate and transpose are required for time-reversal and inversion, respectively). If $|\eta| < 1$, the overlap between the original and the transformed wave functions decays exponentially with the length of the chain and $|\psi\rangle$ is thus not invariant. Given that $|\eta| = 1$, the information about the symmetry-protected topological phase of the system is encoded in the corresponding eigenvector $X_{\beta'\beta}$. We will see that U is related to X, specifically

$$U_{\beta\beta'} = X^*_{\beta'\beta}. \tag{12}$$

[If the iMPS is not obtained in the canonical form, we need to multiply the right-hand side (RHS) by the inverse of the eigenstate of the transfer matrix Eq. (2).]

This convenient expression for finding U can be understood from the symmetry transformation of the Schmidt states $|\alpha R\rangle$ defined in Eq. (5). Figure 1(c) shows the overlap of the Schmidt states $|\alpha R\rangle$ with their transformed partners $\Sigma|\tilde{\alpha} R\rangle$. The overlap corresponds to applying the generalized transfer matrix T^Σ many times; hence only the dominant eigenvector $X_{\beta\beta'}$ remains in the thermodynamic limit. On the other hand, we can apply the transformation Eq. (7) to each transformed matrix and see that only the $U^\dagger$ at the left end remains

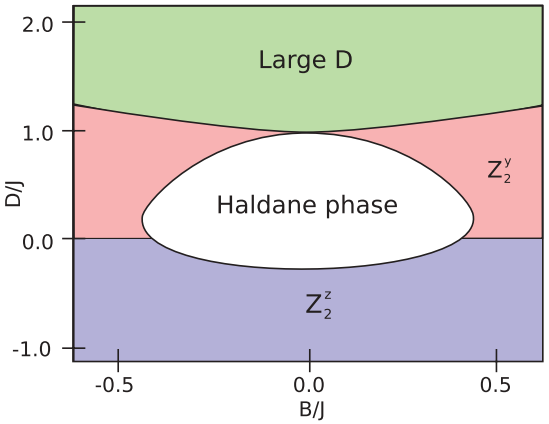

FIG. 3. (Color online) Phase diagram of a spin-1 Heisenberg Hamiltonian in the presence of a single-ion anisotropy D and a transverse magnetic field in the x direction with magnitude B.

[Fig. 1(d)]. Using the fact that the matrices Γ_j and Λ are chosen to be in the canonical form, we can read off that $(U^\dagger)_{\beta\beta'} = X_{\beta\beta'}$ (where we normalize X such that $XX^\dagger = \mathbb{1}$ and ignore a constant phase factor which results from the right end). Thus the U matrices can be obtained by finding the dominant eigenvector of the generalized transfer matrix, i.e., $T^\Sigma U^\dagger = e^{i\theta}U^\dagger$. Once we have obtained the $U^\dagger$ of each symmetry operation, we can read off the factor set [see Eq. (8)] and hence determine in which phase the state is. Furthermore, we can directly see the block structure of the matrices, which is discussed in Ref. 8.

A. Example: Spin-1 chain

In this section we give an example of how we can use this approach to distinguish different symmetric phases. We consider the spin-1 model Hamiltonian

$$H = J\sum_i \vec{S}(i)\cdot\vec{S}(i+1) + B\sum_i S^x(i) + D\sum_i [S^z(i)]^2, \tag{13}$$

in which symmetry-protected topological phases occur. This model is invariant under translation and under spatial inversion as well as under a combined π rotation around the y axis and complex conjugation $[(S^x, S^y, S^z) \to (S^x, -S^y, S^z)]$. The phase diagram has been studied in Ref. 24 and is shown in Fig. 3. The point $D = B = 0$ is the Heisenberg point, around which one finds the gapped Haldane phase. When D increases, there is a transition into another phase which also does not break any symmetry. Even for $B \neq 0$, there is a transition between these two phases (with an intervening phase). At large D, the phase is trivial and can be visualized by a state where all the sites are in the $|S^z = 0\rangle$ state; hence the phase containing the Heisenberg point must be a *nontrivial* topological phase. Furthermore, two antiferromagnetic phases Z_2^y and Z_2^z with spontaneous nonzero expectation values of $\langle S^y\rangle$ and $\langle S^z\rangle$, respectively, are present.

We now show how to use the method introduced in the previous section to distinguish different symmetry-protected topological phases for this model. In the presence of a $Z_2 \times Z_2$ symmetry ($B_x = 0$), we can use the symmetry operations $\mathcal{R}^x = \exp(i\pi S^x)$ and $\mathcal{R}^z = \exp(i\pi S^z)$ (or alternatively any other pair of orthogonal 180° spin rotations) to calculate the $\chi \times \chi$ matrices $U_{\mathcal{R}^x}$ and $U_{\mathcal{R}^z}$ as above. From them we can then define the commutator which distinguishes the different topological phases:

$$\mathcal{O}_{Z_2\times Z_2} = \begin{cases} 0 & \text{if} \quad |\eta_{R^x}| < 1 \text{ or } |\eta_{R^z}| < 1, \\ \frac{1}{\chi}\mathrm{tr}(U_x U_z U_x^\dagger U_z^\dagger) & \text{if} \quad |\eta_{R^x}| = |\eta_{R^z}| = 1. \end{cases} \tag{14}$$

Here η_{R^x} and η_{R^z} are the largest eigenvalues of the generalized transfer matrix Eq. (2). Thus $\mathcal{O}_{Z_2\times Z_2} = 0$ if the state is not $Z_2 \times Z_2$ symmetric, while the two symmetric phases are distinguished by the properties of the U matrices. If U_x and U_z commute ($\mathcal{O}_{Z_2\times Z_2} = 1$) the system is in a trivial phase (i.e., the same class as a site-factorizable state) and if they anticommute ($\mathcal{O}_{Z_2\times Z_2} = -1$), the system is in a nontrivial phase (i.e., the Haldane phase). We proceed in a similar way for the other symmetries. In the presence of inversion symmetry (i.e., $\Gamma \to \Gamma^T$), we define

$$\mathcal{O}_\mathcal{I} = \begin{cases} 0 & \text{if} \quad |\eta_\mathcal{I}| < 1, \\ \frac{1}{\chi}\mathrm{tr}(U_\mathcal{I} U_\mathcal{I}^*) & \text{if} \quad |\eta_\mathcal{I}| = 1. \end{cases} \tag{15}$$

For time-reversal symmetry the matrices transform as $\Gamma_j \to \sum_{j'}[\exp(i\pi S^y)]_{jj'}\Gamma_{j'}^*$ and the corresponding order parameter reads

$$\mathcal{O}_\mathrm{TR} = \begin{cases} 0 & \text{if} \quad |\eta_\mathrm{TR}| < 1, \\ \frac{1}{\chi}\mathrm{tr}(U_\mathrm{TR} U_\mathrm{TR}^*) & \text{if} \quad |\eta_\mathrm{TR}| = 1. \end{cases} \tag{16}$$

These quantities behave similarly to $\mathcal{O}_{Z_2\times Z_2}$, i.e., $\mathcal{O}_{\mathcal{I}/\mathrm{TR}} = 0$ if the symmetry is broken and $\mathcal{O}_{\mathcal{I}/\mathrm{TR}} = \pm 1$ for the two symmetric phases.

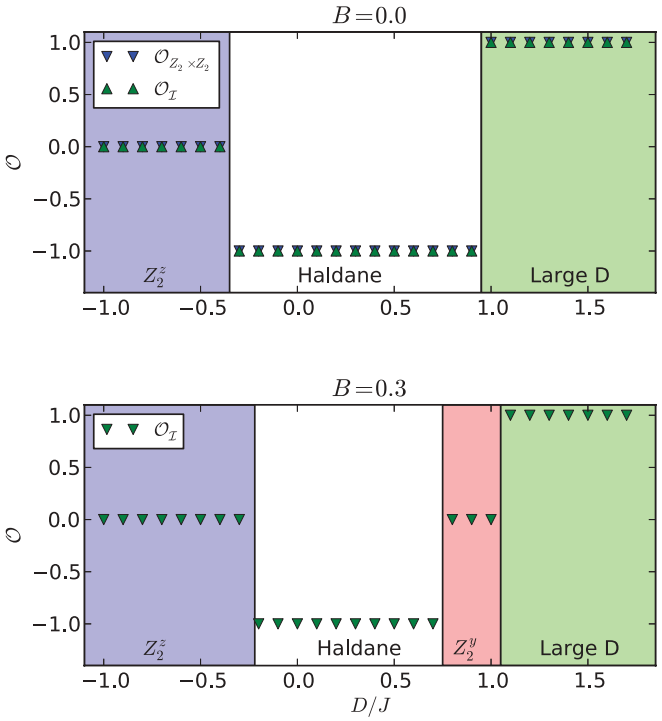

FIG. 4. (Color online) Different phases of Hamiltonian (13) are distinguished by $\mathcal{O}_{Z_2\times Z_2}$ and $\mathcal{O}_\mathcal{I}$ (defined in the text). These quantities are equal to zero if the symmetry is broken and ± 1 distinguishes the trivial and nontrivial phases.

The procedure to calculate the quantities defined above is summarized by Eqs. (10)–(12) and the formulas Eqs. (14)–(16) for the appropriate symmetry. We use the iTEBD method[16] to obtain the ground state of the Hamiltonian Eq. (13) in the desired canonical form. Then we construct the generalized transfer matrices Eq. (10) for the appropriate symmetry operations and find their largest eigenvalues η with corresponding eigenvectors X using sparse matrix diagonalization (the iTEBD algorithm breaks the translational symmetry, yielding two matrices $\Gamma_j^{A/B}$, and thus we construct the transfer matrix using a two-site unit cell). From η and X we can determine the quantities defined in Eqs. (14)–(16). We calculated the $Z_2 \times Z_2$ and inversion order parameters for the spin chain in this way, with the results that are shown in Fig. 4. The phase transition shows up clearly. Interestingly, the sharp distinctions between the phases can be achieved using MPS's with rather small bond dimensions (we used MPS's with up to only $\chi = 50$). For studying the direct vicinity of the critical point it is necessary to use a larger χ because an iMPS ansatz yields a symmetry-broken state when χ is chosen too small.[25]

IV. NONLOCAL ORDER PARAMETERS FROM A WAVE FUNCTION

In the previous section we showed how to detect different phases from an iMPS representation of the ground state. Now we derive expressions which can be evaluated when the wave function is given in another form, for example, using Monte Carlo simulations, or possibly experimentally (as proposed in Ref. 14). The basic idea is to find some operators on the physical Hilbert space which give us some access to the U matrices which exist in the "entanglement Hilbert space."

A. String order in the presence of internal symmetries

Although the spin-1 antiferromagnet is disordered, it has a string order.[7] This is easiest to see at an exactly solvable point in the phase diagram, where the ground state can be found exactly, in the form of a matrix product state, the AKLT state.[5] The state is defined by the matrices $A_{\pm 1} = \pm\sigma_\pm$; $A_0 = -\frac{1}{\sqrt{2}}\sigma_z$. From Eq. (1), any snapshot of the values of the spins S_z on all the sites must have an unusual order: if one discards the sites with an S_z value of 0, then the remaining spins have perfect antiferromagnetic order (as can easily be checked). This is not reflected in an ordinary long-range correlation, however. The mathematical description of this ordering is $S_{z,j}(-1)^{\sum_{j<l<k} S_{z,l}} S_{z,k} = -1$; this operator is called a string operator. Away from this exactly solvable point, the order is no longer perfect, but the expectation value of the string operator is still nonzero: $\mathcal{S}^\alpha_{\mathrm{str}} \equiv \lim_{|j-k|\to\infty} \langle\psi_0| S^\alpha_j e^{i\pi \sum_{j\leqslant l<k} S^\alpha_l} S^\alpha_k |\psi_0\rangle \neq 0$.

Pérez-García *et al.*[12] showed that this string order parameter, which is relevant for $Z_2 \times Z_2$ symmetric spin chains, can be generalized for systems with other symmetry groups. The generalized form for a state which is invariant under symmetry operations $\Sigma(k)$ reads

$$\mathcal{S}(\Sigma, O^A, O^B) = \lim_{n\to\infty} \langle\psi_0| O^A(1) \left(\prod_{k=2}^{n-1} \Sigma(k)\right) O^B(n) |\psi_0\rangle. \tag{17}$$

The nonvanishing of this expression for generic operators means only that the state is symmetric, but does not distinguish among topologically distinct states.

Nevertheless, we will now show that if the operators $O^A(1)$ and $O^B(n)$ are chosen appropriately, this order parameter can distinguish some topological states. However, it is not a complete characterization, and we give a specific example below showing that it does not necessarily work in the presence of more complicated symmetries.

The most basic result about the string-order correlator Eq. (17) is that a phase must be symmetric under Σ for the string order to be nonzero. This criterion does not help to distinguish among topologically different *symmetric* phases. However, there is a second more refined condition for when the string order is nonzero, which *can* distinguish them. For example, the string order defined by $O^A = O^B = S^z$ vanishes in the large-D phase. Why does this occur even though the state is symmetric? The same string order is nonzero in the Haldane phase; hence it seems to be connected to the topological order of the phase, as we will show now.

Intuitively, the string order corresponds to calculating the overlap between the wave function with Σ applied to L consecutive sites and the wave function itself. Since Σ is a symmetry of the wave function, it does not change anything in the bulk of this segment and the overlap should not vanish, generically speaking. A diagrammatic representation of the string order is shown in Fig. 5(a). We represent the symmetry that is sandwiched in the middle using Eq. (7), i.e., $\sum_{j'} \Sigma_{jj'} \Gamma_{j'} = e^{i\theta} U_\Sigma^\dagger \Gamma_j U_\Sigma$. Ignoring the overall phase factor $e^{in\theta}$, we obtain the expression shown in Fig. 5(b). If n is large, the part in between $U_\Sigma^\dagger$ and U_Σ is a product of

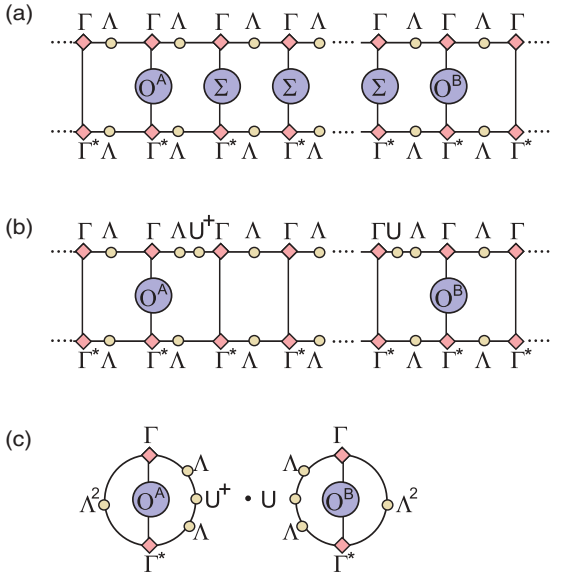

FIG. 5. (Color online) Diagrammatic derivation of the string order $\mathcal{S}$ for a wave function which is symmetric under an internal transformation Σ and represented by an MPS in canonical form: (a) String order involving a segment of transformed sites terminated by operators O^A and O^B. (b) The matrices Γ_j transform according to Eq. (7) and all matrices U and $U^\dagger$ vanish except the ones at the edges. (c) Using the properties of the transfer matrices (defined in the text), the expectation value can be simplified for long segments.

orthogonal Schmidt states of the segment yielding a product of delta functions $\delta_{\alpha\alpha'}$ on the left and $\delta_{\beta\beta'}$ on the right [compare Fig. 5(c)]. That is, the string order is equal to the product $(\mathrm{tr}\Lambda\bar{O}^A\Lambda U_\Sigma^\dagger)(\mathrm{tr}\Lambda\bar{O}^B\Lambda U_\Sigma^T)$, where

$$\bar{O}^A_{\alpha'\alpha} := \langle\alpha' L|O^A|\alpha L\rangle = \sum_\beta \frac{\lambda_\beta^2}{\lambda_\alpha\lambda_{\alpha'}} T^{O^A}_{\beta\beta,\alpha\alpha'} \tag{18}$$

with the generalized transfer matrix T^{O^A} as defined in Eq. (10), and $\bar{O}^B_{\alpha'\alpha} = \langle\alpha' R|O^B|\alpha R\rangle = \sum_\beta T^{O^B}_{\alpha\alpha',\beta\beta}$. This expression is nonzero unless at least one of the two factors is equal to zero. Thus, the string order is generically nonzero in a symmetric phase.

Whether the factors vanish depends on the symmetry of the operators $O^A(1)$ and $O^B(n)$ and can be seen as a selection rule for string order. Such selection rules exist only in the presence of additional symmetry. Thus, suppose that there are two symmetry operations Σ^a and Σ^b which commute but $U_bU_aU_b^\dagger U_a^\dagger = e^{i\phi}$ in the projective representation. We consider the string correlator $\mathcal{S}(\Sigma^a, O^A, O^B)$, and focus on the left end of the interval. The operator O^A can be chosen to have a particular quantum number under Σ^b, i.e., $\Sigma^b O^A(\Sigma^b)^\dagger = e^{i\sigma}O^A$. Then a short calculation shows that $\bar{O}^A$ transforms in the same way under U_b, i.e., $U_b\bar{O}^AU_b^\dagger = e^{i\sigma}\bar{O}^A$. It follows that

$$\mathrm{tr}\Lambda\bar{O}^A\Lambda U_a^\dagger = \mathrm{tr}(U_b\Lambda\bar{O}^A\Lambda U_a^\dagger U_b^\dagger) = e^{i(\sigma-\phi)}\mathrm{tr}\Lambda\bar{O}^A\Lambda U_a^\dagger. \tag{19}$$

Thus we obtain a string-order selection rule: the string-order parameter vanishes if $\sigma \neq \phi$. Without the second symmetry Σ^b, the string order would not vanish. Hence a nonzero string order in a state (although intuitively surprising) is actually not so unusual; it is the *vanishing* of a string order that is the signature of a topological phase. Note that the string order might accidentally vanish (or become very small) at some points even in a phase where $\sigma = \phi$. In that case one would have to find different operators O^A and O^B to distinguish the phases. We refer to the next section for a nonlocal order parameter which does not rely on finding the right operators to unambiguously detect symmetry-protected topological phases. To summarize, the second criterion for the string order is that $\sigma = \phi$ *or else the string order vanishes*.

The string order for the spin-1 Heisenberg chain, for example, can be derived simply in this way. Consider the Heisenberg chain with the symmetries $\mathcal{R}^x = \exp(i\pi S^x)$ and $\mathcal{R}^z = \exp(i\pi S^z)$. Then the selection rule implies that the string order vanishes in the trivial phase if one of the operators O^A,O^B is odd under 180° flips about the x axis. The string order vanishes in the nontrivial phase if one of these operators is *even* (since U^z is odd under flips about the x axis in this phase). Thus, $\langle\psi_0|\mathbb{1}[\prod_{k=2}^{n-1}\mathcal{R}^z(k)]\mathbb{1}|\psi_0\rangle$ vanishes in the nontrivial ($\phi = \pi$) phase and $\langle\psi_0|S^z(1)[\prod_{k=2}^{n-1}\mathcal{R}^z(k)]S^z(n)|\psi_0\rangle$ does not, while the situation is reversed in the trivial ($\phi = 0$) phase. This is different from ordinary ordering transitions such as, e.g., for the Ising model, where even operators have long-range correlations in both phases.

This approach may be used to give an order parameter that is sensitive to certain phase factors, those of the form $U_aU_bU_a^\dagger U_b^\dagger = e^{i\phi}$ for commuting symmetries. In order to determine ϕ systematically, find test operators O with each possible transformation under Σ^b, and then see which of these has a nonzero string correlation. In more detail, note first that $\phi = \frac{2\pi k}{r}$ where r is the order of Σ_b and where k is some integer, and thus finding ϕ is equivalent to finding k. We can then choose "test operators" that are powers of a single operator O_1 that transforms as $(\Sigma^b)^\dagger O_1\Sigma^b = e^{2\pi i/n}O_1$. For $0 \leqslant l \leqslant n-1$ calculate the string order $\mathcal{S}_l = \mathcal{S}(\Sigma^a, O^A, O^B)$ with $O^A = (O_1)^l$, translated to the left end of the segment, and $O^B = (O_1^\dagger)^l$, translated to the right end. The result will be nonzero only for one value of l, namely, $l = k$.

In general, the possible phases of a system with a given symmetry group can be classified by finding all the consistent phase factors for a projective representation [see Eq. (8)]. A phase can thus be identified by measuring the gauge-invariant combinations of these phase factors. The term "gauge-invariant" refers here to phase factors which cannot be removed by rephasing the U matrices.

The procedure just given works for phase factors that arise from a pair of symmetries that commute in the original symmetry group. However, for complicated groups, these might not be the only parameters that one needs. If Σ^a and Σ^b do not commute, e.g., $\Sigma^a\Sigma^b(\Sigma^a)^{-1}(\Sigma^b)^{-1} = \Sigma^x$ (another symmetry), then there can be a phase in the projective representation, $U_aU_bU_a^{-1}U_b^{-1} = e^{i\phi_1}U_x$. This phase cannot be detected using the string-order selection rule, but it also does not matter since it is not gauge invariant: it can be absorbed into U_x. However, a modification of this symmetry group *does* give an example of a *gauge-invariant* phase that cannot be detected by a selection rule. Suppose there is another pair of symmetries Σ^c and Σ^d with the same commutator, i.e., $\Sigma^c\Sigma^d(\Sigma^c)^{-1}(\Sigma^d)^{-1} = \Sigma^x$. Then, in the projective representation, $U_cU_dU_c^{-1}U_d^{-1} = e^{i\phi_2}U_x$. Either ϕ_1 or ϕ_2 may be absorbed into U_x, but not both. In fact, we can write

$$U_aU_bU_a^{-1}U_b^{-1}U_dU_cU_d^{-1}U_c^{-1} = e^{i(\phi_1-\phi_2)}\mathbb{1}. \tag{20}$$

Thus, $e^{i(\phi_1-\phi_2)}$ is an example of a phase factor that is gauge invariant but cannot be detected by the string order just developed. (Appendix A fleshes out the details of this example.) This phase factor *can* be detected by the general approach we started with, of diagonalizing transfer matrices to find the U's and then just calculating the appropriate products of them.

In the next section, we will explain that there is also another type of nonlocal order parameter that is sensitive to these more complicated local phase factors. This type of order parameter can also be used to identify phases protected by time-reversal or inversion symmetry. In fact, these types of order parameter can detect any gauge-invariant phase factor, so they give a complete way to determine what type of symmetry protected topological order a system has.

B. Nonlocal order parameters that measure the phase factors

Phases that are protected by inversion symmetry, time-reversal symmetry, or more complicated internal symmetries (see the example above) cannot be detected using the selection rules. However, there is another type of nonlocal order parameter (for example introduced in Ref. 26 for inversion).

The important aspect of the values of these order parameters is not whether they vanish or not but what their complex phases are; these phases coincide with the phases from the projective representation (such as $U_{\mathcal{I}}^* U_{\mathcal{I}}$). However, they can be measured using the physical degrees of freedom (rather than the ancillary states of a matrix-product representation).

Inversion symmetry. In this case we can define an order parameter by simply reversing a part of the chain with an even length and then calculating the overlap:

$$\mathcal{S}_{\mathcal{I}}(2n) = \langle \psi | \mathcal{I}_{1,2n} | \psi \rangle, \tag{21}$$

where $\mathcal{I}_{1,2n}$ is the inversion on the segment from 1 to $2n$. This expectation value can be evaluated using, e.g., Monte Carlo methods, and it distinguishes the two possible symmetric phases by

$$\lim_{n\to\infty} \mathcal{S}_{\mathcal{I}}(2n) = \pm \mathrm{tr}\Lambda^4, \tag{22}$$

where Λ is a diagonal matrix which contains the Schmidt values (as defined in Sec. II). The *sign* of this quantity determines which of the two inversion-protected phases the chain is in. The expression $\mathcal{S}_{\mathcal{I}}(2n)$ can be described by the following thought experiment: Form pairs of sites that are symmetric about the midpoint of the segment, and perform a measurement of the parity $P_k = \pm 1$ of the state of each pair. Then $\mathcal{S}_{\mathcal{I}}(2n)$ is $\langle \prod_{k=1}^{n} P_k \rangle$. A nonzero value for $\mathcal{S}_I$ means that there is a nonlocal correlation according to which the number of odd pairs is more likely to be either an even or odd number, even when the segment is very long. Generically, one expects that even and odd numbers of pairs with a given parity are equally likely, not because of any symmetry between even and odd numbers but just because of statistical independence: in a million flips of a coin, an even number of heads is almost equally likely to occur as an odd number, even if the coin is unfair, as long as there is no hidden correlation between the coins. In a system with inversion symmetry, however, there will be a correlation of this type. This experiment could even be carried out in practice, but it could be difficult to see the effect, since independent errors in measuring individual pairs will make even and odd numbers equally likely.

We now derive the string order $\mathcal{S}_{\mathcal{I}}(2n)$ formally using the iMPS representation together with the identities defined in Sec. II. The result of reversing a segment and taking the overlap, shown in Fig. 6(a), is that the segments attaching the two chains to each other become twisted. These may be untwisted by reversing the orientation of the segment on the top level of the chain, at the expense of introducing a twist in it [see Fig. 6(b)]; the explicit calculation uses the relationship $\Gamma_j^T = e^{i\theta} U_{\mathcal{I}}^\dagger \Gamma_j U_{\mathcal{I}}$, and so factors of $U_{\mathcal{I}}$ appear in the diagram. Now, each of the ladders is a product of several copies of the transfer matrix T, and so, if n is large, it becomes a projection onto the largest eigenvector of T, which is $\delta_{\alpha\beta}$ [see Eq. (2)], allowing the diagram to be simplified again [see Figs. 6(c) and 6(d)]. Reading along the loop in this figure gives the value of the string-order parameter (the factors of $e^{i\theta}$ cancel):

$$\lim_{n\to\infty} \mathcal{S}_{\mathcal{I}}(n) = \mathrm{tr}\Lambda U_{\mathcal{I}}^T \Lambda^2 U_{\mathcal{I}}^\dagger \Lambda = \mathrm{tr} U_{\mathcal{I}}^T U_{\mathcal{I}}^\dagger \Lambda^4 = \pm \mathrm{tr}\Lambda^4. \tag{23}$$

Note that the line goes backwards through $U_{\mathcal{I}}$ so it is transposed. Unlike the ordinary string order (which vanishes in one phase), it is the sign of this parameter that distinguishes among phases. As a specific example, we calculated $\mathcal{S}_{\mathcal{I}}$ for the spin-1 Heisenberg chain (13) in the presence of a finite transverse field. In this case, the Haldane phase is stabilized by inversion symmetry. The results, which have been obtained using the iTEBD algorithm, are shown in Fig. 7. The order parameter shows a clear distinction between the two phases. As we approach the phase transition, the correlation length gets longer and we have to make the segment longer to see the convergence of $\mathcal{S}_I/\mathrm{tr}\,(\Lambda^4)$ to ± 1.

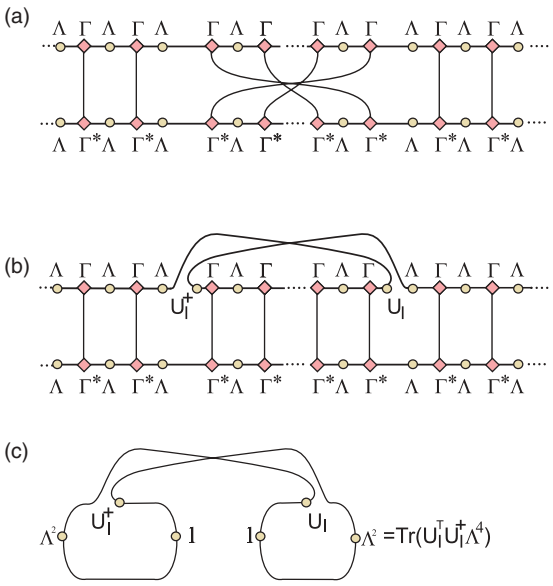

FIG. 6. (Color online) Diagrammatic derivation of the string order $\mathcal{S}_{\mathcal{I}}$ for a wave function which is inversion symmetric and represented by an iMPS in canonical form: (a) Overlap of a wave function with the wave function for an infinite chain in which a segment of n sites has been inverted. (b) The overlap can be untwisted by reversing the segment using the unitaries $U_{\mathcal{I}}$. (c) For large L and n, the expression can be simplified by keeping only the largest-magnitude eigenvector of the transfer matrix T, yielding $\mathcal{S}_{\mathcal{I}}$.

Time-reversal symmetry. A more complicated expectation value can be used to distinguish between phases protected by

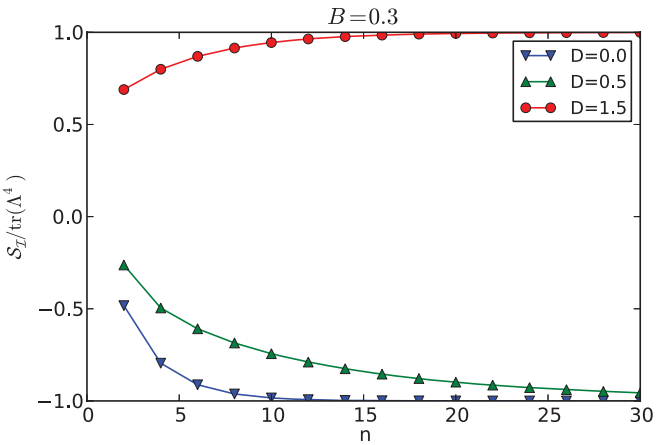

FIG. 7. (Color online) The nonlocal order parameter $\mathcal{S}_{\mathcal{I}}$ distinguishing the Haldane ($D = 0.0, 0.5$) and large-D ($D = 1.5$) phases in the presence of inversion symmetry.

time-reversal symmetry. This order parameter is more subtle to devise because there is no way to apply time reversal to just a portion of a system (as there is for inversion symmetry) since time reversal is antiunitary. For example, consider the state

$$\frac{1}{\sqrt{2}}[(|1\rangle)|0\rangle + (i|0\rangle)|1\rangle] = \frac{1}{\sqrt{2}}[|1\rangle)|0\rangle + |0\rangle(i|1\rangle)] \quad (24)$$

formed from two qubits. One cannot apply time-reversal symmetry to just the first qubit in a unique way, since the result of applying $\mathcal{T}$ to just the first atom comes out differently for the two ways of grouping the factors. However, there is a way to express the overlap on the full chain $\langle\psi|\mathcal{T}|\psi\rangle$ without using antiunitary operators, and this is the starting point for a nonlocal order parameter. Consider first a *single* spin $S = 1$ with $j = -1,0,1$. Then

$$\kappa = \langle\psi|\mathcal{T}|\psi\rangle = \sum_{j,j'} \left[e^{i\pi S^y}\right]_{j'j} \psi_j^* \psi_{j'}^* \quad (25)$$

is not the ordinary expectation value of $e^{i\pi S^y}$ because both factors of ψ have complex conjugates. To relate this to an expectation value, let us take two copies of the spin and introduce the two states

$$|\psi_2\rangle = |\psi\rangle \otimes |\psi\rangle, \quad (26)$$

$$|R\rangle = \frac{1}{\sqrt{3}} \sum_j \left[e^{i\pi S^y}\right]_{jj'} |j\rangle \otimes |j'\rangle, \quad (27)$$

so that $\kappa = \sqrt{3}\langle\psi_2|R\rangle$. The phase of κ is not well defined, since it depends on how one chooses the phase of ψ, so $|\kappa|^2 = 3\langle\psi_2|\,(|R\rangle\langle R|)\,|\psi_2\rangle$ is a more useful quantity. This can be related to an experiment where one takes two unentangled copies of the system and measures their state in a basis including R. The probability that the state is R is then given by $|\kappa^2|/3$.

Now the generalization of $|\kappa|^2$ to an entire chain is useful for testing whether time-reversal symmetry is broken spontaneously, but it does not help to distinguish between different phases. For that, an operator has to be applied over part of the chain in order to create "domain walls" which depend on $U_{\mathcal{T}}$. Therefore, we introduce an entangled state on just n sites,

$$|R_{1n}\rangle = \prod_{k=1}^{n} \left(\frac{1}{\sqrt{3}} \sum_{j_k} [e^{i\pi S^y}]_{j_k j_k'} |j_k\rangle \otimes |j_k'\rangle \right). \quad (28)$$

To define an order parameter that can distinguish different symmetric phases, we also have to introduce a swapping operator (defined as in Ref. 27). Let $\mathrm{Swap}_{n+1,2n}$ swap the parts of the chains between $n+1$ and $2n$. Then we find that

$$\mathcal{S}_{\mathrm{TR}}(n) = d^n \langle\psi_2|\,(|R_{1n}\rangle\langle R_{1n}|)\,\mathrm{Swap}_{n+1,2n}|\psi_2\rangle = \pm(\mathrm{tr}\Lambda^4)^3, \quad (29)$$

where the sign is what we want to measure, $e^{i\phi_{\mathcal{T}}}$. Here d is the local dimension of the Hilbert space. The swapping operator $\mathrm{Swap}_{n+1,2n}$ is introduced because, without it, $\langle\psi_2\,(|R_{1n}\rangle\langle R_{1n}|)\,|\psi_2\rangle$ does not depend on the sign of $U_{\mathcal{T}}U_{\mathcal{T}}^*$ (it is clearly positive). Multiplying by $\mathrm{Swap}_{n+1,2n}$ makes it possible to isolate the phase $e^{i\phi_{\mathcal{T}}}$.

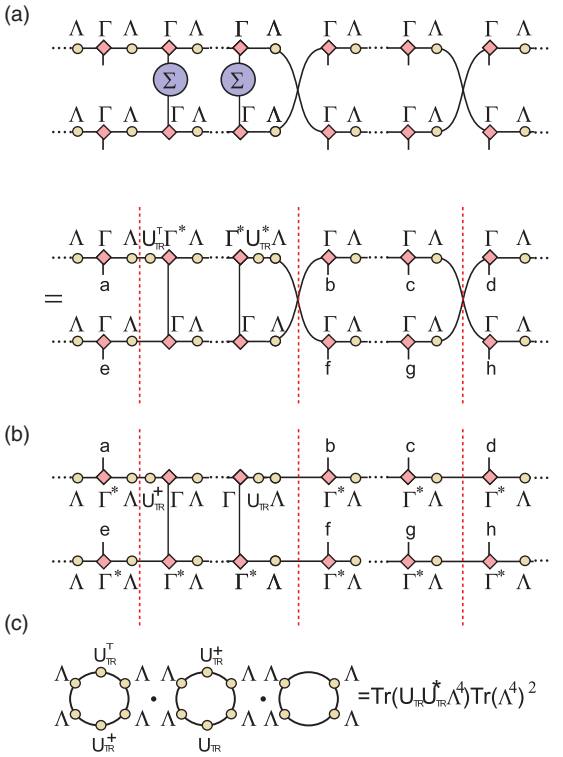

FIG. 8. (Color online) Diagrammatic derivation of the string order $\mathcal{S}_{\mathrm{TR}}$ for a wave function which is time-reversal symmetric and represented by an MPS in canonical form: (a) Representation of the wave function $d^{n/2}\langle R_{1n}|\mathrm{Swap}_{n+1,2n}|\psi_2\rangle$ containing three domain walls, where $\Sigma = \exp(i\pi S^y)/\sqrt{d}$ and d is the physical dimension. The Σ may be replaced by the operator U_{TR} and the complex conjugation of the segment in the upper row. (b) Representation of the wave function $d^{n/2}\langle\psi_2|R_{1n}\rangle$. (c) Contraction of the two wave functions over open indices with the same letter (a–h) and keeping only the largest-magnitude eigenvector of the transfer matrix T yields for larger m,n the order parameter $\mathcal{S}_{\mathrm{TR}}$. The dashed red lines indicate the positions of the domain walls.

Figure 8 shows how to work out the order parameter $\mathcal{S}_{\mathrm{TR}}$. The expectation value is evaluated in two parts: First, we calculate $d^{n/2}\langle R_{1n}|\mathrm{Swap}_{n+1,2n}|\psi_2\rangle$ [Fig. 8(a)] and then $d^{n/2}\langle\psi_2|R_{1n}\rangle$ [Fig. 8(b)]. Since $|R_{1n}\rangle$ extends only over n sites, these are partial inner products, giving a wave function in which n spins have been removed. The short sticks coming out of the other sites represent the sites that have not been contracted yet. Next, we transform Fig. 8(a) using Eq. (7) in the conjugate form $\sum_{j'}[e^{i\pi S^y}]_{jj'}\Gamma_{j'} = U_{\mathrm{TR}}^T\Gamma_j^* U_{\mathrm{TR}}^*$ and take the overlap between Figs. 8(a) and 8(b), by contracting the short sticks with one another. There will be three domain-wall regions that we have to concentrate on (the bonds between $0,1$, $n,n+1$, and $2n,2n+1$); everything else can be simplified by replacing the ladders by projections onto the identity (in the same way as we have done several times before). The three domain walls can be replaced by the product of loops in Fig. 8(c). Contracting these expressions gives $\lim_{n\to\infty}\mathcal{S}_{\mathrm{TR}}(n) = (\mathrm{tr}U_{\mathrm{TR}}^\dagger\Lambda^4 U_{\mathrm{TR}})(\mathrm{tr}U_{\mathrm{TR}}^*\Lambda^4 U_{\mathrm{TR}})(\mathrm{tr}\Lambda^4)$, which is equal to Eq. (29). (If the swap had not been included, the domain wall on the right of the region contracted with R would be proportional to $U_{\mathrm{TR}}^\dagger U_{\mathrm{TR}} = \mathbb{1}$. The swap reverses the orientation of one

of the paths so that $U_{\rm TR}^*$ appears instead of $U_{\rm TR}^\dagger$, yielding the desired phase factor.) This string order is nonzero in both the time-reversal-protected phases, but when it is negative, the phase is nontrivial, just as for the inversion symmetry.

Combinations of multiple local symmetries. For local symmetries, there are also string-order parameters that directly measure the topological phase factors, as in Eq. (22). This type of string order was introduced in Ref. 13. We show that it can identify tricky phase factors like the one in Eq. (20), which ordinary string order cannot. To be general, note that there is a gauge-invariant phase any time there is a sequence of symmetries a_j which can be multiplied together to give the identity in more than one way, $a_1 a_2 \cdots a_m = a_{k_1} a_{k_2} \cdots a_{k_m} = \mathbb{1}$ (where the indices $k_1, \ldots, k_m$ are a permutation of $1, \ldots, m$). When these symmetries are replaced by the U's, a phase factor appears, $U_{k_1} \cdots U_{k_m} = e^{i\phi} U_1 \cdots U_m$, and the phase factor is gauge invariant. For example, in Eq. (20), the symmetries can be multiplied together in the order $aba^{-1}b^{-1}dcd^{-1}c^{-1}$, which gives the identity by assumption, or each symmetry can be grouped with its inverse, which also cancels to $\mathbb{1}$. We will now see that such phase factors can be identified by taking multiple chains and applying symmetries and permutations to them. This order parameter succeeds at identifying phase factors that the string-order selection rule fails to detect. In fact, it gives a complete way to distinguish between topological states, because Schur showed that every gauge-invariant phase factor in a projective representation has this form; see Appendix B.

The string order that isolates such a phase is illustrated in Fig. 9 for $m = 4$. Take m identical copies of the given state and place them side by side. Take three successive long segments L, M, and R. Now apply the symmetries to the middle segment and different permutations to the two ends (similar to the swap operator used in the case of time-reversal symmetry). This causes the U matrices at each of the ends of M to get multiplied together in two orders, which allows one to detect the phase factor. Figure 9 illustrates the order parameter for the simplest case of $U_a U_b U_a^{-1} U_b^{-1}$ (where Σ_a and Σ_b commute). The order parameter and its value are

$$\begin{aligned} \mathcal{S} &= \langle \psi_m | \pi_{(1\ 2 \cdots m-1\ m)}(L) \Sigma^{a_1}(M_1) \Sigma^{a_2}(M_2) \cdots \\ &\quad \times \Sigma^{a_m}(M_m) \pi_{(k_1\ k_2 \cdots k_{m-1}\ k_m)}(R) | \psi_m \rangle \\ &= (\mathrm{tr}\Lambda^{2m})^4 e^{i\phi}. \end{aligned} \tag{30}$$

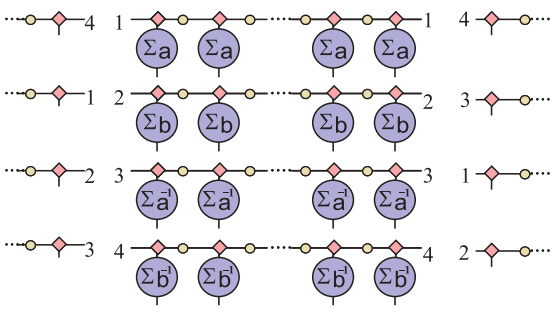

FIG. 9. (Color online) An illustration of a nonlocal order parameter for measuring the phases of local symmetries directly. A segment is chosen from the chains and divided into three consecutive sections. The symmetry operations are applied to the middle sections. The left and right sections are permuted such that the end points with the same number were connected to each other before applying the permutation. The order parameter is then obtained by calculating the overlap with the four original replicas of the state. The labels Γ and Λ have been left out so that the figure does not become too busy; furthermore, there are additional domain walls at the other ends of the segments L and R which are not shown.

Here $\pi_X(L)$ consists of permuting the left segments of the chains according to the permutation X (written as a cycle), $\Sigma^{a_k}(M_k)$ means to apply the symmetry a_k to the middle segment of the kth chain, and $\pi_X(R)$ indicates permuting the right segments. The wave function $|\psi_4\rangle$ is simply a product of m replicas of the ground state. To identify the phase factor in Eq. (20), (which cannot be found from the selection rule, unlike the $m = 4$ example), take $m = 8$ chains, and apply the symmetries $a, b, a^{-1}, b^{-1}, d, c, d^{-1}, c^{-1}$ to the legs of the ladder in the middle segment. Then apply the permutations (12345678) on the left segment and (13245768) on the right one, in order to get the U's to cancel with their inverses on the right and to obtain $(U_a U_b U_a^{-1} U_b^{-1} U_d U_c U_d^{-1} U_c^{-1})^*$ on the left, which is the phase we want to find. (We could also apply a bunch of two-cycles on the right end to get the same phase factor but multiplied by a different combination of Renyi entropies.)

This type of nonlocal order parameter distinguishes between all phases with a local symmetry group. Time-reversal and inversion symmetry phase factors can be determined as in the previous section. By combining all these ideas together, it should also be possible to measure phase factors that arise from combining spatiotemporal symmetries with local symmetries. (We have not yet worked out order parameters for groups that contain either inversion or time-reversal symmetry together with local symmetries, but it looks likely to work.)

V. TOPOLOGY OF NONLOCAL ORDER PARAMETERS

The phase-detecting string order (see Sec. IV B) is actually related to topological surfaces (which gives a justification in hindsight for calling these phases "topological"). It can be represented by a path integral on a topological surface, such as a torus, like the one in Fig. 10(a). To derive such a representation, the ground state is first expressed as

$$|\psi\rangle = \lim_{\beta \to \infty} e^{-\beta H} |\text{arbitrary state}\rangle, \tag{31}$$

i.e., time evolution from time $-\infty$ to zero. This is interpreted as a sum over all possible histories of the system in the half plane $-\infty < \tau < 0$, $-\infty < x < \infty$ (by subdividing time and introducing complete sets of intermediate states, as in the usual derivation of path integrals). Therefore the ground state is a partition function on the half plane with boundary conditions. The procedure for evaluating the wave function is then as follows: The system consists of a half plane with bonds sticking off the upper edge as in Fig. 10(b). The spins on the bonds on the edge are set equal to (j_i) and the partition function $Z(\{j_i\})$ is calculated as a function of these spins. The ground-state wave function is then given by $|\psi\rangle = \sum_{\{j_i\}} Z(\{j_i\}) |\{j_i\}\rangle$.

To evaluate a string operator such as $\langle a_1 a_2 \cdots a_n \rangle$ we sandwich the string between two copies of the wave function and contract all the bonds; see Figs. 10(c) and 10(d). The inner product $\langle \psi | \psi \rangle$ without the a's is represented by a partition function on the whole plane. Inserting the a's modifies the

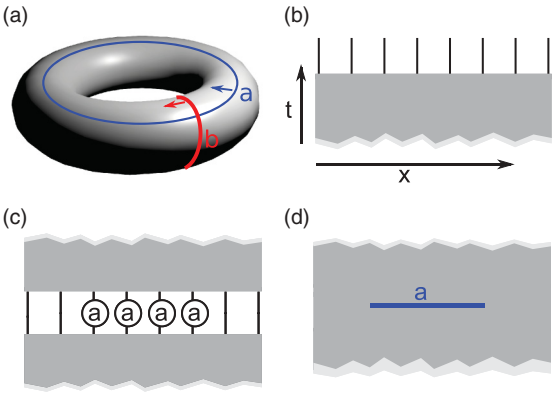

FIG. 10. (Color online) (a) String-order parameters are equivalent to path integrals on topological surfaces. This is derived by piecing different regions together. (b) The ground-state wave function is represented by a partition function on a half plane with bonds sticking off the lower edge. (c),(d) A simple string operator $\prod a_i$ sandwiched between two copies of the wave function is represented by a plane with a branch cut in it. The torus in (a) is derived by a more complicated gluing procedure.

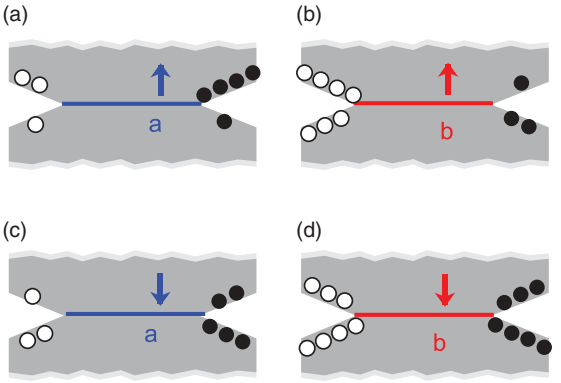

FIG. 11. (Color online) The first step in the gluing. Applying the symmetries to the four copies of the wave functions and then summing over the middle section produces these four patches. Applying the permutation operators and summing over the remaining spins will glue these together into a single surface: the rule for gluing is described by the black and the white dots, which are supposed to be matched with one another. In this figure, the orientation of the arrow represents whether the symmetry is supposed to be a or a^{-1}.

partition function by imposing a boundary condition that the state jumps by the symmetry operation a as the cut is crossed.

String orders that are proportional to topological quantities, as in Eq. (30), are more complicated combinations of strings. This string order can be translated into a geometrical representation by the same method—gluing together half planes in an appropriate way. As the half planes are joined together, they will fit together into a surface such as the torus in Fig. 10(a). The branch cuts will turn out to form closed loops. Such loops can be moved around arbitrarily without changing the value of the partition, which will explain why the partition function represents a topologically stable quantity.

The torus in Fig. 10(a) is built up like a paper model—the permutations play the role of instructions describing which tabs to glue together. We will illustrate this with the following string order:

$$\mathcal{S} = \langle\psi_4|\pi_{(1\ 3)(2\ 4)}(L)\Sigma^a(M_1)\Sigma^b(M_2)\Sigma^{a^{-1}} \times (M_3)\Sigma^{b^{-1}}(M_4)\pi_{(1\ 2\ 3\ 4)(R)}|\psi_4\rangle. \quad (32)$$

This gives the same topological quantity as in Fig. 9 (although it has a slightly different combination of permutations). For simplicity we let L and R extend off to infinity. To visualize the path integral representing $\mathcal{S}$, we will have to glue together eight copies of the wave function (four for the bra and four for the ket). We will start by gluing together these four copies along the *middle* section after applying the appropriate symmetry—see Fig. 11. Next deform all the shapes, as in Figs. 12(a)–12(d). This just prepares the shapes so that they will fit together nicely. Now paste the triangles together; see Fig. 12(e). Last, glue together all the other matching edges—that means gluing opposites sides of the square together so that a torus forms, as in Fig. 10(d); we call the partition function on this torus $Z_{\text{torus}}(a,b)$; it is a function of the group elements on the branch cuts.

We can now understand why the string order is topologically invariant. The partition function, or actually its ratio to

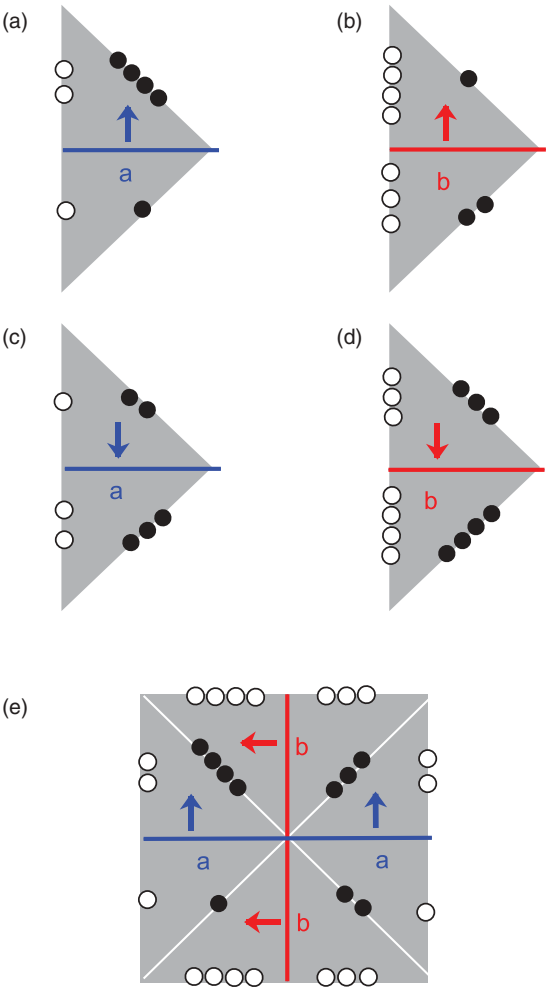

FIG. 12. Middle steps in the gluing. (a)–(d) Distorting the planar regions of the previous step into triangles. (e) Pasting the triangles together to form a square. The last gluings cause the square to be rolled into a torus.

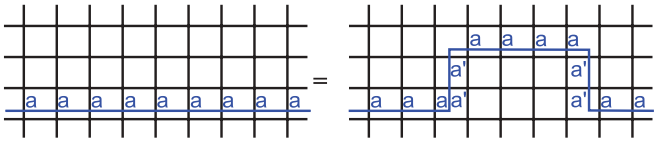

FIG. 13. (Color online) How one proves that the branch cuts can be moved around. The partition function has a microscopic representation as a grid of contracted tensors (each site of the lattice corresponds to a tensor T), and the branch cut is represented by matrices on the bonds of the tensors. The symmetry of each tensor implies that the branch cut can hop over a single site, and iterating this allows it to be transferred anywhere.

the one without branches, $Z_{\text{torus}}(a,b)/Z_{\text{torus}}(1,1)$, is constant in each phase. The branch curves can be moved around with negligible changes in the value of the partition function (as justified below). This implies that changing the Hamiltonian does not affect the ratio either, unless there is a phase transition. The change can be carried out over one part of the surface at a time. If it is changed first over a region that does not overlap the branch lines, then the change affects the numerator and denominator in the same way (because the correlations are short ranged), so the ratio is constant. Then the Hamiltonian can be changed in regions through which branch lines pass—-you can first move the branch line out of the way and then change the Hamiltonian.

That the branch cuts can be moved around depends on three properties. First, the branch cuts, after the surface is pasted, form closed curves (with matching arrows). If they had end points, the end points would not be able to move without changing the partition function. That is why only certain combinations of permutations give *topological* expectation values. Second, the a's must be symmetries of the Hamiltonian. If they are, the string can be moved around: this is easiest to see if the partition function is represented by a tensor network, as in Fig. 13. Each vertex is labeled with a tensor T. Since the system is symmetric, applying the right combination of a and a^{-1} operators to all the legs of T gives T back ($\sum_{u'l'r'd'} a_{uu'}\tilde{a}_{ll'}a^{-1}_{dd'}\tilde{a}^{-1}_{rr'}T_{l'r'u'd'} = T_{lrud}$, where a and $\tilde{a}$ stand for the symmetry on the horizontal and vertical bonds, respectively). Applying this relation allows one to move the string from one site to another, and repeating it many times can move the string anywhere. Third, the symmetries must commute. This is necessary so that the crossing points of the a and b loops can be moved around.

The inversion-symmetry and time-reversal-symmetry string orders also are related to a topological surface (a projective plane). The more general string-order parameters for complicated groups would be described by surfaces with a higher genus and more branch cuts on them. (The branch cuts generally do not have to form closed loops—three branch cuts can come together like branching leaf veins as long as the product of the three group elements on them is the identity.) These partition functions describe a surface with a gauge flux through its holes; this is a foreshadowing of how symmetry-protected phases in two dimensions can be understood by applying gauge fields with the same symmetry group as the phase.[28]

VI. SUMMARY

We have given two ways to distinguish among topological phases in one dimension (phases which cannot be characterized by local order parameters). The first approach is more suitable for numerical calculations: given a wave function in matrix-product form, one can directly calculate the projective representations of the symmetry group (by diagonalizing a transfer matrix), and from that the factor set, which is known to define these phases. Note that, while degeneracies in the entanglement spectrum can indicate a nontrivial topological state, they might also be caused by other effects. Actually calculating the factor set gives definite proof that a state is topological. Furthermore, for a given symmetry group, there may be several distinct topological states, all of which would have similar degeneracies in the entanglement spectrum, but which have distinct factor sets.

The second approach is more physical, as it involves measurements on the actual spins or atoms that make up the system, rather than on the matrix-product state. In this approach, a phase is defined by the value of a nonlocal string order. This characterization provides more insight into the nature of these phases and could be implemented on a state defined by Monte Carlo simulations, or possibly a real system. The ordinary string order of the Haldane phase can be explained using a selection rule that changes at the critical point: there are two types of string order (depending on the operators at the ends of the string) one which vanishes in the trivial phase, and one which vanishes in the nontrivial one. This order parameter can be generalized to many cases, but not to all groups. An alternative order parameter that directly measures the "projective phases" is required to distinguish among phases in general. Such an order parameter works for all cases, including time-reversal and inversion symmetry, and complicated local symmetry groups. Intriguingly, this parameter involves measuring expectation values of string operators on multiple copies of the system, even though these copies are uncorrelated. We show for this generalized nonlocal order parameter how it is actually related to topological surfaces.

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APPENDIX A: EXAMPLE OF A PHASE THAT CANNOT BE DETECTED BY STRING-ORDER SELECTION RULES

Let us assume that a state is invariant under a symmetry group G which fulfills the group algebra $aba^{-1}b^{-1} = x = cdc^{-1}d^{-1}$. (We simplify the expressions by writing $a,b,\ldots$ instead of $\Sigma_a,\Sigma_b,\ldots$.) Then $U_aU_bU_a^{-1}U_b^{-1}U_dU_cU_d^{-1}U_c^{-1} = e^{i\phi}\mathbb{1}$ is gauge invariant and does not look easy to detect by using the selection rule for string order from Sec. IV A. But this is not completely obvious. In fact, if a and b both commute with both c and d, then we can rearrange $aba^{-1}b^{-1}dcd^{-1}c^{-1}$ into $(ad)(bc)(ad)^{-1}(bc)^{-1} = 1$. Thus ad

and bc commute, allowing us to define a phase $\phi_{ad;bc}$ (in general, we define ϕ_{g_1,g_2} for commuting symmetries g_1,g_2 as the phase of $U_{g_1}U_{g_2}U_{g_1}^{-1}U_{g_2}^{-1}$). The phase ϕ can be expressed in terms of it. In fact, rearranging the expression for $e^{i\phi}$ and remembering to keep track of the phases that might arise from exchanging, e.g., U_a and U_c (on account of the topological order), we find that $\phi = \phi_{b;d} - \phi_{a;c} + \phi_{ad;bc}$, so ϕ reduces to simpler phase factors which can all be determined by using the string-order selection rule.

More pairs of symmetries must be noncommuting to ensure that there is no way to simplify ϕ. We will introduce the following group algebra, with c and d relabeled c_1 and c_2:

$$\begin{aligned} &aba^{-1}b^{-1} = x, \quad c_1c_2c_1^{-1}c_2^{-1} = x, \quad ac_1a^{-1}c_1^{-1} = y_1, \\ &ac_2a^{-1}c_2^{-1} = y_2, \quad bc_1b^{-1}c_1^{-1} = bc_2b^{-1}c_2^{-1} = 1. \end{aligned} \tag{A1}$$

Besides the original symmetries a,b,c_1,c_2,x we have introduced additional symmetries y_1,y_2 as the commutators of some of them. Aside from these conditions, we assume that all the generators square to 1. This group has 128 elements. The algebraic relations defining it are complicated generalizations of the quaternion group; for example, the first equation corresponds to the commutator of $i\sigma_x$ and $i\sigma_y$ being $-\mathbb{1}$, which commutes with everything and squares to $\mathbb{1}$ as x does.

Example of "undetectable" projective phase factors for this group. We can write the elements in the group as products of a,b,c_1,c_2 and x,y_1,y_2. The numbers of a,b,c_1,c_2 factors are each the same modulo 2 no matter how we rearrange the factors. So define $n_a(g)$ and $n_b(g)$ to be the number of a's and b's appearing modulo 2. Assume the following projective phase factors:

$$U_{g_1}U_{g_2} = e^{i\rho(g_1,g_2)}U_{g_1g_2} = e^{i\pi n_a(g_2)n_b(g_1)}U_{g_1g_2}. \tag{A2}$$

[To create an example of an undetectable phase factor, we want a minus sign to appear in the first of Eqs. (A1) on replacing the symmetries by their U matrices, and we want this to be the only phase factor that appears. These conditions lead to Eq. (A2).] It is easy to check that this definition is consistent, i.e., that $\rho(g_1g_2,g_3) + \rho(g_1,g_2) = \rho(g_2,g_3) + \rho(g_1,g_2g_3)$ The calculation starts from the linearity of n_a and n_b, e.g., $n_a(g_1g_2) = n_a(g_1) + n_a(g_2)$ (mod 2).

Now let us show first that this is a nontrivial phase (by showing that there is a nontrivial phase factor defined using four symmetries) and second that this phase cannot be detected using a string-order selection rule, because all the commuting pairs of elements g_1 and g_2 also commute in the projective representation. Hence this is a nontrivial phase without any signature in the ordinary string order.

The phase is nontrivial as $U_aU_bU_a^{-1}U_b^{-1} = -U_x$ while $U_{c_1}U_{c_2}U_{c_1}^{-1}U_{c_2}^{-1} = U_x$. Hence the gauge-invariant phase factor from these four symmetries is -1.

However, *all* two-symmetry*phase factors are trivial*. To show this, we have to enumerate (at least partly) all the pairs g,g' of symmetries that commute, and then check that the U's for them also commute. Write $g = za^{n_a}b^{n_b}c_1^{n_1}c_2^{n_2}$ and $g' = z'a^{n'_a}b^{n'_b}c_1^{n'_1}c_2^{n'_2}$, where the n's are each 0 or 1 and the z's are products of some combination of x, y_1, and y_2 (i.e., elements of the center of the group). Since the commutators of any two of a,b,c_1,c_2 are in the center, the commutator of g and g' can be calculated by evaluating the commutators of their factors one pair at a time:

$$gg'g^{-1}g'^{-1} = x^{n_an'_b+n_bn'_a+n_1n'_2+n_2n'_1}y_1^{n_an'_1+n_1n'_a}y_2^{n_an'_2+n_2n'_a}. \tag{A3}$$

We want g and g' to commute, so the exponents of x, y_1, and y_2 must be zero modulo 2. We will then want to calculate $U_gU_{g'}U_g^{-1}U_{g'}^{-1}$, which according to Eq. (A2) is $(-1)^{n_an'_b+n_bn'_a}$.

In order for g and g' to commute, the exponents of the y's must vanish:

$$n_an'_1 + n'_an_1 \equiv n_an'_2 + n'_an_2 \equiv 0 \mod 2. \tag{A4}$$

Consider all four possible combinations of values for n_a and n'_a. First, if $n_a = n'_a = 0$, then U_g and $U_{g'}$ commute because $n_an'_b + n_bn'_a = 0$. Second, if $n_a = 1$ and $n'_a = 0$, then we must have $n'_1 = n'_2 = 0$ by Eq. (A4). This implies that $g' = z'$ or $z'b$. But this commutes with g only in the former case (since g has a factor of a in it and this does not commute with b), while there is a nontrivial phase factor only in the latter case. The remaining two cases are similar.

Hence this group is an example where the regular string-order selection rule we described in Sec. IV A does not help to identify this phase, while the alternative type of order in Sec. IV B does.

APPENDIX B: SCHUR'S THEOREM ON PROJECTIVE REPRESENTATIONS

Schur classified the types of projective representations (which are also known as the "Schur multipliers"); the result[29] implies that all one-dimensional phases, at least those with local symmetry groups, can be recognized using the order parameter of Sec. IV B. Schur's theorem says that the classes of projective representations of a group are in one-to-one correspondence with the characters $e^{i\phi(\gamma)}$ on the group $([F,F] \cap R)/[R,F]$.

We will now explain what these terms mean and how the theorem comes about. The gauge-invariant phase factors we have found involve products such as $U_aU_bU_a^{-1}U_b^{-1}U_dU_cU_d^{-1}U_c^{-1}$ where a,b,c,d are generators of the group. This phase factor can be defined by listing the sequence of group elements that have to be multiplied together: $\{a,b,a^{-1},b^{-1},d,c,d^{-1},c^{-1}\}$, without actually multiplying them. It is convenient to regard such sequences as forming a group (a "free group"): to multiply two sequences, juxtapose them and cancel elements with their inverses when they meet each other. This structure is useful because it makes it possible to break phase factors down to simpler ones (for example, repeating the string just given twice does not give a new phase factor, just the square of the original one).

The sequences that give a gauge-invariant phase factor form a group, which Schur's theorem describes. In general, let the symmetry group be G and let $x_1,\ldots,x_k$ be a set of symmetries that generate it; call the set of sequences of these generators the free group F. Let $[F,F]$ be the group generated by commutators of two elements of F. (Similarly, one can define the commutator of any two subgroups $[A,B]$.) Consider also the set R of sequences whose product is equal to the identity. A sequence that lies in both these subgroups determines a gauge-invariant phase factor; that is, there is a function $e^{i\phi(\gamma)}$

defined on $\gamma \in [F,F] \cap R$. Because γ is an element of R, it gives a phase when the corresponding U's are multiplied together, and these phases are invariant because elements of $[F,F]$ are products of commutators, that is, they have the form $\{a_1,b_1,a_1^{-1},b_1^{-1},\ldots,a_l,b_l,a_l^{-1},b_l^{-1}\}$ where the a's and b's are various elements of F. The theorem of Schur states that all gauge-invariant phase factors are contained in this function. In addition, the theorem finds all the conditions that have to be satisfied by these phases (such as when one of the phases has to be ± 1); the general rule is that $\phi(\gamma) = 0$ when $\gamma \in [R,F]$. Relations such as $e^{i\phi(\gamma)} = \pm 1$ follow: squaring $e^{i\phi(\gamma)}$ gives $e^{i\phi(\gamma^2)}$, which must equal 1 if $\gamma^2 \in [R,F]$. Now all these statements can be recast by saying that $e^{i\phi(\gamma)}$ is a character for the group $([F,F] \cap R)/[R,F]$, and that is essentially Schur's theorem.

For example, consider $Z_2 \times Z_2$. Let a and b be the two generators. Then $x = \{a,b,a^{-1},b^{-1}\}$ is an element of R because a and b commute as elements of the group $Z_2 \times Z_2$. It is also an element of $[F,F]$, so it defines a phase factor $e^{i\phi_{ab}}$. Now the second part of the theorem implies that this phase factor is equal to ± 1. To see this, we will show that $x^2 \in [R,F]$, which implies $(e^{i\phi(x)})^2 = e^{i\phi(x^2)} = 1$. That $x^2 \in [R,F]$ is implied by the following relationship (where the commas represent multiplication in the free group): $x^2 = (\{x,a,x^{-1},a^{-1}\},\{a^2,b,a^{-2},b^{-1}\})$. This is in $[R,F]$ because x and a^2 are both in R.

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