



Entanglement spectrum of a topological phase in one dimension

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We show that the Haldane phase of $S=1$ chains is characterized by a double degeneracy of the entanglement spectrum. The degeneracy is protected by a set of symmetries (either the dihedral group of π rotations about two orthogonal axes, time-reversal symmetry, or bond centered inversion symmetry), and cannot be lifted unless either a phase boundary to another, “topologically trivial,” phase is crossed, or the symmetry is broken. More generally, these results offer a scheme to classify gapped phases of one-dimensional systems. Physically, the degeneracy of the entanglement spectrum can be observed by adiabatically weakening a bond to zero, which leaves the two disconnected halves of the system in a finitely entangled state.

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I. INTRODUCTION

A topological phase is a phase of matter which cannot be characterized by a local order parameter, and thus falls beyond the Landau paradigm of condensed matter physics. Topological phases are often characterized by a gap separating excitations from the ground state in the bulk and by the presence of gapless edge modes. The existence of edge excitations implies that a topological phase cannot be deformed continuously into a conventional, topologically trivial phase without going through a phase transition, in which the gap closes and the edge mode merges with the bulk.

The Haldane phase of integer spin chains^{1,2} is an example of a “symmetry protected topological phase” in one dimension.³ This phase appears also in other one-dimensional systems, such as chains of interacting bosons⁴ and fermions.⁵ These gapped phases lack a local order parameter, and are not amenable to a description by a site factorizable wave function. Alternatively, in certain cases, the Haldane phase can be characterized by the existence of fractionalized edge excitations, by a nonvanishing nonlocal “string” order parameter or, as recently proposed, by a quantized Berry phase.^{6–8}

However, in the most general case, the description of the Haldane phase in terms of a string order parameter or spin- $\frac{1}{2}$ edge states is insufficient. As we will demonstrate below, slightly deforming the Hamiltonian can destroy the string order parameter (which is known to be fragile to small perturbations⁹) and lift the degeneracy of the edge states. Yet, as long as an appropriate set of symmetries is preserved, the Haldane phase is stable,^{3,10} in the sense that it is still separated from other, topologically trivial phases by a thermodynamic phase transition in which the gap closes. This stability, by itself, can be used as an operational definition of the Haldane phase. However, it is desirable to find a definition which can be stated in terms of the ground-state wave func-

tion of a single Hamiltonian. Recently, it has been proposed that topological phases can be characterized by their “entanglement spectrum,” obtained by arbitrarily dividing the system into two parts, tracing out one half and diagonalizing the reduced density matrix of the other.^{11–16} This creates artificial edges, without disrupting inversion symmetry. For example, the entanglement spectrum of the Affleck-Kennedy-Lieb-Tasaki (AKLT) state¹⁷ consists of two degenerate nonzero eigenvalues, which mimic the doubly degenerate energy edge spectrum of a system with a physical boundary.¹⁸

In this paper, we show that the Haldane phase is characterized by a double degeneracy of the entire entanglement spectrum. This degeneracy is caused by the same set of symmetries which protect the stability of the Haldane phase, applied to the eigenstates of the reduced density matrix. If the Hamiltonian is deformed while keeping these symmetries intact, the degeneracy remains until a phase boundary is crossed. This symmetry-protected double degeneracy can be used to define the Haldane phase in the most general situation, when both gapless edge states and a string order parameter are absent.

The most surprising result of the analysis is that inversion symmetry alone is enough to preserve the degeneracy of the entanglement spectrum. If this is the only symmetry present, there are no gapless edge modes, since edges break inversion symmetry. There is also no conventional string order, either.¹⁹

This approach can be used to classify the phases of any one-dimensional system, given its symmetry group. For a given set of symmetries, there are several types of gapped phases. One of them is the “nondegenerate” (or “trivial”) phase, in which the eigenvalues of the density matrix can be nondegenerate. Besides this, there can be several types of “degenerate” (“nontrivial”) phases. The entanglement spectrum in any one of the latter phases has at least twofold

degeneracy. In this case, the density-matrix eigenstates transform in a nontrivial way under a *projective* representation of the symmetry group.

The entanglement spectrum, although being associated with a partition of the system at a certain point in space, actually carries highly nonlocal information about the ground-state wave function. We show that the double degeneracy of the entanglement spectrum has a simple physical consequence. If one of the bonds of the system is adiabatically weakened until its strength reaches zero, the symmetry of the Hamiltonian continues to retain the degeneracy in the entanglement spectrum across the weakened bond. Hence, the von Neumann entropy of the partition in the final state is equal to $\ln(2)$ once the bond is broken. This is a physical reflection of the entanglement in the ground state and can, in principle, be used to identify it in experiment.

This paper is organized as follows. First we introduce in Sec. II a spin-1 model Hamiltonian which has a Haldane phase for a certain parameter range. In Sec. III, we briefly review some properties of matrix-product states, which we use to study properties of the entanglement spectrum, and show how matrix-product states transform under symmetry operations. The main result of this paper, namely, the degeneracy of the entanglement spectrum in the Haldane phase, is derived in Sec. IV. Numerical results for several model Hamiltonians with different symmetries are shown in Sec. V. In Sec. VI we briefly outline the generalization of these results toward a classification scheme of gapped phases in one dimension. A more detailed discussion is deferred to a later publication.²⁰ A numerical experiment, which sheds light on the physical consequences of the degeneracy of the entanglement spectrum, is presented in Sec. VII. Finally, the results and conclusions are summarized in Sec. VIII. Some details, concerning the application of the above results to generalizations of the Haldane phase and a derivation of the properties of the Haldane phase under inversion, are discussed in the appendices.

II. MODEL HAMILTONIANS

In order to study the stability of the Haldane phase, we will mainly focus on various spin-1 model Hamiltonians with different symmetries. As we will prove in Sec. IV, the Haldane phase is protected by certain symmetries. One of them is a symmetry under a bond-centered spatial inversion

$$S_j^{x,y,z} \rightarrow S_{-j+1}^{x,y,z}, \quad (1)$$

where $S_j^{x,y,z}$ are the spin-1 operators at site j . Other possible symmetries are the time reversal (TR) symmetry

$$S_j^{x,y,z} \rightarrow -S_j^{x,y,z} \quad (2)$$

or the symmetry with respect to spin rotations by π about a pair of orthogonal axes. As long as *at least one* of these symmetry groups is not broken, the entire entanglement spectrum remains doubly degenerate. Therefore, the Haldane phase maintains its identity and cannot evolve adiabatically to another phase.

For concreteness, throughout most of this paper we consider the following spin-1 model Hamiltonian:

$$H_0 = J \sum_j \vec{S}_j \cdot \vec{S}_{j+1} + B_x \sum_j S_j^x + U_{zz} \sum_j (S_j^z)^2. \quad (3)$$

The symmetries of this model include translation, spatial inversion, a rotation by π around the x axis, and a combination of a rotation by π around the y axis and time-reversal $e^{-i\pi S^y} \times \text{TR}$ (which takes $S_j^{x,z} \rightarrow S_j^{x,z}, S_j^y \rightarrow -S_j^y$).

The phase diagram has been studied in Ref. 3. At large U_{zz} , we find a trivial insulator phase which can be described by a caricature state where all the sites are in the $|S^z=0\rangle$ state. Furthermore, we find 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. $U_{zz}=B_x=0$ is the Heisenberg point, for which one finds the gapped Haldane phase. Even when nonzero U_{zz} and B_x values are introduced into this Hamiltonian, the Haldane phase is separated from the “nondegenerate phases” by phase transitions. Here, we investigate the question of what defines the Haldane phase and thus protects these transitions from becoming smooth crossovers. We will later add different terms to H_0 which break various symmetries, and show explicitly for which classes of perturbations the Haldane phase remains well defined.

III. MATRIX PRODUCT STATE REPRESENTATION

A. Definitions

In order to prove the above statements, we will use a matrix product state (MPS) representation²¹ of the ground-state wave function. We also use this representation to compute the ground-state properties numerically, using the infinite time-evolving block decimation (iTEBD) method.²² The iTEBD method is a descendent of the density-matrix renormalization-group method.²³ For the sake of completeness, we now review some of the properties of MPS's. A translationally invariant MPS for a chain of length L can formally be written in the following form:²⁴

$$|\Psi\rangle = \sum_{\{m_j\}} \text{tr}[\Gamma_{m_1} \Lambda \dots \Gamma_{m_L} \Lambda] |m_1 \dots m_L\rangle. \quad (4)$$

Here, Γ_m are $\chi \times \chi$ matrices with χ being the dimension of the matrices used in the MPS. The index $m = -S, \dots, S$ is the “physical” index, e.g., enumerating the spin states on each site, and Λ is a $\chi \times \chi$, real, diagonal matrix with non-negative matrix elements. Ground states of one-dimensional gapped systems can be efficiently approximated by matrix-product states,^{25–27} 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 $L \rightarrow \infty$. We therefore think of χ as being a finite (but arbitrarily large) number.

The matrices Γ, Λ can be chosen such that they satisfy the canonical conditions for an infinite MPS (Refs. 28 and 29)

$$\sum_m \Gamma_m \Lambda^2 \Gamma_m^\dagger = \sum_m \Gamma_m^\dagger \Lambda^2 \Gamma_m = 1. \quad (5)$$

These equations can be interpreted as stating that the transfer matrix

$$T_{\alpha\alpha':\beta\beta'} = \sum_m \Gamma_{m\beta}^\alpha (\Gamma_{m\beta'}^{\alpha'})^* \Lambda_\beta \Lambda_{\beta'} \quad (6)$$

has a right eigenvector $\delta_{\beta\beta'}$ with eigenvalue $\lambda=1$. (* denotes complex conjugation.) Similarly, $\tilde{T}_{\alpha\alpha':\beta\beta'} = \sum_m (\Gamma_{m\beta'}^{\alpha'})^* \Gamma_{m\beta}^\alpha \Lambda_\alpha \Lambda_{\alpha'}$ has a left eigenvector $\delta_{\alpha\alpha'}$ with $\lambda=1$. We further require that $\delta_{\alpha\alpha'}$ is the *only* eigenvector with eigenvalue $|\lambda| \geq 1$ (which is equivalent to the requirement that $|\psi\rangle$ is a pure state³⁰).

The considerations given here become most intuitive when one considers, formally, an infinite chain. If the chain is infinite and has open ends, it may be partitioned at a certain bond. The wave function can then be Schmidt decomposed³¹ in the form

$$|\Psi\rangle = \sum_\alpha \lambda_\alpha |\alpha L\rangle |\alpha R\rangle, \quad (7)$$

where $|\alpha L\rangle$ and $|\alpha R\rangle$ ($\alpha=1, \dots, \chi$) are orthonormal basis vectors of the left and right partitions, respectively. In the limit $L \rightarrow \infty$, and under the canonical conditions [Eq. (5)], the Schmidt eigenvalues λ_α are simply the entries of the Λ matrix, $\Lambda_\alpha, \lambda_\alpha^2$ are the eigenvalues of the reduced density matrix of either of the two partitions, and are referred to as the *entanglement spectrum*. The entanglement entropy is $S = -\sum_\alpha \lambda_\alpha^2 \ln \lambda_\alpha^2$. This corresponds to the von Neumann entropy of the reduced density matrix. 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, e.g., if the broken bond is between sites 0 and 1, $|\alpha L\rangle = \sum_{\{m_j\}, j=0} [\prod_{k=0} \Lambda \Gamma_{m_k}]_{\gamma\alpha} |\dots m_{-2} m_{-1} m_0\rangle$. 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. 29 and 32.

B. Symmetries in matrix product states

In order to study the consequences of symmetries of the wave functions, it is useful to first study how these symmetries are reflected in the MPS representation. If $|\Psi\rangle$ is invariant under a *local symmetry*, which is represented in the spin basis as a unitary matrix $\sum_{mm'}$, then the Γ matrices can be shown to satisfy³⁰

$$\sum_{m'} \sum_{mm'} \Gamma_{m'} = e^{i\theta_\Sigma} U_\Sigma^\dagger \Gamma_m U_\Sigma, \quad (8)$$

where U_Σ is a unitary matrix which commutes with the Λ matrices, and $e^{i\theta_\Sigma}$ is a phase. Thus, the matrices U_Σ form a χ -dimensional (projective) representation of the symmetry group of the wave function. In close analogy to the derivation in Ref. 30, we can derive a similar relation to Eq. (8) for time-reversal and inversion symmetry. For a time-reversal transformation $\Gamma_{m'}$ is replaced by $\Gamma_{m'}^*$ (complex conjugate) on the left-hand side. Finally, in the case of inversion symmetry $\Gamma_{m'}$ is replaced by $\Gamma_{m'}^T$ (transpose) on the left-hand side of Eq. (8).

IV. DEGENERACIES IN THE ENTANGLEMENT SPECTRUM

We now turn to derive our main result, namely, the degeneracies in the entanglement spectrum of the wave function in the Haldane phase. Our strategy is to determine when the transformation law for the Schmidt eigenstates under the symmetry operations of the system is nontrivial. From Eq. (8), the Schmidt eigenstates of the left half of the system, $|\alpha L\rangle$, transform under a symmetry operation Σ according to the following rule:

$$\Sigma |\alpha L\rangle = \sum_\beta (U_\Sigma)_{\beta\alpha} |\beta L\rangle. \quad (9)$$

Similarly, the right Schmidt states $|\alpha R\rangle$ transform by the conjugate matrix. Thus, the Schmidt eigenstates transform according to a projective representation of the symmetry group of the system. The phases of the matrices U_Σ are not uniquely determined by Eq. (8), or by Eq. (9). The phase ambiguities turn out to be the key to proving the degeneracies of the entanglement spectrum. We will show that for certain symmetries, there can be situations where *the irreducible representations present in U_Σ are all multidimensional*. In these cases, which are identified with the Haldane phase (or a generalization of it), the entire entanglement spectrum has nontrivial degeneracies.

A. Inversion symmetry

As a first example, let us consider a system which is symmetric under spatial inversion. The transformation law of Γ is written as

$$\Gamma_m^T = e^{i\theta_I} U_I^\dagger \Gamma_m U_I, \quad (10)$$

where U_I is a unitary matrix and $\theta_I \in [0, 2\pi)$ is a phase. Iterating this relation twice gives

$$\Gamma_m = e^{2i\theta_I} (U_I U_I^\dagger)^\dagger \Gamma_m U_I U_I^*. \quad (11)$$

Now, the relation implies that

$$\sum_m \Gamma_m^\dagger \Lambda U_I U_I^* \Lambda \Gamma_m = e^{2i\theta_I} U_I U_I^*, \quad (12)$$

where we have used Eq. (5) and the fact that $[U_I, \Lambda]=0$. Thus $U_I U_I^*$ is an eigenvector of the transfer matrix T [Eq. (6)] with eigenvalue $e^{2i\theta_I}$. Since by our assumption, the only unimodular eigenvalue of T is $\lambda=1$ and this eigenvalue is unique, we find that $e^{2i\theta_I}=1$ and $U_I U_I^* = e^{i\phi_I}$ where ϕ_I is a phase. Hence $U_I^T = U_I e^{-i\phi_I}$. Repeating this relation twice, we find that $e^{-2i\phi_I}=1$, i.e., $\phi_I=0$ or π .

If $\phi_I=\pi$, then U_I is an antisymmetric matrix. From this we find that all the eigenvalues Λ_α are *at least* doubly degenerate. Moreover, the corresponding multiplicity k_α is even for all α . This follows from the fact that U_I transforms the k_α -dimensional subspace of states with eigenvalue Λ_α within itself. Therefore, the matrix U_I^α (projected into subspace α) satisfies $\det U_I^\alpha = \det [(U_I^\alpha)^T] = \det (-U_I^\alpha) = (-1)^{k_\alpha} \det U_I^\alpha$. But since U_I^α is unitary, $\det U_I^\alpha \neq 0$ and therefore $(-1)^{k_\alpha}=1$.

The fact that, in the presence of inversion symmetry, the phase ϕ_I can only take discrete values (0 or π), leads to

phase transitions between states when one would not expect them on the basis of the Landau paradigm of broken symmetry. If an inversion-symmetric wave function evolves continuously, its characteristic phase $\phi_{\mathcal{T}}$ cannot change discontinuously, and therefore its value is fixed. The only way $\phi_{\mathcal{T}}$ can change is through a critical point, where either the correlation length diverges because the transfer matrix T has a pair of unimodular eigenvectors (and the main relation, $U_I^* U_I = e^{i\phi_{\mathcal{T}}}$ cannot be proven) or there is simply a discontinuous change in the ground-state wave function (i.e., a first-order transition). We can therefore identify two distinct states, characterized by $\phi_{\mathcal{T}}=0, \pi$. The state with $\phi_{\mathcal{T}}=\pi$ can be identified with the Haldane phase. To show this, we consider the AKLT state with $\Gamma_a = \sigma_a$, $\Lambda = \frac{1}{\sqrt{2}}\mathbb{1}$, where σ_a ($a=x, y, z$) are Pauli matrices. We are here using the time-reversal invariant spin basis $|x\rangle = \frac{1}{\sqrt{2}}(|1\rangle - |-1\rangle)$, $|y\rangle = \frac{i}{\sqrt{2}}(|1\rangle + |-1\rangle)$, and $|z\rangle = |0\rangle$. Under inversion, $\sigma_a \rightarrow \sigma_a^T = -\sigma_y \sigma_a \sigma_y$, and thus $U_{\mathcal{T}} = \sigma_y$ and $\theta_{\mathcal{T}} = \pi$. Since $\sigma_y \sigma_y^* = -\mathbb{1}$, we find that $e^{i\phi_{\mathcal{T}}} = -1$. The AKLT state is known to describe the same phase as the Haldane phase.¹⁷ Therefore, we conclude that the Haldane phase is characterized by $e^{i\theta_{\mathcal{T}}} = -1$ and $e^{i\phi_{\mathcal{T}}} = -1$, and a doubly degenerate entanglement spectrum. The wave function cannot evolve continuously if the phases $\theta_{\mathcal{T}}$ or $\phi_{\mathcal{T}}$ change discontinuously. This implies that changes in $\theta_{\mathcal{T}}$ or $\phi_{\mathcal{T}}$ between 0 and π are always accompanied by a phase transition. Consequently, the degeneracy in the Haldane phase can only be lifted by a phase transition. The full argument for the existence of a transition in such cases appears in Ref. 33.

In the discussion above, we have assumed that the system is invariant under both inversion and translation [see Eq. (4)]. However, in fact, inversion symmetry alone is sufficient to protect the double degeneracy in the entanglement spectrum, as long as it is bond centered. To show this, one can imagine adding a general commensurate perturbation to the Hamiltonian, such that the unit cell is enlarged. One can still write the ground-state wave function in a translationally invariant form [Eq. (4)] where each site represents a single unit cell. If the unit cell is defined such that it ends at an inversion-symmetric bond, the new system is also inversion symmetric, and the entanglement spectrum degeneracy remains protected. Since the size of the unit cell can be arbitrarily large, it is clear that translational symmetry cannot be essential for this argument to hold. The same argument can be made in the case of local symmetries, such as the ones described in Secs. IV B and IV C.

B. Time-reversal symmetry

The transformation of the MPS wave function Γ matrices under TR has the form

$$\sum_{m'} (\Sigma_{\mathcal{T}})_{mm'} \Gamma_{m'}^* = e^{i\theta_{\mathcal{T}}} U_{\mathcal{T}}^\dagger \Gamma_m U_{\mathcal{T}}. \quad (13)$$

Here we have used the S^z basis for the spins ($m = -1, 0, 1$) and $\Sigma_{\mathcal{T}} = e^{i\pi S^y}$. From this, one can derive (in close analogy with the case of spatial inversion) that $U_{\mathcal{T}} U_{\mathcal{T}}^* = e^{i\phi_{\mathcal{T}}}$, where $\phi_{\mathcal{T}}$ can be either 0 or π . If $e^{i\phi_{\mathcal{T}}} = -1$, then the double degen-

eracy of the entanglement spectrum follows (precisely as in the previous section). The AKLT state Γ matrices transform as $\Gamma_m \rightarrow \sigma_y \Gamma_m \sigma_y$. Thus $U_{\mathcal{T}} = \sigma_y$ and time-reversal symmetry is sufficient to protect the double degeneracy of the entanglement spectrum in the Haldane phase. Note that $\theta_{\mathcal{T}}$ is not well-defined because it depends on the phase of the wave function.

The transformation of the MPS wave function Γ matrices under $e^{-i\pi S^y} \times \text{TR}$ corresponds to a complex conjugation (\mathcal{CC}) of the wave function and has the form

$$\Gamma_m^* = e^{i\theta_{\mathcal{CC}}} U_{\mathcal{CC}}^\dagger \Gamma_m U_{\mathcal{CC}}. \quad (14)$$

From this, one can derive that $U_{\mathcal{CC}} U_{\mathcal{CC}}^* = e^{i\phi_{\mathcal{CC}}}$, where $\phi_{\mathcal{CC}}$ can be either 0 or π . The AKLT state Γ matrices transform as $\Gamma_m \rightarrow \Gamma_m$. It follows that $U_{\mathcal{CC}} = \mathbb{1}$ and thus $e^{-i\pi S^y} \times \text{TR}$ alone is *not sufficient* to protect the double degeneracy of the entanglement spectrum in the Haldane phase. Physically, this means that it is possible to add to the Hamiltonian a perturbation which is invariant under $e^{-i\pi S^y} \times \text{TR}$ but destroys the Haldane phase, in the sense that it is no longer separated from an unentangled product state by a phase transition. This perturbation has to break all other symmetries that may protect the Haldane phase (an example of such a perturbation can be found in Sec. V).

C. Sets of rotations

A symmetry of rotation about a single axis by $\frac{2\pi}{n}$, where n is an integer, does not lead to any classification of phases. If Σ is a rotational symmetry of order n , one can show that $U_\Sigma^n = e^{i\phi}$ as in the previous section. Rescaling U_Σ by $e^{i\phi/n}$ leaves Eq. (8) satisfied, and shows that ϕ has no significance. However, when there are multiple symmetries, there is also a phase for each pair of symmetries Σ_1 and Σ_2 . This phase is defined by noting that the transformation of Schmidt states corresponding to $\Sigma_1 \Sigma_2$ can differ by a phase from the product of the Schmidt state representations of Σ_1 and Σ_2

$$U_{\Sigma_1} U_{\Sigma_2} = e^{i\rho(\Sigma_1, \Sigma_2)} U_{\Sigma_1 \Sigma_2}. \quad (15)$$

If the phase $\rho(\Sigma_1, \Sigma_2)$ cannot be gauged away by redefining the phases of $U_{\Sigma_{1,2}}$, then the combined symmetry can lead to a protected Haldane phase.

A concrete example is a system with symmetry under the dihedral group D_2 of π rotations about three orthogonal axes (say, x , y , and z axes). Since the product of π rotations about the x and z axes $\mathcal{R}_x \mathcal{R}_z$ or $\mathcal{R}_z \mathcal{R}_x$ give a π rotation about the y axis \mathcal{R}_y , the group is equivalent to $Z_2 \times Z_2$. Thus it is sufficient to consider the action of two generators, say \mathcal{R}_x and \mathcal{R}_z . For \mathcal{R}_x ,

$$\sum_{m'} (\Sigma_x)_{mm'} \Gamma_{m'} = e^{i\theta_x} U_x^\dagger \Gamma_m U_x, \quad (16)$$

where $\Sigma_x = e^{i\pi S^x}$. Repeating this relation twice, we get $\Gamma_m = e^{2i\theta_x} (U_x^\dagger)^2 \Gamma_m U_x^2$. From this it follows [analogously to the arguments below Eq. (12)] that $e^{2i\theta_x} = 1$ and $U_x^2 = e^{i\phi_x}$. The phase factor $e^{i\phi_x}$ is not important, since it can be absorbed in U_x . Therefore we can assume that $U_x^2 = \mathbb{1}$. Similarly for \mathcal{R}_z ,

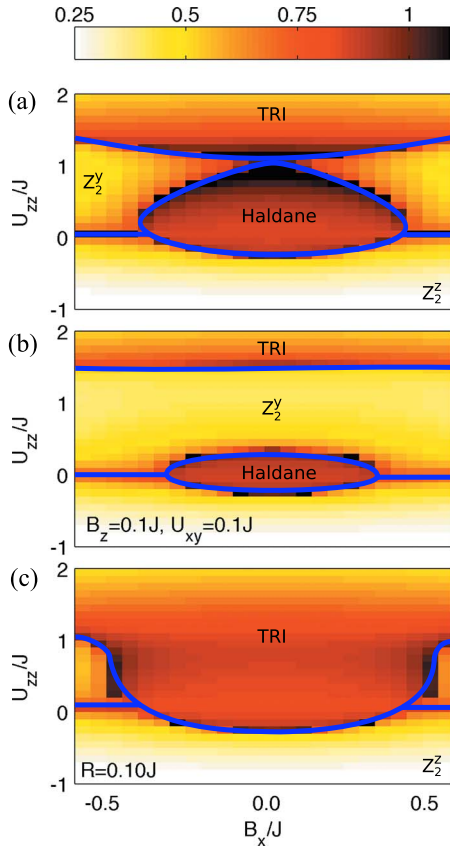


FIG. 1. (Color online) The colormaps show the entanglement entropy S for different spin-1 models: Panel (a) shows the data for Hamiltonian H_0 in Eq. (3), panel (b) for H_0 plus a term which breaks the $e^{-i\pi S^y} \times \text{TR}$ symmetry [Eq. (17)], and panel (c) for H_0 plus a term which breaks inversion symmetry [Eq. (18)]. The blue lines indicate a diverging entanglement entropy as a signature of a continuous phase transition. The phase diagrams contain four different phases: a TRI phase for large U_{zz} , two symmetry breaking antiferromagnetic phases Z_2^y and Z_2^z , and a Haldane phase (which is absent in the last panel).

we arrive at $U_z^2=1$. The combined operation $\mathcal{R}_x\mathcal{R}_z$, however, may give rise to a nontrivial phase factor. By repeating this symmetry twice, the associated unitary matrix U_xU_z can be shown (in the same way as above) to satisfy $U_xU_z = e^{i\phi_{xz}}U_zU_x$. Since the phases of U_x and U_z have been defined, the phase factor $e^{i\phi_{xz}}$ is *not* arbitrary, and can have a physical meaning. Clearly $e^{i\phi_{xz}} = \pm 1$. If $e^{i\phi_{xz}} = -1$, then the spectrum of Λ is doubly degenerate, since Λ commutes with the two unitary matrices U_x and U_z which anticommute among themselves. For the AKLT state, $U_x = \sigma_x$ and $U_z = \sigma_z$, therefore $U_xU_z = -U_zU_x$, and the Haldane phase is protected if the system remains symmetric under both \mathcal{R}_x and \mathcal{R}_z .

V. EXAMPLES

We now demonstrate how the symmetries discussed above stabilize the Haldane phase. We use the iTEBD method to numerically calculate the ground state of the model given by Eq. (3), augmented by various symmetry-breaking perturbations. We used MPS's with a dimension of

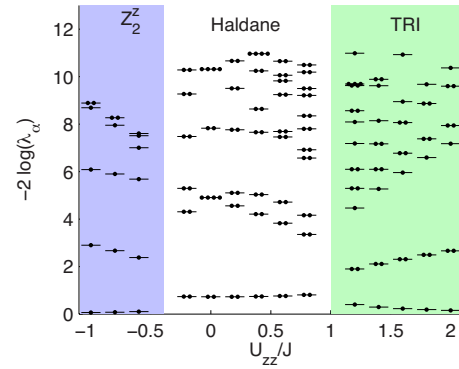


FIG. 2. (Color online) Entanglement spectrum of Hamiltonian H_0 in Eq. (3) for $B_x=0$ (only the lower part of the spectrum is shown). The dots show the multiplicity of the Schmidt values, which is even in the entire Haldane phase.

$\chi=80$ for the simulations. The double degeneracy of the entanglement spectrum is used to identify the Haldane phase.

Example 1. We begin with the original Hamiltonian H_0 in Eq. (3). This model is translation invariant, invariant under spatial inversion, under $e^{-i\pi S^x}$ and under $e^{-i\pi S^y} \times \text{TR}$. Using the above argument, we know that inversion symmetry alone is sufficient to protect a Haldane phase. The phase diagram is shown in Fig. 1(a) and agrees with the results of Ref. 3. A diverging entanglement entropy indicates a phase transition (see, for example, Ref. 34) and we use observables such as S_y and S_z to reveal the nature of the phases. In our approach, the Haldane phase can be easily identified by looking at the degeneracy of the entanglement spectrum as shown in Fig. 2: the even degeneracy of the entanglement spectrum occurs in the entire phase.

In the entanglement spectrum of the trivial insulating (TRI) phase, there are both singly and multiply degenerate levels. We have checked that the multiple degeneracies in the TRI spectrum can be lifted by adding symmetry-breaking perturbations to the Hamiltonian (while preserving inversion symmetry). In the Haldane phase, on the other hand, the double degeneracy of the entire spectrum is robust to adding such perturbations.

The colormap in Fig. 3(a) shows the difference of the two largest Schmidt values for the whole B_x - U_{zz} phase diagram. In the Haldane phase, the whole spectrum is at least twofold degenerate and thus the difference is zero.

Example 2. The Hamiltonian H_0 has, in fact, more symmetries than are needed to stabilize the Haldane phase. To demonstrate this, we add a perturbation H_1 of the form

$$H_1 = B_z \sum_j S_j^z + U_{xy} \sum_j (S_j^x S_j^y + S_j^y S_j^x). \quad (17)$$

H_1 is translation invariant and symmetric under spatial inversion, but breaks the $e^{-i\pi S^x}$ and the $e^{i\pi S^y} \times \text{TR}$ symmetry. The phase diagram for fixed $B_z=0.1J$ and $U_{xy}=0.1J$ as a function of B_x and U_{zz} is shown in Fig. 1(b). As predicted by the symmetry arguments above, we find a finite region of stability for the Haldane phase. This region is characterized, as before, by a twofold degeneracy in the entanglement spectrum, as shown in Fig. 3(b).

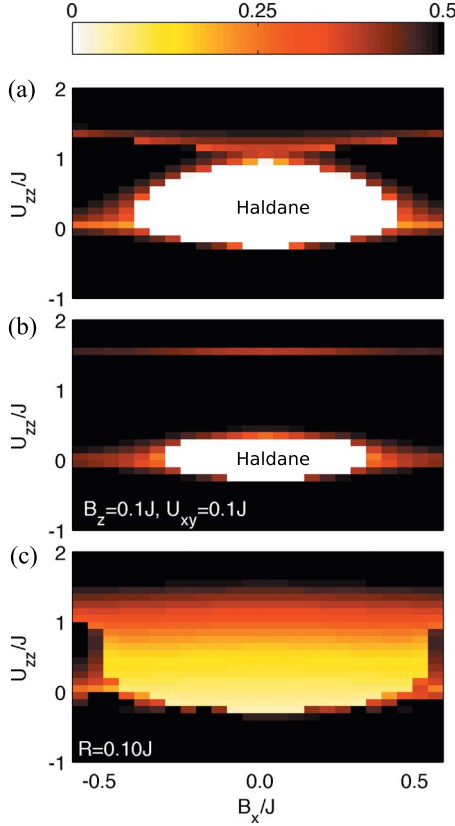


FIG. 3. (Color online) The colormaps show the difference between the two largest Schmidt values $|\lambda_1 - \lambda_2|$ for different spin-1 models. Panel (a) corresponds to the original Hamiltonian H_0 in Eq. (3), panel (b) to H_0 plus a term that breaks $e^{i\pi S^y} \times \text{TR}$ [Eq. (17)], and panel (c) to H_0 plus a term which breaks inversion symmetry [Eq. (18)]. The quantity $|\lambda_1 - \lambda_2|$ is zero only in the Haldane phase.

Example 3. In this example, we consider a case in which there is no symmetry that protects the Haldane phase. We add the following inversion symmetry-breaking term:

$$H_1 = R \sum_j [\mathcal{S}_j^z (\mathcal{S}_j^x \mathcal{S}_{i+1}^x + \mathcal{S}_j^y \mathcal{S}_{j+1}^y) - \mathcal{S}_{j+1}^z (\mathcal{S}_j^x \mathcal{S}_{j+1}^x + \mathcal{S}_j^y \mathcal{S}_{j+1}^y) + \text{H.c.}] \quad (18)$$

Note that this term is invariant under $e^{i\pi S^y} \times \text{TR}$. The phase diagram for the parameter $R=0.1J$ is shown in Fig. 1(c). As predicted by the symmetry arguments above, we do *not* find a Haldane phase with a twofold degeneracy [see Fig. 3(c)]. The Haldane phase region is continuously connected to the TRI phase. The same scenario appears if we consider very small R .

Example 4. Another example in which the Haldane phase and the TRI phase are continuously connected is recently given in Eq. (6) of Ref. 35. The model studied is related to the thin-torus limit of the fractional quantum Hall effect. The model also does not have any of the symmetries which protects the Haldane phase. Thus their finding is consistent with our analysis.

VI. CLASSIFICATION OF GAPPED PHASES IN ONE DIMENSION

In Sec. IV we have identified several ϕ parameters, such as $\phi_{\mathcal{T}}$, $\phi_{\mathcal{I}}$, and ϕ_{xz} , which parametrize the phase ambiguities in the symmetry operations acting on the Schmidt eigenstates of the wave function. When one of these parameters is non-zero, the entanglement spectrum is degenerate, and a non-trivial (Haldane-type) degenerate phase is stable over a finite range in parameter space.

When more than one symmetry is present, the nontrivial (degenerate) phases may be classified into several families depending on the combination of values taken by the corresponding ϕ 's. In fact, there are even more phases than this argument would naively suggest.²⁰ Most generally, given the symmetry group of the system, the phases can be classified according to all the possible inequivalent projective representations of the symmetry group. The general classification scheme of one-dimensional gapped phases will not be described in detail in this work, but will be deferred to a later publication Ref. 20.

In Appendix A, we consider various generalizations of the Haldane phase, which are protected by different symmetries. In a $S=1$ antiferromagnetic chain with Dzyaloshinskii-Moriya interactions in a magnetic field, we show that there is a stable Haldane-type phase which is protected by a modified inversion symmetry. The extended Bose-Hubbard model also has a generalized Haldane phase.⁴ This phase is shown to be inequivalent to the usual Haldane phase of spin-1 chains, which is also supported by the symmetry group of this system.

VII. ADIABATIC BOND WEAKENING

The doubly degenerate entanglement spectrum is a unique feature of the Haldane phase, which can be used to distinguish it from other phases. However, since the entanglement spectrum is a highly nonlocal property, one may wonder whether it has any physical consequences, which can be accessed in experiments.

In the introduction, we discussed an adiabatic process in which a single bond in the system is slowly weakened to zero. The degree of correlation remaining across this bond can be measured by the entanglement entropy. We will show that, if the system starts in the Haldane phase and inversion symmetry about the weakened bond is preserved throughout the process, the minimum value of the entanglement entropy of the two halves is $\ln(2)$. This is because the entanglement spectrum eigenvalues remain doubly degenerate. The minimum entropy is reached if just one pair of entanglement eigenvalues is nonzero.

This property of the Haldane phase can be used, in principle, to identify it in an experiment. It means that, starting from the Haldane phase and separating it adiabatically into two halves A and B , some degree of entanglement between A and B must remain in the final state, as long as the symmetry that protects the Haldane phase is respected. This manifests itself in physical correlation functions between the two halves. Namely, there must exist a pair of physical operators \mathcal{O}_A and \mathcal{O}_B belonging to subsystems A and B , respectively,

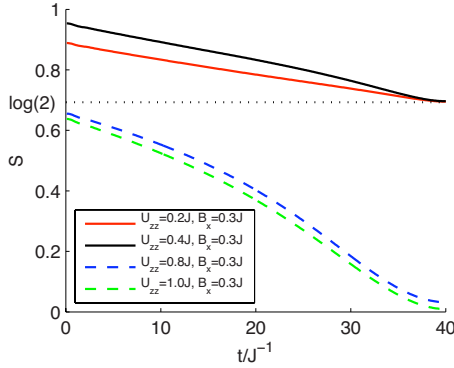


FIG. 4. (Color online) Half-chain entanglement entropy of the model Hamiltonian (3) at a bond which is slowly weakened as a function of time $J_{\text{weak}}=J-t\Gamma$ and $\Gamma=J^2/40$. The entanglement entropy of the resulting state is $\ln 2$ in the Haldane phase and zero otherwise.

such that the disconnected correlation function $C_{A,B}=\langle\mathcal{O}_A\mathcal{O}_B\rangle-\langle\mathcal{O}_A\rangle\langle\mathcal{O}_B\rangle$ remains nonzero, even when the two subsystems are completely disconnected. Starting from a nondegenerate phase, on the other hand, the final state can be completely disentangled across the cut bond.³⁶

To simulate the weakening of one bond numerically, we start by preparing ground states of Hamiltonian (3) for different parameters using the iTEBD algorithm with a unit cell of size $L=80$ which is large compared to the correlation length. We then evolve this state in time while decreasing the strength of one bond in between two half chains, J_{weak} , according to $J_{\text{weak}}=J-t\Gamma$. For the rate $\Gamma=J^2/40$ and $t=0, \dots, 40J^{-1}$, we found that this time evolution is essentially adiabatic. We calculate the entanglement entropy at the middle bond as a function of time. The result for $B_x=0.3J$ and various values for U_{zz} is shown in Fig. 4. Within the Haldane phase ($U_{zz}=0.2J$ and $0.4J$) the entanglement entropy at the end of the weakening process is equal to $\ln(2)$. In the TRI phase ($U_{zz}=0.8J$ and $1.0J$), the entanglement entropy decreases monotonically to zero.

The robustness of the degeneracy in the entanglement spectrum of the Haldane phase has an intuitive explanation, as follows. Let us examine the Schmidt decomposition of the ground-state wave function corresponding to dividing the system along the weakened bond. Initially, since $\phi_{\mathcal{I}}=\pi$, the Schmidt states appear in doublets. As we show in Appendix B, the Schmidt decomposition can be written as

$$|\Psi\rangle=\sum_{\alpha=1}^{\chi/2}\lambda_{2\alpha-1}(|\alpha,1\rangle|\overline{\alpha,2}\rangle-|\alpha,2\rangle|\overline{\alpha,1}\rangle), \quad (19)$$

where $\lambda_{2\alpha-1}$ are the Schmidt eigenvalues, $|\alpha, i\rangle$ with $i=1, 2$ are Schmidt states of the left subsystem, and $|\overline{\alpha, i}\rangle=\mathcal{I}|\alpha, i\rangle$ are the inversion-related states on the right subsystem. $|\Psi\rangle$ is odd under inversion, as can be seen by applying the inversion operator \mathcal{I} . Since the Hamiltonian remains symmetric under inversion throughout the bond-weakening process, $|\Psi\rangle$ has to remain antisymmetric. Thus, at the end of the adiabatic evolution, the system is in the ground state of the *antisymmetric sector*, which generally differs from the true

ground state (unless the ground state of each of the disconnected halves is degenerate). This is because the true ground state, a product state, is symmetric under inversion. The antisymmetric sector ground state can be written as $\frac{1}{\sqrt{2}}(|0\rangle|\overline{1}\rangle-|1\rangle|\overline{0}\rangle)$. Here $|0\rangle$ and $|1\rangle$ are, respectively, the ground state and first excited state of the left subsystem and $|\overline{0}\rangle$ and $|\overline{1}\rangle$ are the ground state and first excited state of the right subsystem, which are related by inversion to the corresponding states on the left. Thus the entanglement spectrum remains doubly degenerate, and entanglement entropy in the final state is $\ln(2)$.

Note that this property of the Haldane phase is not associated with the existence of zero-energy edge states. (The two states $|0\rangle$ and $|1\rangle$ do not have to be degenerate.) In particular, the Hamiltonian H_0 [Eq. (3)] does not have any zero-energy edge state at an open boundary.

VIII. SUMMARY

In this work, we have considered the Haldane phase of $S=1$ chains as an example of a “topological” phase in one dimension. It has been known for a long time that this phase cannot be characterized by any local symmetry-breaking order parameter, and that its unusual character only shows up in nonlocal properties, such as zero-energy fractionalized edge states and nonlocal string order parameters. When perturbing away from the $SU(2)$ symmetric point, both the edge states and the string order can be eliminated. Remarkably, the Haldane phase can still remain stable, given that certain symmetries are preserved. That is, the nontrivial topological character of the Haldane phase is protected by symmetry, even though the Haldane phase itself does not break any symmetry spontaneously.

We have shown that the nontrivial topological nature of the Haldane phase of $S=1$ chains is reflected by a double degeneracy of the entire entanglement spectrum. The degeneracy is protected by the same set of symmetries which protects the Haldane phase and cannot be lifted unless either a phase boundary to another, “topologically trivial” phase is crossed, or the symmetry is broken. The Haldane phase is protected by any of the following symmetries: spatial inversion symmetry, time-reversal symmetry, or the dihedral symmetry D_2 (rotations by π about a pair of orthogonal axes). This result on the symmetry protection is completely consistent with what was obtained from different arguments.³³ The degeneracy of the entanglement spectrum can be used to characterize the Haldane phase in the most general situation, in which edge modes and string order may be absent (see Table I).

The degeneracy of the entanglement spectrum in the Haldane phase is proven by examining how the Schmidt eigenstates transform under a projective representation of the symmetry group of the system. The transformation laws contain phase factors, which are constrained to take discrete values by symmetry. If these phase factors are nontrivial, they require a degeneracy in the entanglement spectrum. Depending on which phase factors take nontrivial values, several distinct “Haldane-type” states are possible. This offers a scheme to classify all possible gapped phases of a one-

TABLE I. The different symmetries which can stabilize the Haldane phase. For each class of symmetries, the table shows whether string order, edge states, or the degeneracy of the entanglement spectrum are necessarily present. The symmetry under π rotations about a pair of orthogonal axes is represented by the dihedral group D_2 .

Symmetry	String order	Edge states	Degeneracy
$D_2 (=Z_2 \times Z_2)$	Yes	Yes	Yes
Time reversal	No	Yes	Yes
Inversion	No	No	Yes

dimensional system, given its symmetry group. Such a general classification will be the subject of a forthcoming paper.²⁰

The degeneracy of the entanglement spectrum is a highly nonlocal property, and is not easily related to physical observables. Nevertheless, the degeneracy of the entanglement spectrum has direct physical consequences. It means that in the Haldane phase, the entanglement of the system across any cut cannot drop below the minimum value of $\ln(2)$. This can be observed, for example, by adiabatically weakening a bond to zero. In the Haldane phase, if inversion symmetry is preserved throughout this process, it leaves the two disconnected halves of the system in a finitely entangled state. In a topologically trivial state, on the other hand, the two halves can be completely decoupled and form an unentangled product state after the process has ended. The nonzero residual entanglement is reflected in correlation functions of physical observables belonging to the two halves of the system. Such an adiabatic weakening process could, at least, in principle, serve as a way to experimentally distinguish the Haldane phase from other, topologically trivial phases.

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APPENDIX A: GENERALIZATION OF THE SYMMETRY-PROTECTED HALDANE PHASE

We have seen above that the Haldane phase of spin-1 antiferromagnetic chains can be characterized by a double degeneracy of the entanglement spectrum, which can be traced back to the nontrivial transformation law of its Schmidt eigenstates under certain symmetry operations. The double degeneracy of the Haldane phase is protected by any one of the three symmetries (dihedral group of π rotations about two orthogonal axes, time-reversal symmetry, or bond-

centered inversion symmetry). In fact, there are various generalizations of the Haldane phase, which are protected by modified symmetries.

For example, in magnetism, the Dzyaloshinskii-Moriya (DM) interaction generally arises if the system lacks inversion symmetry about the center of bond. In the case of the one-dimensional chain, the DM interaction is given as

$$\sum_j \vec{D}_j \cdot (\vec{S}_j \times \vec{S}_{j+1}). \quad (\text{A1})$$

The following two cases often appear in models of magnetism: a uniform DM interaction $\vec{D}_j = \vec{D}$ and a staggered DM interaction $\vec{D}_j = (-1)^j \vec{D}$. Let us assume $\vec{D} = (0, 0, D)$ (parallel to z axis).

The DM interaction, which is also known as antisymmetric exchange interaction, clearly breaks inversion symmetry about the bond. Here we consider the Hamiltonian of a $S=1$ chain

$$H_{\text{DM}} = J \sum_j \vec{S}_j \cdot \vec{S}_{j+1} + B_z \sum_j S_j^z + \sum_j \eta^j \vec{D} \cdot (\vec{S}_j \times \vec{S}_{j+1}), \quad (\text{A2})$$

where $\eta=1$ for the uniform and $\eta=-1$ for the staggered DM interaction case. This model breaks all the three symmetries we have discussed above, if $B_z, \vec{D} \neq 0$. Thus one might expect that the Haldane phase is no longer well defined in this model. However, it turns out that the double degeneracy of the entanglement spectrum, and thus the well-defined Haldane phase, survives for $D > 0$. This can be simply understood because the Hamiltonian can be transformed^{37,38} to

$$\tilde{H}_{\text{DM}} = U_G^\dagger H_{\text{DM}} U_G \quad (\text{A3})$$

$$= J \sum_j S_j^z S_{j+1}^z + J_\perp \sum_j (S_j^x S_{j+1}^x + S_j^y S_{j+1}^y) + B_z \sum_j S_j^z. \quad (\text{A4})$$

Here, $J_\perp = \sqrt{J^2 + D^2}$, if we choose

$$U_G = e^{i \sum_j j \alpha S_j^z}, \quad (\text{A5})$$

for the uniform DM interaction, and

$$U_G = e^{i \sum_j (-1)^j (\alpha/2) S_j^z}, \quad (\text{A6})$$

for the staggered DM interaction, with $\alpha = \tan^{-1}(D/J)$. The resulting Hamiltonian is simply the standard XXZ antiferromagnetic chain in an magnetic field B_z . The inversion symmetry of the model guarantees a double degeneracy in the entanglement spectrum, and hence protects the Haldane phase.

In the context of the original Hamiltonian, however, the symmetry that protects the double degeneracy is somewhat obscured. The inversion \mathcal{I} acts on the transformed Hamiltonian as

$$\tilde{H}_{\text{DM}} \rightarrow \mathcal{I}^\dagger \tilde{H}_{\text{DM}} \mathcal{I}. \quad (\text{A7})$$

Here we define the inversion \mathcal{I} as usual so that site j goes to site $1-j$. We find that the modified symmetry of the original Hamiltonian is the invariance under

$$H_{\text{DM}} \rightarrow \mathcal{I}'^\dagger H_{\text{DM}} \mathcal{I}', \quad (\text{A8})$$

where

$$\mathcal{I}' = U_G \mathcal{I} U_G^\dagger = \begin{cases} e^{i\alpha \sum_j (2j-1) S_j^z \mathcal{I}} & (\text{uniform DM}) \\ e^{i\alpha \sum_j (-1)^j S_j^z \mathcal{I}} & (\text{staggered DM}) \end{cases}. \quad (\text{A9})$$

Namely, it is the invariance under inversion with an appropriate ‘‘twist’’ (rotation of each spin about z axis).

The invariance under \mathcal{I}' , which protects the Haldane phase, is not a generic symmetry and may be broken rather easily by perturbations which could occur naturally. For example, if the uniform magnetic field were applied to the x direction instead of the z direction in the Hamiltonian (A2), it is clear that the model is no longer invariant under \mathcal{I}' .

For example, for a staggered DM interaction, a uniform field in the x direction leaves a staggered magnetic field $\propto \sum_j (-1)^j S_j^x$ after the transformation. The staggered field breaks inversion symmetry about the bond center and thus eliminates the degeneracy in the entanglement spectrum. That a staggered field destroys the Haldane phase was noticed earlier.³⁹

As another example of physical interest, let us discuss the ‘‘Haldane-insulator’’ (HI) phase in the extended Bose-Hubbard model (EBHM). We will show that the HI phase is protected by a similar mechanism. The model Hamiltonian of the EBHM reads

$$H_{\text{BH}} = -t \sum_j (b_j^\dagger b_{j+1} + \text{H.c.}) + \frac{U}{2} \sum_j n_j (n_j - 1) + V \sum_j n_j n_{j+1} \quad (\text{A10})$$

where b_j^\dagger creates a boson at site j , $n_j = b_j^\dagger b_j$, and we assume a filling of one boson per site ($\langle n_j \rangle = 1$) and $t, U, V > 0$. In Ref. 10, it has been shown that the EBHM has a phase which is analogous to the Haldane phase. This phase was termed a HI.

The symmetries of the EBHM are translation, time-reversal, inversion, and particle conservation. It is useful to consider an effective spin-1 model by truncating the Hilbert space of each site to states with $n=0, 1, 2$, which is strictly justified in the large U limit. This modification is not expected to be important in this limit, since states with $n > 2$ are higher in energy. The corresponding effective pseudospin Hamiltonian reads

$$H_{\text{eff}} = -t \sum_j (S_j^+ S_{j+1}^- + \text{H.c.}) + \frac{U}{2} \sum_j (S_j^z)^2 + V \sum_j S_j^z S_{j+1}^z + H', \quad (\text{A11})$$

where we have introduced the pseudospin operator $S^z = n - 1$, and H' contains other terms which break the ‘‘particle-hole’’ symmetry of H_{eff} , which is represented in the pseudospin language by a π rotation about the x axis. This spurious symmetry is not crucial for the stability of the HI phase, as we shall show below.

Ignoring H' , the Hamiltonian H_{eff} is very similar to H_0 in Eq. (3), with the exception that the $S_j^+ S_{j+1}^- + \text{H.c.}$ (‘‘hopping’’) term is of opposite sign. As a result, the HI phase of Eq.

(A11) is not protected by inversion symmetry (\mathcal{I}). The phase $e^{i\phi_{\mathcal{I}'}}$, which is the parity of the ground state under inversion about a bond (see next appendix), is equal to +1 in this case; the ground state of a system with the ordinary, negative, sign for the kinetic energy cannot have nodes.

However, the HI phase is protected by a modified symmetry instead. The effective Hamiltonian can be mapped to the antiferromagnetic spin Hamiltonian (3) by a staggered rotation of spins by $\pm \pi/2$ about z axis, alternatingly on even and odd sites. The staggered rotation is given by the unitary transformation of the same form as Eq. (A6), but now with $\alpha = \pi$. (We note that, if we increase the DM interaction from zero to infinity for the antiferromagnetic chain, $|\alpha|$ changes from zero to $\pi/2$. Thus the present case is distinct from the antiferromagnetic chain with DM interactions.) The transformation changes the sign of the hopping term to negative; in the spin chain context this makes in-plane exchange interaction antiferromagnetic as in Eq. (3).

Following the discussion for a staggered DM interaction, and using $\alpha = \pi$, we find that the HI phase is protected by invariance under the operation

$$\mathcal{I}' = e^{i\pi \sum_j S_j^z \mathcal{I}}. \quad (\text{A12})$$

As an interesting example, a staggered field in the x direction is now invariant under \mathcal{I}' (and thus does not break the double degeneracy of the entanglement spectrum), while a uniform field in the same direction is not.

In terms of the discussion in Sec. IV, the HI phase is characterized by $\phi_{\mathcal{I}'} = \pi$ and $\phi_{\mathcal{I}} = 0$, and is thus distinct from the usual Haldane phase of H_0 , with $\phi_{\mathcal{I}'} = 0$ and $\phi_{\mathcal{I}} = \pi$. This shows that these two states cannot be connected adiabatically while preserving either \mathcal{I} or \mathcal{I}' .

APPENDIX B: SCHMIDT DECOMPOSITION OF A $\phi_{\mathcal{I}} = \pi$ STATE

Let us prove Eq. (19). We consider an inversion-symmetric MPS $|\Psi\rangle$ defined on a finite chain of an even length $2L$ and assume that $|\Psi\rangle$ is characterized by $\phi_{\mathcal{I}} = \pi$. The MPS is written as

$$|\Psi\rangle = \sum_{\{m_j\}} V_L^T \Gamma_{m_1} \Lambda \dots \Gamma_{m_L} \Lambda \times \Gamma_{m_{L+1}} \Lambda \dots \Gamma_{m_{2L}} V_R |m_1 \dots m_{2L}\rangle. \quad (\text{B1})$$

Since we are interested in bulk properties in the limit $L \rightarrow \infty$, we assume a sufficiently long chain with position-independent matrices Γ_m . V_L and V_R are χ -dimensional column vectors which define the boundary conditions (to be specified later). Describing the boundary conditions in this way is possible as long as there are no edge modes, which is generically true when only inversion symmetry is present (Otherwise, the edges states of the two ends may require some extra care.). Since $|\Psi\rangle$ is invariant under inversion, the matrices Γ_m satisfy Eq. (10). Applying this relation to the matrices $\Gamma_{m_{L+1}} \dots \Gamma_{m_{2L}}$, we get

$$\begin{aligned}
 |\Psi\rangle &= e^{-iL\theta} \sum_{\{m_j\}} V_L^T \Gamma_{m_1} \Lambda \dots \Gamma_{m_L} \Lambda \\
 &\times U_T \Gamma_{m_{L+1}}^T \Lambda \dots \Gamma_{m_{2L}}^T U_T^\dagger V_R |m_1 \dots m_{2L}\rangle. \quad (\text{B2})
 \end{aligned}$$

Now, we choose boundary conditions such that $V_R = U_T V_L$. The wave function $|\Psi\rangle$ can be written as

$$|\Psi\rangle = e^{-iL\theta} \sum_{\alpha,\beta} \lambda_\alpha (U_T)_{\alpha\beta} |\alpha\rangle |\beta\rangle, \quad (\text{B3})$$

where

$$|\alpha\rangle = \sum_{\{m_j\}} (V_L^T \Gamma_{m_1} \Lambda \dots \Gamma_{m_L})_\alpha |m_1 \dots m_L\rangle. \quad (\text{B4})$$

Since $\phi_T = \pi$, the Schmidt eigenvalues λ_α are all doubly degenerate (see Sec. IV A). Let us order the λ_α 's such that

$\lambda_{2\alpha-1} = \lambda_{2\alpha}$ for every $1 \leq \alpha \leq \chi$. The matrix $U_{\alpha\beta}$ commutes with Λ . Therefore, it must have a block-diagonal form with 2×2 blocks on the diagonal. Since $U^T = -U$ (which follows from $\phi_T = \pi$, as shown in Sec. IV A), the blocks on the diagonal of U are all of the form $e^{i\eta_\alpha} \sigma_2$, where η_α is a phase. Therefore, we write $|\Psi\rangle$ as

$$|\Psi\rangle = \sum_{\alpha=1}^{\chi/2} \lambda_{2\alpha-1} (|\alpha, 1\rangle |\overline{\alpha, 2}\rangle - |\alpha, 2\rangle |\overline{\alpha, 1}\rangle), \quad (\text{B5})$$

where $|\alpha, j\rangle \equiv e^{i(\eta_\alpha - L\theta_T/2)} |2\alpha - 1 + j\rangle$ ($j=1, 2$) and $|\overline{\alpha, j}\rangle \equiv \mathcal{I}|\alpha, j\rangle$. In the limit $L \rightarrow \infty$, the states $|\alpha, j\rangle$ become orthonormal [as can be shown from the canonical conditions in Eq. (5)], and therefore Eq. (B5) is the Schmidt decomposition of $|\Psi\rangle$. This concludes our proof.

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