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# Symmetry protection of topological phases in one-dimensional quantum spin systems

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We discuss the characterization and stability of the Haldane phase in integer spin chains on the basis of simple, physical arguments. We find that an odd-$S$ Haldane phase is a topologically nontrivial phase which is protected by any one of the following three global symmetries: (i) the dihedral group of $\pi$ rotations about the $x$, $y$, and $z$ axes, (ii) time-reversal symmetry $S^{x,y,z} \to -S^{x,y,z}$, and (iii) link inversion symmetry (reflection about a bond center), consistent with previous results [Phys. Rev. B **81**, 064439 (2010)]. On the other hand, an even-$S$ Haldane phase is not topologically protected (i.e., it is indistinct from a trivial, site-factorizable phase). We show some numerical evidence that supports these claims, using concrete examples.

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## I. INTRODUCTION

States of matter can be classified into different phases, which are often distinguished by (local) order parameters. Identification of phases generally requires certain symmetries. For example, the ordered and the disordered phases of the Ising model are sharply distinct only in the presence of the $Z_2$ symmetry of spin reversal. In the absence of the symmetry, the two phases can be connected without a phase transition and thus cannot be distinguished uniquely. This phase transition corresponds to the spontaneous breaking of the $Z_2$ symmetry. Therefore, it is natural that the $Z_2$ symmetry is required in this example to protect the ordered phase as a well-defined phase distinct from the disordered phase.

Even if there is no symmetry which distinguishes the two phases, they can still be separated by a transition. However, it is generically first order and terminates at a critical end point. Thus, as in the case of liquid and gas phases, there is a smooth path which connects the two phases, without any phase transition. In this sense, in the absence of protection due to symmetry, phase transitions can still exist but they do not generally *define* essentially distinct phases,

On the other hand, even when there is no local order parameter or spontaneous breaking of a global symmetry, we sometimes find distinct quantum phases separated by quantum phase transitions. We then attribute the distinction to a nontrivial or "topological phase." While there are several known characterizations of topological phases, the complete understanding in general dimensions is still lacking. The related question, what kind of symmetry, if any, is required to protect the topological phase, is much less obvious compared to the case of a standard spontaneous symmetry breaking. In this paper, we will consider one-dimensional systems (1D) to establish some intuition about this question.

One of the simplest examples of a topological phase is the Haldane phase in quantum spin chains.[1,2] As predicted by Haldane, the Heisenberg antiferromagnetic (HAF) chain with an integer spin $S$,

$$\mathcal{H}_{\mathrm{HAF}} = J \sum_j \vec{S}_j \cdot \vec{S}_{j+1}, \tag{1}$$

where $J > 0$, has a nonzero excitation gap and exponentially decaying spin correlation functions, while the same model is gapless and has power-law correlations for a half integer $S$.

Following Haldane's prediction, Affleck, Kennedy, Lieb, and Tasaki (AKLT) presented model Hamiltonians for which the ground state can be obtained exactly.[3,4] In addition to providing a tractable model in which the Haldane conjecture can be tested, the ground state (AKLT state) was later found to exhibit several unexpected properties, such as a nonlocal "string order" and edge states, which extend also to states within the same phase.[5]

On the other hand, despite the relative simplicity of quantum spin chains and intensive study over several decades, the framework for describing their topological properties has just recently been understood. In fact, it was only recently that the importance of inversion (parity) symmetry in the Haldane phase was pointed out. Based on a field-theory (bosonization) analysis of a related boson model, Berg *et al.* pointed out in Ref. 6 that the $S = 1$ Haldane phase is distinct from other phases only in the presence of inversion symmetry. Next, based on the Tensor Entanglement Filtering Renormalization Group (TEFR) approach, Gu and Wen stated that the $S = 1$ Haldane phase is protected by the *combination* of the translation, complex conjugation ("time reversal"), and inversion symmetry.[7,8] Gu and Wen pointed out that the combined symmetry above protects the topological phase, even when the existing characterizations (edge states and string order) do not work. It turns out that the symmetry protection can be understood in terms of "fractionalization" of symmetry operations at the edges and is reflected by nontrivial degeneracies in the entanglement spectrum.[9,10] The fractionalization is described precisely using projective representations of the symmetry group. This approach was then generalized to any gapped 1D system and shown to give a complete procedure in one dimension for identifying the topological phase of such systems.[11–13] Several 1D models in which symmetry fractionalization plays an important role have been studied recently—see, for example, Refs. 14–17.

In this paper, we illustrate the behavior of topological order in one dimension by reexamining spin systems and the robustness of their topological phases on the basis of

 

simple, physical arguments and discuss a number of concrete examples. We say that the topological phase around the AKLT state is robust if it cannot be adiabatically connected to another, "topologically trivial" state, without going through a phase transition. Here, "topologically trivial" means that the state is site-factorizable, namely, that the state is given by a single tensor product of local states. An example of such a topologically trivial state is

$$|\mathcal{D}\rangle = |0\rangle_1 \cdots |0\rangle_L, \tag{2}$$

which is the ground state of a chain with single-ion anisotropy $D(S^z)^2$ in the limit of $D \to +\infty$. (For a precise mathematical definition of the robustness of the topological phases in one dimension, see also Refs. 11 and 12.) We show that for odd values of the spin $S$, our results are consistent with those of Refs. 6 and 9: The AKLT state is robust as long as *any one* of the three symmetries mentioned in the abstract ($\pi$ rotation of the spin about the $x$, $y$, $z$ axes, and time reversal or inversion symmetry) is respected. Surprisingly, these arguments suggest that other systems, such as even-spin AKLT states and $S = 1$ spin ladders with an even number of legs, are *not* topologically protected, even if all the symmetries are respected. In particular, the $S = 2$ AKLT phase is indistinct from a trivial state, even if full SU(2) symmetry is maintained. We show here how to transform such states into one another, giving numerical evidence that there are no phase transitions along the way.

This paper is organized as follows: We begin by discussing the stability of the Haldane phase owing to a hidden discrete symmetry in Sec. II, with a clarification of the required symmetry. We then generalize the Haldane phase in Sec. III to different symmetries and discuss the concept of symmetry protected topological phases. In Sec. IV we demonstrate concrete examples in the form of matrix-product states and present numerical simulations to support and illustrate our arguments. In particular, we construct explicit paths which smoothly connect the $S = 2$ AKLT state to various site-factorizable states, demonstrating that the former state is trivial. Our results are summarized in Sec. V.

## II. HALDANE PHASE IN THE PRESENCE OF GLOBAL $D_2$ SYMMETRY

First let us briefly discuss the hidden order and edge states in the context of a hidden $Z_2 \times Z_2$ symmetry. Although this concept had been developed in the early 1990's, to the best of our knowledge, the symmetry of the Hamiltonian required for this mechanism has not been discussed explicitly. Here we also clarify the required symmetry, which could be understood as one of the symmetries protecting the Haldane phase as a distinct, topological phase.

It is believed that the ground state of the standard Heisenberg chain belongs to the Haldane phase, which also includes the translationally invariant Affleck-Kennedy-Lieb-Tasaki (AKLT) state. The $S = 1$ AKLT state exhibits the following two remarkable properties: (I) Free $S = \frac{1}{2}$ degree of freedom appearing at each end of the chain in the case of open boundary conditions. Namely, the ground state of the AKLT Hamiltonian is fourfold degenerate due to the $2^2$ edge states, although the ground state is unique in the case of periodic boundary conditions. (II) A nonlocal order measured by the string order parameter[5]

$$O^{\alpha}_{\mathrm{str}} \equiv \lim_{|j-k|\to\infty} \left\langle S^{\alpha}_j e^{i\pi \sum_{j\leqslant l<k} S^{\alpha}_l} S^{\alpha}_k \right\rangle. \tag{3}$$

These two features turned out to be characteristics of not only the AKLT state, but rather of the $S = 1$ "Haldane phase," which includes the ground states of the AKLT model and the $S = 1$ antiferromagnetic Heisenberg chain. In fact, the degeneracy due to the edge states is split for a generic open chain in the Haldane phase, with a finite length. However, the splitting is exponentially small for longer chains, resulting in fourfold quasidegenerate ground states below the Haldane gap.[18] Numerical calculations have shown that the string order parameter is also nonvanishing within the Haldane phase.

Kennedy and Tasaki[19] unified these two apparently unrelated features as consequences of hidden symmetry breaking. This concept is introduced as follows. We introduce a nonlocal unitary transformation defined by (see also Ref. 20)

$$U_{\mathrm{KT}} = \prod_{j<k} \exp\left(i\pi S^z_j S^x_k\right). \tag{4}$$

This transforms spin operators as

$$U_{\mathrm{KT}} S^x_j U^{-1}_{\mathrm{KT}} = S^x_j \exp\left(i\pi \sum_{k>j} S^x_k\right), \tag{5}$$

$$U_{\mathrm{KT}} S^y_j U^{-1}_{\mathrm{KT}} = \exp\left(i\pi \sum_{k<j} S^z_k\right) S^y_j \exp\left(i\pi \sum_{k>j} S^x_k\right), \tag{6}$$

$$U_{\mathrm{KT}} S^z_j U^{-1}_{\mathrm{KT}} = \exp\left(i\pi \sum_{k<j} S^z_k\right) S^z_j. \tag{7}$$

Although these are nonlocal operators with "strings," the Heisenberg chain Hamiltonian (1) is transformed into a Hamiltonian with only short-range interactions:

$$\tilde{H} = \sum_j \left\{ S^x_j \exp\left(i\pi S^z_{j+1}\right) S^x_{j+1} + S^y_j \exp\left[i\pi\left(S^z_j + S^x_{j+1}\right)\right] S^y_{j+1} + S^z_j \exp\left(i\pi S^z_j\right) S^z_{j+1} \right\}. \tag{8}$$

This is thanks to a cancellation of string factors similar (although not identical) to that in Jordan-Wigner transformation.

The transformation (4) can be applied to a wide class of spin chain Hamiltonians. For the transformation to be useful, the transformed Hamiltonian must have only short-range interactions. We point out that the sufficient and necessary condition the Hamiltonian must satisfy for the transformed Hamiltonian to have local interactions is that it has to have a global discrete symmetry with respect to rotation by angle $\pi$ about the $x$, $y$, and $z$ axes [i.e., $\prod_j \exp(i\pi S^x_j)$, and similar for $y$ and $z$]. This symmetry group, sometimes called the dihedral group $D_2$, is equivalent to $Z_2 \times Z_2$, since the product of $\pi$ rotations about the $x$ and $z$ axes gives the $\pi$ rotation about the $y$ axis. We note that, although global $D_2$ invariant models and time-reversal invariant ones have a large overlap, they are not identical. For example, the anisotropic perturbation $\sum_j (S^z_j S^z_{j+1} + S^z_j S^x_{j+2})$ is time-reversal invariant but not $D_2$ invariant. On the other hand, $\sum_j S^x_j S^y_{j+1} S^z_{j+2}$ is $D_2$ invariant but not time-reversal invariant.

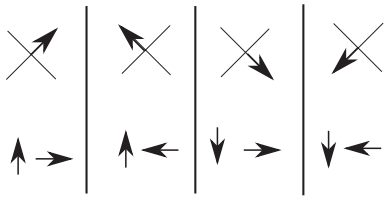

FIG. 1. Four symmetry broken states (upper panel) which are obtained by applying the nonlocal transformation $U_{\rm KT}$ to the degenerate edge states (lower panel). Note that the arrows in the upper panel represent the spin polarization in the bulk, while in the lower panel they represent the spin polarization at the edges.

The transformed *Hamiltonian* $U_{\rm KT}\mathcal{H}U_{\rm KT}^{-1}$ has the same $Z_2 \times Z_2$ symmetry as the original one. This is because the $\pi$ rotations around the $x, y$, and $z$ transform into themselves under $U_{\rm KT}$ (e.g., $e^{i\pi S_l^z}$ commutes with each of the factors $e^{i\pi S_z^j S_x^k}$) However, as the states of the spins are transformed in a nonlocal way, a state without any broken global symmetry may be transformed into a state with long-range ferromagnetic order; that is, there may be *hidden* symmetry breaking.

The symmetry breaking in the transformed system is an indication of edge states in the original Hamiltonian. Note that edge states on a finite chain can break the $Z_2 \times Z_2$ symmetry. Although this symmetry breaking occurs only at the ends, the nonlocal transformation spreads this symmetry breaking through the entire bulk. In fact, the $Z_2 \times Z_2$ symmetry is broken completely in the bulk, implying a fourfold degenerate set of ground states with magnetization along diagonal directions as illustrated in Fig. 1. The $z$ and $x$ components of the magnetization in the bulk after the nonlocal transformation determine the $z$ component of the spin $\frac{1}{2}$ at the left end and the $x$ component of the spin at the right end in the original system, respectively. The string order of the original system(1) is also simple to understand in terms of the hidden breaking of the symmetry: It is the result of applying the Kennedy-Tasaki transformation (4) to the usual ferromagnetic order parameter.

To understand the correspondence between the edge states and the broken symmetry in the bulk, it is easiest to consider the AKLT state. The four degenerate states which transform into the four symmetry-broken states are defined by giving the $z$ component of the free spin $\frac{1}{2}$ at the left end and the $x$ component of the spin $\frac{1}{2}$ at the right end definite values. To see this, start by fixing just the spin at the left end to $S_{z,\rm left} = +\frac{1}{2}$. Then expand this state in terms of $S_z$ eigenstates. The string order is perfect in the AKLT state, meaning that in every component of the wave function, if we erase the sites with $S_z = 0$, we get a chain with a perfect antiferromagnetic order, $|\ldots, -1, +1, -1, +1, \ldots\rangle$.[3,4] Thus the first nonzero spin must be $+1$ in each term and from then on the nonzero $S_z$'s alternate between $\pm 1$. When $U_{\rm KT}$ is applied, it flips the direction of every second nonzero spin, so that all the sites end up in either the $|S_z = +1\rangle$ or $|S_z = 0\rangle$ state. When the $x$ component of the spin $\frac{1}{2}$ at the right end is also fixed, one can likewise argue that each site is in the $|S_x = +1\rangle$ state or the $|S_x = 0\rangle$ state (working in the $S_x$ basis instead). But these two conditions together uniquely determine the state of every site. Note that the only spinor that has only $+1$ and 0 states in both the $x$ and $z$ basis is $\sqrt{\frac{2}{3}}|S_x = 1\rangle + \sqrt{\frac{1}{3}}|S_x = 0\rangle = i(\sqrt{\frac{2}{3}}|S_z = 1\rangle + \sqrt{\frac{1}{3}}|S_z = 0\rangle)$. So after applying the *nonlocal* transformation $U_{\rm KT}$, the wave function is just a product state with this state on every site, spontaneously breaking the symmetry all along the chain.

Similar arguments can be applied to relate any of the four polarizations of the edge states to the four broken symmetry states after the nonlocal transformation, as shown in Fig. 1. A closely related analysis from a different perspective was recently discussed in Ref. 21.

The stability of the Haldane phase for $S > 1$ has been less understood. Once the transformation is written as Eq. (4), it can be readily applied to any integer $S$, and the transformation of the Hamiltonian and the string order parameter remain the same. However, it turns out that the hidden $Z_2 \times Z_2$ symmetry is spontaneously broken in the translationally invariant AKLT state only if $S$ is odd, but unbroken if $S$ is even.[20] This can also be seen by counting the degeneracy of the edge states. Therefore, with regard to the hidden $Z_2 \times Z_2$ symmetry, the even-$S$ AKLT states are indistinguishable from a trivial disordered state. However, the physical meaning of this finding was not well understood; it was unclear if the even-$S$ AKLT states are really indistinguishable from a trivial state, or whether they are distinct from a trivial state by another, unknown criterion.

## III. STABILITY OF THE HALDANE PHASE

In the following, we discuss different ways to understand topological phases in one-dimensional quantum spin systems without referring to the hidden $Z_2 \times Z_2$ symmetry. We find that the odd-$S$ and even-$S$ AKLT states differ in the robustness of the topological phase, as was suggested, in retrospect, by the hidden $Z_2 \times Z_2$ symmetry analysis.

### A. Characterization by edge states in the presence of time-reversal symmetry

Let us now discuss the topological phase, from the viewpoint of "edge physics." Here we apply the idea similar to what was used to characterize the quantum spin Hall insulator.[22] As long as the gap does not close in the bulk, we may focus on the nearly degenerate ground states corresponding to the edge states. The spin-$S$ AKLT state with open boundary conditions has a spin-$S/2$ edge degree of freedom at each end, and thus $(S + 1)$-fold degeneracy at each end. In general, if we introduce a perturbation to the Hamiltonian, the edge degeneracy is expected to be lifted. However, if the edge spin is half integer, namely, for the odd-$S$ AKLT state, as long as the Hamiltonian has time-reversal symmetry, the twofold Kramers degeneracy at each edge should remain. As a consequence, the odd-$S$ AKLT state must be separated from a trivial disordered state by a quantum phase transition. In this sense, the topological phase in the odd-$S$ AKLT state is robust and protected by time-reversal symmetry.

On the other hand, for the even-$S$ AKLT state, the edge spin is an integer. Thus the degeneracy is lifted by a generic perturbation even if the Hamiltonian is invariant under time reversal, because there is no Kramers degeneracy. If the

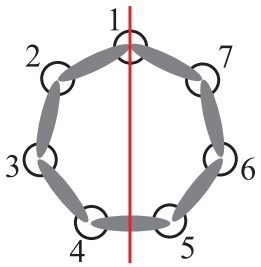


FIG. 2. (Color online) The $S = 1$ AKLT state on a ring with $L = 7$ sites. The connecting lines represent spin-$\frac{1}{2}$ singlets. We consider the lattice inversion about the vertical line.

Hamiltonian is SU(2) invariant, the lowest $S + 1$ degeneracy related to the edge should remain up to a finite strength of the perturbation. However, as a function of the perturbation strength, there is always a possibility that a $S = 0$ state separates from the bulk, crosses the $S + 1$ multiplet, and becomes the ground state. Note that in such a process, the bulk gap need not close anywhere. Thus, it seems that an even-$S$ AKLT state is, strictly speaking, *indistinct* from a trivial state, regardless of the presence of time reversal or SU(2) symmetries. We demonstrate this explicitly in Sec. IV, where we show that the $S = 2$ AKLT state can be smoothly connected to a fully dimerized state.

### B. Inversion symmetry of a ring

We will now argue that the odd-$S$ Haldane phase is also protected just by link inversion symmetry (lattice inversion about the center of a bond). To illustrate the point, it is convenient to consider first an AKLT state on a chain of *odd* length $L$ with periodic boundary conditions. Although the system is frustrated for odd $L$, the ground state of the AKLT model is still unique, reflecting the short-range spin correlations. For example, we discuss the $S = 1$ AKLT state for $L = 7$ as shown in Fig. 2, and inversion $\mathcal{I}$ about the vertical line.

Let us recall the original AKLT construction, starting from two $S = \frac{1}{2}$'s per site, and denote a valence bond (singlet of two $S = \frac{1}{2}$'s) between sites $j$ and $k$ by $|(j,k)\rangle$. The valence bond $|(j,k)\rangle$ is antisymmetric under inversion, namely, the exchange of $j$ and $k$. Thus, under inversion $\mathcal{I}$, the valence bond $|(4,5)\rangle$ crossing the line changes sign: $\mathcal{I}|(4,5)\rangle = -|(4,5)\rangle$. The other valence bonds are flipped as well, for example, $\mathcal{I}|(3,4)\rangle = -|(5,6)\rangle$. However, being paired with $\mathcal{I}|(5,6)\rangle = -|(3,4)\rangle$, we find $\mathcal{I}|(3,4)\rangle|(5,6)\rangle = |(3,4)\rangle|(5,6)\rangle$. The symmetrization operation in the AKLT construction is also invariant under $\mathcal{I}$. Thus we obtain

$$\mathcal{I}\left|\Psi^{\mathrm{AKLT}}_{S=1}\right\rangle_{L=7} = -\left|\Psi^{\mathrm{AKLT}}_{S=1}\right\rangle_{L=7}. \tag{9}$$

(For a related discussion in a different setting, see Ref. 23.) The same argument can be easily applied to higher-spin AKLT states: An odd-$S$ AKLT state is odd under inversion on a ring with any odd length $L$ because there are an odd number of valence bonds on every link. Even if we introduce perturbations to the odd-$S$ AKLT model, the ground state on the odd length ring should still be odd under inversion, as long as the Hamiltonian respects inversion symmetry and the gap does not close. On the other hand, a trivial state given by a tensor product of local states, such as $|\mathcal{D}\rangle$ defined in Eq. (2), is even under $\mathcal{I}$. Therefore we conclude that there must be a phase transition between the odd-$S$ AKLT state and the trivial $|\mathcal{D}\rangle$ state, if inversion symmetry is kept. That is, the odd-$S$ Haldane phase is a topological phase protected just by inversion symmetry. We emphasize that the topological phase is characterized by the odd parity under inversion but *not* by a spontaneous symmetry breaking.

In contrast, an even-$S$ AKLT state is even under inversion, regardless of the length of the chain because there is an even number of valence bonds on the links. This argument suggests that inversion does not protect the phase represented by the even-$S$ AKLT state. Together with the previous section, this supports our conjecture that the even-$S$ AKLT state is, in fact, indistinct from a trivial state.

### C. Argument based on the matrix-product state representation

The above heuristic argument, based on the global properties of the ground state under inversion, requires the ring to have an odd length $L$. However, this is not essential, as can be seen in the following more general formulation[9,10] based on matrix product states[24,25] (MPS). For completeness, we repeat the argument of Ref. 9 below. Let us consider an inversion-symmetric system. Although our analysis does not depend essentially on translation symmetry, here we also assume a translation invariant MPS as in Eq. (10), for the sake of simplicity. On a chain of length $L$ with periodic boundary conditions, a translation invariant MPS is given by

$$|\Psi\rangle = \sum_{m_1,\ldots,m_L} \mathrm{Tr}\left(A_{m_1}\cdots A_{m_L}\right)|m_1,\ldots,m_L\rangle, \tag{10}$$

where $A_m$ are $\chi \times \chi$ matrices, and $|m_j\rangle$ represents a local state at site $j$. We shall refer to the matrix dimension $\chi$ as the ancilla dimension. We assume that the ground state $|\Psi_0\rangle$ fulfills the following conditions: (a) $|\Psi_0\rangle$ can be well approximated by the MPS Eq. (10) with finite dimensional matrices $A_m$, (b) the matrices $A_m$ evolve continuously as we change a parameter of the Hamiltonian, and (c) $|\Psi_0\rangle$ is not a "cat state," i.e., a superposition of two states that are not connected by any local operator (in analogy with Schrödinger's cat or any superposition of two macroscopically different states).[26] The correlation length of a MPS state can be determined from the eigenvalue spectrum of the completely positive map acting on the space of $\chi \times \chi$ matrices[26]

$$\mathcal{E}(X) = \sum_m A_m X A_m^\dagger. \tag{11}$$

This map can be interpreted as a transfer matrix which determines correlation functions. The largest eigenvalue of $\mathcal{E}$ for a normalized MPS is always equal to one. The second largest (in terms of absolute value) eigenvalue $\epsilon_2$ determines the largest correlation length

$$\xi = -\frac{1}{\ln|\epsilon_2|} \tag{12}$$

for a state that is not a cat state.

It is useful to write the matrices $A_m$ in a canonical form as $A_m = \Gamma_m \Lambda$, where $\Lambda$ is a diagonal matrix containing the

square roots of the eigenvalues of the reduced density matrix. The matrices $\Gamma_m$ and $\Lambda$ are then chosen to satisfy[27,28]

$$\sum_m \Gamma_m^\dagger \Lambda^2 \Gamma_m = \mathbb{1} \text{ and } \sum_m \Gamma_m \Lambda^2 \Gamma_m^\dagger = \mathbb{1}. \quad (13)$$

This implies that the transfer matrix Eq. (11) has an eigenvector $\mathbb{1}$ with eigenvalue $\lambda = 1$, and if condition (c) is fulfilled, all other eigenvalues have smaller magnitudes.[29]

A reflection corresponds to transposing all matrices $\Gamma_m \to \Gamma_m^T$. This transformation preserves the canonical form of the MPS. Since we assume the state to be invariant under inversion, we know from Refs. 9 and 29 that there exists a unitary $U_\mathcal{I}$ with $[U_\mathcal{I}, \Lambda] = 0$ such that

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

By iterating this relation twice, we arrive at $\Gamma_m = e^{2i\theta_\mathcal{I}} (U_\mathcal{I} U_\mathcal{I}^*)^\dagger \Gamma_m U_\mathcal{I} U_\mathcal{I}^*$. Combining this relation with Eq. (13), we obtain $\sum_m \Gamma_m^\dagger \Lambda U_\mathcal{I} U_\mathcal{I}^* \Lambda \Gamma_m = e^{2i\theta_\mathcal{I}} U_\mathcal{I} U_\mathcal{I}^*$, i.e., the matrix $U_\mathcal{I} U_\mathcal{I}^*$ is an eigenvector of the transfer matrix with an eigenvalue $e^{2i\theta_\mathcal{I}}$. Since we assume that all eigenvectors with unimodular eigenvalues are proportional to $\mathbb{1}$ with eigenvalue $\lambda = 1$, $\theta_\mathcal{I}$ is either 0 or $\pi$, and $U_\mathcal{I} U_\mathcal{I}^* = e^{-i\phi_\mathcal{I}} \mathbb{1}$, or $U_\mathcal{I}^T = e^{i\phi_\mathcal{I}} U_\mathcal{I}$. Iterating the latter relation twice, we find that $\phi_\mathcal{I}$ can be either 0 or $\pi$, i.e., $U_\mathcal{I}$ is either symmetric or antisymmetric. Equation (14) implies that, for $\Gamma_m$ to evolve continuously, $U_\mathcal{I}$ has to be continuous (up to a phase) and therefore must remain symmetric or antisymmetric. Therefore, the only way in which $\phi_\mathcal{I}$ and $\theta_\mathcal{I}$ can change is through a phase transition in which one of the assumptions above breaks down. For example, second-order phase transitions through conformal critical points are characterized by a diverging entanglement entropy and thus violate (a).[30] A violation of (b) corresponds to a first-order (discontinuous) phase transition. Violations of (c) correspond to a level crossing in the spectrum of the transfer matrix $T$ which implies a quantum phase transition, as discussed in detail in Ref. 31.

In the $S = 1$ AKLT state, we can represent the state by a MPS with $\Gamma_a = \sigma_a/\sqrt{2}$. Here $\sigma_a$ $(a = x, y, z)$ are Pauli matrices and we use the time-reversal invariant spin basis $|x\rangle = \frac{1}{\sqrt{2}}(|1\rangle - |-1\rangle)$, $|y\rangle = \frac{i}{\sqrt{2}}(|1\rangle + |-1\rangle)$, $|z\rangle = |0\rangle$. Under reflection of the system, the matrices transform as $\sigma_a \to \sigma_a^T = -\sigma_y \sigma_a \sigma_y$. Therefore $U_\mathcal{I} = \sigma_y$ and $\theta_\mathcal{I} = \phi_\mathcal{I} = \pi$. We also find $\theta_\mathcal{I} = \phi_\mathcal{I} = \pi$ for other odd $S$ while $\theta_\mathcal{I} = \phi_\mathcal{I} = 0$ for even $S$. The state $|\mathcal{D}\rangle$, on the other hand, transforms simply as $\Gamma_m^T = \Gamma_m$ (since the $\Gamma_m$ are scalars) and thus $\theta_\mathcal{I} = \phi_\mathcal{I} = 0$. Consequently, the system has to undergo a phase transition when going from the odd-$S$ AKLT state to the trivial state $|\mathcal{D}\rangle$, in agreement with the heuristic argument of Sec. III B.

## IV. TRIVIALITY OF THE EVEN-$S$ AKLT STATE

We now complete the discussion by demonstrating that, on the other hand, the even-$S$ AKLT state is in the same phase as trivial states when a number of different symmetries are imposed. We begin by describing a state, formed by a MPS similar to the one proposed in Ref. 13, which shows that the $S = 2$ AKLT state is smoothly connectable to the trivial state with $S^z = 0$ on every site. In this example, translation, time-reversal, and inversion symmetries are maintained throughout the path, but SU(2) symmetry is broken. We continue by studying an SU(2) preserving example, in which we interpolate smoothly from the $S = 2$ AKLT state to a fully dimerized state. The same construction fails for $S = 1$, suggesting that in this case the topological phase is protected in the presence of sufficient symmetry, in agreements with our conclusion that the odd-spin and even-spin states are distinct phases. Finally, we analyze a spin ladder example, in which an interpolation from an $S = 2$ AKLT state to a trivial state without breaking any symmetry is possible.

### 1. From $S = 2$ AKLT to large-$D$ limit

Let us present an explicit interpolation between the trivial state $|\mathcal{D}\rangle$ [Eq. (2)] and an even-$S$ AKLT state, in terms of MPS. We focus on the $S = 2$ case as the simplest example. We take the standard $S^z$ basis so that $m_j = -2, -1, 0, 1, 2$ can be identified with the eigenvalue of $S_j^z$. We take $\chi = 3$ as for the $S = 2$ AKLT state and choose the matrices $A_m$ as a function of a parameter $t$:

$$A_m(t) \equiv t A_m^{\text{AKLT}} + (1-t)\delta_{m,0} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \quad (15)$$

Here, $A_m^{\text{AKLT}}$ is the MPS representation for the $S = 2$ AKLT state:[32]

$$\sum_m A_m^{\text{AKLT}} |m\rangle = \frac{1}{\sqrt{10}} \begin{pmatrix} |0\rangle & \sqrt{3}|1\rangle & \sqrt{6}|2\rangle \\ -\sqrt{3}|-1\rangle & -2|0\rangle & -\sqrt{3}|1\rangle \\ \sqrt{6}|-2\rangle & \sqrt{3}|-1\rangle & |0\rangle \end{pmatrix}. \quad (16)$$

By construction, the resulting MPS state $|\Psi(t)\rangle$ coincides with the $S = 2$ AKLT state at $t = 1$, and reduces to the trivial state $|\mathcal{D}\rangle$ at $t = 0$. $|\Psi(t)\rangle$ is not invariant under the global SU(2) symmetry, except at $t = 1$. On the other hand, it respects $U(1)$ symmetry (conservation of total $S^z$), translation symmetry, global $D_2$ symmetry, time-reversal symmetry, and inversion symmetry. Although $A_m(t)$ itself is not in the canonical form[26] of the MPS, for $0 < t \leqslant 1$, it can be transformed to it.

Thus, if $|\epsilon_2| < 1$ holds for $t$ in this range, the correlation length remains finite and the path represents an adiabatic evolution without a phase transition. On the other hand, if $|\epsilon_2| = 1$ occurs at a value of $t$ in $0 < t < 1$, the correlation length diverges, signaling a phase transition.

The eigenvalue spectrum of $\mathcal{E}$ for the interpolating MPS (15) can be obtained analytically as a function of $t$, using MATHEMATICA. (The explicit expressions are lengthy and thus omitted here.) The analytic expressions are plotted in Fig. 3. The largest eigenvalue (without degeneracy) is unity for all values of $t$, as expected. Clearly, the absolute value of all the other eigenvalues are smaller than 1. Thus the correlation length remains finite for $0 \leqslant t \leqslant 1$ and has no discontinuities, implying that the $S = 2$ AKLT state is connected adiabatically to the trivial state $|\mathcal{D}\rangle$, without crossing any quantum phase transition. Moreover, the general theorem of Ref. 26 ensures that $|\Psi(t)\rangle$ is the unique ground state of a Hamiltonian with only short-range interactions and there is a nonvanishing excitation gap. Thus the apparent nontrivial structure in the even-$S$ AKLT states is rather fragile; these states can be adiabatically connected to a trivial state even while preserving

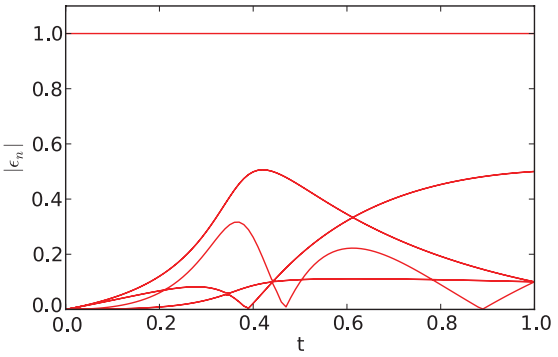


FIG. 3. (Color online) Eigenvalue spectrum of the transfer matrix [completely positive map (11)] for the interpolating MPS defined in (15). Except for the largest eigenvalue (unity), all the eigenvalues have an absolute value smaller than 1 for $0 \leqslant t \leqslant 1$, implying finite correlation length. Thus the trivial state $|\mathcal{D}\rangle$ at $t = 0$ and the $S = 2$ AKLT state at $t = 1$ are adiabatically connected without any phase transition.

inversion, $D_2$, and time-reversal symmetries. This is in sharp contrast to the odd-$S$ case.

### 2. From the AKLT state to a dimerized phase

In the particular example above we used an SU(2)-breaking path to connect the $S = 2$ AKLT state adiabatically to a trivial state. As explained in Secs. III A and III B, however, we expect that even if SU(2) symmetry is respected, an even-$S$ AKLT state can be adiabatically connected to a trivial state, if translational symmetry is broken. (Note that as long as translational symmetry is retained, there is no path connecting the AKLT state to a site-factorizable one, but for a trivial reason: There is no site-factorizable state with SU(2) symmetry for $S > 0$.)

We demonstrate this by constructing a continuous path in MPS space between an $S = 2$ AKLT state and a fully dimerized state. The explicit form of the MPS $|\Psi(t)\rangle$ used to interpolate between the dimerized state at $t = 0$ and a uniform AKLT state for $t = 1$ is given for general spin $S$ in the Appendix [see Fig. 4 (a)]. The state $|\Psi(t)\rangle$ is invariant under SU(2) and inversion for any value of $t$. To show that the correlation length remains finite throughout the path, we have diagonalized numerically the transfer matrix corresponding to $|\Psi_t\rangle$ [Eq. (14)], for a range of values between $t = 0$ and 1. The results for the are shown in Fig. 4(b). As can be seen in the figure, although the correlation length is large, it remains finite for any $0 \leqslant t \leqslant 1$.

### 3. Spin ladders

In order to illustrate the arguments in an especially intuitive way, we contrast $S = \frac{1}{2}$ and $S = 1$ two-leg ladder systems. The Hamiltonian is given by

$$H = J_{\text{leg}} \sum_i \{\mathbf{S}_{1,i} \cdot \mathbf{S}_{1,i+1} + \mathbf{S}_{2,i} \cdot \mathbf{S}_{2,i+1}\} + J_{\text{rung}} \sum_i \mathbf{S}_{1,i} \cdot \mathbf{S}_{2,i}, \tag{17}$$

with the rung and leg couplings $J_{\text{rung}}$ and $J_{\text{leg}}$, respectively. This Hamiltonian has been studied extensively in the literature for both $S = \frac{1}{2}$ and $S = 1$ (for example, see Refs. 33–37). Here, we are interested in the case where we continuously

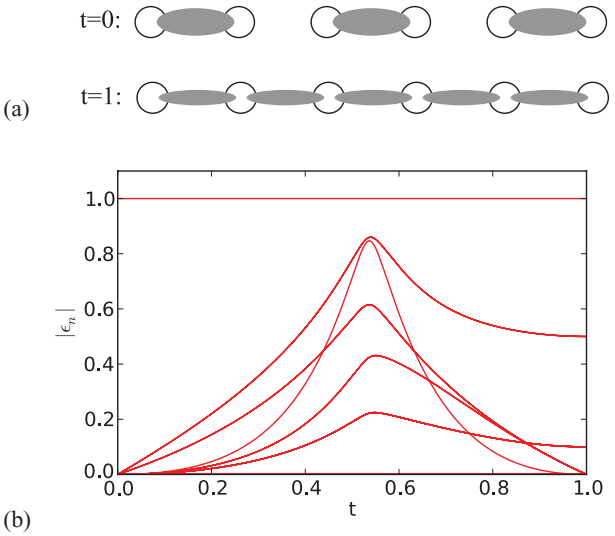


FIG. 4. (Color online) (a) Dimerized state of spin-$S$ singlets on every second bond at $t = 0$ and the AKLT state formed by $S/2$ singlets on every bond at $t = 1$. (b) Eigenvalue spectrum of the two-site transfer matrix along the path connecting the fully dimerized state and the AKLT state for the spin $S = 2$ chain (see text for details).

tune the coupling $J_{\text{rung}}$ on the rungs from negative to positive values while we keep the coupling on the legs constant ($J_{\text{leg}} = 1$). In the limit of $J_{\text{rung}} \to -\infty$, the system maps to a $2S$ Heisenberg model. If $J_{\text{rung}} \to \infty$, the spins form rung singlets, and the ground state is a product state. In the $S = \frac{1}{2}$ case, the point $J_{\text{rung}} = 0$ is a critical point because the systems corresponds to two decoupled $S = \frac{1}{2}$ Heisenberg chains, each having gapless excitations. Thus the two limits cannot be connected adiabatically, at least through this path. In the $S = 1$ case, the point $J_{\text{rung}} = 0$ corresponds to two decoupled $S = 1$ Heisenberg chains which are gapped. Furthermore, previous Monte Carlo studies[35] have shown that the correlation length remains finite along the entire path. Thus the two limits are connected adiabatically. This is in agreement with the above arguments: The $S = 1$ Heisenberg model cannot be connected to a trivial product state while the $S = 2$ Heisenberg point can.

We used the infinite time evolving block decimation (iTEBD)[27] algorithm to numerically calculate the entanglement spectrum along the path connecting the two limits (see Fig. 5). The results are presented as a function of $R = J_{\text{rung}}/(J_{\text{leg}} + |J_{\text{rung}}|)$ for $J_{\text{leg}} > 0$. In the case of $S = \frac{1}{2}$, we clearly observe the predicted twofold degeneracy in the Haldane phase.[9] At the critical point $R = 0$, the entanglement spectrum collapses to one point, and for positive $R$, the entanglement spectrum has no double degeneracies anymore.

In the $S = 1$ case, the systems remains gapped along the entire path and no divergence occurs, in agreement with the results of Ref. 35. Note that, in this case, the lowest entanglement level is threefold degenerate for $R < 0$, corresponding to an effective $S = 1$ edge state, as expected in an $S = 2$ AKLT state. However, this edge degeneracy is not sufficient to distinguish the AKLT state from the trivial (rung singlet) phase. Indeed, at $R = 0$, a level crossing occurs in the entanglement spectrum, and for $R > 0$ the lowest entanglement level is singly degenerate, and the gap in the entanglement spectrum

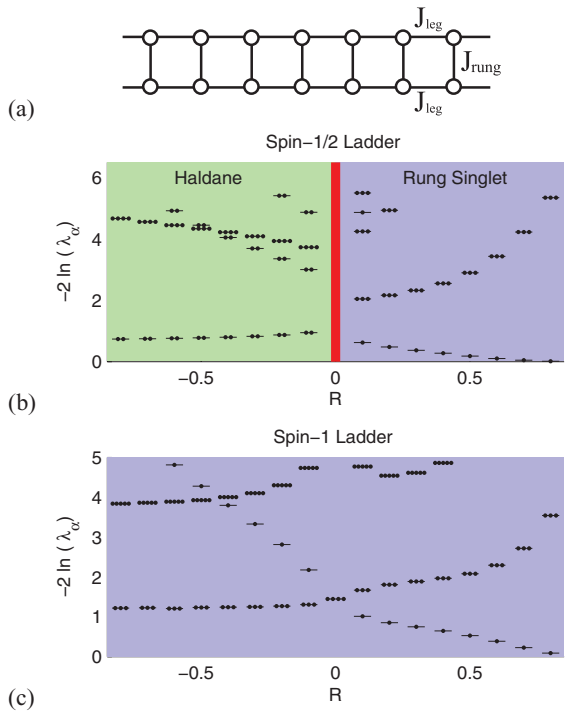


FIG. 5. (Color online) (a) Ladder geometry used for the calculation. Entanglement spectra for (b) $S = \frac{1}{2}$ and (c) $S = 1$ ladders. The entanglement spectrum is plotted vs the ratio $R = J_{rung}/(J_{leg} + |J_{rung}|)$ for $J_{leg} > 0$. Thus $R = -1$ corresponds to infinite ferromagnet coupling on the rungs and $R = 1$ to infinite antiferromagnet couplings. The number of dots on each level indicates its degeneracy.

increases monotonically with $R$, reaching that of the trivial state for $R \to \infty$. Such a level crossing in the entanglement spectrum can occur without a bulk phase transition. In this sense, the existence of an edge state generally does *not* define a phase.

The difference between the two situations can be summarized as in Fig. 6. In the Haldane phase, the entire entanglement spectrum is at least doubly degenerate.[9] Therefore, even if level crossings occur, the lowest entanglement level is always doubly degenerate. This degeneracy is related to an edge state, in the presence of global $D_2$ or time-reversal symmetry. Such an edge state is robust and signals a distinct phase. In the presence of time-reversal symmetry, the protection of the edge state could also be understood as a consequence of the Kramers degeneracy at the edge; all the energy levels at the edge are doubly degenerate and thus the edge state persists even in the presence of a level crossing at the boundary. The degeneracy of the lowest entanglement level or the edge state can be eliminated only via a bulk phase transition (in the presence of an appropriate symmetry), such as the critical point $R = 0$ of the two-leg $S = \frac{1}{2}$ ladder. This difference between robust and nonrobust edge states is also useful in understanding more complicated systems such as spin tubes.[38]

As a final remark, we comment on the relation of our results to those of Anfuso and Rosch.[39] They constructed a path in the parameter space of a fermionic spin-$\frac{1}{2}$ two-leg ladder model which adiabatically connects the $S = 1$ Heisenberg point (described as a Mott insulator with strong ferromagnetic interactions across the rungs) with a trivial product state (a

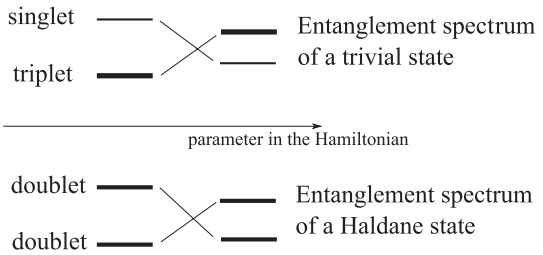


FIG. 6. Schematic diagrams of evolution of entanglement spectra. In the trivial phase (upper panel), the degeneracy of the lowest entanglement level can change, for example, between unity and 3 (which is indeed the case when $R$ changes sign, in the $S = 1$ two-leg ladder discussed in the text). This means that the edge state with $S = 1$ can appear and disappear without a bulk phase transition. In contrast, in the Haldane phase (lower panel), the entire entanglement spectrum is doubly degenerate. Thus the lowest entanglement level is always doubly degenerate, which implies existence of an edge state. The edge state can be removed only via a bulk phase transition (in the presence of an appropriate symmetry described in the text).

band insulator). The Hamiltonian along this path is time-reversal and $D_2$ symmetric, in apparent contradiction with our results for the odd-$S$ AKLT state. (Their model breaks inversion symmetry explicitly along the path.) The reason for this discrepancy is that the model of Anfuso *et al*. includes the possibility of charge fluctuations; i.e., the elementary objects are not odd-$S$ spins, but mobile $S = \frac{1}{2}$ fermions. In that case, one cannot define uniquely the parity of $\frac{S}{2}$ on a given site; even in the Mott insulator phase, virtual fluctuations in the fermion number can switch the site from integer to half integer $S$. Therefore, the arguments presented above for protection by time-reversal or $D_2$ symmetries, which relied crucially on the fact that every site has a well-defined spin, break down. In contrast, in the models we consider here, we assume that the particles are immobile, and therefore the local spin is well defined. On the other hand, in the presence of a lattice inversion symmetry, we expect that the Haldane phase is still robust as a topological phase, even in fermionic models. This does not contradict with Ref. 39, as their model breaks the inversion symmetry explicitly.

## V. CONCLUSIONS

To summarize, we have shown that the topological phase in the odd-$S$ AKLT state is protected as long as either time-reversal, link-centered inversion, or global $D_2$ rotational symmetry is preserved. This symmetry protection, which has been argued before[9] on the basis of properties of the entanglement states, is shown to follow from simple physical arguments: The $D_2$ protection is a result of the hidden symmetry breaking in the AKLT state;[19] protection by time-reversal symmetry is related to the Kramers degeneracy due to the effective half-integer edge spin in an odd-$S$ AKLT state; and the protection by link inversion follows from the odd parity of this state under inversion. Note that none of the above arguments depends on translational symmetry.

In contrast, we argue that even-$S$ AKLT states are fundamentally different. Even in the presence of all the above-mentioned symmetries, this state is adiabatically connectable to a trivial state, as we demonstrated explicitly using a path

in the MPS space. A similar adiabatic connection between the $S = 2$ AKLT state and a trivial state is suggested recently in the analysis of finite-length $S = 2$ chains with both exchange and single-ion anisotropy.[40] Even if the full SU(2) invariance is maintained along the path, we have demonstrated that an even-$S$ AKLT state is adiabatically connectable to a trivial dimerized state with broken translational symmetry.

Our analysis can be extended to more general one-dimensional quantum spin systems, such as chains with bond alternation, spin ladders, and tubes. In the AKLT-type construction based on valence bonds, when a "cut" (such as the vertical line in Fig. 2) is crossed by an odd number of valence bonds, the state has a robust topological phase protected by either time-reversal or link-inversion symmetry, thanks, respectively, to the edge Kramers degeneracy or the odd parity with respect to link inversion. For example, the $n$-leg $S = 1$ Heisenberg ladder, in the weak rung coupling limit (where each chain becomes independent), is topologically distinct from a product state when $n$ is odd. The topological phase survives at a finite rung coupling (persisting until the system passes through a quantum transition) provided that either time-reversal or link inversion is kept.

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## APPENDIX: MPS PATH FROM A DIMERIZED STATE TO THE AKLT STATE

In this Appendix, we construct a path between a fully dimerized state (a broken translational symmetry state in which every pair of spins are coupled in a singlet) and an AKLT state, for general spin $S$, which remains gapped when the spin is even. The path is parametrized by a parameter $t$, where $t = 0$ corresponds to the fully dimerized state and $t = 1$ corresponds to the AKLT state. The MPS along the path is of the form

$$|\Psi\rangle = \sum_{m_1,\ldots,m_L} \mathrm{Tr}\big[A_{m_1}(t)B_{m_2}(t)\cdots A_{m_{L-1}}(t)B_{m_L}(t)\big] \times |m_1,\ldots,m_L\rangle, \tag{A1}$$

where the matrices $A_m(t)$, $B_m(t)$ are given by

$$A_m(t) = \begin{pmatrix} tA_m^{11} & t(1-t)A_m^{12} \\ t(1-t)A_m^{21} & (1-t)A_m^{22} \end{pmatrix},$$

$$B_m(t) = \begin{pmatrix} tB_m^{11} & t(1-t)B_m^{12} \\ t(1-t)B_m^{21} & (1-t)B_m^{22} \end{pmatrix}.$$

Here, $A_m^{11}$ is an $(S+1)\times(S+1)$ matrix, $A_m^{12}$ is $(S+1)\times 1$, $A_m^{21}$ is $(2S+1)\times(S+1)$, and $A_m^{22}$ is $(2S+1)\times 1$. The dimensions of $B_m^{ij}$ are the same as those of $(A_m^{ji})^T$.

As $t$ varies from 1 to 0, the state evolves from the AKLT state, which corresponds to the upper left blocks of the $A$ and $B$ matrices, into the dimerized state, which is defined by the lower right block of $A$, $B$. For intermediate values of $t$, the off-diagonal blocks $A^{12}$, $A^{21}$, $B^{12}$, $B^{21}$ mix these two states together.

The matrix elements of the matrices $A_m^{11}, B_m^{11}$ are given by

$$\big[A_m^{11}\big]_{\alpha,\beta} = \big[B_m^{11}\big]_{\alpha,\beta} = (-1)^{\beta}\langle S/2,\alpha,S/2,\beta;S,m\rangle, \tag{A2}$$

where $\langle j_1,m_1,j_2,m_2;J,M\rangle$ are Clebsch-Gordan coefficients, and we index the matrix elements by $\alpha,\beta = -S/2,\ldots,S/2$. The matrices $A_m^{11}, B_m^{11}$ are exactly the matrices of the AKLT state in Eq. (16).

Similarly, the matrix elements of the other matrices are

$$\big[A_m^{12}\big]_{\alpha,\beta} = \big[B_m^{21}\big]_{\alpha,\beta} = 0, \tag{A3}$$

$$\begin{aligned} [A^{21}]_{\alpha,\beta} &= (-1)^{\beta}\langle S,\alpha,S/2,\beta;S,m\rangle, \\ \big[B_m^{12}\big]_{\alpha,\beta} &= (-1)^{\beta}\langle S/2,\alpha,S,\beta;S,m\rangle, \end{aligned} \tag{A4}$$

$$\begin{aligned} [A^{22}]_{\alpha,\beta} &= (-1)^{\beta}\langle S,\alpha,0,\beta;S,m\rangle, \\ \big[B_m^{22}\big]_{\alpha,\beta} &= (-1)^{\beta}\langle 0,\alpha,S,\beta;S,m\rangle. \end{aligned} \tag{A5}$$

Now for odd $S$, this path fails (as we expect) to be continuous. The matrix $A^{21}$ vanishes because it is not possible to make a spin $S$ state (which is an integer) out of integer- and half-integer spin particles $S$ and $S/2$. Thus, the AKLT state and the dimerized state are not combined with one another in any way, and the transition is discontinuous. The state is just $t^N|\mathrm{AKLT}\rangle + (1-t)^N|\mathrm{Dimerized}\rangle$; at a certain value of $t = t_c$, the two terms have equal weights. Everywhere else, one of the two terms is exponentially bigger than the other, so the correlation functions change discontinuously from the AKLT state's correlation functions to the dimerized state's correlation function. [The correlation length of the MPS cannot be calculated using Eq. (12) in this case because the state is not a pure state in the sense of Ref. 31.]

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