Gapped quantum phases for the $S = 1$ spin chain with D_{2h} symmetry

Zheng-Xin Liu,[1] Min Liu,[1] and Xiao-Gang Wen[2,1]
[1]Institute for Advanced Study, Tsinghua University, Beijing, 100084, P. R. China
[2]Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA
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We study different quantum phases in integer spin systems with on-site $D_{2h} = D_2 \otimes Z_2$ and translation symmetry. We find four distinct nontrivial phases in $S = 1$ spin chains despite the fact that they all have the same symmetry. All four phases have gapped bulk excitations, doubly degenerate end states, and the doubly degenerate entanglement spectrum. These nontrivial phases are examples of symmetry-protected topological (SPT) phases introduced by Gu and Wen [Phys. Rev. B **80**, 155131 (2009)]. One of the SPT phases corresponds to the Haldane phase and the other three are new. These four SPT phases can be distinguished experimentally by their different responses of the end states to weak external magnetic fields. According to the Chen–Gu–Wen classification, the D_{2h} symmetric spin chain can have a total of 64 SPT phases that do not break the symmetry. Here we constructed seven nontrivial phases from the seven classes of nontrivial projective representations of the D_{2h} group. Four of these are found in $S = 1$ spin chains and studied in this paper.

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I. INTRODUCTION

Topological order was introduced to distinguish different phases which cannot be separated by symmetry-breaking orders.[1] Using a definition of phase and phase transition based on local unitary transformations, Ref. 2 shows that what topological order really describes is actually the pattern of long-range entanglements in gapped quantum systems.

For a long time, the Haldane phase[3] for $S = 1$ spin chains was regarded as a simple example of topological order. The existence of string order (or hidden $Z_2 \otimes Z_2$ symmetry breaking), nearly degenerate end states, and gapped excitations were considered the hallmarks of the Haldane phase.[4] However, it was shown that even after we break the spin-rotation symmetry which destroys the string order and gaps the end states, the Haldane phase can still exist (i.e., it is still distinct from the trivial phase). Furthermore, it was shown that the Haldane phase has no long-range entanglements.[5,6] In fact, all one-dimensional (1D) gapped ground states have no long-range entanglements.[7] Thus there are no intrinsic topologically ordered states in gapped 1D systems.[6] This raises a question: What is the order in the Haldane phase?

It turns out that when Hamiltonians have some symmetries, even short-range entangled states with the same symmetry can belong to different phases.[2,5] Such phases are called "symmetry-protected topological (SPT) phases" by Gu and Wen.[5] In fact, the Haldane phase is not an intrinsically topologically ordered phase, but actually an example of SPT phase protected by translation and $SO(3)$ spin-rotation symmetries. This result is supported by a recent realization that the existence of the Haldane phase requires symmetry (such as parity, time-reversal, or spin-rotational symmetry).[5,8] In other words, if the necessary symmetries are absent, the Haldane phase can continuously connect to the trivial phase without any phase transition. We would like to mention that the topological insulators[10–15] are not intrinsically topologically ordered phases either. They are other examples of SPT phases protected by time-reversal symmetry.

In this paper, we will study new SPT phases of a spin chain protected by translational symmetry and on-site $D_{2h} = D_2 \otimes Z_2$ symmetry, where D_2 is a point group composed of discrete spin rotations and Z_2 is generated by the time-reversal operation T. Here we assume that the physical spin forms a linear representation of D_2 and $T^2 = 1$. To see an example of the new SPT phases, we study a simple spin-1 model with those symmetries:

$$H = \sum_i [\cos\theta S_{x,i} S_{x,i+1} + \sin\theta[\cos\phi(S_{y,i} S_{y,i+1} + S_{z,i} S_{z,i+1}) + \sin\phi(S_{xz,i} S_{xz,i+1} + S_{xy,i} S_{xy,i+1})]], \quad (1)$$

where $S_{mn} = S_m S_n + S_n S_m$ $(m,n = x,y,z)$. As shown in Fig. 1, this model has three phases, the Néel phase, the T_0 phase, and the T_x phase. The Néel phase breaks the D_{2h} symmetry, and the other two phases do not break any symmetry. We can use sublattice spin magnetization as an order parameter to distinguish the Néel phase. However, the remaining two phases cannot be distinguished through local order parameters such as sublattice spin magnetization. Further, in both phases, the entanglement spectrum[9] is doubly degenerate, so both of them are nontrivial. However, the entanglement spectrum is not a good order parameter to separate them. Therefore, we need a new tool to distinguish these two nontrivial phases that cannot be described by symmetry breaking and the entanglement spectrum. It turns out that the new tool is the projective representation of the symmetry group. The two phases can be distinguished since their doubly degenerate end states form different projective representations of D_{2h}. This has a physical consequence: The doubly degenerate end states respond differently to a weak external magnetic field.

To be more precise, the doubly degenerate end states can be viewed as an effective spin-1/2 spin with asymmetric g factors: g_x, g_y, and g_z describing the coupling of the end spin to an external magnetic field in the x, y, and z directions. We find that $g_x, g_y, g_z \neq 0$ in the T_0 phase and $g_x \neq 0, g_y = g_z = 0$ in the T_x phase. We would like to stress that such a property is robust against any perturbations that do not break the D_{2h}

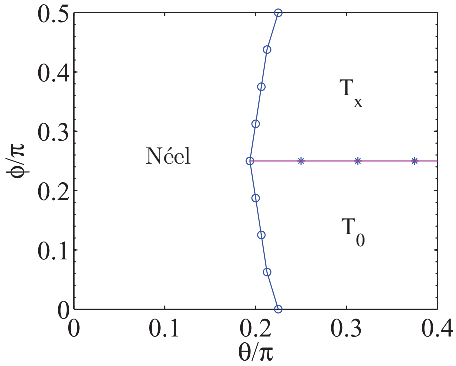


FIG. 1. (Color online) The phase diagram of model (1). The transition between the Néel phase and the SPT phases are second order, and the transition between T_0 and T_x is first order.

symmetry (the perturbation may even break the translation symmetry).

The D_{2h} symmetric 1D spin system has very rich quantum phases. It is shown that it can have 64 different gapped phases that do not break the D_{2h} and the translation symmetry.[16] In fact, it is the projective representation theory that allows one to find all the nontrivial SPT phases beyond the symmetry-breaking description. In this paper, we will not study all of them. We will use only eight classes of projective representations of the D_{2h} group to construct eight gapped no-symmetry-breaking phases; one is trivial and the other seven are nontrivial SPT phases. We find that four of the seven SPT phases (labeled as T_0, T_x, T_y, and T_z) can be realized in an $S = 1$ spin chain. Here T_0 is the usual Haldane phase (because it includes the Heisenberg point), and T_x, T_y, T_z are the new SPT phases. The states in different SPT phases cannot be smoothly connected to each other without explicitly breaking the D_{2h} symmetry in the Hamiltonian. The remaining three SPT phases cannot be realized for $S = 1$ chains; we will not focus on them in the present paper.

The four SPT phases are experimentally distinguishable due to the different behaviors of their end states. In the T_0 phase, the end states can be considered as spin-1/2 free spins. So the weak magnetic field couples to the end spins and lifts the ground-state degeneracy at linear order. However, in the T_x phase, the end states can no longer be considered as normal spin-1/2 spins because they behave differently under time reversal. As mentioned above, their g factors $g_y, g_z = 0$, which means that B_y and B_z cannot split the degenerate ground states in the T_x phase at linear order. Similarly, the end states of T_y (or T_z) respond to only B_y (or B_z). According to these properties, we propose an experimental scenario to distinguish these four phases.

This paper is organized as follows. In Sec. II, we introduce the four SPT phases for the $S = 1$ spin-chain models. In Sec. III, we focus on the interaction of the end states to weak external magnetic fields and propose an experimental method to distinguish different SPT phases. In Sec. IV we briefly summarize the relationship between the SPT phases and the classes of projective representations, and leave detailed derivations to the Appendices. Section V is devoted to conclusions and discussions.

II. THE MODEL AND SPT PHASES

The D_{2h} group has eight group elements, $D_{2h} = \{E, R_x, R_y, R_z, T, R_xT, R_yT, R_zT\}$, which is a direct product of the 180° spin-rotation group $D_2 = \{E, R_x = e^{-i\pi S_x}, R_y = e^{-i\pi S_y}, R_z = e^{-i\pi S_z}\}$ and time-reversal symmetry group $Z_2 = \{E, T\}$. Note that T inverts the spin $(S_x, S_y, S_z) \to (-S_x, -S_y, -S_z)$ and is anti-unitary. D_{2h} has eight 1D linear representations (as shown in Table VI in Appendix B). Since T is anti-unitary, the bases $|\phi\rangle$ and $i|\phi\rangle$ have different time-reversal parities. This subtle property yields more than one SPT phase.

The most general Hamiltonian for an $S = 1$ spin chain with D_{2h} symmetry and with only a nearest-neighbor interaction is given by

$$\begin{aligned} H_{D_{2h}} = \sum_i \big[& a_1 S_{x,i}^2 S_{x,j}^2 + a_2 \big(S_{x,i}^2 S_{y,j}^2 + S_{y,i}^2 S_{x,j}^2\big) \\ & + a_3 S_{y,i}^2 S_{y,j}^2 + a_4 \big(S_{x,i}^2 S_{z,j}^2 + S_{z,i}^2 S_{x,j}^2\big) \\ & + a_5 S_{z,i}^2 S_{z,j}^2 + a_6 \big(S_{y,i}^2 S_{z,j}^2 + S_{z,i}^2 S_{y,j}^2\big) \\ & + b_1 S_{x,i} S_{x,j} + b_2 S_{yz,i} S_{yz,j} + c_1 S_{y,i} S_{y,j} \\ & + c_2 S_{xz,i} S_{xz,j} + d_1 S_{z,i} S_{z,j} + d_2 S_{xy,i} S_{xy,j} \\ & + e_1 S_{x,i}^2 + e_2 S_{y,i}^2 + e_3 S_{z,i}^2 \big], \end{aligned} \tag{2}$$

where $j = i + 1$, $S_{mn} = S_m S_n + S_n S_m$ $(m,n = x,y,z)$, and $a_1, a_2, \ldots, e_1, e_2, e_3$ are constants. We are interested in the parameter regions within which the excitations are gapped and the ground states respect the D_{2h} symmetry.

In general, for 1D systems with translation symmetry and on-site symmetry group G, a gapped ground state that does not break any symmetry can be approximately written as a matrix product state (MPS)

$$|\psi\rangle = \sum_{\{m_1,\ldots,m_N\}} \mathrm{Tr}(A^{m_1} \ldots A^{m_N}) |m_1 \ldots m_N\rangle, \tag{3}$$

which varies in the following way under the symmetry group

$$\sum_{m'} u(g)_{mm'} A^{m'} = \alpha(g) M(g)^\dagger A^m M(g), \tag{4}$$

where $g \in G$ is a group element and $\alpha(g)(M(g))$ is its linear (projective) representation matrix. Thus it is concluded that the SPT phases are classified by (ω, α), where ω is the element of the second cohomology group $H^2(G, U(1))$ (which describes different classes of projective representations of the symmetry group G).[6]

So in our case, the ground state can be generally written in the forms of the MPS shown in Eq. (3). The requirement of $|\psi\rangle$ being invariant under D_{2h} is equivalent to the condition in Eq. (4). The main task of this paper is to try to find different kinds of states that satisfy this condition. In this paper, we consider only the case $\alpha(g) = 1$. The full classification (with a different approach from this paper) is given in Ref. 16.

Let us first consider the on-site terms in Eq. (2). When $|e_1|$, $|e_2|$, or $|e_3|$ is large, the ground state of $H_{D_{2h}}$ is simple. For instance, when $e_3 \to -\infty$, the ground state is a long-range ordered state which breaks the D_{2h} symmetry; when $e_3 \to \infty$, the ground state is a product state $|\psi\rangle = \prod_i \otimes |0\rangle_i$, which is trivial.[17] Since we are interested in the nontrivial SPT phases, we will set $e_1 = e_2 = e_3 = 0$ in the following discussion.

A. Exactly solvable models

The Affleck–Kennedy–Lieb–Tasaki (AKLT) model[18] is an exactly solvable model with $SO(3)$ symmetry that falls in the Haldane phase. The AKLT model contains all the physical properties of the Haldane phase, and all other states in this phase can smoothly deform into the AKLT state. Since the ground-state wave function of this exactly solvable model is a simple matrix product (sMP) state[19] and is known in advance, studying this model is relatively easy and helps us to understand the physics of the Haldane phase.

In this section, we will introduce four classes of exactly solvable models that have D_{2h} symmetry. Analogous to the of AKLT state, the ground states of these exactly solvable models are nontrivial sMP states satisfying Eq. (4). We will show that different classes of sMP states cannot be smoothly connected, which indicates that each class corresponds to a phase.

The first example is a direct generalization of the AKLT model. The ground state of the AKLT state is represented by $A^x = \sigma_x$, $A^y = \sigma_y$, $A^z = \sigma_z$, which has $SO(3)$ symmetry. When generalized to D_{2h} symmetry, we obtain

$$A^x = a\sigma_x, \quad A^y = b\sigma_y, \quad A^z = c\sigma_z, \tag{5}$$

where a,b,c are nonzero real numbers (the same below). When $a = b = c = 1$, the above state reduces to the AKLT state. For this reason, we say that this model also belongs to the Haldane phase. We label this phase as T_0. Similar to the AKLT model, the parent Hamiltonian of the above state is composed of projectors (for details see Appendices A and B):

$$\begin{aligned} H_0 = \sum_i \bigg[&\left(\frac{1}{4} + b^2c^2\gamma\right) S_{x,i}S_{x,j} + \left(\frac{1}{4} + a^2c^2\gamma\right) S_{y,i}S_{y,j} \\ &+ \left(\frac{1}{4} + a^2b^2\gamma\right) S_{z,i}S_{z,j} + \left(\frac{1}{4} - b^2c^2\gamma\right) S_{yz,i}S_{yz,j} \\ &+ \left(\frac{1}{4} - a^2c^2\gamma\right) S_{xz,i}S_{xz,j} + \left(\frac{1}{4} - a^2b^2\gamma\right) S_{xy,i}S_{xy,j} \bigg] \\ &+ h_0, \end{aligned} \tag{6}$$

where $\gamma = \frac{1}{2(a^4+b^4+c^4)}$ and

$$\begin{aligned} h_0 = -\sum_i \big[&c^4\gamma\left(S_{x,i}^2 S_{y,j}^2 + S_{y,i}^2 S_{x,j}^2\right) + b^4\gamma\left(S_{x,i}^2 S_{z,j}^2 \right. \\ &\left. + S_{z,i}^2 S_{x,j}^2\right) + a^4\gamma\left(S_{y,i}^2 S_{z,j}^2 + S_{z,i}^2 S_{y,j}^2\right)\big]. \end{aligned}$$

At open boundary conditions, Hamiltonian (6) has exactly fourfold degenerate ground states independent of the chain length. The uniqueness of the ground state can be proved following the AKLT model.[18] The above exactly solvable model is frustration free, that is, the expectation value of the Hamiltonian is minimized locally in the ground states. The excitations are gapped and all correlation functions of local operators are short ranged. Furthermore, if a,b,c are normalized, $a^2 + b^2 + c^2 = 1$, then it is easily checked that

$$\sum_m A^m (A^m)^\dagger = I, \quad \sum_m (A^m)^\dagger \Lambda^2 A^m = \Lambda^2;$$

here $\Lambda = I$, indicating that the entanglement spectrum of the ground states is doubly degenerate. This informs us that the state of Eq. (5) is nontrivial. Actually, the models in the vicinity of Eq. (6) (the phase T_0) have very similar properties unless gap closing (second-order phase transition) or level crossing (first-order phase transition) happens.

Now we consider another example of the sMP state,

$$A^x = ia\sigma_x, \quad A^y = b\sigma_y, \quad A^z = c\sigma_z. \tag{7}$$

Above the sMP state is also invariant under D_{2h} group. As will be shown later, it cannot be continuously connected to Eq. (5) without breaking the D_{2h} symmetry. This means that it belongs to another phase which we label as T_x phase. The parent Hamiltonian of Eq. (7) is given by

$$\begin{aligned} H_x = \sum_i \bigg[&\left(\frac{1}{4} + b^2c^2\gamma\right) S_{x,i}S_{x,j} + \left(\frac{1}{4} - a^2c^2\gamma\right) S_{y,i}S_{y,j} \\ &+ \left(\frac{1}{4} - a^2b^2\gamma\right) S_{z,i}S_{z,j} + \left(\frac{1}{4} - b^2c^2\gamma\right) S_{yz,i}S_{yz,j} \\ &+ \left(\frac{1}{4} + a^2c^2\gamma\right) S_{xz,i}S_{xz,j} + \left(\frac{1}{4} + a^2b^2\gamma\right) S_{xy,i}S_{xy,j} \bigg] \\ &+ h_0. \end{aligned} \tag{8}$$

Similarly, the third example

$$A^x = a\sigma_x, \quad A^y = ib\sigma_y, \quad A^z = c\sigma_z, \tag{9}$$

belongs to the T_y phase and its parent Hamiltonian is

$$\begin{aligned} H_y = \sum_i \bigg[&\left(\frac{1}{4} - b^2c^2\gamma\right) S_{x,i}S_{x,j} + \left(\frac{1}{4} + a^2c^2\gamma\right) S_{y,i}S_{y,j} \\ &+ \left(\frac{1}{4} - a^2b^2\gamma\right) S_{z,i}S_{z,j} + (\frac{1}{4} + b^2c^2\gamma) S_{yz,i}S_{yz,j} \\ &+ \left(\frac{1}{4} - a^2c^2\gamma\right) S_{xz,i}S_{xz,j} + \left(\frac{1}{4} + a^2b^2\gamma\right) S_{xy,i}S_{xy,j} \bigg] \\ &+ h_0. \end{aligned} \tag{10}$$

The last example

$$A^x = a\sigma_x, \quad A^y = b\sigma_y, \quad A^z = ic\sigma_z, \tag{11}$$

belongs to the T_z phase with its parent Hamiltonian given by

$$\begin{aligned} H_z = \sum_i \bigg[&\left(\frac{1}{4} - b^2c^2\gamma\right) S_{x,i}S_{x,j} + \left(\frac{1}{4} - a^2c^2\gamma\right) S_{y,i}S_{y,j} \\ &+ \left(\frac{1}{4} + a^2b^2\gamma\right) S_{z,i}S_{z,j} + \left(\frac{1}{4} + b^2c^2\gamma\right) S_{yz,i}S_{yz,j} \\ &+ \left(\frac{1}{4} + a^2c^2\gamma\right) S_{xz,i}S_{xz,j} + \left(\frac{1}{4} - a^2b^2\gamma\right) S_{xy,i}S_{xy,j} \bigg] \\ &+ h_0. \end{aligned} \tag{12}$$

Above we have given four special models that belong to different SPT phases. In the next subsection, we will show that if one keeps the D_{2h} symmetry, phase transitions must happen when connecting these models.

B. Transitions between different SPT phases

To justify the four SPT phases, we will use a numerical method to study more general Hamiltonians. The method we adopt is one version of the tensor renormalization group (RG) approach developed in one dimension by Vidal[20] and later generalized to two dimensions by Jiang *et al.*[21] In this method, the ground state is approximated by a MPS. For

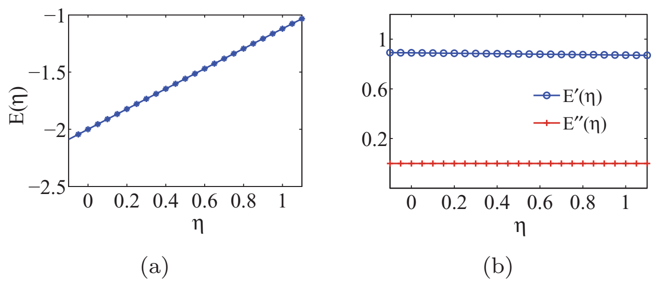


FIG. 2. (Color online) (a) The energy curve $E(\eta)$, (b) the first and second derivatives of $E(\eta)$. All these curves are smooth, indicating that these states are in the same phase.

an arbitrarily initialized state, we can act the (infinitesimal) imaginary time-evolution operator $U(\delta\tau) = e^{-H\delta\tau}$ for infinite times, finally obtaining the fixed-point matrix A^m. If the dimension D of A^m is not too small, the corresponding MPS is very close to the true ground state. In one dimension, the ground-state energy, correlation functions, density matrix, and entanglement spectrum can be calculated directly from the matrix A^m.

We have checked our tensor RG method by the simple transverse Ising model $H = \sum_i \sigma_i^z \sigma_{i+1}^z + B\sigma_i^x$. From the analytic result, the transition point is at $B = 1$. Our numerical result shows a high accuracy for this transition point, with an error of less than 1% when we set $D = 16$. So we can use the tensor RG method to distinguish different SPT phases given in last section.

Notice that h_0 is a common term in the four exactly solvable models, which indicates that it is unimportant and can be dropped. This can be numerically verified. For this purpose, we add a perturbation to the models, such as in Eq. (8),

$$H(\eta) = H_x - \eta h_0, \tag{13}$$

where $\eta \in [0,1]$. As shown in Fig. 2, the ground-state energy $E(\eta)$ and its derivatives $E'(\eta), E''(\eta)$ are all smooth functions, indicating that all the Hamiltonians $H(\eta)$ belong to the same phase. Using the same method, one can also check that the Hamiltonians (with D_{2h} symmetry) in the vicinity of an exactly solvable model fall in the same phase. For instance, the Heisenberg model and H_0 in Eq. (6) are in the same phase.

Now the question is whether the ground states of different exactly solvable models can be smoothly transformed into each other. To this end, we consider a more realistic model of Eq. (1) which connects two exactly solvable models, such as H_0 and H_x. We are interested in the antiferromagnetic cases and will focus on the parameter region $\theta,\phi \in [0,\frac{\pi}{2}]$. The point $(\frac{\pi}{4},0)$ is the Heisenberg model. From the result of the last paragraph, the Heisenberg model is in the same phase as Eq. (6), and similarly $(\frac{\pi}{4},\frac{\pi}{2})$ is in the same phase as Eq. (8). If these two points cannot be smoothly connected (i.e., if gap closing or level crossing will unavoidably happen), then Eqs. (6) and (8) belong to different phases.

Using the tensor RG method, we can calculate the ground-state energy of Eq. (1) and the phase diagram is shown in Fig. 1. When θ is less then 0.21π, the ground state is Néel ordered. When θ increases, a second-order phase transition occurs and we enter the SPT phases. Figure 3 shows the entanglement spectrum, the energy curve, and its first and second derivatives at $\phi = \frac{\pi}{8}$ (or $\phi = \frac{3\pi}{8}$), which illustrate this transition. Near the transition point, the trial energy decreases with increasing D, which indicates that the ground state at the transition point is described by a MPS with diverging dimension D. Consequently, the ground-state entanglement entropy diverges, which is a feature of second-order phase transition.

The region $\phi \in [0,\frac{\pi}{4})$ belongs to the T_0 phase and $\phi \in (\frac{\pi}{4},\frac{\pi}{2}]$ belongs to the T_x phase. A first-order phase transition between them happens at $\phi = \frac{\pi}{4}$.

The first-order phase transition occurs exactly at $\phi = \frac{\pi}{4}$. This is because the whole phase diagram is symmetric above and below the line $\phi = \frac{\pi}{4}$. This symmetry can be seen in the Hamiltonian. Notice that, under a unitary matrix U, we get

$$U^\dagger S_x U = S_x, \quad U^\dagger S_y U = -S_{xz}, \quad U^\dagger S_z U = S_{xy}, \tag{14}$$

where $U = \begin{pmatrix} \frac{1}{\sqrt{2}e^{i\frac{\pi}{4}}} & 0 & \frac{1}{\sqrt{2}}e^{-i\frac{\pi}{4}} \\ 0 & 1 & 0 \\ \frac{1}{\sqrt{2}}e^{-i\frac{\pi}{4}} & 0 & \frac{1}{\sqrt{2}}e^{i\frac{\pi}{4}} \end{pmatrix}$.[22] This means that Hamiltonian (1) satisfies $(\prod_i \otimes U_i)^\dagger H(\theta,\phi)(\prod_i \otimes U_i) = H(\theta,\frac{\pi}{2}-\phi)$, which yields $E(\theta,\phi) = E(\theta,\frac{\pi}{2}-\phi)$, and their ground states are transformed by the (local) unitary transformation $\prod_i \otimes U_i$. But this unitary transformation is not invariant under time reversal T, so the behavior of the ground state also changes under time reversal. As a result, the state after the transformation belongs to a different phase.

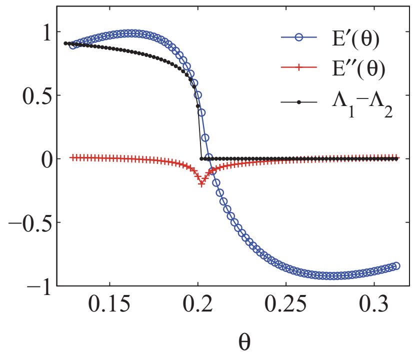
The entanglement spectrum of the ground states can also be obtained programmatically. We find that in both T_0 and T_x phases the entanglement spectrum is doubly degenerate [see Fig. 3(a)]. This shows that the T_0 and T_x phases are indeed nontrivial. Similar to model (1), the phase transition between T_0 and T_y or between T_0 and T_z can also be illustrated.

Now we will show that first-order phase transition also exists between any two of T_x,T_y,T_z. As an example, we consider the model that contains the transition between T_x and T_z phases:

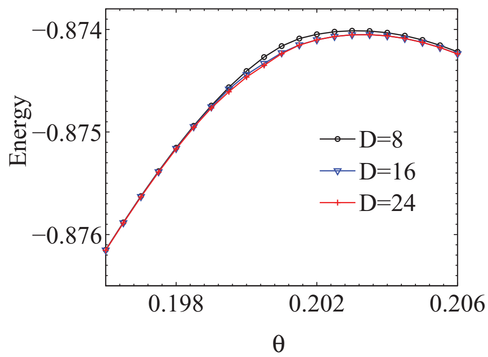
$$H = \sum_i \left[\frac{1}{6}S_{y,i}S_{y,j} + \frac{5}{6}S_{xz,i}S_{xz,j} + \cos\theta(S_{x,i}S_{x,j} + S_{xy,i}S_{xy,j}) + \sin\theta(S_{z,i}S_{z,j} + S_{yz,i}S_{yz,j})\right]. \tag{15}$$

When $\theta = \tan^{-1}\frac{1}{5}$, the above Hamiltonian is in the same phase as H_x as shown in Eq. (13), and when $\theta = \tan^{-1}5$, it is in the same phase as H_z. The ground-state energy of Eq. (15) as a function of θ can be obtained using the tensor RG method, and the result is shown in Fig. 4. A first-order transition at $\theta = \frac{\pi}{4}$ manifests itself. For the reason similar to that of Eq. (14), the model also has a symmetry $E(\theta) = E(\frac{\pi}{2}-\theta)$.

From the above analysis, we can conclude that the four exactly solvable models really stand for four distinct SPT phases. All these SPT phases are protected by the D_{2h} symmetry. As will be shown in Sec. IV, no more SPT phases exist for $S = 1$ spin chain models with D_{2h} symmetry. Furthermore, Eqs. (1) and (15) show that these SPT phases can be obtained by much simpler Hamiltonians, which is hopefully realized experimentally.



(a)



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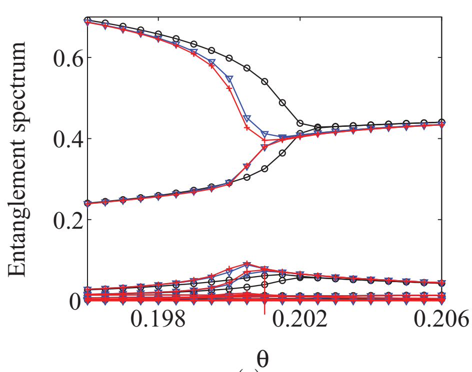

(c)

FIG. 3. (Color online) (a) The first-order derivative (line with circles) and the second-order derivative (line with crosses) of $E(\theta)$ at $\phi = \frac{\pi}{8}$ (or $\phi = \frac{3\pi}{8}$). We have set $D = 16$. The dotted line is the difference between the two biggest weights of the entanglement spectrum $\Lambda_1 - \Lambda_2$. Since $E'(\theta)$ is continuous but $E''(\theta)$ is not, the transition is second order. The degeneracy of Λ_1 and Λ_2 indicates that the T_0 (and T_x) phase is nontrivial. (b) The refined energy curve $E(\theta)$ near the transition point with $D = 8,16,24$. The trial energy decreases with increasing D, which is evidence of the factor that at the transition point the ground state is a MPS with infinite D. (c) The entanglement spectrum with different D. The black circles are for $D = 8$, blue triangles for $D = 16$, and red crosses for $D = 24$. At the transition point, the entanglement entropy increases with D and diverges when D goes to infinity.

Now an interesting question arises: How do we distinguish these SPT phases in a practical way? It is impossible to distinguish these phases by linear response in the bulk since it is gapped. However, the end "spins" localized at open boundaries may have different behaviors in different SPT phases. In the next section, we will propose an experimental method to detect each SPT phase.

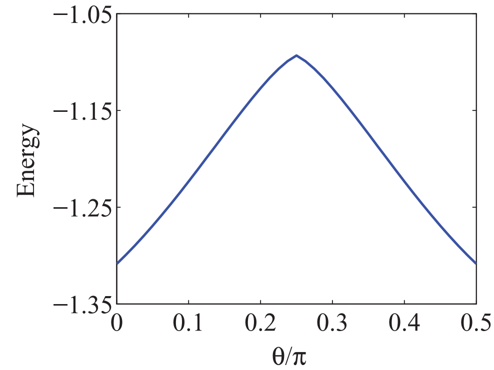

FIG. 4. (Color online) The ground-state energy for the model described by Eq. (15). A first-order phase transition is obvious.

III. DISTINGUISHING DIFFERENT SPT PHASES

We expect to distinguish the four SPT phases through their different physical properties. Experimentally, all measurable physical quantities are response functions, or susceptibilities. So we need to add small perturbations and expect that (the "end spins" of) different phases have different responses. The simplest perturbation for a spin system is magnetic field $H' = g_L \mu_B \mathbf{B} \cdot \tilde{\mathbf{S}}$; here $\tilde{\mathbf{S}} = \sum_i \mathbf{S}_i$, g_L is the Landé factor, and μ_B is the Bohr magneton. We will study the linear response to small $\mathbf{B}$.

Since the states in the same phase have the same universal properties, we will focus on the exactly solvable models first. For simplicity, we consider the AKLT model, namely, H_0 with $a = b = c = 1$. In the MPS picture, the physical $S = 1$ spin is divided into two $J = 1/2$ virtual spins. In the AKLT state, the virtual spins pair into singlets (called valence bonds) on each link between neighboring sites. Under open boundary conditions, a free $J = 1/2$ spin at each end remains unpaired. The two end spins account for the exact fourfold degeneracy of the ground states. In this picture, it is easy to calculate the total spin in the ground-state Hilbert space. The singlets in the bulk have no contributions to $\tilde{\mathbf{S}}$; only the two end spins $\mathbf{j}_1$ and $\mathbf{j}_2$ contribute and, as aresult $\tilde{\mathbf{S}} = \mathbf{j}_1 + \mathbf{j}_2$. In this sense, the end spins can be considered as *impurity spins* of a paramagnetic material. Since the total spin of an open chain is $\frac{1}{2} \otimes \frac{1}{2} = 0 \oplus 1$, we expect that the eigenvalue of $\tilde{S}_x, \tilde{S}_y, \tilde{S}_z$ should be $1, -1, 0, 0$. This can be verified by the exact diagonalizing of a short chain. We denote these four degenerate ground states as $|\psi_1\rangle, |\psi_2\rangle, |\psi_3\rangle, |\psi_4\rangle$. Then the matrix element of $\tilde{S}_m$ in the ground-state Hilbert space is given by

$$\tilde{S}_m^{\alpha\beta} = \langle \psi_\alpha | \tilde{S}_m | \psi_\beta \rangle, \ \ \alpha,\beta = 1,2,3,4. \qquad (16)$$

The eigenvalues of the matrices $(\tilde{\mathbf{S}}^{\alpha\beta})$ are exactly $1, -1, 0, 0$, and these values are independent of the length of the chain. Thus a small magnetic field along any direction $H' = g_L \mu_B B_x S_x$ or $g_L \mu_B B_y S_y$ or $g_L \mu_B B_z S_z$ will split the ground-state degeneracy and give rise to a finite magnetization.

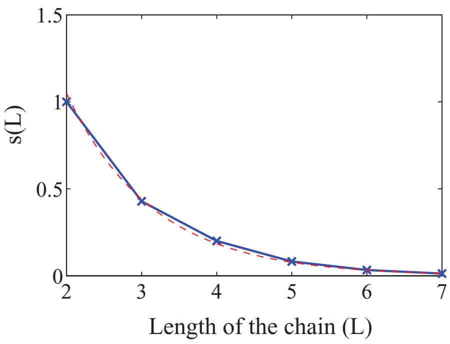

FIG. 5. (Color online) The eigenvalues of $\tilde{S}_y$ and $\tilde{S}_z$ are s, $-s$,0,0. The magnitude of s exponentially decays with the length of the chain in the T_x phase. The dashed line is an exponential fit. The results are obtained by exact diagonalization and we calculate only up to seven sites.

At finite temperature, the susceptibility satisfies the Curie law and is given by[23]

$$\chi(T) \simeq \frac{Ng^2\mu_B^2}{3k_BT}, \tag{17}$$

where N is the number of end spins, $g = \sqrt{J(J+1)}g_L$, $J = 1/2$, and g_L is the Landé g factor. If the spin-1 chains in the sample are broken into long separate segments, then N can be a considerable number. We also note that, in real samples, the susceptibility also contains a temperature-independent part coming from the bulk.

We see that, for the AKLT model, the spin susceptibility diverges at low temperature along all directions. For a general model in the T_0 phase, the divergence of $\chi_x(T),\chi_y(T),\chi_z(T)$ still holds, except that it is no longer isotropic.

However, in phase T_x, the end "spins" have absolutely different physical properties. We consider the model H_x in Eq. (8), and set $a = b = c = 1$. Then we calculate the eigenvalues of operators $\tilde{S}_x,\tilde{S}_y$ and $\tilde{S}_z$ in the ground-state Hilbert space as before. We find that the eigenvalues of $(\tilde{S}^{\alpha\beta})_x$ are still $1,-1,0,0$, meaning that along the x direction the spin-1/2 end spins still exist and $\chi_x(T)$ diverges at $T = 0$. The eigenvalues of $(\tilde{S}^{\alpha\beta})_y$ and $(\tilde{S}^{\alpha\beta})_z$ also have the structure s, $-s$,0,0, but the magnitudes of the nonzero eigenvalues s exponentially decay to zero with the increasing of the length of the chain (see Fig. 5). This means that in the y and z directions, there are no free spins coupled to the magnetic field. In Appendix D we will show that this property is determined by the projective representation carried by the virtual spins. In this case, $\chi_y(T)$ and $\chi_z(T)$ are given by Eq. (17) with $g_y,g_z \approx 0$. The results that $\chi_x(T)$ follows Curie law and $\chi_y(T)$, $\chi_z(T)$ has effective $g_y,g_z \approx 0$ are universal properties of all the models in the T_x phase.

Similarly, one can check that only $\chi_y(T)$ follows Curie law in the T_y phase with the usual $g_y \approx \sqrt{J(J+1)}g_L$ ($g_x,g_z \approx 0$), and similarly only $\chi_z(T)$ follows Curie law in the T_z phase with the usual $g_z \approx \sqrt{J(J+1)}g_L$ ($g_x,g_y \approx 0$). Therefore, by measuring the temperature dependence of susceptibility and the effective g in x,y,z directions, we are able to distinguish the four SPT phases.

IV. PROJECTIVE REPRESENTATIONS AND SPT PHASES

In previous sections, we have given four SPT phases of model (2) and studied their physical properties. In this section, we will explain how the D_{2h} symmetry supports the existence of these phases. Then we will discuss other possible SPT phases of spin systems with D_{2h} symmetry.

The ground state of a gapped phase is written as Eq. (3). If we require that the ground state MPS be invariant under the symmetry group D_{2h}, namely, $g|\psi\rangle = |\psi\rangle$ ($g \in D_{2h}$), then under the action of the symmetry group the matrix A^m must vary in the following way.

(1) g is unitary, $g \in \{E,R_x,R_y,R_z\}$,

$$\sum_{m'} u(g)_{mm'}A^{m'} = M(g)^\dagger A^m M(g); \tag{18}$$

(2) g is anti-unitary, $g \in \{T,R_xT,R_yT,R_zT\}$,

$$\sum_{m'} u(g)_{mm'}KA^{m'} = M(g)^\dagger A^m M(g). \tag{19}$$

Here $u(g)$ and $M(g)$ are representations of the symmetry group D_{2h}. The matrices $u(g)$ satisfy the same multiplication law of the D_{2h} group and are called *linear representations*. The physical spin freedoms are linear representations of D_{2h}. $M(g)$ and $M(g)e^{i\theta}$ are equivalent and belong to the same presentation. Up to a phase factor (which depends on the group elements), $M(g)$ satisfy the multiplication law of D_{2h}, and this kind of presentation is called a *projective representation*. The virtual spins (and the end states) are projective representations of D_{2h}. More knowledge about projective representation can be found in Refs. 6 and 24.

The D_{2h} group has eight 1D linear representations (see Table VI) and eight (and only eight) classes of projective representations labeled by (111), (11-1),(1-11),(1-1-1),(-111),(-11-1),(-1-11) and (-1-1-1) (see Table VII). The first class of projective representation (111) is the eight 1D linear representations, which are trivial (an example of the the corresponding trivial phase is the case $e_3 \to \infty$). The other seven projective representations are two-dimensional (2D) and nontrivial. Since states supporting different projective representations (or virtual spins) cannot be smoothly transformed into each other, each projective representation corresponds to a SPT phase. This means that there should be at least seven different nontrivial SPT phases for spin systems respecting D_{2h} symmetry. [In fact, when considering different $\alpha(g)$ there are more nontrivial SPT phases for spin systems respecting D_{2h} symmetry.[16]]

How can we obtain the projective representations? Mathematically, finding the projective representations of a group G is equivalent to finding the linear representations of its cover group, which is a central extension of G and is called representation group $R(G)$.[24] The representation group $R(D_{2h})$ is available in literature,[24] so we can calculate the matrix elements of all the projective representations of D_{2h} (see Table VII).

Once the matrices of the projective representations are obtained, we can calculate the Clebsch-Gordan (CG) coefficients for decomposing the direct product of two projective representations. From the CG coefficients, we can construct sMP states and their parent Hamiltonians.[25] Models (6), (8), (10), and (12) are constructed accordingly and correspond to the (-1-1-1),(-1-11),(-11-1), (-111) representations, respectively. From these models we can know what kinds of interactions are essential for each SPT phase.

As shown in Appendix B, the remaining three SPT phases of (1-11),(11-1),(1-1-1) cannot be realized for $S = 1$ spin chains. The reason is that the physical freedom is not sufficient to support the direct product of two such projective representations. However, these phases might be realized in $S = 1$ spin ladders or $S = 2$ models, and this will be our upcoming work.

V. CONCLUSION AND DISCUSSION

In summary, we have found four nontrivial SPT phases T_0, T_x, T_y, T_z of $S = 1$ spin chains which have on-site D_{2h} symmetry. These SPT phases have similar properties as the usual Haldane phase, such as the bulk excitation gap, short-range correlations, existence of end spins, and entanglement spectrum degeneracy. However, the different projective representations of the end spin under D_{2h} indicate that they do belong to different phases. The SPT order that distinguishes them is the class of projective representations [or the group elements of the second cohomology $H^2(D_{2h}, U(1))$] corresponding to the ground states (or the matrices A^m).

We find that different SPT phases can be distinguished by experimental method. The magnetic susceptibilities χ_x, χ_y, χ_z obey Curie law and diverge at zero temperature. In the T_0 phase the effective g factors of the end spin have the usual values for magnetic fields in the x, y, and z directions. But in the T_x (or T_y or T_z) phase, the effective $g \approx \sqrt{J(J+1)} g_L$ has the usual value only for the magnetic field in the x direction (or y direction or z direction). The effective $g = 0$ [see Eq. (17)] for the magnetic field in the other two directions. We suggest other numerical methods, such as the density matrix renormalization group (DMRG), to verify the existence of these SPT phases and their different responses to magnetic field.

The T_0 phase (or the usual Haldane phase) can be realized experimentally. The antiferromagnetic Heisenberg model, which is the microscopic Hamiltonian of many quantum magenets, belongs to the T_0 phase. The T_0 phase is robust when the continuous spin-rotation symmetry is reduced to D_{2h} (by small anisotropic exchanging, single-ion anisotropy term, easy-axis term, etc.). However, as shown in Sec. II, the other three T_x, T_y, T_z phases require remarkable biquadratic interactions. Currently, materials with such kind of interactions seems not to be found. However, if the system has spin-orbital interaction, it is possible that the ground state belongs to one of these nontrivial phases.

From the seven nontrivial projective representations of the D_{2h} group, we constructed seven SPT phases. Four of them are discussed above. The other three may be realized in $S = 1$ spin ladders or spin $S = 2$ models and are not discussed in this paper. Some conclusion in this paper can be generalized to larger spin systems and higher dimensions.

TABLE I. Multiplication table of D_2

	E	R_x	R_y	R_z
E	E	R_x	R_y	R_z
R_x	R_x	E	R_z	R_y
R_y	R_y	R_z	E	R_x
R_z	R_z	R_y	R_x	E

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APPENDIX A: SPIN CHAIN WITH D_2 SYMMETRY

In this Appendix, we will first study $S = 1$ spin systems with D_2 symmetry. The same method can be applied to the D_{2h} case.

1. General Hamiltonian with D_2 point group symmetry

The point group D_2 has only four elements, $D_2 = \{E, R_x, R_y, R_z\}$. The multiplication table is shown in Table I.

It has four 1D linear representations, whose matrix elements and bases of representations are shown in Table II. From quantum mechanics, we know that the $2S + 1$ bases of integer spin S span an irreducible linear representation space of $SO(3)$ group. This Hilbert space is reduced to a direct sum of $2S + 1$ 1D irreducible linear representation spaces of D_2. For example, when $S = 1$ (a vector), the bases

$$|x\rangle = \frac{1}{\sqrt{2}}(|-1\rangle - |1\rangle),$$
$$|y\rangle = \frac{1}{\sqrt{2}} i(|-1\rangle + |1\rangle),$$
$$|z\rangle = |0\rangle$$

form the B_3, B_2, B_1 representations of D_2, respectively.

Here we focus on the $S = 1$ model with nearest-neighbor interaction. The general Hamiltonian with D_2 symmetry is given by

$$H_{D_2} = H_{D_{2h}} + f_1(S_{x,i} S_{yz,j} + S_{yz,i} S_{x,j}) + f_2(S_{y,i} S_{xz,j} + S_{xz,i} S_{y,j}) + f_3(S_{z,i} S_{xy,j} + S_{xy,i} S_{z,j}), \quad \text{(A1)}$$

where f_1, f_2, f_3 are constants and $H_{D_{2h}}$ is given in Eq. (2). The above Hamiltonian H_{D_2} also has translational symmetry and spatial inversion symmetry. The additional f_1, f_2, f_3 terms are

TABLE II. Linear representations of D_2

	E	R_x	R_y	R_z	Bases or operators		
A	1	1	1	1	$\|0,0\rangle$		S_x^2, S_y^2, S_z^2
B_1	1	−1	−1	1	$\|1,z\rangle$	S_z	S_{xy}
B_2	1	−1	1	−1	$\|1,y\rangle$	S_y	S_{xz}
B_3	1	1	−1	−1	$\|1,x\rangle$	S_x	S_{yz}

TABLE III. Multiplication table of $R_1(D_2)$. Notice that $P^4 = Q^4 = E$, $P^2 = Q^2$ and $QP = P^3Q$.

	E	P^2	P^3	P	Q	P^2Q	PQ	P^3Q
E	E	P^2	P^3	P	Q	P^2Q	PQ	P^3Q
P^2	P^2	E	P	P^3	P^2Q	Q	P^3Q	PQ
P^3	P^3	P	P^2	E	P^3Q	PQ	Q	P^2Q
P	P	P^3	E	P^2	PQ	P^3Q	P^2Q	Q
Q	Q	P^2Q	PQ	P^3Q	P^2	E	P	P^3
P^2Q	P^2Q	Q	P^3Q	PQ	E	P^2	P^3	P
PQ	PQ	P^3Q	P^2Q	Q	P^3	P	P^2	E
P^3Q	P^3Q	PQ	Q	P^2Q	P	P^3	E	P^2

TABLE IV. Multiplication table of $R_2(D_2)$. Notice that $P^4 = Q^2 = E$ and $QP = P^3Q$.

	E	P^2	P^3	P	Q	P^2Q	PQ	P^3Q
E	E	P^2	P^3	P	Q	P^2Q	PQ	P^3Q
P^2	P^2	E	P	P^3	P^2Q	Q	P^3Q	PQ
P^3	P^3	P	P^2	E	P^3Q	PQ	Q	P^2Q
P	P	P^3	E	P^2	PQ	P^3Q	P^2Q	Q
Q	Q	P^2Q	PQ	P^3Q	E	P^2	P^3	P
P^2Q	P^2Q	Q	P^3Q	PQ	P^2	E	P	P^3
PQ	PQ	P^3Q	P^2Q	Q	P	P^3	E	P^2
P^3Q	P^3Q	PQ	Q	P^2Q	P^3	P	P^2	E

odd under time reversal and break the T symmetry of H_{D_2}. To study the SPT phases, we need to obtain the projective representations of D_2.

2. Projective representation and CG coefficients of D_2

From Ref. 24, determining the projective representation of a point group G is equivalent to determining the linear representation of its representation group(s) $R(G)$ (which cover G integer times). There are two nonisomorphism representation groups of D_2, namely, $R_1(D_2)$ and $R_2(D_2)$, both of which have two generators P, Q and eight group elements. Their multiplication tables are listed in Tables III and IV. In the following, we will mainly discuss the covering group $R_1(D_2)$, and leave the discussion about $R_2(D_2)$ to the end of this section.

To obtain all the irreducible representations, we only need to block diagonalize the canonical representation matrices of the two generators P and Q. In the canonical representation, the group space itself is also the representation space. Each group element g_1 is considered as an operator $\hat{g}_1$:

$$\hat{g}_1(g_2) = g_1g_2. \tag{A2}$$

Here g_2 and g_1g_2 are two vectors in the representation space and $\hat{g}_1$ becomes a matrix.

The canonical representation matrices of the generators of R_1 can be read from Table III:

$$P = \begin{pmatrix} 0&0&1&0&0&0&0&0\\ 0&0&0&1&0&0&0&0\\ 0&1&0&0&0&0&0&0\\ 1&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&1\\ 0&0&0&0&0&0&1&0\\ 0&0&0&0&1&0&0&0\\ 0&0&0&0&0&1&0&0 \end{pmatrix},$$

$$Q = \begin{pmatrix} 0&0&0&0&0&1&0&0\\ 0&0&0&0&1&0&0&0\\ 0&0&0&0&0&0&0&1\\ 0&0&0&0&0&0&1&0\\ 1&0&0&0&0&0&0&0\\ 0&1&0&0&0&0&0&0\\ 0&0&1&0&0&0&0&0\\ 0&0&0&1&0&0&0&0 \end{pmatrix}.$$

To simultaneously block diagonalize the above matrices, we need to identify the base vectors (or wave function) of each irreducible representation (these base vectors form a unitary matrix which block diagonalize P and Q simultaneously). In quantum mechanics, we use good quantum numbers (eigenvalues of commuting quantities) to label different states. For example, $|S,m\rangle$ symbolize a spin state, where $S(S+1)$ is the eigenvalue of the Casimir operator of the $SO(3)$ group and m is the eigenvalue of the Casimir operator of its subgroup $SO(2)$. A similar method has been applied to the representation theory of groups.[26] What we need to do is to find all the commuting quantities, or the complete set of commuting operators (CSCO).[26]

The Casimir operators of discrete groups are their class operators. For $R_1(D_2)$, there are five classes (hence there are five different irreducible linear representations), and the corresponding five class operators are given as:

$$C = \{E,\ P^2,\ P + P^3,\ Q + P^2Q,\ PQ + P^3Q\}.$$

The class operators commute with each other and all other group elements. This set of class operators C is called CSCO-I in Ref. 26. The eigenvalues of the class operators are greatly degenerate, which can only be used to distinguish different irreducible representations (IRs). To distinguish the bases in each IR, we can use the class operators of its subgroup(s). Group R_1 has a cyclic subgroup

$$C(s) = \{E, P, P^2, P^3\};$$

each element forms a class. The set of class operators of the subgroup is written as $C(s)$. The operator set $[C, C(s)]$ is called CSCO-II, which can be used to distinguish all the bases if every IR occurs only once in the reduced canonical representation.

However, in the reduced canonical representation, a d-dimensional representation occurs d times and it has the same eigenvalues for CSCO-II. To lift this degeneracy, we need more commuting operators. Fortunately, we can use the class operators of the "intrinsic group" $\bar{R}_1$, whose group elements are defined as

$$\hat{\bar{g}}_1(g_2) = g_2g_1. \tag{A3}$$

Notice that $\hat{\bar{g}}$ commutes, with $\hat{g}$ as defined in Eq. (A2). The class operators of $\bar{R}_1$ are identical to those of R_1, $\bar{C} = C$. The set of class operators for the intrinsic subgroup

$$\bar{C}(s) = \{\bar{E}, \bar{P}, \bar{P}^2, \bar{P}^3\}$$

is noted as $\bar{C}(s)$. The eigenvalues of $\bar{C}(s)$ provide a different set of "quantum numbers" to each identical IR.

Now we obtain the complete set of class operators $(C, C(s), \bar{C}(s))$, which is called CSCO-III. The common eigenvectors of the operators in CSCO-III are the orthonormal bases of the irreducible representations, and each eigenvector has a unique "quantum number".

To obtain the bases, we need to simultaneously diagonalize all the operators in CSCO-III and get their eigenvectors. Actually, we need only a few of these operators; for example, we can choose $Q + P^2 Q$ in C, P in $C(s)$, and $\bar{P}$ in $\bar{C}(s)$. The matrices of these operators of $R_1(D_2)$ are given below:

$$Q + P^2 Q = \begin{pmatrix} 0&0&0&0&1&1&0&0\\ 0&0&0&0&1&1&0&0\\ 0&0&0&0&0&0&1&1\\ 0&0&0&0&0&0&1&1\\ 1&1&0&0&0&0&0&0\\ 1&1&0&0&0&0&0&0\\ 0&0&1&1&0&0&0&0\\ 0&0&1&1&0&0&0&0 \end{pmatrix},$$

$$P = \begin{pmatrix} 0&0&1&0&0&0&0&0\\ 0&0&0&1&0&0&0&0\\ 0&1&0&0&0&0&0&0\\ 1&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&1\\ 0&0&0&0&0&0&1&0\\ 0&0&0&0&1&0&0&0\\ 0&0&0&0&0&1&0&0 \end{pmatrix},$$

$$\bar{P} = \begin{pmatrix} 0&0&1&0&0&0&0&0\\ 0&0&0&1&0&0&0&0\\ 0&1&0&0&0&0&0&0\\ 1&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&1&0\\ 0&0&0&0&0&0&0&1\\ 0&0&0&0&0&1&0&0\\ 0&0&0&0&1&0&0&0 \end{pmatrix}.$$

Practically, we can diagonalize a linear combination $\hat{O} = (Q + P^2 Q) + aP + b\bar{P}$, where a,b are arbitrary constants ensuring that all the eigenvalues of $\hat{O}$ are nondegenerate. From the nondegenerate eigenvectors (column vectors) of $\hat{O}$, we obtain an unitary matrix U:

$$U = \begin{pmatrix} \frac{1}{\sqrt{8}} & \frac{1}{\sqrt{8}} & \frac{1}{\sqrt{8}} & \frac{1}{\sqrt{8}} & \frac{1}{2} & 0 & 0 & \frac{1}{2}\\ \frac{1}{\sqrt{8}} & \frac{1}{\sqrt{8}} & \frac{1}{\sqrt{8}} & \frac{1}{\sqrt{8}} & -\frac{1}{2} & 0 & 0 & -\frac{1}{2}\\ \frac{1}{\sqrt{8}} & \frac{1}{\sqrt{8}} & -\frac{1}{\sqrt{8}} & -\frac{1}{\sqrt{8}} & -\frac{1}{2}i & 0 & 0 & \frac{1}{2}i\\ \frac{1}{\sqrt{8}} & \frac{1}{\sqrt{8}} & -\frac{1}{\sqrt{8}} & -\frac{1}{\sqrt{8}} & \frac{1}{2}i & 0 & 0 & -\frac{1}{2}i\\ \frac{1}{\sqrt{8}} & -\frac{1}{\sqrt{8}} & \frac{1}{\sqrt{8}} & -\frac{1}{\sqrt{8}} & 0 & -\frac{1}{2}i & -\frac{1}{2}i & 0\\ \frac{1}{\sqrt{8}} & -\frac{1}{\sqrt{8}} & \frac{1}{\sqrt{8}} & -\frac{1}{\sqrt{8}} & 0 & \frac{1}{2}i & \frac{1}{2}i & 0\\ \frac{1}{\sqrt{8}} & -\frac{1}{\sqrt{8}} & -\frac{1}{\sqrt{8}} & \frac{1}{\sqrt{8}} & 0 & -\frac{1}{2} & \frac{1}{2} & 0\\ \frac{1}{\sqrt{8}} & -\frac{1}{\sqrt{8}} & -\frac{1}{\sqrt{8}} & \frac{1}{\sqrt{8}} & 0 & \frac{1}{2} & -\frac{1}{2} & 0 \end{pmatrix}, \quad \text{(A4)}$$

The matrix U is the transformation that block diagonalizes P and Q simultaneously:

$$U^\dagger P U = \begin{pmatrix} 1&0&0&0&0&0&0&0\\ 0&1&0&0&0&0&0&0\\ 0&0&-1&0&0&0&0&0\\ 0&0&0&-1&0&0&0&0\\ 0&0&0&0&-i&0&0&0\\ 0&0&0&0&0&i&0&0\\ 0&0&0&0&0&0&-i&0\\ 0&0&0&0&0&0&0&i \end{pmatrix}, \quad \text{(A5)}$$

$$U^\dagger Q U = \begin{pmatrix} 1&0&0&0&0&0&0&0\\ 0&-1&0&0&0&0&0&0\\ 0&0&1&0&0&0&0&0\\ 0&0&0&-1&0&0&0&0\\ 0&0&0&0&0&i&0&0\\ 0&0&0&0&i&0&0&0\\ 0&0&0&0&0&0&0&i\\ 0&0&0&0&0&0&i&0 \end{pmatrix}. \quad \text{(A6)}$$

There are four 1D IRs and one 2D IR (which occurs twice) in the reduced canonical representation:

$$P_2 = \begin{pmatrix} -i & 0\\ 0 & i \end{pmatrix} = -i\sigma_z, \quad Q_2 = \begin{pmatrix} 0 & i\\ i & 0 \end{pmatrix} = i\sigma_x. \quad \text{(A7)}$$

So there is a total of five independent representations.

The eight elements in R_1 can be projected onto D_2, as shown in Table V. And the linear representations of R_1 correspond to the projective representations of D_2. The four 1D IRs correspond to the linear IRs of D_2, and the 2D IR stands for a nontrivial projective IR of D_2. Up to a phase factor, these 2D matrices are the 180° rotation operators of a spin with $J = 1/2$ [which is a projective IR of the $SO(3)$ group].

Now let's look at the direct product of the projective IRs of D_2. For the 1D linear IRs, the direct products are still 1D IRs, which satisfy the following law:

$$A \times B_1 = B_1, \quad A \times B_2 = B_2, \quad A \times B_3 = B_3,$$
$$B_1 \times B_2 = B_3, \quad B_1 \times B_3 = B_2, \quad B_2 \times B_3 = B_1.$$

The direct product of 1D and 2D IRs are still 2D projective IRs of D_2. The direct product of two 2D projective IRs is interesting. It reduces to four 1D linear IRs. Using the CSCO-II, we can diagonalize the 4×4 matrices $P_2 \otimes P_2$ and $Q_2 \otimes$

TABLE V. Projection from $R_1(D_2)$ to D_2

$R_1(D_2)$	E P^2	P P^3	Q $P^2 Q$	PQ $P^3 Q$
D_2	E	R_z	R_x	R_y
Rotation π of $J = 1/2$\$up to a phase factor)	I	$i\sigma_z$	$i\sigma_x$	$i\sigma_y$

Q_2 with the following unitary matrix (the column vectors are just the CG coefficients):

$$U_4 = \begin{pmatrix} -\frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 0 & 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} & 0 & 0 \end{pmatrix},$$

$$U_4^\dagger (P_2 \otimes P_2) U_4 = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

$$U_4^\dagger (Q_2 \otimes Q_2) U_4 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

These CG coefficients of the projective IRs of D_2 are analogous to the decoupling of the direct product of two spins with $J = 1/2$, $\frac{1}{2} \otimes \frac{1}{2} = 1 \otimes 0$ except the three-dimensional(3D) IR of spin 1 becomes a direct sum of three 1D IRs. If we label the bases of the 2D projective representation of D_2 as $|\uparrow\rangle, |\downarrow\rangle$, then the CG coefficients are given as

$$\begin{aligned} |x\rangle &= \frac{1}{\sqrt{2}}(|\downarrow_1\downarrow_2\rangle - |\uparrow_1\uparrow_2\rangle), \\ |y\rangle &= \frac{i}{\sqrt{2}}(|\downarrow_1\downarrow_2\rangle + |\uparrow_1\uparrow_2\rangle), \\ |z\rangle &= \frac{1}{\sqrt{2}}(|\uparrow_1\downarrow_2\rangle + |\downarrow_1\uparrow_2\rangle), \\ |\text{singlet}\rangle &= \frac{1}{\sqrt{2}}(|\uparrow_1\downarrow_2\rangle - |\downarrow_1\uparrow_2\rangle). \end{aligned} \tag{A8}$$

Repeating the above procedure, we obtain the IRs of $R_2(D_2)$. The four 1D IRs are the same as that of $R_1(D_2)$, while the 2D IR is given as:

$$P_2' = \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix} = -i\sigma_z, \quad Q_2' = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \sigma_x, \tag{A9}$$

The above representations and Eqs. (A7) differ only by a gauge transformation $P_2' = P_2$ and $Q_2' = iQ_2$, so they belong to the same projective representation of D_2. The CG coefficients for the 2D IRs are obtained easily:

$$\begin{aligned} |x\rangle &= \frac{1}{\sqrt{2}}(|\downarrow_1\downarrow_2\rangle + |\uparrow_1\uparrow_2\rangle), \\ |y\rangle &= \frac{i}{\sqrt{2}}(|\downarrow_1\downarrow_2\rangle - |\uparrow_1\uparrow_2\rangle), \\ |z\rangle &= \frac{1}{\sqrt{2}}(|\uparrow_1\downarrow_2\rangle - |\downarrow_1\uparrow_2\rangle), \\ |\text{singlet}\rangle &= \frac{1}{\sqrt{2}}(|\uparrow_1\downarrow_2\rangle + |\downarrow_1\uparrow_2\rangle). \end{aligned} \tag{A10}$$

A. sMP state with D_2 symmetry and its parent Hamiltonian

Before studying the model with D_2 symmetry, let's review the $S = 1$ AKLT model[18] [which has $SO(3)$ symmetry] first. The AKLT state is a sMP state given by $A^x = \sigma_x, A^y = \sigma_y, A^z = \sigma_z$. The A^m matrices are 2×2, meaning that the physical spin $S = 1$ is viewed as a symmetric combination of two $J = 1/2$ virtual spins [essentially projective representations of $SO(3)$]. Alternatively, we can write the state as

$$|\phi\rangle = \text{Tr}(W_1 W_2 \ldots W_N), \tag{A11}$$

where $W_i = A^x|x\rangle_i + A^y|y\rangle_i + A^z|z\rangle_i$. According to Ref. 25, the matrices A^m of a sMP state can be obtained by

$$A^m = B^T (C^m)^*, \tag{A12}$$

where B is the CG coefficient combining two virtual spins into a singlet $|0,0\rangle = B_{m_1 m_2}|\frac{1}{2}, m_1; \frac{1}{2}, m_2\rangle$, and C^m is the CG coefficient combining two virtual spins into a triplet $|1,m\rangle = C^m_{m_1 m_2}|\frac{1}{2}, m_1; \frac{1}{2}, m_2\rangle$.

Now we can generalize this formalism to the D_2 case, where the three states of $S = 1$ become a direct sum of three IRs of D_2. The D_2 group has a 2D nontrivial projective representation, and the direct product of two such projective IRs can be reduced using the CG coefficients (B and $C^{x,y,z}$) in Eqs. (A8). Similar to the $SO(3)$ case, we can consider the two 2D projective IRs as "virtual spins". From Eq. (A12), we can construct the following matrix (a similar sMP state has been studied in Ref. 27):

$$W = a\sigma_x|x\rangle + b\sigma_y|y\rangle + c\sigma_z|z\rangle, \tag{A13}$$

where a,b,c are arbitrary nonzero *complex* constants. The corresponding sMP state is given by $|\phi\rangle = \text{Tr}(W_1 W_2 \ldots W_N)$, which is invariant under the group D_2. Notice that the CG coefficients in Eqs. (A10) give the same sMP state (up to some gauge transformations). Notice also that Eqs. (A13) are different from Eqs. (5), (7), (9), or (11). If a,b, and c are to be arbitrary complex numbers, they are not invariant under T.

The above sMP state is injective, and the parent Hamiltonian can be obtained by projection operators. We consider a block containing two spins; the four matrix elements of $W_i W_{i+1}$ span a four-dimensional Hilbert space. Suppose the orthonormal bases are $|\psi_{1,2,3,4}\rangle_i$; then we can construct a projector

$$P_i = 1 - \sum_{\alpha=1}^{4} |\psi_\alpha\rangle\langle\psi_\alpha|_i, \tag{A14}$$

and the Hamiltonian $H = \sum_i P_i$. It can be easily checked that the sMP state is the unique ground state of this Hamiltonian.

The projector P_i is a 9×9 matrix that can be written in forms of spin operators. Notice that any Hermitian operator of site i,j can be expanded by the 81 generators of $U(9) = U(3)_i \otimes U(3)_j$, i.e., $\lambda_{\alpha i}\lambda_{\beta j}$ $(\alpha,\beta = 1,\ldots,9)$. So, we have

$$P_i = \sum_{\alpha,\beta=1}^{9} \xi_{\alpha\beta}\lambda_{\alpha i}\lambda_{\beta j}, \tag{A15}$$

where $\xi_{\alpha\beta}$ are constants. Further, the generators of $U(3)$ can be written as polynomials of spin operators.

$$\lambda_1 = (S_x + S_{xz})/\sqrt{2},$$
$$\lambda_6 = (S_x - S_{xz})/\sqrt{2},$$
$$\lambda_2 = (S_y + S_{yz})/\sqrt{2},$$
$$\lambda_7 = (S_y - S_{yz})/\sqrt{2},$$
$$\lambda_4 = S_x^2 - S_y^2,$$
$$\lambda_5 = S_{xy},$$
$$\lambda_3 = \left(S_z + 3S_z^2\right)/2 - I,$$
$$\lambda_8 = \left(3S_z - 3S_z^2 + 2I\right)/2\sqrt{3},$$
$$\lambda_9 = \sqrt{\frac{2}{3}}I = \sqrt{\frac{1}{6}}\left(S_x^2 + S_y^2 + S_z^2\right),$$

where $S_{mn} = S_m S_n + S_n S_m, (m,n = x,y,z)$ and $\lambda_1 \sim \lambda_8$ are the Gellmann matrices of $SU(3)$ generators. Finally, we can write the Hamiltonian in the form of spin operators. For simplicity, we first assume that a,b,c are real numbers; then the Hamiltonian is given in Eq. (6), which is invariant under T. The T symmetry goes away when a,b, or c becomes an arbitrary complex number. For instance, if $a \to ae^{i\theta}$, then Hamiltonian (6) becomes

$$\begin{aligned} H = \sum_i \Bigg[&\left(\frac{1}{4} + \frac{b^2c^2/2}{a^4+b^4+c^4}\right) S_{x,i}S_{x,j} \\ &+ \left(\frac{1}{4} + \frac{\cos 2\theta a^2c^2/2}{a^4+b^4+c^4}\right) S_{y,i}S_{y,j} \\ &- \frac{\sin 2\theta a^2c^2/2}{a^4+b^4+c^4}(S_{y,i}S_{xz,j} + S_{xz,i}S_{y,j}) \\ &+ \left(\frac{1}{4} + \frac{\cos 2\theta a^2b^2/2}{a^4+b^4+c^4}\right) S_{z,i}S_{z,j} \\ &+ \frac{\sin 2\theta a^2b^2/2}{a^4+b^4+c^4}(S_{z,i}S_{xy,j} + S_{xy,i}S_{z,j}) \\ &+ \left(\frac{1}{4} - \frac{\cos 2\theta a^2b^2/2}{a^4+b^4+c^4}\right) S_{xy,i}S_{xy,j} \\ &+ \left(\frac{1}{4} - \frac{b^2c^2/2}{a^4+b^4+c^4}\right) S_{yz,i}S_{yz,j} \\ &+ \left(\frac{1}{4} - \frac{\cos 2\theta a^2c^2/2}{a^4+b^4+c^4}\right) S_{xz,i}S_{xz,j} \Bigg] + h_0. \end{aligned} \quad \text{(A16)}$$

When $\sin 2\theta \neq 0$ the above Hamiltonian does not have T symmetry.

Varying the values of a,b,c, we can transform the ground state of the above Hamiltonian into that of the AKLT model smoothly without breaking D_2 symmetry. This means that above sMP state also belongs to the Haldane phase. In Appendix B we will consider the models with additional time-reversal symmetry.

APPENDIX B: SPIN CHAIN WITH D_{2h} SYMMETRY

In the last section we have studied the spin chain with on-site D_2 symmetry. Now we consider a $S = 1$ spin chain with additional spin-inversion (or time-reversal) symmetry. The complete on-site symmetry now becomes $D_{2h} = \{E, R_x, R_y, R_z, T, R_xT, R_yT, R_zT\}$. It has eight 1D linear real IRs, as listed in Table VI. Notice the time reversal operator $T = e^{-i\pi S_y}K$ is anti-unitary, so the states $|m\rangle$ and $i|m\rangle$ $(m = x,y,z)$ belong to different linear representations; the former is odd under T and is noted by index u, and the latter is even under T and noted by g. So we need to introduce six bases $|x\rangle,|y\rangle,|z\rangle$ and $i|x\rangle,i|y\rangle,i|z\rangle$. To construct a sMP state, at least one of the pair $|x\rangle$, $i|x\rangle$ (and also the pairs $|y\rangle$, $i|y\rangle$ and $|z\rangle$, $i|z\rangle$) should be present in the physical bases.

To obtain the projective IRs of D_{2h}, we need to study the linear IRs of the representation group $R(D_{2h})$, which also has three generators P,Q,R (corresponding to R_z, R_x, T) satisfying $P^4 = Q^4 = R^4 = E$ and $P^3Q = QP, Q^3R = RQ, R^3P = PR$.[24] The total number of elements in $R(D_{2h})$ is 64. It has 8 1D representations (corresponding to the eight linear IRs of D_{2h}) and 14 2D representations (corresponding to the seven classes of projective IRs of D_{2h}). To obtain the IRs of $R(D_{2h})$, we only need to know the representation matrix of the three generators P,Q,R. Using the same method given in the last section, we obtain all the IRs of $R(D_{2h})$ (see Table VII).

Now we give the CG coefficients that reduce the direct product of two projective IRs to a direct sum of linear IRs of D_{2h}.

$$\begin{aligned}
&E_1 \otimes E_1 = E_2 \otimes E_2 = A_g \oplus B_{1g} \oplus A_u \oplus B_{1u}; && C^{A_g} = \sigma_x,\ C^{B_{1g}} = \sigma_z,\ C^{A_u} = i\sigma_y,\ C^{B_{1u}} = I;\\
&E_3 \otimes E_3 = E_4 \otimes E_4 = A_g \oplus B_{3g} \oplus A_u \oplus B_{3u}; && C^{A_g} = I,\ C^{B_{3g}} = i\sigma_y,\ C^{A_u} = \sigma_z,\ C^{B_{3u}} = \sigma_x;\\
&E_5 \otimes E_5 = E_6 \otimes E_6 = A_g \oplus B_{1g} \oplus B_{2g} \oplus B_{3g}; && C^{A_g} = \sigma_x,\ C^{B_{1g}} = i\sigma_y,\ C^{B_{2g}} = \sigma_z,\ C^{B_{3g}} = I;\\
&E_7 \otimes E_7 = E_8 \otimes E_8 = B_{1g} \oplus B_{3g} \oplus B_{1u} \oplus B_{3u}; && C^{B_{1g}} = \sigma_z,\ C^{B_{3g}} = i\sigma_y,\ C^{B_{1u}} = I,\ C^{B_{3u}} = \sigma_x;\\
&E_9 \otimes E_9 = E_{10} \otimes E_{10} = B_{1g} \oplus B_{2g} \oplus A_u \oplus B_{3u}; && C^{A_u} = \sigma_x,\ C^{B_{3u}} = I,\ C^{B_{1g}} = i\sigma_y,\ C^{B_{2g}} = \sigma_z;\\
&E_{11} \otimes E_{11} = E_{12} \otimes E_{12} = B_{2g} \oplus B_{3g} \oplus A_u \oplus B_{1u}; && C^{A_u} = i\sigma_y,\ C^{B_{1u}} = \sigma_x,\ C^{B_{2g}} = I,\ C^{B_{3g}} = \sigma_z;\\
&E_{13} \otimes E_{13} = E_{14} \otimes E_{14} = A_g \oplus B_{2g} \oplus B_{1u} \oplus B_{3u}; && C^{A_g} = i\sigma_y,\ C^{B_{2g}} = I,\ C^{B_{1u}} = \sigma_x,\ C^{B_{3u}} = \sigma_z;
\end{aligned} \quad \text{(B1)}$$

and

$$\begin{aligned}
E_1\otimes E_2 &= B_{2g}\oplus B_{3g}\oplus B_{2u}\oplus B_{3u}; \quad C^{B_{3g}}=\sigma_x,\ C^{B_{2g}}=\sigma_z,\ C^{B_{3u}}=i\sigma_y,\ C^{B_{2u}}=I;\\
E_3\otimes E_4 &= B_{1g}\oplus B_{2g}\oplus B_{1u}\oplus B_{2u}; \quad C^{B_{1g}}=I,\ C^{B_{2g}}=i\sigma_y,\ C^{B_{1u}}=\sigma_z,\ C^{B_{2u}}=\sigma_x;\\
E_5\otimes E_6 &= A_u\oplus B_{1u}\oplus B_{2u}\oplus B_{3u}; \quad C^{A_u}=\sigma_x,\ C^{B_{1u}}=i\sigma_y,\ C^{B_{2u}}=\sigma_z,\ C^{B_{3u}}=I;\\
E_7\otimes E_8 &= A_g\oplus B_{2g}\oplus A_u\oplus B_{2u}; \quad C^{A_g}=\sigma_z,\ C^{B_{2g}}=i\sigma_y,\ C^{A_u}=I,\ C^{B_{2u}}=\sigma_x;\\
E_9\otimes E_{10} &= A_g\oplus B_{3g}\oplus B_{1u}\oplus B_{2u}; \quad C^{A_g}=\sigma_x,\ C^{B_{3g}}=I,\ C^{B_{1u}}=i\sigma_y,\ C^{B_{2u}}=\sigma_z;\\
E_{11}\otimes E_{12} &= A_g\oplus B_{1g}\oplus B_{2u}\oplus B_{3u}; \quad C^{A_g}=i\sigma_y,\ C^{B_{1g}}=\sigma_x,\ C^{B_{2u}}=I,\ C^{B_{3u}}=\sigma_z;\\
E_{13}\otimes E_{14} &= B_{1g}\oplus B_{3g}\oplus A_u\oplus B_{2u}; \quad C^{A_u}=i\sigma_y,\ C^{B_{2u}}=I,\ C^{B_{1g}}=\sigma_x,\ C^{B_{3g}}=\sigma_z.
\end{aligned} \tag{B2}$$

Here all the coefficients are chosen to be real.

Now we construct sMP states from the CG coefficients of Eqs. (B1), (B2), and (A12). Since all the CG coefficients are real, the constructed matrices $A^m = B^T(C^m)^*$ are also real (here $B = C^{A_g}$, $m = B_{1g}, B_{1u}...B_{3u}$), and are invariant under the anti-unitary operator K. However, the bases $|B_{1g}\rangle = i|z\rangle, |B_{2g}\rangle = i|y\rangle$ or $|B_{3g}\rangle = i|z\rangle$ contain a factor i; this factor i may be combined with A^m when writing the matrix $W = \sum_m A^m|m\rangle$. So the definition of A^m depends on the choice of base. If we choose $|m\rangle = |x\rangle,|y\rangle,|z\rangle$ as the physical bases, then A^m will absorb the factor i (if existent) and may be either real or purely imaginary. This convention is adopted in the main part of this paper. On the other hand, if we just choose $|m\rangle = |B_{1g}\rangle,|B_{1u}\rangle,...|B_{3u}\rangle$ as the physical bases (and forget about the fact that some bases, such as B_{1g} and B_{1u}, are linearly dependent), then all the matrices A^m are real. In the following discussion, we will adopt the second convention.

Notice that the combinations $E_5\otimes E_5$, $E_9\otimes E_{10}$, $E_{11}\otimes E_{12}$, and $E_{13}\otimes E_{13}$ contain all the bases of $S=1$ ($|B_1\rangle,|B_2\rangle,|B_3\rangle$) and the singlet state ($|A_g\rangle$), we can construct the sMP state by using these combinations. We will study them case by case.

(1)$E_5\otimes E_5$

Up to an overall phase, the local matrix W is given by $W = a\sigma_x|x\rangle + ib\sigma_y|y\rangle + c\sigma_z|z\rangle$; here a,b,c are real numbers. The Hamiltonian can be constructed using the method given in Appendix A, and the result is given in Eq. (10).

(2)$E_9\otimes E_{10}$

Up to an overall phase, the local matrix W is given by $W = a\sigma_x|x\rangle + b\sigma_y|y\rangle + ic\sigma_z|z\rangle$, and the Hamiltonian is shown in Eq. (12).

(3)$E_{11}\otimes E_{12}$

Up to an overall phase, the local matrix W is given by $W = ia\sigma_x|x\rangle + b\sigma_y|y\rangle + c\sigma_z|z\rangle$, and the Hamiltonian is given in Eq. (8).

(4)$E_{13}\otimes E_{13}$

The local matrix W is given by $W = a\sigma_x|x\rangle + b\sigma_y|y\rangle + c\sigma_z|z\rangle$, and the Hamiltonian is given in Eq. (6).

With the D_{2h} symmetry kept, the ground states of the above four exactly solvable models cannot be smoothly transformed into each other, which indicates they belong to different SPT phases (see Sec. III).

According to Ref. 6, there should be seven SPT phases since there are seven classes of projective representations.

However, in the other three projective IRs, the reduced Hilbert space of the direct product of two virtual "spins" contains only one of the three bases for the physical $S=1$ states (notice that the singlet $|A_g\rangle$ is necessary to construct a sMP state), which means that these three SPT phases cannot be realized in $S=1$ systems.

TABLE VI. Linear representations of D_{2h}

	E	R_x	R_y	R_z	T	R_xT	R_yT	R_zT	Bases	Operators
A_g	1	1	1	1	1	1	1	1	$\vert 0,0\rangle$	S_x^2,S_y^2,S_z^2
B_{1g}	1	−1	−1	1	1	−1	−1	1	$i\vert 1,z\rangle$	S_{xy}
B_{2g}	1	−1	1	−1	1	−1	1	−1	$i\vert 1,y\rangle$	S_{xz}
B_{3g}	1	1	−1	−1	1	1	−1	−1	$i\vert 1,x\rangle$	S_{yz}
A_u	1	1	1	1	−1	−1	−1	−1	$i\vert 0,0\rangle$	
B_{1u}	1	−1	−1	1	−1	1	1	−1	$\vert 1,z\rangle$	S_z
B_{2u}	1	−1	1	−1	−1	1	−1	1	$\vert 1,y\rangle$	S_y
B_{3u}	1	1	−1	−1	−1	−1	1	1	$\vert 1,x\rangle$	S_x

APPENDIX C: INVARIANCE OF THE SMP STATE UNDER THE SYMMETRY GROUP

First, we assume that all the operators of the symmetry group G are *unitary*. The CG coefficients (of the representation group) are defined as

$$\begin{aligned}
|m\rangle &= \sum_{\alpha,\beta} C^m_{\alpha\beta}|\alpha,\beta\rangle,\\
|\text{singlet}\rangle &= \sum_{\alpha,\beta} B_{\alpha\beta}|\alpha,\beta\rangle,
\end{aligned} \tag{C1}$$

where $|m\rangle$ belong to nontrivial linear IRs and $|\text{singlet}\rangle$ is a trivial linear IR and α,β are bases of some 2D projective IR. We will show that the sMP state given by Eq. (A12) is invariant under the representation group $R(G)$ (and hence the symmetry group G). Suppose that g is a group element of $R(G)$, and $u(g)/N(g),M(g)$ is the representation matrix for the physical spin/virtual "spins", then

$$\begin{aligned}
\hat g|m\rangle &= u_{m'm}|m'\rangle,\\
\hat g|\alpha\rangle &= N_{\alpha'\alpha}|\alpha'\rangle,\\
\hat g|\beta\rangle &= M_{\beta'\beta}|\beta'\rangle.
\end{aligned} \tag{C2}$$

From Eqs. (C1) and (C2), we obtain

$$\sum_{m'} u_{m'm}C^{m'} = NC^mM^T. \tag{C3}$$

TABLE VII. Projective representations of D_{2h}. The numbers α,β,γ are obtained by $\alpha = P^2$, $\beta = Q^2$, $\gamma = R^2$. The three generators P,Q,R of $R(D_{2h})$ will project to R_z,R_x,T of D_{2h}, respectively.

	$P(R_z)$	$Q(R_x)$	$R(T)$	...	$\alpha = P^2$, $\beta = Q^2$, $\gamma = R^2$
A_g	1	1	1	...	
B_{1g}	1	−1	1	...	
B_{2g}	−1	−1	1	...	
B_{3g}	−1	1	1	...	1 1 1
A_u	1	1	−1	...	
B_{1u}	1	−1	−1	...	
B_{2u}	−1	−1	−1	...	
B_{3u}	−1	1	−1	...	
E_1	I	$i\sigma_z$	σ_y	...	1 -1 1
$E_2 = E_1 \otimes B_{3g}$	-I	$i\sigma_z$	σ_y	...	
E_3	σ_z	I	$i\sigma_y$	...	1 1 -1
$E_4 = E_3 \otimes B_{1g}$	σ_z	-I	$i\sigma_y$	...	
E_5	$i\sigma_z$	σ_x	I	...	−1 1 1
$E_6 = E_5 \otimes A_u$	$i\sigma_z$	σ_x	-I	...	
E_7	σ_z	$i\sigma_z$	$i\sigma_x$	...	1 −1 −1
$E_8 = E_7 \otimes B_{1g}$	σ_z	-$i\sigma_z$	$i\sigma_x$	...	
E_9	$i\sigma_z$	σ_x	$i\sigma_x$	...	−1 1 -1
$E_{10} = E_9 \otimes A_u$	$i\sigma_z$	σ_x	-$i\sigma_x$	...	
E_{11}	$i\sigma_z$	$i\sigma_x$	σ_z	...	−1 -1 1
$E_{12} = E_{11} \otimes B_{3g}$	$i\sigma_z$	$i\sigma_x$	-σ_z	...	
E_{13}	$i\sigma_z$	$i\sigma_x$	$i\sigma_y$	...	−1 −1 −1
$E_{14} = E_{13} \otimes A_u$	$i\sigma_z$	$i\sigma_x$	-$i\sigma_y$	...	

The complex conjugate of above equation is

$$\sum_{m'} u^{\dagger}_{mm'}(C^{m'})^* = N^*(C^m)^* M^{\dagger}. \tag{C4}$$

Since the representation matrix $u(g)$ [$N(g)$, $M(g)$] is unitary, the representation matrix of $\hat{g}^{-1}$ is $[u(g)]^{\dagger}([N(g)]^{\dagger},[M(g)]^{\dagger})$. Replacing $\hat{g}$ by $\hat{g}^{-1}$ in Eqs. (C2)–(C4), we obtain

$$\sum_{m'} u_{mm'}(C^{m'})^* = N^T(C^m)^* M. \tag{C5}$$

Similar to Eq. (C3), we also have

$$B = NBM^T,$$

or equivalently $B^T = MB^TN^T$. Thus we have

$$M^{\dagger}B^T = B^TN^T. \tag{C6}$$

From Eqs.(C5) and (C6), we have

$$\begin{aligned}\hat{g}\left(\sum_m A^m|m\rangle\right) &= \sum_{m,m'} u_{m'm}A^m|m'\rangle \\ &= \sum_{m,m'} B^T u_{m'm}(C^m)^*|m'\rangle \\ &= \sum_{m'} B^TN^T(C^{m'})^*M|m'\rangle \\ &= \sum_m M^{\dagger}B^T(C^m)^*M|m\rangle \\ &= \sum_m M^{\dagger}A^mM|m\rangle. \end{aligned} \tag{C7}$$

The above equation is nothing but Eq. (4), which indicates that the sMP state constructed by $A^m = B^T(C^m)^*$ is really invariant under the group $R(G)$ (or equivalently, the symmetry group G).

Now we consider the case that some group elements, such as the time reversal operator T, of G are *anti-unitary*. Suppose that by properly choosing the phases of $|\alpha\rangle$ and $|\beta\rangle$, all the CG coefficients B and C^m are *real*. In this case, the anti-unitary operators behave as unitary operators when acting on A^m, and Eq. (C7) also holds for anti-unitary operators.

To obtain the complete representation of the anti-unitary operators, we introduce an unitary transformation to the bases $|\alpha\rangle,|\beta\rangle$ of the virtual "spins" so that A^m transforms into a complex matrix:

$$\begin{aligned}|\alpha\rangle &= V_{\alpha'\alpha}|\alpha'\rangle, \\ |\beta\rangle &= U_{\beta'\beta}|\beta'\rangle;\end{aligned} \tag{C8}$$

then

$$\begin{aligned}|m\rangle &= C^m_{\alpha\beta}|\alpha\beta\rangle = C^m_{\alpha\beta}V_{\alpha'\alpha}U_{\beta'\beta}|\alpha'\beta'\rangle \\ &= (VC^mU^T)_{\alpha'\beta'}|\alpha'\beta'\rangle = C'^m_{\alpha'\beta'}|\alpha'\beta'\rangle,\end{aligned} \tag{C9}$$

which gives $C'^m = VC^mU^T$. Similarly, we have $B' = VBU^T$. Since $A^m = B^T(C^m)^*$, so we get $A'^m = UA^mU^{\dagger}$. When unitary operator $\hat{g}_u$ acts on $A'^m|m\rangle$, Eq. (C7) holds as expected:

$$\begin{aligned}\hat{g}_u\left(\sum_m A'^m|m\rangle\right) &= U\hat{g}_u\left(\sum_m A^m|m\rangle\right)U^{\dagger} \\ &= \sum_m UM^{\dagger}A^mMU^{\dagger}|m\rangle \\ &= \sum_m (M')^{\dagger}A'^mM'|m\rangle,\end{aligned}$$

TABLE VIII. Correspondence between physical operators and effective operators in the T_0 phase according to their transformation property (parities) under D_{2h}.

Linear IR $\eta(g)$	B_{3u}	B_{2u}	B_{1u}
Operators $\hat{O}_m$	σ_x	σ_y	σ_z
Physical operators	$\tilde{S}_x$	$\tilde{S}_y$	$\tilde{S}_z$

where $M' = UMU^\dagger$. Now let us see what happens if an anti-unitary operator $\hat{g}_a$ acts on $A'^m|m\rangle$:

$$\hat{g}_a\left(\sum_m A'^m|m\rangle\right) = \hat{g}_a\left[U(\sum_m A^m|m\rangle)U^\dagger\right]$$
$$= U^*\hat{g}_a\left(\sum_m A^m|m\rangle\right)U^T$$
$$= \sum_m U^*M^\dagger A^m M U^T|m\rangle$$
$$= \sum_m (\tilde{M}')^\dagger A'^m \tilde{M}'|m\rangle,$$

where $\tilde{M}' = UMU^T = U(MK)U^\dagger$. Here we have used the factor that A^m are real matrices. So Eq. (C7) still holds for anti-unitary operators, except that the representation matrix $M(g_a)$ transforms into $\tilde{M}'(g_a)$ instead of $M'(g_a)$, or equivalently, $M(g_a)$ is replaced by $M(g_a)K$. Thus for an anti-unitary operator $\hat{g}$, we have

$$u(g)K(A^m) = KM^\dagger A^m MK. \tag{C10}$$

This result will be used in Appendix D.

Notice that, to obtain a sMP state that is invariant under a symmetry group G containing anti-unitary operators, the only condition we require is that the CG coefficients B and C^m (for the unitary projective IRs of G) can be transformed into real numbers by choosing proper phases.

APPENDIX D: EFFECTIVE OPERATORS IN THE GROUND-STATE HILBERT SPACE

From the projective representation, we can study the effective operator of a usual operator (which acts on the physical spin Hilbert space) on the ground-state Hilbert space, or equivalently, the end "spins". Naturally, the usual operator and its effective operator should vary in the same way, or respect the same linear representation, under the group D_{2h}. So we will study the effective operators from the symmetry point of view.

TABLE IX. Correspondence between physical operators and effective operators in the T_x phase according to their transformation property (parities) under D_{2h}.

Linear IR $\eta(g)$	B_{3u}	B_{2g}	B_{1g}
Operators $\hat{O}_m$	σ_x	σ_y	σ_z
Physical operators	$\tilde{S}_x$	$\tilde{S}_{xz}$	$\tilde{S}_{xy}$

If the spin chain is long enough, the two end "spins" are free (i.e., the interaction between them is neglectable). So we expect that the effective operators on the end "spins" are single-body operators instead of two-body interactions. Notice that all the nontrivial projective representations of D_{2h} are 2D; we have only three choices of the effective operators, the Pauli matrices. We will study them one by one.

First, we study the T_0 phase, which corresponds to the projective IR $(-1\ -1\ -1)$. Under symmetry operation g, the operator $\hat{O}_m$ varies in the following way:

$$M(g)^\dagger \hat{O}_m M(g) = \eta(g)_{mm'}\hat{O}_{m'}, \tag{D1}$$

where $M(g)$ is the projective IR for the end "spin". From the conclusion in Appendix C and Table VII, we get $M(R_z) = i\sigma_z$, $M(R_x) = i\sigma_x$, $M(T) = i\sigma_y K$. $\eta(g)$ is a linear representation of D_{2h}, which equals either 1 or -1. Actually, $\eta(g)$ is the parity of $\hat{O}_m$ under g. For instance, $\eta(T) = -1$ means that $\hat{O}_m$ has odd parity under time-reversal transformation and vice versa. After simple algebra, we obtain the correspondence in Table VIII: the operators in the same column transform in the same way.

From Table VIII, we find that σ_m and $\tilde{S}_m$ $(m = x,y,z)$ have the same symmetry (or the same parity under symmetry operations), so the former can be considered as the effective operator of the latter. Since σ_m is the spin operator of the end spins, the system will respond to a weak external magnetic field (along any direction) effectively through the end spins.

However, things are different in the T_x phase, which corresponds to the projective IR (-1-11). From Table VII, we can substitute $M(R_z) = i\sigma_z$, $M(R_x) = i\sigma_x$, $M(T) = \sigma_z K$ into Eq. (D1) and obtain the results in Table IX.

Notice that the end "spin" operators $\sigma_y(\sigma_z)$ do not have the same symmetry as that of $\tilde{S}_y(\tilde{S}_z)$ because they have different time-reversal parities. Since there are no single-body effective operators corresponding to $\tilde{S}_y$ and $\tilde{S}_z$, the models in the T_x phase will not response to weak external magnetic fields along the y and z directions.

Similar results can be obtained for the T_y and T_z phases and will not be repeated here.

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