Symmetry fractionalization: symmetry-protected topological phases of the bond-alternating spin-1/2 Heisenberg chain

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Abstract

We study different phases of the one-dimensional bond-alternating spin-1/2 Heisenberg model by using the symmetry fractionalization mechanism. We employ the infinite matrix-product state representation of the ground state (through the infinite-size density matrix renormalization group algorithm) to obtain inequivalent projective representations and commutation relations of the (unbroken) symmetry groups of the model, which are used to identify the different phases. We find that the model exhibits trivial as well as symmetry-protected topological phases. The symmetry-protected topological phases are Haldane phases on even/odd bonds, which are protected by the time-reversal (acting on the spin as \( \sigma \rightarrow -\sigma \)), parity (permutation of the chain about a specific bond), and dihedral (\( \pi \)-rotations about a pair of orthogonal axes) symmetries. Additionally, we investigate the phases of the most general two-body bond-alternating spin-1/2 model, which respects the time-reversal, parity, and dihedral symmetries, and obtain its corresponding twelve different types of the symmetry-protected topological phases.

Keywords: symmetry fractionalization, symmetry-protected topological phases, bond-alternating spin-1/2 Heisenberg chain, entanglement spectrum

(Some figures may appear in colour only in the online journal)

1. Introduction

For many years, Landau–Ginzburg theory of phase transitions was the dominant paradigm for characterization of different phases of matter [1]. In this theory the characterization is based on the breaking of a symmetry associated with a local order parameter. Over the past decade, however, the emergence of some exotic phases such as the Haldane phase [2] in one dimension, \( Z_2 \) spin liquids [3], topological insulators [4], and quantum Hall states [5] (which all elude Landau–Ginzburg theory) has attracted a renewed interest in characterization of quantum phases. In particular, in one dimension, it has been proven that quantum phase transitions between the so-called ‘symmetry-protected topological’ (SPT) phases are not accompanied by any symmetry breaking [6]. Thus providing powerful methods for reliable classification of phases is still much needed and of fundamental importance. Recently, based on symmetries of a given model and corresponding transformation of matrix-product state (MPS) representation of its ground state, a ‘symmetry fractionalization’ scheme to classify phases has been proposed in [6, 7]. Later, by combining the symmetry-breaking mechanism of Landau–Ginzburg theory and the symmetry fractionalization technique, a unified formalism for identification of phases of one-dimensional gapped systems was developed [8, 9]. In one dimension, this picture is
complete, but in the case of higher dimensions it is not. In brief, this method employs the projective representations\(^4\) and commutation relations of the (unbroken) symmetry groups of the underlying model to assign a set of unique labels for each phase—for a short review, see appendix.

Finding appropriate order parameters to identify SPT phases has been the subject of vast recent investigations [10–14]. Most of the proposed order parameters cannot determine crucial characteristics of SPT phases, but still may show the presence or absence of a SPT phase. To fully characterize SPT phases, a direct calculation of inequivalent classes of projective representations of the symmetry groups of the system of interest is required. In particular, in [15] an order parameter based on iMPS representation of ground state has been introduced, which can find fractionalizations of (unbroken) symmetry groups. It has been argued that this order parameter is sufficiently strong in order to specify any SPT phases—for another strong order parameter, see [12, 16].

Here, we employ the iMPS representation of the ground state to study the spin-1/2 bond-alternating Heisenberg chain and find the associated entanglement spectrum (the eigenvalues of the half-system reduced density matrix). This spectrum shows a significant change in the behavior of the model through a potential quantum phase transition point, observed in the form of evenness and oddness of the entanglement spectrum degeneracy. However, the entanglement spectrum is insufficient to provide a picture in which all phases are specified. This goal, in fact, requires the stronger symmetry fractionalization technique. We incorporate the known symmetries of the model in the iMPS representation, and calculate its phase labels. Specifically, we demonstrate that the model has two SPT phases and a symmetry-broken ferromagnetic (FM) phase. These two SPT phases are due to the existence of two different types of bonds (called ‘odd’ and ‘even’, or ‘red’ and ‘blue’, respectively) corresponding to the two couplings of the model (\(J\) and \(J'\), respectively). The labels of these phases are evidently different; however, part of this label set in each is exactly equal to the labels of the Haldane phase (throughout the paper, the Haldane phase is referred to the phase characterized by the ground state of the spin-1 Heisenberg chain or equivalently to the Affleck–Kennedy–Lieb–Tasaki (AKLT) model [17]). Next, we study the most general spin-1/2 bond-alternating model respecting the time-reversal \((T)\), parity \((P)\), and dihedral \((D_2)\) symmetries, and classify twelve different kinds of SPT phases among several possible phases. To see that whether there is any hidden symmetry responsible for the obtained phase diagram, we perturb the bond-alternating Hamiltonian with three different symmetry-breaking terms. As a result, we conclude that the phase portrait obtained through the \([TPD_2]\) symmetries is already complete.

This paper is organized as follows. In section 2 we describe the model and how an iMPS representation for its ground state can be constructed. Next in section 3 we identify the associated phases of the model by the symmetry fractionalization. We also use the iMPS representation in order to obtain the entanglement spectrum. To see how general and rich the phase landscape of the model can be, we also investigate the SPT phases of the most general bond-alternating model. In addition, we discuss how the phases are protected by the \(P\), \(T\), and \(D_2\) symmetries. Section 4 concludes the paper, and summarizes our main findings. Appendix includes details of the symmetry fractionalization technique and its application to the bond-alternating model.

2. Bond-alternating spin-1/2 Heisenberg model

2.1. Hamiltonian

The bond-alternating spin-1/2 Heisenberg model on a one-dimensional chain is defined by the following Hamiltonian:

\[
H = \sum_{i=1}^{\infty} J \sigma_i^{(2i-1)} \cdot \sigma_i^{(2i)} + J' \sigma_i^{(2i)} \cdot \sigma_i^{(2i+1)},
\]

where \(\sigma = (\sigma_x, \sigma_y, \sigma_z)\) are the Pauli operators, and \(J\) and \(J'\) are the exchange couplings. We argue later that the ratio of the very couplings controls a topological phase transition. The excitation spectrum of the model and its connection to the spin-Peierls transition has been studied in [19], where it has been shown that the gapless phase of the homogeneous spin-1/2 Heisenberg chain \((J = J')\) is unstable against an addition of bond-alternation to a gapped spin-Peierls state. Figure 1 shows a sketch of the phase diagram of the model, which has been obtained by implementing iMPS with the infinite time-evolving block decimation (iTEBD) method [18]. Suitable string order parameters [20] have indicated two distinct phases

![Figure 1. Phase diagram of the one-dimensional bond-alternating spin-1/2 Heisenberg model [18]. Here \(J\) and \(J'\) are the exchange couplings associated to the even and odd bonds, respectively. In the boundary of the odd- and even-Haldane phases a topological phase transition occurs. The labels \((0,1,0,0,1,0),(1,1,1,-1,-1,-1),(−1,−1,1,1,1,1)\) identify the trivial (FM), odd-Haldane, and even-Haldane phases, respectively—see section 3.2.](image-url)
for the blue and red regions of figure 1 separated by a quantum phase transition at the gapless line \( J = J' > 0 \), where the central charge \( c \approx 1 \) implies a Gaussian transition there. Since the string order parameters have exactly the form of string order parameter of the Haldane phase, the phases were named even- and odd-Haldane phases.

Nevertheless, it should be noted that string order parameters are not reliable labels for phases, since they are not necessarily stable in the Haldane phase [6]. In addition, nonzero string order parameters usually show the preservation of the symmetry and surprisingly if we choose them according to the projective representation of the symmetries they become zero (the signature of the phases [15]).

The model also represents a FM phase when both \( J \) and \( J' \) become negative, shown by the yellow region in figure 1 separated by the solid-green lines from the even- or odd-Haldane phases. The transition to the FM phase is accompanied by the spontaneous breaking of the SU(2) to U(1) symmetry, which is defined by the magnetization order parameter.

Therefore, to identify the different phases of the model we need to specify the symmetry fractionalization of the model. To this end, we obtain inequivalent projective representations and commutation relations of the symmetry groups of the Hamiltonian (1), which include \([TPD_2]\) and the two-site translational invariance \((TI)\).

Remark.—It has been known that spin-1/2 models with the \( T \) and one-site \( TI \) symmetries cannot have any SPT phase; they only show symmetry breaking (degenerate ground states) or gapless phases [8]. Thus to observe the SPT phases in the spin-1/2 models we need to explicitly break the \( TI \) symmetry (as occurred in equation (1)) or use three-body interactions, e.g. as appeared in cluster Hamiltonians [21].

2.2. iMPS representation of the ground state

We use an iMPS representation scenario to obtain the ground state of the Hamiltonian (1). This type of representation has been proven reliable for the ground state of one-dimensional gapped Hamiltonians [22]. To minimize the energy, there exist several algorithms (all resulting an iMPS representation) such as iTEBD [23], infinite-size density matrix renormalization group (iDMRG) [24–26], and matrix-product operator representations [27, 28]. Although iTEBD is the dominant method used to enhance the convergence of the algorithm, because of some valuable features of iDMRG, especially fast convergence and no need to apply the Trotter-Suzuki approximation, we adopt iDMRG here (as outlined in [24]). According to the iDMRG algorithm, the ground state of the \( N \)-site system is given by

\[
|\Psi\rangle = \sum_{m_1,\ldots,m_N} \text{Tr}[\Gamma_{m_1,\Lambda} \cdots \Gamma_{m_N,\Lambda}] |m_1\ldots m_N\rangle,
\]

where \(\Lambda\)s are some diagonal positive matrices, and \(\Gamma_{m,\Lambda}\)s are some \(\chi \times \chi\) matrices associated to site \(\ell\). It is evident that the Hamiltonian (1) and its corresponding ground state have the two-site \(TI\) symmetry, whereby two pairs \((\Lambda, \bar{\Lambda})\) and \((\Gamma, \bar{\Gamma})\) are needed within the iMPS representation of the ground state. These symbols are shown by blue and red colors in figure 2(a), respectively. We also assume that the two-site transfer matrix \(\mathcal{T}_{\Lambda\bar{\Lambda}}(\eta) = \sum_{m,n} \langle \bar{\Lambda}_{m}\bar{\Lambda}_{n}\Lambda_{m}\Lambda_{n}\rangle_{\eta}^{\Lambda\bar{\Lambda}}\) satisfies the following conditions: (i) \(\sum_{i,j} \mathcal{T}_{\Lambda\bar{\Lambda}}(\eta)_{ij} = \eta \delta_{\Lambda\bar{\Lambda}}\), and (ii) the eigenvalue \(\eta\) is non-degenerate and maximum—see appendix and figure A1(a). In this case, the iMPS representation of the ground state is called the ‘canonical short-range correlated form’. In the canonical short-range correlated iMPSs, \((\Lambda, \bar{\Lambda})\) are the diagonal positive matrices which represent the density matrices of the semi-infinite chain. Note that \(\eta = \Lambda\Lambda^\dagger (\bar{\eta} = \bar{\Lambda}\bar{\Lambda}^\dagger)\) shows the density matrix when the chain is partitioned into two parts from the blue (red) bonds of the iMPS representation of figure 2(a).

3. Classification of phases

3.1. Entanglement spectrum

The entanglement spectrum has proven to be a proper candidate to identify the SPT phases without prior knowledge of the symmetry, since the different projective representations of the symmetry manifest themselves in the degeneracy of entanglement spectrum pattern. For example, the presence of the SPT phases results in an even degeneracy of the entanglement spectrum [6]. Figure 3(a) shows the entanglement spectrum of \(\varrho_b\) and \(\varrho_r\) versus \(J/J'\). In the \(J/J' < 1\) region, the degeneracies of the eigenvalues of \(\varrho_b\) and \(\varrho_r\) are, respectively, odd and even, and remain unchanged throughout this region. Here one can conclude that the entanglement of the bonds which possess even degeneracy cannot be removed by using any local unitary transformation unless the system undergoes a phase transition. In contrast, one can adiabatically transform the bonds possessing odd degeneracy to a product state (trivial phase). Right after crossing \(J/J' = 1\), the degeneracies on the bonds change to even (for blue) and odd (for red), which signals a quantum
characterize the SPT phases. Therefore, we implement the SPT phase transitions here, it is in general insufficient to eigenvalues of density matrices ϱ. The system passes through the critical point (J/J′ = −1, 0) (orange solid line).

We now label the phases with the even-Haldane (J/J′ < 1) and odd-Haldane (J/J′ > 1), which will be clearer in the next subsection. Another phase transition can be characterized for J, J′ < 0, where the odd/even degeneracy of the entanglement spectrum disappears, and the entanglement spectrum indicates a dominant single eigenvalue (called the FM phase), as depicted in figure 3(b). This pattern illustrates either a trivial or a symmetry broken phase. In fact, in the FM phase the T and D2 symmetries are broken, while P is preserved.

Although the entanglement spectrum reliably signals the SPT phase transitions here, it is in general insufficient to characterize the SPT phases. Therefore, we implement the symmetry fractionalization to identify the SPT phases.

3.2. Symmetry fractionalization

Here we use the symmetry fractionalization mechanism to obtain unique labels for the phases of the bond-alternating spin-1/2 Heisenberg chain. We employ the procedure of appendix to calculate numerically inequivalent projective representations and commutation relations of the symmetries of the model, which include T, P, D2, and two-site T1.

We first look for inequivalent projective representations of the D2 symmetry. If we denote u(x) = σx and u(z) = σz, then the representation of the symmetry group D2 is defined by G_{D2} = {u(x) ⊗ u(x), u(z) ⊗ u(z)}. Here (· · · ) denotes the group, which satisfy u(x)u(z) = −u(z)u(x) and u(x)u(x) = u(z)u(z) = I. To preserve the D2 symmetry in the iMPS representation of the ground state with the two-site T1, Γ and Γ̅ are required to satisfy

\begin{align*}
\sum_i u_{ji}(g)\Gamma_i & = \beta(g)Z^{-1}(g)\Gamma_j X(g), \\
\sum_i u_{ji}(g)\Gamma_{\bar{i}} & = \beta'(g)X^{-1}(g)\Gamma_j Z(g).
\end{align*}

where g ∈ [x, z], and β(g) and β′(g) are arbitrary phases. The inequivalent projective representations of D2 and two-site T1 are given by X(x)X(z) = ±X(z)X(x) and Z(x)Z(z) = ±Z(z)Z(x), which introduce four different classes of projective representation of the symmetries. Within each specific phase, one of the above projective representations holds, and it can change to the other ones only through a quantum phase transition. Therefore, the ± signs actually provide a unique label for the phases. To determine the projective representation (within each phase), we need to calculate the corresponding ± signs of the projective representations. Accordingly, we define the parameters

\begin{align*}
\Pi^{b}_{D2} & = \begin{cases} 0 & \text{if } |\eta| < 1 \\
(1/\chi)^{\text{Tr}[X(x)X(z)X^{-1}(x)X^{-1}(z)]} & \text{if } |\eta| = 1,
\end{cases} \\
\Pi_{D2} & = \begin{cases} 0 & \text{if } |\eta| < 1 \\
(1/\chi)^{\text{Tr}[X(x)X(z)Z^{-1}(x)Z^{-1}(z)]} & \text{if } |\eta| = 1.
\end{cases}
\end{align*}

(Here ‘r’ and ‘b’ indicate even and odd bonds, respectively). Throughout the even-Haldane phase we have Π_{D2} = 1 and Π_{D2} = 10, and upon the quantum phase transition at J = J′ > 0, these parameters change to Π_{D2} = 1 and Π_{D2} = −1. In the FM phase, the D2 symmetry is broken, which means we have a degeneracy in the ground state.

A straightforward justification for our results can be obtained by considering the states of figures 2(b) and (c). These states faithfully represent the odd-Haldane and even-Haldane phases, respectively. If the singlet states on the blue lines in figure 2(b) are put into the canonical iMPS form, we obtain

\begin{align*}
\Gamma_0 & = (0 \ 1), \quad \Gamma_1 = (-1 \ 0), \\
\Gamma_0 & = (1 \ 0)^T, \quad \Gamma_1 = (0 \ 1)^T, \\
\Lambda & = \mathbb{I}/\sqrt{2}, \quad K = 1.
\end{align*}

To calculate the parameters, we start by calculating \lim_{\chi \to \infty}\langle |\psi|\chi^{N(g)}|\psi\rangle = \lim_{\chi \to \infty}(\eta)^{N(g)} to see the state possesses the symmetry or not. In the SPT phases we find, up to accuracy of machine, the ground states preserve the symmetries. After that we calculate some quantities such as \text{Tr}[X(x)X^{-1}(x)X^{-1}(z)]/\chi expected to be ±1. Since the iMPS representation provides a faithful description of the gapped systems, the accuracy of calculation of the mentioned quantities is again equal to the accuracy of machine. In all parts of our computations we use \chi \leq 80.
Using equations (3) and (4) we find \( X(x) = \sigma_x \), \( X(z) = \sigma_z \), and \( Z(x) = Z(z) = 1 \), which confirm the numerical result of table 1. The same procedure for the red lines in figure 2(c) leads to \( Z(x) = X(z) = 1 \), which are again in agreement with the numerical result of table 1.

In a similar manner, one can show that to preserve parity and two-site TI, the above equations need to be changed to

\[
(\Gamma_i)^T = \theta_p N_b^{-1} T_i N_r, \quad (\overline{T})^T = \theta_p N_r^{-1} T_i N_b, \tag{5}
\]

where \( N_b = \pm N^T \), \( N_r = \pm N^T \), and \( \theta_p \theta_p = \pm 1 \). Each of these signs (±) defines a unique label for the phases. Thus, the model with the \( P \) and two-site TI symmetries can only show eight phases. Similarly, the parameter of the symmetry is

\[
\Pi^{(b)}_p = \begin{cases} 0 & \text{if } |\eta| < 1 \\ (1/\chi) \text{Tr}[N(b)N^*_r] & \text{if } |\eta| = 1 \end{cases}
\]

The parameter \( \Pi^{(b)}_p \) in the even-Haldane phase is \(-1(1)\), and flips to \(-1(-1)\) for the odd-Haldane phase. The singlet states of figures 2(b) and (c) lead to \( N_b = \sigma_x \), \( N_r = 1 \), \( \theta_p \theta_p = -1 \), and \( N_r = \sigma_y \), \( N_b = 1 \), \( \theta_p \theta_p = -1 \), respectively, which agree with our numerical results. Note that unlike the dihedral and time-reversal symmetries, parity is preserved in the FM phase.

To preserve the time-reversal symmetry, we have

\[
\sum_i v_{ji}(\Gamma_i)^* = M^*_r T_i M_b, \tag{6}
\]

\[
\sum_i v_{ji}(\overline{T})^* = M^*_b T_i M_r, \tag{7}
\]

where \( v \) \(* v = -I \). Distinct phases are identified by \( M_r = \pm M_r^T \) and \( M_b = \pm M_b^T \). The parameter associated to this symmetry is

\[
\Pi^{(b)}_T = \begin{cases} 0 & \text{if } |\eta| < 1 \\ (1/\chi) \text{Tr}[M(b)M^*_r] & \text{if } |\eta| = 1 \end{cases}
\]

The value of \( \Pi^{(b)}_T \) changes from \(-1(1)\) in the even-Haldane phase to \(-1(-1)\) in the odd-Haldane phase. One can simply obtain \( (M_r = 1, M_b = \sigma_x) \) and \( (M_r = \sigma_y, M_b = 1) \) for the states of figures 2(b) and (c), respectively.

According to the inequivalent projective representations of the [\( TP D_2 \)] symmetries, we assign the label

\[
\Pi = (\Pi^{(b)}_d, \Pi^{(b)}_p, \Pi^{(b)}_T, \Pi^{(b)}_{D_2}, \Pi^{(b)}_{P}, \Pi^{(b)}_{T})
\]

to each phase. Therefore, the labels for even-Haldane, odd-Haldane, and FM phases are respectively \((-1, -1, 1, 1, 1, 1), (1, 1, 1, -1, -1, -1), (0, 1, 0, 0, 1, 0)\)—see figure 1.

To obtain a comprehensive classification of different phases, we also need to consider all symmetries together. The combination of the symmetries can produce new labels for the phases, which are specified by projective commutation relations between their representations. The combinations of equations (3)–(7) lead to the following commutation relations:

\[
N^{-1}_x Z(g)N_r = \gamma^0_x(g) Z^*(g), \tag{8}
\]

\[
N^{-1}_r X(g)N_b = \gamma^0_r(g) X^*(g), \tag{9}
\]

\[
M^{-1}_r Z(g)M_r = \gamma^0_r(g) Z^*(g), \tag{10}
\]

\[
M^{-1}_b X(g)M_b = \gamma^0_b(g) X^*(g), \tag{11}
\]

where \( g \in \{x, z\} \). Furthermore, if we fix the arbitrary phases of \( X(x) \) and \( Z(z) \) by imposing \( X^2(x) = Z^2(z) = 1 \) and \( X^2(z) = Z^2(z) = 1 \), we arrive at the following labels:

\[
\gamma(x) = (\gamma^0_x(x), \gamma^0(x), \gamma^0_z(x), \gamma^0_z(x)), \tag{12}
\]

\[
\gamma(z) = (\gamma^0_x(z), \gamma^0_b(z), \gamma^0_r(z), \gamma^0_r(z)), \tag{13}
\]

whose elements could be \( \pm 1 \). These labels are added to the ones obtained previously for a complete classification.

Throughout the even-Haldane phase we obtain \( \gamma(x) = (1, 1, 1, 1, 1, 1) \), upon the quantum phase transition at \( J = J' > 0 \), for the odd-Haldane phase \( \gamma(x) \) and \( \gamma(z) \) becomes \( (1, 1, 1, 1, 1, 1) \), which are listed in table 2. One can simply obtain the same result for the states of figures 2(b) and (c). Therefore, up to the [\( TP D_2 \)] symmetries, the labels \( \Pi, \gamma(x) \), and \( \gamma(z) \)—tables 1 and 2—provide a complete classification of the phases of the bond-alternating spin-1/2 Heisenberg model.

Finally, we can now compare the labels of Haldane phase of spin-1 Heisenberg chain with the labels \( \Pi, \gamma(x), \) and \( \gamma(z) \). It can be shown that for the Haldane phase, which has the one-site TI symmetry [6, 15],

\[
\Pi^{D_2} = \Pi^{P} = -1, \quad \Pi^{P} = \Pi^{T} = -1
\]

\[
\gamma^0(x) = \gamma^0_b(x) = -1, \quad \gamma^0_r(z) = \gamma^0_r(z) = -1,
\]

\[
\gamma^0_r(x) = \gamma^0_b(x) = -1, \quad \gamma^0_r(z) = \gamma^0_r(z) = -1.
\]

By comparison of our labels with these labels, we conclude that the symmetry fractionalization of the red and blue bonds of the even-(odd-)Haldane phase are akin to the Haldane (trivial) and trivial (Haldane) phases, respectively.

### 3.3 General bond-alternating model

We now investigate SPT phases of the most general two-body bond-alternating spin-1/2 Hamiltonian, which respects the [\( TP D_2 \)] symmetries. This general Hamiltonian reads

\[
H_{BA} = \sum_{i=1}^{3} (J_i \sigma_i^{2} \sigma^{2i+1} + J'_i \sigma_i^{2i+1} \sigma^{2i+2}). \tag{12}
\]
Table 3. Inequivalent projective representations and commutation relations of the symmetries of the most general two-body bond-alternating spin-1/2 model with the \([TPD_2]\) symmetries (equation (12)).

| Phase          | \(\Pi_p^b/\Pi_p^d\) | \(\Pi_l^b/\Pi_l^d\) | \(\Pi_p/\Pi_p^d\) | \(\gamma_f(\chi)\gamma_f(\chi)\) | \(\gamma_f(\chi)\gamma_f(\chi)\) | \(\gamma_f(\chi)\gamma_f(\chi)\) |
|----------------|----------------------|----------------------|----------------------|----------------------|----------------------|----------------------|
| Trivial        | 1/1                   | 1/1                   | 1/1                   | 1/1                   | 1/1                   | 1/1                   |
| Even-Haldane   | -1/1                  | -1/1                  | -1/1                  | -1/1                  | -1/1                  | -1/1                  |
| \(T_x\)        | 1/1                   | -1/1                  | -1/1                  | -1/1                  | -1/1                  | -1/1                  |
| \(T_y\)        | 1/1                   | -1/1                  | 1/1                   | 1/1                   | 1/1                   | 1/1                   |
| \(T_z\)        | 1/1                   | -1/1                  | 1/1                   | 1/1                   | 1/1                   | 1/1                   |
| \(T_{xx}\)     | 1/1                   | -1/1                  | 1/1                   | 1/1                   | 1/1                   | 1/1                   |

where \(J = J(\sin(\theta)\cos(\varphi), \sin(\theta)\sin(\varphi), \cos(\theta))\) (and similarly for \(J'\)). Within the space of the coupling parameters \((J_x = J/J', \vartheta, \vartheta', \varphi')\) we want to find (numerically) the phases respecting the following conditions: (i) nonvanishing gap and (ii) respecting the \([TPD_2]\) symmetries. We use the procedure of appendix to find the symmetry fractionalization of the phases of the Hamiltonian (12).

A remark is in order here. Results of iDMRG calculations may produce states resembling properties of SPT phases while indeed belonging to a symmetry-breaking class. For example, the ground state of the one-dimensional Ising model can be a cat state, that shows even degeneracy in the entanglement spectrum. Thereby, one may erroneously consider the corresponding phase as a SPT phase. To avoid such cases, we employ the following two methods to authenticate the SPT phases: (i) perturbing the SPT phase with proper perturbative terms, and (ii) initializing the iDMRG algorithm with different states.

We calculate \(\Pi, \gamma(x),\) and \(\gamma(z)\) numerically for the most general two-body bond-alternating spin-1/2 model defined in equation (12). In this respect, we sweep the coupling parameter space for \(-2 \leq J_x \leq 2\) with \(\Delta J_x = 0.2, 0 \leq \vartheta, \vartheta' \leq \pi\) with \(\Delta \vartheta = \Delta \vartheta' = 0.3,\) and \(0 \leq \varphi, \varphi' \leq 2\pi\) with \(\Delta \varphi = \Delta \varphi' = 0.5\). Additionally, our iDMRG calculations are performed with \(\chi = 16,\) which lead to the results presented in table 3. Hence, the general Hamiltonian (12) exhibits symmetry-breaking phases (with degenerate ground states), gapless phases, and twelve different types of SPT phases. Table 3 shows the symmetry fractionalization of six SPT phases of the model (the other six SPT phases can be obtained by replacing \((r, b) \rightarrow (b, r)\)). These SPT phases are labelled with T-index similar to the notation of [29]. Here the commutation relation between \(T\) and \(D_2\) distinguishes the phases \(T_x, T_y, T_z,\) and \(T_{xx}.\) However, we do not claim that table 3 necessarily shows all possible SPT phases of the Hamiltonian (12), because it really depends on the specific values of the coupling parameters. For example, there might still be an SPT phase within a tiny area of the phase diagram, which needs a more fine-tuned coupling parameters and a more careful implementation of iDMRG.

3.4. Stability of the SPT phases

Here we study the stability of the SPT phases of the bond-alternating spin-1/2 Heisenberg model under the breaking of the \([TPD_2]\) symmetries. In particular, we would like to clarify whether these symmetries already suffice to protect the SPT phases of the model—or perhaps another hidden symmetry is responsible for this. To answer this question, we examine how the addition of three different terms \((H_1, H_2,\) and \(H_3)\) to the model may affect the SPT phases.

3.4.1. \(P\) protection. Let us add the following perturbative cluster-like term to the Hamiltonian (1):

\[
H_1 = \sum_i \kappa_1 \delta_i^{(2)} \sigma_i^{(2)} \sigma^{(2)}_i + \kappa_2 \delta_i^{(2)} \sigma_i^{(2)} \sigma^{(2)}_i + \kappa_3 \delta_i^{(2)} \sigma_i^{(2)} \sigma^{(2)}_i.
\]

(13)

All \([TPD_2]\) symmetries are broken for any nonzero values of \(\kappa_1 \neq \kappa_2,\) while the \(P\) symmetry is retrieved when \(\kappa_1 = \kappa_2.\) For \(\kappa_1 \neq \kappa_2, H_1\) destroys the even degeneracy of the red (blue) bonds in the even-(odd-)Haldane phase, which verifies that the mentioned symmetries are necessary to protect both even- and odd-Haldane phases. We would like to add that when \(\kappa_1 = \kappa_2, P\) is preserved, and the even degeneracy of the entanglement spectrum appears immediately. Therefore, \(P\) alone can protect the SPT phase. Moreover, adding a cluster term with \(\kappa_1 \neq \kappa_2\) prevents the model from exhibiting any quantum phase transition in the whole \(J\) region. In fact, the cluster term obstructs the gap closing on the critical line \(J = J'.\) To show this explicitly, we plot the von Neumann entropy

\[
S = -\sum_{i=1}^{\chi} (|\chi_i|) \log(|\chi_i|)
\]

versus \(J/J'\) in figure 4(a). It is expected that entropy diverges as \(S \propto \log(\chi)\) [30] whenever a model encounters a quantum phase transition. Figure 4(a) shows that for \((\kappa_1, \kappa_2) = (0.1, 0.2), S\) remains almost equal for different values of \(\chi,\) which demonstrates that we encounter a single phase. This is a result of the cluster term, which breaks all necessary symmetries to protect the SPT phases. However, for \((\kappa_1, \kappa_2) = (0.1, 0.1),\) the \(P\) symmetry is retrieved, and a finite entanglement effect at \(J = J'\) appears, where \(S\) shows increasing values for different \(\chi,\) resembling a divergent like behavior—see the inset of figure 4(a).

3.4.2. \(T\) protection. We examine another perturbation as below to emphasize the protection by the \(T\) symmetry,

\[
H_2 = \sum_i \left[ \delta_1 (\sigma_i^{(2)} \sigma_i^{(2)} + \sigma_i^{(2)} \sigma_i^{(2)}) + \delta_2 (\sigma_i^{(2)} + \sigma_i^{(2)}) \right].
\]

(15)

This Hamiltonian breaks the \([TPD_2]\) symmetries given nonzero values for \(\delta_1\) and \(\delta_2,\) whereas it only respects the \(T\)
symmetry if $\delta_2 = 0$. For $\delta_2 \neq 0$, the entanglement spectrum loses the structure of even degeneracy (not shown here), which is a manifestation of no SPT phase. As shown in figure 4(b), $S$ remains constant when $\chi$ increases, which denotes that the model does not undergo a quantum phase transition. However, if we choose $\delta_2 = 0$, in which the $T$ symmetry is preserved, finite entanglement effects on $S$ appear at $J = J'$, confirming a quantum phase transition between two SPT phases—see the inset of figure 4(b).

3.4.4. $D_2$ protection. The addition of the third Hamiltonian as below indicates the protection by the $D_2$ symmetry,

$$H_3 = a_1 \sum_i (\sigma_i^{(2^1)} \sigma_i^{(2^2)} + \sigma_i^{(2^2)} \sigma_i^{(2^1)}) + a_2 \sum_i (\sigma_i^{(2^1)} + \sigma_i^{(2^1)}).$$

Nonzero values for $a_1$ and $a_2$ break the $[TPD_2]$ symmetries, while it keeps only $D_2$ for $a_1 \neq 0$ and $a_2 = 0$. We have plotted the von-Neumann entropy for various $J/J'$ for $(a_1, a_2) = (0.1, 0.2)$ in figure 4(c), which does not show a signature of quantum phase transition. In the absence of symmetry, there is no SPT phase, and the model is in a single phase. However, for $a_2 = 0$ the revival of the $D_2$ symmetry imposes the presence of two SPT phases, which are separated by a quantum phase transition at $J = J'$, as shown in the inset of figure 4(c).

Thus we conclude that any of the $P$, $T$, and $D_2$ symmetries protects the both even- and odd-Haldane phases on the spin-1/2 bond-alternating Heisenberg chain.

4. Summary and conclusions

We have studied the phases of the bond-alternating spin-1/2 Heisenberg chain. Our main tool in doing so has been the recently introduced symmetry fractionalization technique. This technique is based on implementing the known symmetries of the model in the matrix-product representation of the ground state. A set of labels have been obtained from the inequivalent projective representations and commutation relations of the symmetries (here the time-reversal, parity, and dihedral). These labels can help uniquely identify the phases of the model.

We have calculated the associated phase labels of this model by employing an infinite-size density-matrix renormalization algorithm and an exhaustive search in the space of Hamiltonian parameters. We identified three phases for this model, one (topologically) trivial phase corresponding to a FM state and two symmetry-protected topological phases. We demonstrated that these topological phases naturally resemble a Haldane phase (which originally appeared as the ground state of the spin-1 Heisenberg chain or equivalently being in the form of the ground state of the Affleck–Kennedy–Lieb–Tasaki model). As a supporting tool, we also calculated the entanglement spectrum of the model. In addition, by employing the same symmetry fractionalization technique, we also studied the most general one-dimensional bond-alternating model respecting similar symmetries as our model, and found that this model can exhibit twelve different symmetry-protected topological phases. Robustness of the phases of the model against breaking of the time-reversal, parity, and dihedral symmetries have also been investigated. In particular, we perturbed the bond-alternating Hamiltonian with three symmetry-breaking terms in the forms of cluster-like three-body Hamiltonian and two-body interactions of mixed types. Protection of the obtained phases for the model against such perturbations indicated that the set of the symmetries of the system (time-reversal, parity, and dihedral) already suffice to completely characterize the phases.

Two remarks are in order here. i.e. Employing the symmetry fractionalization technique, we discerned two odd-Haldane and even-Haldane phases, which have distinct phase labels. The observation of these two different phases is in complete agreement with the results of [18] (albeit obtained with a different toolkit). In addition, it is straightforward to see that connecting the two $J_1 < J_2$ and $J_1 > J_2$ regimes (which exhibit odd- and even-Haldane phases, respectively) smoothly is not possible. In fact, we need to cross the $J_1 = J_2$ line where the system becomes the conventional antiferromagnetic spin-1/2 Heisenberg model, which is gapless. Here, response functions such as second-order derivative of the ground-state energy and string order parameters show singularity. This is
another clear signature of that the two sides of this critical line belong to different phases. ii. We would like to stress that the symmetry fractionalization method we have employed here uses the iDMRG technique, which is by construction an ‘infinite-size’ method. That is, no finite-size boundary effect in phase characterization of the underlying model would show up in this picture.

The bond-alternating spin-1/2 Heisenberg chain is a prototype model to demonstrate the spin-Peierls transition and Su–Shrieffer–Heeger model of polyacetylene [31]. Hence, our classification in terms of (inequivalent) projective representations of the symmetries is also valid for these models. In other words, the spin-Peierls transition of the spin-1/2 Heisenberg chain is the quantum phase transition between two symmetry-protected topological phases, which could be a result of phonon coupling or disorder in the system. Moreover, the one-dimensional representations of the underlying symmetries could be a classified expression for the Zak phase [32], which has recently been experimentally observed [33].

Our study of complete phase characterization emphasizes the power of the symmetry fractionalization technique for phase identification in one-dimensional gapped systems. We hope that our findings can spur similar investigations on other models of quantum systems. It is evident that developing methods and tools for identification of phases of quantum matter in higher dimensions is certainly an important goal for the next step.

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Appendix. Numerical calculation of the inequivalent projective representations of a symmetry

We briefly review how one can employ the iMPS representation of the ground state to completely classify one-dimensional gapped phases. Next, we elaborate on numerical calculations of the inequivalent projective representations and commutation relations of the symmetries of the phases.

Assume that an iMPS representation is symmetric under the two-site TI and \( u(g) \), where \( u(g) \) is a projective unitary representation of some group \( G \). iMPS generally requires two matrices \((\Gamma, \overline{\Gamma})\) to preserve the two-site TI, and preservation of \( u(g)^{\otimes N} \) imposes the following condition on \((\Gamma, \overline{\Gamma})\):

\[
\sum_j u_{ji}(g) \Gamma_j = \beta(g) Z^{-1}(g) \Gamma_j X(g), \quad (A.1)
\]

\[
\sum_j u_{ji}(g) \overline{\Gamma}_j = \beta'(g) X^{-1}(g) \overline{\Gamma}_j Z(g), \quad (A.2)
\]

where \( \beta'(g) \) and \( \beta(g) \) are arbitrary phases. The combination of equations (A.1) and (A.2) yields

\[
\sum_m u_{mn}(g) u_{ji}(g) \Gamma_m \Gamma_n = \alpha(g) Z^{-1}(g) \Gamma_j \Gamma_m Z(g), \quad (A.3)
\]

\[
\sum_m u_{mn}(g) u_{ji}(g) \overline{\Gamma}_m \Gamma_n = \alpha(g) X^{-1}(g) \overline{\Gamma}_j \Gamma_m X(g), \quad (A.4)
\]

where \( \alpha(g) = \beta(g) \beta'(g) \). Since iMPSs are short-range correlated states (see figure A1(a)), sufficiently long consecutive sites of \( \Gamma_j \Gamma_j \) can span the space of \( \chi \times \chi \) matrices. This is called the ‘injectivity’ property [34]. If \( u(g) \otimes u(g) \) forms a unitary representation of the group \( G \), using the injectivity condition, equations (A.3) and (A.4), we conclude that inequivalent projective representations of \( X(g) \) and \( Z(g) \) would specify different phases. Moreover, \( \alpha(g) \) forms a
one-dimensional representation of $G'$, which could be another label for the phases.

To gain further insight, we first give an example of the $D_2$ symmetry. If we denote $u(x) = \sigma_x$ and $u(z) = \sigma_z$, the representation group of the $D_2$ symmetry is defined by $G_{D_2} = \{u(x) \otimes u(z), u(z) \otimes u(x)\}$, where $(\cdots)$ denotes the generators of the group, which satisfy $u(x)u(z) = -u(z)u(x)$ and $u(x)u(x) = u(z)u(z) = I$. Equations (A.3) and (A.4) are written in the following forms:

$$\sum_{ni} u_{mn}(z)u_{ji}(z)\Gamma_j\Gamma_n = \alpha(z)Z^{-1}(-z)\Gamma_j\Gamma_nZ(z),$$

(A.5)

$$\sum_{ni} u_{mn}(z)u_{ji}(z)\Gamma_j\Gamma_n = \alpha(z)X^{-1}(z)\Gamma_j\Gamma_nX(z),$$

(A.6)

which also hold for the $x$ index. Using the properties of $G_{D_2}$ and the injectivity condition on $G_{D_2}$, one obtains $\alpha(x) = \pm 1$, $\alpha(z) = \pm 1$, $X(x)Z(x) = \pm X(x)Z(x)$, and $Z(z)Z(z) = \pm Z(z)Z(x)$. The first and the second outcomes indicate different one-dimensional representations of the $D_2$ symmetry, and the last ones show different projective representations of $D_2$. Therefore, four one-dimensional and four projective representation of $D_2$ introduce overall sixteen phases.

We can obtain a more complete classification of the phases by considering the commutation relation between different symmetries. To clarify this, suppose that the system maintains the $D_2$, $P$, $T$, and two-site $TI$ symmetries. To preserve these symmetries, in addition to equations (A.5) and (A.6), the following equations must be satisfied:

$$\sum_i \gamma_{ji}(\Gamma_j)^* = M^{-1}\Gamma_jM,$$

(A.7)

$$\sum_i \gamma_{ji}(\Gamma_j^*)^* = M^{-1}\Gamma_j^*M,$$

(A.8)

$$(\Gamma_j)^T = \theta P N^{-1}\Gamma_j N,$$

(A.9)

$$(\Gamma_j^*)^T = \theta^* P N^{-1}\Gamma_j N,$$

(A.10)

If we combine equations (A.5)-(A.10) we find

$$N^{-1}XN = \gamma' p(x)X'(x),$$

(A.11)

$$M^{-1}XN = \gamma'' p(x)X'(x),$$

(A.12)

$$N^{-1}ZN = \gamma_1(x)Z'(x),$$

(A.13)

$$M^{-1}ZM = \gamma_2(x)Z'(x),$$

(A.14)

where $\gamma(x) = (\gamma'_p(x), \gamma''_p(x), \gamma_1(x), \gamma_2(x))$ are some arbitrary phases. Similar relations to equations (A.11)-(A.14) are obtained for $z$ instead of $x$. To uniquely define $\gamma(x)$ and $\gamma(z)$, we fix the arbitrary phases of $X$ and $Z(x)$ according to $X^2(x) = X^2(x) = I$ and $Z^2(z) = Z^2(z) = I$. Under these conditions, $\gamma(x)$ and $\gamma(z)$ can only take $\pm 1$, which is another unique label for the phases [9]. Therefore, the commutation relation of $D_2$, $P$, $T$, and the two-site $TI$ can produce $16 \times 16$ different phases.

To extract numerically the inequivalent projective representation of the underlying symmetries we should obtain a reliable iMPS representation of the ground state to follow the procedure (figure A1). Introducing an appropriate parameter, one can identify inequivalent projective representations of the symmetries and also the commutation relations between them. For instance, the following parameter shows inequivalent projective representation of $D_2$:

$$\Pi = \begin{cases} 0 & \text{if } |\eta'| < 1 \\ \left(1/\chi\right)\text{Tr}[X(x)X(z)X^{-1}(x)X^{-1}(z)] & \text{if } |\eta'| = 1. \end{cases}$$

(A.15)

The commutation relations between $D_2$ and $P$ symmetries can be obtained by the following parameter:

$$\gamma(x) = (1/\chi)\text{Tr}[N^{-1}X(x)NX^T(x)],$$

(A.16)

by imposing the constraint $X^2(x) = I$.

References

[1] Goldenfeld N 1992 Lectures on Phase Transitions and the Renormalization Group (Reading, MA: Perseus Books)

[2] Haldane F D M 1983 Continuum dynamics of the 1D Heisenberg antiferromagnet: identification with the o(3) nonlinear sigma model Phys. Lett. A 93 464

[3] Read N and Sachdev S 1991 Large-N expansion for frustrated quantum antiferromagnets Phys. Rev. Lett. 66 1773–6

[4] Kane C L and Mele E J 2005 Quantum spin hall effect in graphene Phys. Rev. Lett. 95 226801

[5] Tsui D C, Stormer H L and Gossard A C 1982 2D magnetotransport in the extreme quantum limit Phys. Rev. Lett. 48 1559–62

[6] Pollmann F, Turner A M, Berg E and Oshikawa M 2010 Detection of two dimensional symmetry enriched topological phases in one dimension Phys. Rev. B 81 064439

[7] Turner A M, Pollmann F and Berg E 2011 Topological phases of one-dimensional fermions: an entanglement point of view Phys. Rev. B 83 075102

[8] Chen X, Gu Z C and Wen X G 2011 Classification of gapped symmetric phases in one-dimensional spin systems Phys. Rev. B 83 035107

[9] Chen X, Gu Z C and Wen X G 2011 Complete classification of one-dimensional symmetry protected topological phases in commuting spin systems Phys. Rev. B 84 235128

[10] Cui J, Amico L, Fan H, Gu M, Hamma A and Vedral V 2013 Local characterization of one-dimensional topologically ordered states Phys. Rev. B 88 125117

[11] Marvian I 2013 Symmetry protected topological entanglement arXiv:1307.6617

[12] Hagemeister J, Perez-Garcia D, Cirac I and Schuch N 2012 Order parameter for symmetry-protected phases in one dimension Phys. Rev. Lett. 109 050402

[13] Zaletel M P 2013 Detecting two dimensional symmetry protected topological order in a ground state wave function arXiv:1309.7387

[14] Huang C-Y, Chen X and Pollmann F 2014 Detection of symmetry enriched topological phases Phys. Rev. B 90 045142

[15] Pollmann F and Turner A M 2012 Detection of symmetry-protected topological phases in one dimension Phys. Rev. B 86 125441

[16] Langari A, Pollmann F and Sinahtgar M 2013 Ground-state fidelity of the spin-1 Heisenberg chain with single ion anisotropy: quantum renormalization group and exact diagonalization approaches J. Phys.: Condens. Matter 25 406002

[17] Affleck I, Kennedy T, Lieb E H and Tasaki H 1987 Rigorous results on valence-bond ground states in antiferromagnets Phys. Rev. Lett. 59 799–802
[18] Wang H T, Li B and Cho S Y 2013 Topological quantum phase transition in bond-alternating spin-1/2 heisenberg chains Phys. Rev. B 87 054402
[19] Bonner J C and Blöte H W J 1982 Excitation spectra of the linear alternating antiferromagnet Phys. Rev. B 25 6059–80
[20] Hida K 1992 Crossover between the haldane-gap phase and the dimer phase in the spin-1/2 alternating Heisenberg chain Phys. Rev. B 45 2207
[21] Montes S and Hamma A 2012 Phase diagram and quench dynamics of the cluster-xy spin chain Phys. Rev. E 86 021101
[22] Hastings M B 2007 An area law for one-dimensional quantum systems J. Stat. Mech. P09024
[23] Vidal G 2007 Classical simulation of infinite-size quantum lattice systems in one spatial dimension Phys. Rev. Lett. 98 070201
[24] McCulloch I P 2008 Infinite size density matrix renormalization group, revisited, arXiv:0804.2509
[25] Kjäll J A, Zaletel M P, Mong R S K, Bardarson J H and Pollmann F 2013 Phase diagram of the anisotropic spin-2 xxx model: infinite-system density matrix renormalization group study Phys. Rev. B 87 235106
[26] Schollwöck U 2011 The density-matrix renormalization group in the age of matrix product states Ann. Phys. 326 96
[27] Pirvu B, Murg V, Cirac J and Verstraete F 2010 Matrix product operator representations New J. Phys. 12 025012
[28] Liu C, Wang L, Sandvik A W, Su Y C and Kao Y J 2010 Symmetry breaking and criticality in tensor-product states Phys. Rev. B 82 060410
[29] Liu Z X, Chen X and Wen X G 2011 Symmetry-protected topological orders of one-dimensional spin systems with $D_3 + t$ symmetry Phys. Rev. B 84 195145
[30] Vidal G, Latorre J I, Rico E and Kitaev A 2003 Entanglement in quantum critical phenomena Phys. Rev. Lett. 90 227902
[31] Su W P, Schrieffer J R and Heeger A J 1979 Solitons in polyacetylene Phys. Rev. Lett. 42 1698–701
[32] Zak J 1989 Berry’s phase for energy bands in solids Phys. Rev. Lett. 62 2747–50
[33] Atala M, Aidelsburger M, Barreiro J T, Abanin D, Kitagawa T, Demler E and Bloch I 2013 Direct measurement of the zak phase in topological bloch bands Nat. Phys. 9 795–800
[34] Perez-Garcia D, Verstraete F, Wolf M M and Cirac J I 2007 Matrix product state representations Quantum Inform. Comput. 7 401–30
[35] Orús R and Vidal G 2008 Infinite time-evolving block decimation algorithm beyond unitary evolution Phys. Rev. B 78 155117
[36] Sanderson C 2010 Armadillo: an open source C++ linear algebra library for fast prototyping and computationally intensive experiments Technical Report NICTA