

Competing magnetic and topological orders in the spin-1 Kitaev-Heisenberg chain with single-ion anisotropy

Sahinur Reja¹ and Satoshi Nishimoto^{2,3}

¹Department of Physics, *Jadavpur University*, Kolkata 700032, West Bengal, India

²Department of Physics, *Technical University Dresden*, 01069 Dresden, Germany

³Institute for Theoretical Solid State Physics, *IFW Dresden*, 01069 Dresden, Germany



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We investigate the ground-state phase diagram of the spin-1 Kitaev–Heisenberg (KH) chain in the presence of uniaxial single-ion anisotropy D_z using the density-matrix renormalization-group method. The relative strength of the Heisenberg and Kitaev interactions is parametrized by a coupling angle ϕ , defined by $J = \cos \phi$ and $K = \sin \phi$. By combining energy-based diagnostics with finite-size extrapolations of order parameters and correlation functions, we obtain a comprehensive phase diagram as a function of ϕ and D_z . The phase diagram contains ferromagnetic and Néel ordered phases, collinear states with four-site spin modulation, magnetically disordered or critical regimes, two Kitaev-dominated spin-liquid-like regions, and a topological Haldane phase near the Heisenberg limit. We find that the Kitaev-dominated disordered regions acquire finite parameter widths in the spin-1 model, whereas the Haldane phase is fragile against Kitaev-type anisotropy, especially for $D_z < 0$. Positive D_z generally suppresses magnetic order and expands nonmagnetic regimes, while negative D_z enhances Ising-like magnetic order. At $D_z = 0$, we also identify an exactly solvable point at $\tan \phi = -2(\phi/\pi \simeq 1.6476)$, which gives rise to a first-order transition between the Néel- z state and a four-site collinear state. We further contrast these findings with the spin-1/2 KH chain and with the spin-1 honeycomb KH model, highlighting the distinct roles of single-ion anisotropy and dimensionality in Kitaev-type magnets.

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I. INTRODUCTION

Frustrated quantum magnets in low dimensions provide a fertile arena for unconventional phases and exotic excitations, including quantum spin liquids (QSLs) featuring fractionalization and topological order [1–4]. Among the theoretical platforms, the Kitaev model with bond-dependent anisotropic exchange has played a central role in elucidating such physics [5]. In realistic materials, however, conventional Heisenberg interactions are typically present as well, motivating extensive studies of the Kitaev–Heisenberg (KH) model in one and two dimensions. The resulting phase diagrams host highly entangled ground states with fractionalized excitations and topological order in certain parameter regimes, and are widely discussed in connection with topological quantum computation and emergent gauge structures [6–8].

While most prior work has focused on spin-1/2 systems [9,10], recent experimental progress has broadened the search to higher-spin magnets, including spin-1 candidates such as $\text{Na}_2\text{Ni}_2\text{TeO}_6$ [11–13], $\text{A}_3\text{Ni}_2\text{SbO}_6$ ($A = \text{Li, Na}$) [14–16], $\text{Na}_3\text{Ni}_2\text{BiO}_6$ [17], and KNiAsO_4 [18]. For $S > 1/2$, the physics is richer and more challenging. In contrast to the $S = 1/2$ case, the pure $S = 1$ Kitaev model is not exactly solvable,

and no exact solution in terms of free Majorana fermions coupled to a static $\mathbb{Z}_2$ gauge field is known. Accordingly, a variety of numerical and analytical approaches have been employed to clarify the fundamental properties of the spin-1 Kitaev model [19–37]. Notably, compared to the spin-1/2 case where the Kitaev spin-liquid (KSL) regime can be broad [38], spin-1 systems typically display enhanced stability of magnetically ordered phases due to reduced quantum fluctuations [27].

An efficient route toward understanding the ground-state properties of two-dimensional (2D) KH systems is to study their one-dimensional (1D) analogs, since many ordered states in the 2D spin-1/2 KH model can be understood by analogy with the corresponding 1D KH chain [39–41], which allows substantially more accurate numerical analysis. Along these lines, several theoretical works have investigated the spin-1 KH chain [42–45]. Spin-1 chains additionally support the topological Haldane phase protected by hidden symmetry [46,47]. The overall phenomenology resembles that of the spin-1/2 KH chain, except that the Tomonaga–Luttinger liquid (TLL) near the Heisenberg limit is replaced by the Haldane phase and the KSL regimes are suggested to acquire finite parameter widths rather than remaining isolated points [42].

Another important ingredient specific to $S > 1/2$ systems is uniaxial single-ion anisotropy (SIA). In Mott insulators, onsite interactions can generate nonlinear spin terms of the form $D_z \sum_i (S_i^z)^2$, where D_z controls easy-plane ($D_z > 0$) versus easy-axis ($D_z < 0$) tendencies. Recent studies of spin-1 Kitaev materials incorporating SIA have attracted increasing

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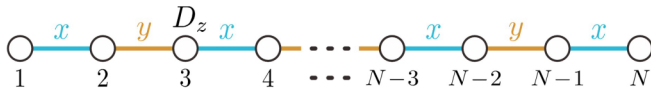


FIG. 1. Lattice structure of the spin-1 KH chain with SIA under OBC. The Kitaev bond type alternates as $x, y, x, y, \dots$, starting from an x bond at the left edge. For the open chains with even N used in the present calculations, and in particular for the $N = 4n$ chains used to define the LLRR order parameters, the rightmost bond is also an x bond.

attention [26,34,48]. In general, positive D_z suppresses magnetic order and tends to broaden KSL and/or nonmagnetic sectors, whereas negative D_z stabilizes Ising-like Néel- z and ferromagnetic (FM)- z orders. In 2D systems, SIA can also promote more exotic textures; for instance, in the spin-1 honeycomb KH model, large positive D_z favors vortex states with enlarged magnetic unit cells that erode the KSL region [34]. Despite the clear relevance of SIA to spin-1 Kitaev candidates [14–16,18], the combined effect of Kitaev, Heisenberg, and SIA terms in spin-1 chains remains comparatively unexplored.

In this paper, we accurately determine the ground-state phase diagram of the spin-1 KH chain with SIA by using the density-matrix renormalization-group (DMRG) method. We express the Heisenberg and Kitaev exchanges with a single parameter ϕ as $J = \cos \phi$ and $K = \sin \phi$ and map out the ϕ - D_z plane by first locating putative transitions from the second derivative of the ground-state energy on periodic chains of $N = 24$. We then diagnose the phases via relevant order parameters and correlation functions for open chains with up to $N = 144$ and determine accurate phase boundaries by thermodynamic extrapolations of these order parameters. Our calculations reveal four magnetically long-range-ordered (LRO) phases [FM- z , FM- xy , a two-sublattice collinear (LLRR2) state, and Néel- z], two magnetically short-range-ordered (SRO) regions (Néel- xy and LLRR1), and a topological Haldane phase, together with antiferromagnetic (AFM) and FM KSL regimes, hereafter referred to as AFM-KSL and FM-KSL, which acquire *finite* parameter widths in the spin-1 case. We further identify an exactly solvable point at $\tan \phi = -2(\phi/\pi \simeq 1.6476)$ for $D_z = 0$, which enforces a first-order boundary between Néel- z and LLRR2.

The rest of the paper is organized as follows. In Sec. II, we describe the model. In Sec. III, we provide details of the numerical techniques and define the order parameters used to identify the phases and their boundaries. In Sec. IV, we present the numerical results leading to the ϕ - D_z phase diagram. Finally, we provide discussion and summary in Secs. V and VI, respectively.

II. MODEL

We consider the spin-1 KH chain with SIA, described by the Hamiltonian

$$\mathcal{H} = \sum_i [J \mathbf{S}_i \cdot \mathbf{S}_{i+1} + K S_i^x S_{i+1}^x + D_z (S_i^z)^2], \quad (1)$$

where $\mathbf{S}_i = (S_i^x, S_i^y, S_i^z)$ is the spin-1 operator on site i , and $\gamma = x$ or y depending on the bond type (see Fig. 1). In our 1D setup, we impose a two-site unit cell, where the

bond-dependent Kitaev interactions alternate between x and y bonds along the chain. Explicitly, the bond type γ is assigned as

$$\gamma = \begin{cases} x & \text{if } i \text{ is odd,} \\ y & \text{if } i \text{ is even,} \end{cases} \quad (2)$$

so that the chain starts with an x bond at the left edge under open boundary conditions (OBC). We define the order parameters corresponding to various magnetic phases according to this convention (see below). The alternation of x and y bonds reproduces the bond-directional structure of the Kitaev exchange on the honeycomb lattice projected onto a 1D geometry.

The parameters J and K denote the isotropic Heisenberg and anisotropic Kitaev exchange couplings, respectively. The SIA D_z controls the energetic cost of nonzero S^z components, favoring easy-plane ($D_z > 0$) or easy-axis ($D_z < 0$) behavior, depending on its sign. To comprehensively explore the ground-state properties of our model (1) as a function of the exchange parameters J and K , we parametrize them as

$$J = \cos \phi, \quad K = \sin \phi, \quad (3)$$

so that the model can be analyzed over the full circle $\phi \in [0, 2\pi)$. This parametrization allows us to smoothly interpolate between various limiting cases, including the pure Heisenberg ($K = 0$) and pure Kitaev ($J = 0$) chains, as well as mixed regimes where the two interactions compete. Unless otherwise stated, we set the overall exchange energy scale to $\sqrt{J^2 + K^2} = 1$.

III. METHOD

In this section, we summarize our DMRG setup and explain how we combine periodic- and open-boundary calculations to construct the phase diagram and to identify each phase.

A. Numerical technique

To investigate the ground-state properties of the model (1), we employ the DMRG method [49], which provides high accuracy for 1D systems with short-range interactions. We use both periodic boundary conditions (PBC) and open boundary conditions (OBC); their roles are complementary, as described below.

For bulk quantities such as the ground-state energy E_0 , the total spin S_{tot} , and the static spin structure factor $S(q)$, we perform PBC calculations on $N = 24$ -site rings. Since PBC calculations are more demanding, we retain up to $m = 4000$ density-matrix eigenstates and perform up to 20 sweeps to ensure convergence. The typical discarded weight (truncation error) is less than 10^{-8} .

For nonlocal probes (e.g., string correlations) and for evaluating order parameters corresponding to various magnetic phases, we perform OBC calculations, which yield higher accuracy at comparable computational cost. In OBC calculations, we may employ weak boundary pinning fields or symmetry-broken initial states to select a representative ordered configuration, thereby enabling the direct identification of magnetic order through local expectation values (e.g., $\langle S_i^z \rangle$)

in the bulk. We study OBC chains with $N = 24$ –144 sites, retain up to $m = 4000$ states, with final discarded weights typically $\lesssim 10^{-8}$. To minimize boundary-induced Friedel oscillations, OBC observables are evaluated in a central window of sites, far from the edges. This choice reduces finite-size corrections and improves the stability of the subsequent finite-size scaling analyses. Order parameters obtained for various system sizes are extrapolated to the thermodynamic limit. Unless stated otherwise, all results are converged with respect to m , the number of sweeps, and system sizes.

Additional convergence checks are presented in Appendix E. There we show the bond-dimension dependence of the energy and discarded weight at the most demanding parameter point, $\phi/\pi = 0.6$ and $D_z = 0$, the dependence of representative order parameters on the boundary pinning field h , and the spatial periodicity of the converged PBC wave function for $N = 24$. These results confirm that the numerical data used in the main text are well converged and that the extrapolated bulk order parameters are essentially independent of the pinning-field strength.

B. Investigation procedure

We first obtain a global characterization of the ground-state phases by systematically varying the coupling angle ϕ [Eq. (3)] and scanning the SIA strength D_z . The phase diagram is initially mapped on a small PBC cluster ($N = 24$ -site ring) by evaluating the following bulk diagnostics: (i) the ground-state energy per site E_0/N , (ii) the total spin per site S_{tot}/N , where S_{tot} is determined from $\langle S_{\text{tot}}^2 \rangle = S_{\text{tot}}(S_{\text{tot}} + 1)$, and (iii) the static spin structure factor

$$S^{\alpha\alpha}(q) = \frac{1}{N} \sum_{i,j} e^{iq(r_i - r_j)} \langle S_i^\alpha S_j^\alpha \rangle \quad (\alpha = x, y, z), \quad (4)$$

whose peak position diagnoses magnetic periodicity via a characteristic wave vector q . This strategy provides a reliable starting point for locating magnetic phase boundaries in related KH models [39,50,51].

Once a coarse phase diagram is obtained, we refine the phase boundaries and determine the nature of each phase (LRO vs. SRO) by performing higher-accuracy OBC calculations on longer chains. Specifically, we compute real-space correlations $\langle S_i^\alpha S_{i+r}^\alpha \rangle$ and evaluate order parameters that distinguish topological order, magnetic order, and symmetry breaking. The order parameters used to identify the phases summarized in Fig. 2 are defined below.

C. Order parameters

To characterize the ground-state phases of the Hamiltonian in Eq. (1), we introduce appropriate order parameters for the relevant candidate phases. Phases with spontaneous symmetry breaking are identified by conventional magnetic order parameters, whereas topological and disordered phases require nonlocal quantities or bond-energy-based observables. Within DMRG simulations on open chains, these order parameters are constructed from local spin expectation values and correlation functions, taking advantage of the open boundary conditions. In particular, open edges explicitly break both spin-rotational and translational symmetries,

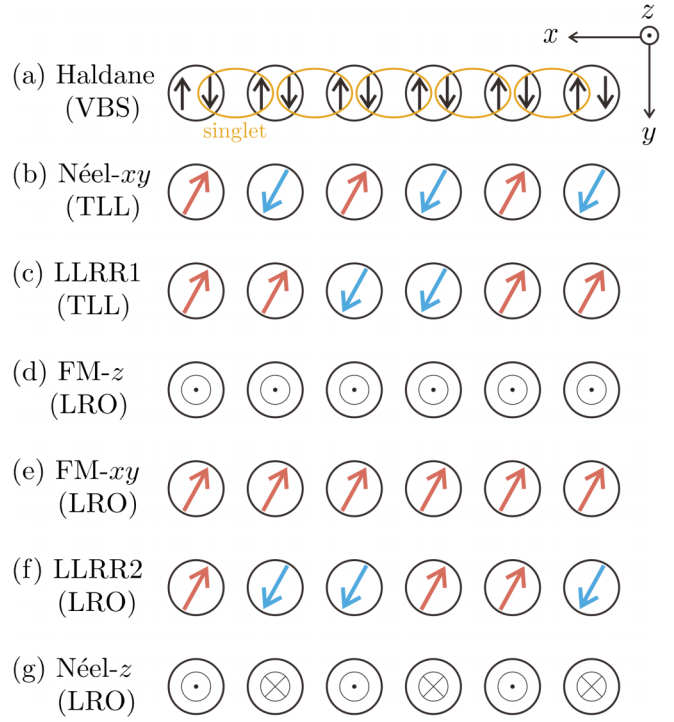


FIG. 2. Schematic representations of the seven phases realized in the 1D spin-1 KH model, excluding the KSL regimes. We do not include the KSL states here because they do not exhibit a simple semiclassical spin pattern associated with local symmetry breaking. In the ideal Kitaev limit, spin correlations are extremely short-ranged (only nearest-neighbor bond correlations remain finite), which further complicates a schematic real-space depiction.

thereby selecting a preferred ordering direction. This controlled symmetry breaking enables accurate evaluation of local order parameters and reliable finite-size scaling analyses. In the following, we define the specific order parameters used to distinguish the phases summarized in Fig. 2.

Here, the abbreviation LLRR stands for a “left-left-right-right” spin pattern, referring to a four-site modulation in which two neighboring spins point predominantly in one direction and the next two point predominantly in the opposite direction. The labels LLRR1 and LLRR2 are used to distinguish two such four-site-modulated regimes with different relative phases and different long-distance behavior.

In the following definitions, N is assumed to be even. For the LLRR1 and LLRR2 order parameters, we further choose $N = 4n$, with n being an integer, so that the four-site modulation is compatible with the chain length and the central four sites are defined unambiguously.

1. Haldane phase

The Haldane phase does not exhibit conventional magnetic order, but it can be characterized as a topological valence bond solid (VBS) state with hidden $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry breaking [52–54]. This phase is typically identified by evaluating the

nonlocal string correlation function

$$C_{\text{str}}(i, j) = \left\langle S_i^z \exp \left(i\pi \sum_{k=i+1}^{j-1} S_k^z \right) S_j^z \right\rangle, \quad (5)$$

whose asymptotic value $|C_{\text{str}}(-\infty, \infty)|$ serves as a string order parameter that characterizes the Haldane phase. In practical simulations, we define the string order parameter around the center of the system as

$$\mathcal{O}_{\text{str}} = \lim_{N \rightarrow \infty} \left| C_{\text{str}} \left(\frac{N}{4}, \frac{3N}{4} \right) \right|. \quad (6)$$

For the spin-1 Heisenberg chain ($\phi = 0$), this parameter takes the value $|C_{\text{str}}(-\infty, \infty)| \approx 0.3743$ [55].

2. Néel-xy phase

The Néel-xy phase is characterized by alternating spin alignment in the xy plane. We define the corresponding order parameter from the local spin expectation values at the chain center as

$$\mathcal{O}_{\text{Néel-xy}} = \lim_{N \rightarrow \infty} \frac{1}{2} \left| \langle S_{N/2}^x \rangle - \langle S_{N/2+1}^x \rangle \right|. \quad (7)$$

To induce symmetry breaking and stabilize a preferred orientation, staggered boundary fields are applied along the x axis, $h_1^x = -h_N^x = h$. Although strong edge fields polarize spins near the boundaries, the bulk value of $\mathcal{O}_{\text{Néel-xy}}$ converges to a well-defined limit independent of h as $N \rightarrow \infty$, allowing reliable extraction from the central region.

Because of the remaining spin-rotational symmetry in the xy plane, an equivalent definition can be given using the y component,

$$\mathcal{O}_{\text{Néel-xy}} = \lim_{N \rightarrow \infty} \frac{1}{2} \left| \langle S_{N/2}^y \rangle - \langle S_{N/2+1}^y \rangle \right|, \quad (8)$$

with $h_1^y = -h_N^y = h$. In practice, the open boundaries spontaneously select one direction, so either choice is valid in numerical simulations.

3. Néel-z phase

The Néel-z phase is defined analogously, but the spin symmetry is broken only along the z axis. The corresponding order parameter is uniquely given by

$$\mathcal{O}_{\text{Néel-z}} = \lim_{N \rightarrow \infty} \frac{1}{2} \left| \langle S_{N/2}^z \rangle - \langle S_{N/2+1}^z \rangle \right|, \quad (9)$$

where staggered boundary fields $h_1^z = -h_N^z = h$ are applied to stabilize the symmetry-broken state.

4. FM-xy phase

The FM-xy phase is characterized by uniform FM alignment in the xy plane. Assuming that the spontaneous magnetization points along the x axis, the order parameter is defined from the bulk magnetization as

$$\mathcal{O}_{\text{FM-xy}} = \lim_{N \rightarrow \infty} \left| \langle S_{N/2}^x \rangle \right|. \quad (10)$$

To stabilize the symmetry-broken state, uniform boundary fields are applied along the x axis, $h_1^x = h_N^x = h$.

5. FM-z phase

The FM-z phase exhibits FM order along the z axis. The corresponding order parameter is given by

$$\mathcal{O}_{\text{FM-z}} = \lim_{N \rightarrow \infty} \left| \langle S_{N/2}^z \rangle \right|, \quad (11)$$

with uniform boundary fields $h_1^z = h_N^z = h$ applied to select the ordered state.

6. LLRR1 phase

The LLRR1 order parameter is designed to detect a four-site left-left-right-right spin modulation appearing on the $J < 0$, $K > 0$ side, close to the AFM Kitaev limit, where $|J| \ll K \simeq 1$. Assuming that the selected spin direction is along the x axis, the dominant interaction on the x bonds favors AFM alignment, whereas the weaker interaction on the y bonds favors FM alignment. This alternation of AFM and FM tendencies gives rise to a four-site modulation. For open chains with $N = 4n$, we define the order parameter using the four central sites:

$$\mathcal{O}_{\text{LLRR1}} = \lim_{N \rightarrow \infty} \frac{1}{4} \left| \langle S_{N/2-1}^x \rangle - \langle S_{N/2}^x \rangle - \langle S_{N/2+1}^x \rangle + \langle S_{N/2+2}^x \rangle \right|. \quad (12)$$

Boundary fields are applied as $h_1^x = h_N^x = h$.

7. LLRR2 phase

The LLRR2 order parameter detects a related four-site modulation on the $J > 0$, $K < 0$ side, close to the FM Kitaev limit, where $J \ll |K| \simeq 1$. Assuming that the selected spin direction is along the x axis, the dominant interaction on the x bonds favors FM alignment, whereas the weaker interaction on the y bonds favors AFM alignment. This produces a four-site pattern shifted in phase relative to LLRR1. The order parameter is defined as

$$\mathcal{O}_{\text{LLRR2}} = \lim_{N \rightarrow \infty} \frac{1}{4} \left| \langle S_{N/2-1}^y \rangle + \langle S_{N/2}^x \rangle - \langle S_{N/2+1}^y \rangle - \langle S_{N/2+2}^x \rangle \right|. \quad (13)$$

This is similar in form to the LLRR1 order parameter but shifted by a relative phase of $\pi/2$. The boundary fields are applied as $h_1^x = -h_N^x = h$.

8. Kitaev spin-liquid phase

The KSL phase does not exhibit any magnetic long-range order. However, it can be identified by the absence of conventional order parameters and the presence of short-range entanglement, the basic characteristic of quantum spin liquids. In our model, we quantify the bond-dependent correlations associated with the alternating x and y Kitaev interactions by introducing the following dimer order parameter

$$\mathcal{O}_{\text{dim}}^\gamma = \lim_{N \rightarrow \infty} \left| \langle S_i^\gamma S_{i+1}^\gamma \rangle - \langle S_{i+1}^\gamma S_{i+2}^\gamma \rangle \right|, \quad (14)$$

where $\gamma = x, y$ denotes the Kitaev component associated with the corresponding bond type, and i is chosen near the center of the chain. In the Kitaev-dominated regime, this quantity remains finite and size independent, thereby serving as a diagnostic of the Kitaev-dominated spin-liquid-like phase.

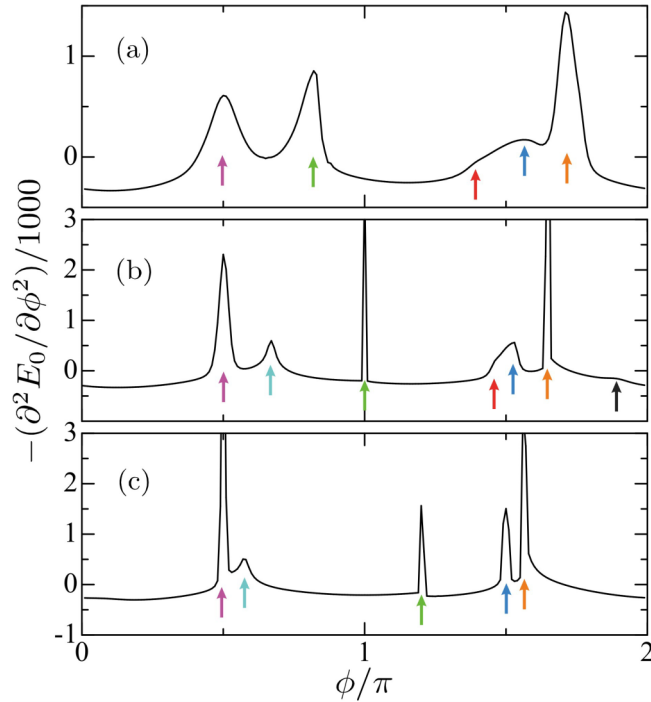


FIG. 3. Second derivative of the ground-state energy E_0 with respect to ϕ for fixed (a) $D_z = 0.6$, (b) 0.0 , and (c) -0.6 . The arrows indicate possible phase boundaries.

IV. NUMERICAL RESULTS

A. Second derivative of the energy

To establish the basic structure of the phase diagram in the ϕ - D_z plane, we start by evaluating the second derivative of the ground-state energy E_0 with respect to the tuning parameter ϕ for several fixed values of D_z . This quantity serves as a sensitive finite-size diagnostic for identifying candidate phase boundaries. In general, peaks or shoulders in this quantity indicate the locations of phase boundaries. Figures 3(a)–3(c) display the second derivative of E_0 as a function of ϕ/π for three representative values of $D_z = 0.6, 0.0$, and -0.6 respectively, obtained for a periodic chain of $N = 24$ sites. The positions of these anomalies—indicated by arrows—are taken as estimates of the transition points.

We also note that in Fig. 3(a) a weak shoulder is visible on the high- ϕ side of the second peak. This feature may be associated with the nearby Néel- z –Haldane boundary. However, for this value of D_z , it is not clearly separated from the main peak in the $N = 24$ PBC energy-curvature data, and we therefore do not assign an independent boundary to it. When the corresponding anomaly becomes clearly separated for smaller D_z , such as the peak near $\phi/\pi \simeq 2$ at $D_z = 0$, we identify it as a phase boundary in combination with the order-parameter analysis.

To determine which phases are separated by these transitions, we examine the color maps of the total spin S_{tot} , the momentum q_{max} at which the spin structure factor $S^{\alpha\alpha}(q)$ attains its maximum, and the corresponding peak intensity I_{max} , as depicted respectively in Figs. 4(a)–4(c). These quantities are plotted as functions of ϕ/π and D_z , together with the transition points extracted from Fig. 3. Based on these

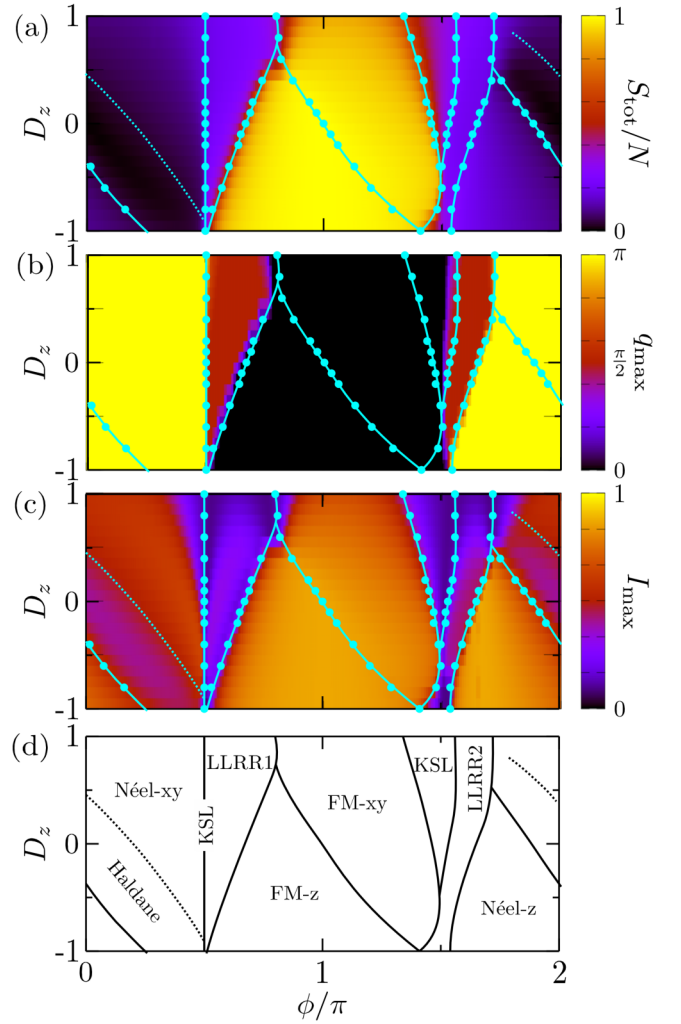


FIG. 4. Color maps of (a)–(c) the total spin S_{tot} , the momentum q_{max} at which the spin structure factor $S^{\alpha\alpha}(q)$ attains its maximum, and the corresponding peak intensity I_{max} , plotted as functions of ϕ/π and D_z . The transition points extracted from Fig. 3 are also indicated. (d) Ground-state phase diagram in the ϕ - D_z plane, obtained from the analysis of the second derivative of the energy. The dotted line is approximately evaluated from I_{max} (see text).

results, the overall phase diagram as a function of ϕ/π and D_z is presented in Fig. 4(d). We note that the phase boundary between the Haldane and Néel- z phases does not produce a pronounced peak in the second derivative of the ground-state energy. We therefore estimate this boundary approximately from the behavior of I_{max} : in the Haldane phase, spin–spin correlations decay exponentially with distance, resulting in a comparatively small peak intensity of $S^{\alpha\alpha}(q)$, see Fig. 4(c).

However, this approach has limited sensitivity to transitions between magnetically disordered phases, where conventional order parameters do not exhibit singular behavior. In our model, this limitation is the most evident near the boundaries separating the AFM Kitaev phase from its neighboring Néel- xy and LLRR1 phases, as well as at the transition between the Haldane and Néel- xy regions, as mentioned above. Nevertheless, previous studies have demonstrated that phase diagrams inferred from the second derivative of the ground-state energy,

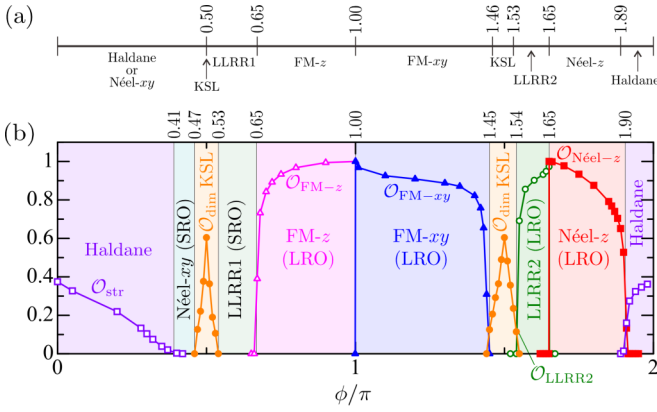


FIG. 5. Ground-state phase diagram vs ϕ/π at $D_z = 0$, obtained from (a) the second derivative of the energy for a 24-site PBC cluster and (b) extrapolated order parameters in the thermodynamic limit.

even for moderately large finite systems, provide a reliable approximation to the thermodynamic limit for magnetically ordered phases. Motivated by this observation, we use the tentative phase boundaries identified here as a starting point for a more detailed analysis of the order parameters characterizing each phase. These analyses are presented in the following subsections.

B. Phase diagram at $D_z = 0$

1. Comparison between the second-derivative and order-parameter approaches

We first focus on the $D_z = 0$ case. As a reference, Fig. 5(a) shows the phase diagram as a function of ϕ/π obtained from the above analysis on an $N = 24$ PBC cluster. We further compute the relevant order parameters for open chains with up to $N = 144$ sites and extrapolate them to the thermodynamic limit; the extrapolated values of the order parameters are summarized in Fig. 5(b). Details of the finite-size scaling analyses are provided in Appendix A.

As expected, the phase boundaries between magnetically ordered phases, as well as those between ordered and disordered phases, agree quantitatively well between the two methods. However, for boundaries between magnetically disordered phases, the situation is somewhat different. In particular, the phase diagram obtained from the order parameters reveals an additional boundary between the Haldane and Néel-xy phases, which was not captured by the analysis of the second derivative of the energy. Moreover, while the second-derivative approach suggested a single transition point near $\phi/\pi = 0.5$, the order-parameter analysis shows that the KSL phase actually occupies a finite parameter region.

2. Order-parameter behavior for magnetically ordered phases

We now turn to a more detailed quantitative examination of each order parameter. We begin with four phases exhibiting magnetic LRO: FM-z ($0.65 \lesssim \phi/\pi < 1.00$), FM-xy ($1.00 \lesssim \phi/\pi < 1.45$), LLRR2 ($1.54 \lesssim \phi/\pi < 1.65$), and Néel-z ($1.65 \lesssim \phi/\pi < 1.90$). In each case, the corresponding order parameter— $\mathcal{O}_{FM-z}$, $\mathcal{O}_{FM-xy}$, $\mathcal{O}_{LLRR2}$, or $\mathcal{O}_{Néel-z}$ —extrapolates to a finite value in the thermodynamic limit. The

FM-z and FM-xy phases, as well as the LLRR2 and Néel-z phases, are directly adjacent to each other, and the transitions between them are of first-order character, as evidenced by discontinuous jumps in the order parameters depicted in Fig. 5(b). Each of these ordered phases also borders a disordered phase.

Near the phase boundaries ($\phi/\pi \approx 0.65, 1.45, 1.54, 1.90$), the corresponding order parameters change rapidly but remain continuous within the system sizes studied. We therefore do not infer the order of these transitions solely from the order-parameter behavior. Instead, we use the pronounced anomalies in the second derivative of the ground-state energy as finite-size indicators of candidate phase boundaries, and determine the phases on both sides by independent order-parameter and correlation-function analyses [cf. Fig. 5(a)].

Ferromagnetic phases. To understand the phases better, we use the fact that the Hamiltonian in Eq. (1) without the SIA term can be decomposed as $\mathcal{H} = \mathcal{H}_{\text{Ising}} + \mathcal{H}_{\text{ex}} + \mathcal{H}_{\text{dsf}}$, where $\mathcal{H}_{\text{ex},i} = \frac{2J+K}{4}(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+)$, $\mathcal{H}_{\text{dsf},i} = \frac{K}{4}(-1)^i(S_i^+ S_{i+1}^+ + S_i^- S_{i+1}^-)$, and $\mathcal{H}_{\text{Ising},i} = JS_i^z S_{i+1}^z$.

Since the coefficients of both $\mathcal{H}_{\text{ex}}$ and $\mathcal{H}_{\text{Ising}}$ are negative in the region $0.65 \lesssim \phi/\pi \lesssim 1.5$, FM order is naturally expected. In fact, at $D_z = 0$, we find a FM phase for $0.65 < \phi/\pi < 1.45$. At the spin-isotropic point $\phi/\pi = 1$, the system is equivalent to the spin-1 FM Heisenberg chain. Thus, the spins can align along an arbitrary direction owing to SU(2) rotational symmetry, and the corresponding order parameters satisfy $\mathcal{O}_{FM-xy} = \mathcal{O}_{FM-z} = 1$, as shown in Fig. 5(b). Away from the isotropic point, the SU(2) symmetry is broken. For $\phi/\pi < 1$, the effective easy-axis character favors magnetization along the z direction, whereas for $\phi/\pi > 1$, the magnetization lies in the xy plane. Within this plane, the magnetization direction can freely rotate, reflecting the residual U(1) rotational symmetry.

Exactly solvable point. At $D_z = 0$, in addition to the isotropic FM point ($\phi/\pi = 1$), the model has a special point at $\phi = \phi_0$, where $\phi_0/\pi \simeq 1.6476$ and $\tan \phi_0 = -2$. At this point, $J_0 = \cos \phi_0 > 0$ and $K_0 = \sin \phi_0 = -2J_0$, so that the exchange part $\mathcal{H}_{\text{ex}}$ vanishes.

The nature of this point can be understood most transparently by a four-sublattice spin rotation. We define the rotated spin operators by

$$S_i^\alpha = \eta_i^\alpha \tilde{S}_i^\alpha, \quad (15)$$

where the site-dependent signs are chosen as

$$(\eta_i^x, \eta_i^y, \eta_i^z) = \begin{cases} (+1, +1, +1), & i = 4m + 1, \\ (+1, -1, -1), & i = 4m + 2, \\ (-1, -1, +1), & i = 4m + 3, \\ (-1, +1, -1), & i = 4m + 4. \end{cases} \quad (16)$$

with integer m . This corresponds to local π rotations of the spin axes on three of the four sublattices. For an x bond, the signs satisfy

$$\eta_i^x \eta_{i+1}^x = +1, \quad \eta_i^y \eta_{i+1}^y = \eta_i^z \eta_{i+1}^z = -1, \quad (17)$$

whereas for a y bond they satisfy

$$\eta_i^y \eta_{i+1}^y = +1, \quad \eta_i^x \eta_{i+1}^x = \eta_i^z \eta_{i+1}^z = -1. \quad (18)$$

Therefore, at $K = -2J$,

$$JS_i \cdot S_{i+1} + KS_i^\gamma S_{i+1}^\gamma = -J\tilde{S}_i \cdot \tilde{S}_{i+1} \quad (19)$$

for both $\gamma = x$ and $\gamma = y$ bonds. Thus, for $J > 0$, the model is mapped onto a ferromagnetic spin-1 Heisenberg chain,

$$H = -J \sum_i \tilde{S}_i \cdot \tilde{S}_{i+1}. \quad (20)$$

Thus, the exact ground-state manifold is the fully polarized FM manifold in the rotated basis. Different choices of the polarization direction correspond, in the original spin basis, to different ordered configurations. For example, a polarization along the z direction gives the full-moment Néel- z product state, $|\uparrow\downarrow\uparrow\downarrow\cdots\rangle_z$ and its spin-reversed partner. On the other hand, a polarization along the x direction gives the LLRR2 configuration, $|\rightarrow\rightarrow\leftarrow\leftarrow\rightarrow\rightarrow\leftarrow\leftarrow\cdots\rangle_x$, where $|\rightarrow\rangle_x$ and $|\leftarrow\rangle_x$ denote the $S^x = +1$ and $S^x = -1$ states, respectively. In this sense, the Néel- z and LLRR2 states are different representatives of the same hidden FM ground-state manifold at $\phi = \phi_0$. An infinitesimal deviation from this point selects one of these competing ordered states, producing the first-order transition between the Néel- z and LLRR2 phases. Correspondingly, the order parameter reaches its full value on each side of the transition, as shown in Fig. 5(b).

There is another point satisfying $2J + K = 0$, namely $\phi/\pi \simeq 0.6476$, where $J < 0$ and $K > 0$. The same four-sublattice rotation maps this point onto an antiferromagnetic spin-1 Heisenberg chain, because the effective coupling $-J$ is then positive. Therefore, it does not yield the same simple product-state ground-state manifold as the point $\phi/\pi \simeq 1.6476$.

3. Order-parameter behavior for magnetically disordered phases

Next, we consider five phases that do not display magnetic LRO: the Haldane phase ($-0.10 \lesssim \phi/\pi < 0.41$), the Néel- xy phase ($0.41 \lesssim \phi/\pi < 0.47$), the AFM-KSL phase ($0.47 \lesssim \phi/\pi < 0.53$), the LLRR1 phase ($0.53 \lesssim \phi/\pi < 0.65$), and the FM-KSL phase ($1.45 \lesssim \phi/\pi < 1.54$).

Haldane phase. The Haldane phase is characterized by a finite string order parameter $\mathcal{O}_{\text{str}}$. Although this order reflects a hidden AFM structure, it does not correspond to conventional magnetic LRO. At $\phi = 0$, the system is equivalent to the spin-1 AFM Heisenberg chain, and $\mathcal{O}_{\text{str}}$ reaches its maximal value of 0.3711. This value decreases gradually as ϕ moves away from zero. Toward the boundary with the Néel- xy phase at $\phi/\pi = 0.41$, $\mathcal{O}_{\text{str}}$ decays continuously in a manner consistent with a Berezinskii–Kosterlitz–Thouless transition. If the Néel- xy phase is interpreted as an XY-like TLL, providing a power-law decay of the spin–spin correlations, this behavior is consistent with previous studies for the spin- $\frac{1}{2}$ KH chain [39]. Since the Haldane phase is a gapped VBS state, the spin–spin correlations decay exponentially. A detailed analysis of this behavior is presented in Appendix B.

We would like to emphasize that we avoid using the entanglement-spectrum degeneracy as the primary criterion for locating the Haldane phase in the present finite-size open-chain calculations. In finite open Haldane chains, the physical spin-1/2 edge degrees of freedom and finite-size effects can obscure the simple even-fold degeneracy expected in the

thermodynamic or infinite-MPS limit. Indeed, even the $S = 1$ Heisenberg chain with open boundaries shows an entanglement spectrum dominated by integer-spin multiplet structures for the system sizes considered here. We therefore use the nonlocal string order parameter and the exponential decay of spin correlations as the more robust diagnostics of the Haldane phase.

KSL and adjacent phases. The AFM-KSL and FM-KSL phases are identified by a nonzero dimer order parameter. In contrast, the Néel- xy and LLRR1 phases exhibit short-range spin patterns [Figs. 2(b) and 2(c), respectively], but their associated order parameters $\mathcal{O}_{\text{Néel-xy}}$ and $\mathcal{O}_{\text{LLRR1}}$ vanish in the thermodynamic limit (see Appendix A). This indicates that they correspond to disordered or critical phases, which can be classified as TLLs. The Haldane–Néel- xy , Néel- xy –AFM-KSL, and AFM-KSL–LLRR1 boundaries separate magnetically disordered or critical regimes and are not associated with discontinuous magnetic order parameters in our calculations. In the present finite-size PBC analysis, these boundaries produce only weak or broad features in the second derivative of the ground-state energy, making them difficult to locate reliably from the energy curvature alone. We therefore identify these boundaries primarily from the behavior of the relevant order parameters and correlation functions, together with their finite-size scaling.

Néel- xy phase. In the Néel- xy phase, spins form an antiferromagnetic pattern in the xy plane while preserving continuous spin-rotational symmetry. Since the extrapolated Néel- xy order parameter vanishes in the thermodynamic limit, this regime does not exhibit true dipolar LRO in 1D. Nevertheless, dominant staggered transverse correlations are clearly visible in the spin structure factor. As shown in Fig. 12(b) in Appendix B, the spin–spin correlation exhibits a power-law decay, which is characteristic of a TLL-like critical regime.

This identification is further supported by the spin structure factor shown in Fig. 12(c). Here, $S(q)$ is evaluated from the full spin correlation function $\langle S_i \cdot S_j \rangle$, with the site pair chosen so that each distance $r = |i - j|$ straddles the center of the open chain. The resulting $S(q)$ exhibits a pronounced peak at $q = \pi$, reflecting dominant staggered spin correlations. To examine whether this peak corresponds to true long-range order, we plot $S(\pi)$ as a function of $1/N^{0.44}$ in Fig. 12(d). The exponent 0.44 is obtained from a numerical fit to the power-law decay of the real-space spin correlation in the Néel- xy regime and is used here as an empirical scaling variable for the finite-size extrapolation of the peak intensity. The extrapolation to zero indicates that the Néel- xy regime does not possess dipolar long-range order, but is instead characterized by quasi-long-range staggered correlations.

LLRR1 phase. While both LLRR1 and LLRR2 phases show similar local spin patterns, their long-distance behavior differs significantly. The LLRR2 phase exhibits true long-range order in this order parameter, remaining finite in the thermodynamic limit. In contrast, the order parameter in the LLRR1 phase decays with increasing system size, indicating the absence of long-range order. This distinction suggests that LLRR2 corresponds to a symmetry-breaking phase, whereas LLRR1 should be regarded as a disordered or critical phase with strong short-range modulation. This interpretation is further supported by the spin structure factor. As shown in

Fig. 12(e), $S(q)$ in the LLRR1 regime has a dominant peak at $q = \pi/2$, reflecting the four-site modulation characteristic of the LLRR pattern. The scaling variable $1/N^{0.29}$ used in Fig. 12(f) is determined in the same way from the numerical power-law decay of the corresponding real-space spin correlation in the LLRR1 regime. The peak intensity $S(\pi/2)$ extrapolates to zero in the thermodynamic limit, indicating the absence of true dipolar long-range order. Thus, the LLRR1 regime exhibits dominant quasi-long-range four-site correlations, but not true dipolar long-range order. Since the LLRR1 regime is magnetically disordered or critical, we also checked whether it hides quadrupolar long-range order. As shown in Appendix D, the connected quadrupolar correlations are enhanced by positive D_z , but they still decay to zero at long distances, providing no evidence for quadrupolar long-range order.

The difference between LLRR1 and LLRR2 can be understood from the sign of the effective interaction in a hidden, rotated basis. Although both regimes exhibit a similar four-site modulation in local spin correlations, they are located on opposite sides of the Kitaev-dominated parameter space. Near the $K = -2J$ point, a four-sublattice rotation maps the Hamiltonian to an effective spin-1 Heisenberg chain. For the LLRR2 side ($J > 0$ and $K < 0$), this effective model is ferromagnetic, and its ferromagnetic order appears in the original spin basis as the four-site LLRR2 long-range order. In contrast, for the LLRR1 side ($J < 0$ and $K > 0$), the corresponding effective model is antiferromagnetic and does not support conventional dipolar long-range order. This explains why the LLRR1 regime can exhibit strong four-site correlations while its order parameter vanishes in the thermodynamic limit. Thus, the distinction between LLRR1 and LLRR2 is not the local modulation wave vector itself, but whether the four-site modulation develops into true symmetry-breaking long-range order.

Differences from previous work. The main differences between our results and those of the previous study [43] are summarized as follows. First, at $D_z = 0$, Ref. [43] identified most of the region with $J > 0$ ($-0.5 < \phi/\pi < 0.5$), specifically $-0.35 \lesssim \phi/\pi \lesssim 0.47$, as belonging to the Haldane phase. In contrast, our analysis reveals that the interval $-0.35 \lesssim \phi/\pi \lesssim -0.10$ should be classified as the Néel- z phase, while $0.41 \lesssim \phi/\pi \lesssim 0.47$ corresponds to the Néel- xy phase. This finding indicates that the Haldane phase is fragile against Kitaev-type anisotropy, particularly for $D_z < 0$. Furthermore, although the LLRR1 and LLRR2 phases exhibit very similar four-site periodic spin patterns, we find that the LLRR2 phase possesses magnetic LRO, whereas the LLRR1 phase shows only quasi-long-range correlations without true LRO. This distinction was not captured in Ref. [43].

C. D_z dependence of phases

1. Haldane phase

Figure 6 shows the D_z dependence of the string order parameter in the thermodynamic limit for $\phi/\pi = 0.2$ and 0.3 . Since the Haldane state is a gapped VBS phase, it is favored by nearly isotropic spin interactions that stabilize effective singlet formation between fractionalized spin-1/2 degrees of freedom. Consequently, deviations from the isotropic limit—either by introducing the bond-dependent Kitaev term (finite

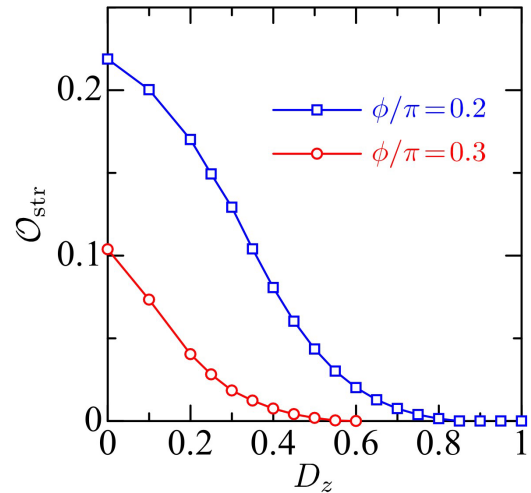


FIG. 6. D_z dependence of the string order parameter for $\phi/\pi = 0.2$ (blue squares) and 0.3 (red circles).

ϕ) or by applying a single-ion anisotropy D_z —are expected to weaken the Haldane phase. Indeed, $\mathcal{O}_{\text{str}}$ at $\phi/\pi = 0.3$ is smaller than that at $\phi/\pi = 0.2$, and in both cases it decreases monotonically with increasing D_z . The string order parameter smoothly approaches zero upon crossing into the Néel- xy phase, consistent with a continuous transition. This trend is analogous to that observed in Fig. 5(b) when ϕ/π is increased at fixed $D_z = 0$.

For sufficiently large positive D_z , the system is expected to cross over into the so-called large- D_z phase [56], in which the spins are predominantly in the $S^z = 0$ state (a trivial product state in the $D_z \rightarrow +\infty$ limit).

2. Néel- z phase

We now turn to the D_z dependence of the Néel- z phase. For $D_z > 0$, the $|\uparrow\rangle$ and $|\downarrow\rangle$ components of the spin-1 basis become progressively less populated compared with the $|0\rangle$ component. As D_z increases, the energy gain from forming a Néel state along the z axis is therefore reduced. Figure 7(a) shows $\mathcal{O}_{\text{Néel-}z}$ as a function of D_z for $\phi/\pi = 1.75, 1.80$, and 1.85 . As ϕ/π increases, the critical value of D_z decreases, as expected. Near $D_z = 0$, the initial rate of decrease of $\mathcal{O}_{\text{Néel-}z}$ is

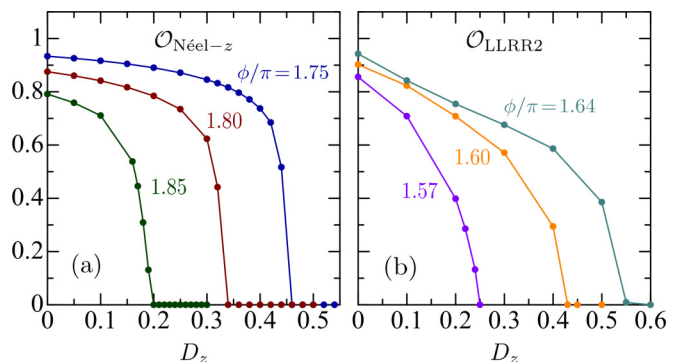


FIG. 7. D_z dependence of (a) the Néel- z order parameter $\mathcal{O}_{\text{Néel-}z}$ for $\phi/\pi = 1.75, 1.80$, and 1.85 , and (b) the LLRR2 order parameter $\mathcal{O}_{\text{LLRR2}}$ for $\phi/\pi = 1.57, 1.60$, and 1.64 .

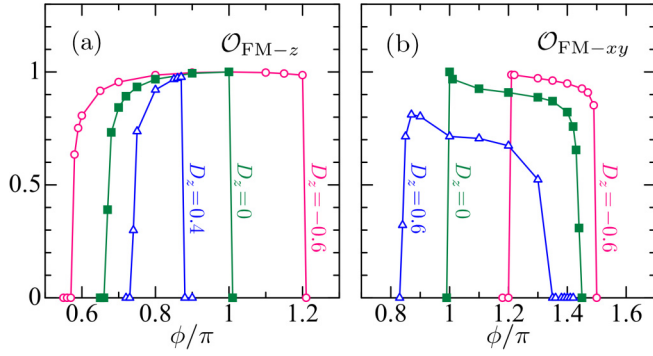


FIG. 8. D_z dependence of the ferromagnetic order parameters. (a) $\mathcal{O}_{\text{FM}-z}$ as a function of ϕ/π for $D_z = -0.6, 0$, and 0.4 . (b) $\mathcal{O}_{\text{FM}-xy}$ as a function of ϕ/π for $D_z = -0.6, 0$, and 0.6 .

slightly larger for larger ϕ/π , reflecting the reduced stability of the Néel- z order. However, $\mathcal{O}_{\text{Néel}-z}$ drops sharply to zero only when approaching the phase boundary with the Haldane phase.

Although we do not show the data here, for negative D_z the $|\uparrow\rangle$ and $|\downarrow\rangle$ components become more populated, and the spin-1 degrees of freedom effectively reduce to an Ising-like form. In the large negative- D_z limit, the Hamiltonian essentially reduces to $\mathcal{H}_{\text{Ising}}$. As a result, the entire parameter regions $0 < \phi/\pi < 0.5$ and $1.5 < \phi/\pi < 2.0$ are occupied by the Néel- z phase in the ground-state phase diagram.

3. LLRR2 phase

The stability of the LLRR2 order is similar to that of the Néel- z phase. As discussed above for $D_z = 0$ case, the order parameter $\mathcal{O}_{\text{LLRR2}}$ reaches its maximum value of 1 at $\tan \phi = -2(\phi/\pi \simeq 1.6476)$ and decreases as ϕ/π is reduced, dropping sharply to zero near the boundary with the FM-KSL phase at $\phi/\pi \approx 1.54$. Figure 7(b) shows $\mathcal{O}_{\text{LLRR2}}$ as a function of D_z for $\phi/\pi = 1.57, 1.60$, and 1.64 . Compared with $\mathcal{O}_{\text{Néel}-z}$, the stronger quantum fluctuations in the LLRR2 phase lead to a more rapid suppression of $\mathcal{O}_{\text{LLRR2}}$ as D_z increases. The critical value of D_z at which $\mathcal{O}_{\text{LLRR2}}$ vanishes increases with ϕ/π , reflecting the higher intrinsic stability of the LLRR2 order for larger ϕ/π . Importantly, even after $\mathcal{O}_{\text{LLRR2}}$ becomes zero, the short-range four-site periodic spin structure remains intact. This indicates that the transition driven by D_z can be interpreted as a change from LLRR2 LRO to LLRR2 SRO.

4. Ferromagnetic states

As the nature of magnetization axes differ between FM- z and FM- xy phases, the D_z dependence of these phases also shows distinct behaviors. Figure 8(a) depicts $\mathcal{O}_{\text{FM}-z}$ as a function of ϕ/π for $D_z = -0.6, 0$, and 0.4 . For $D_z > 0$, spin polarization along the z axis becomes energetically unfavorable. Consequently, the FM- z region for $D_z = 0.4$ is significantly reduced compared with that for $D_z = 0$. In contrast, for $D_z < 0$, polarization along the z axis yields an energy gain, and the FM- z region for $D_z = -0.6$ is substantially enhanced relative to that at $D_z = 0$. In the limit $D_z \rightarrow -\infty$, the Hamiltonian effectively reduces to $\mathcal{H} = \mathcal{H}_{\text{Ising}} = J \sum_i S_i^z S_{i+1}^z$.

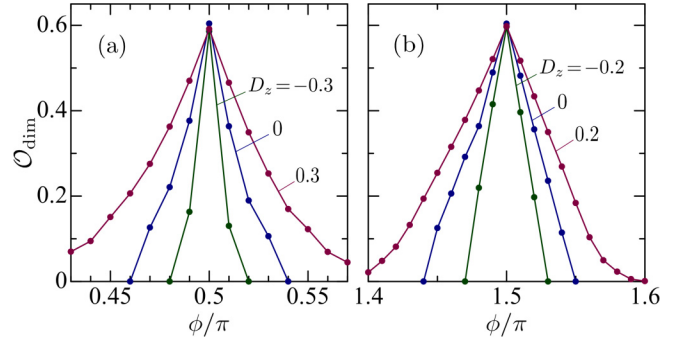


FIG. 9. Dimer order parameter as a function of ϕ/π for several values of D_z near (a) the AFM-KSL region ($\phi/\pi \approx 0.5$) and (b) the FM-KSL region ($\phi/\pi \approx 1.5$).

As a result, the entire region with negative J ($0.5 < \phi/\pi < 1.5$) becomes FM ordered along the z direction.

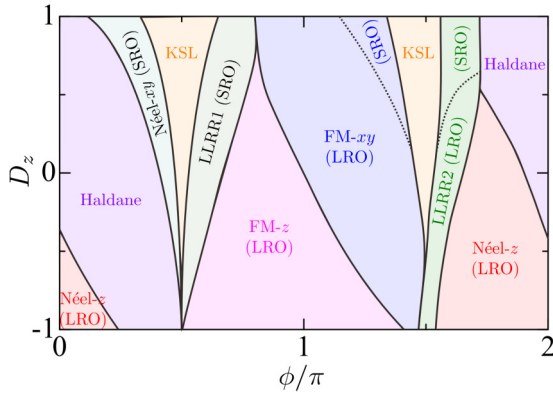
Let us now consider the FM- xy phase. Figure 8(b) shows $\mathcal{O}_{\text{FM}-xy}$ as a function of ϕ/π for $D_z = -0.6, 0$, and 0.6 . The overall extent of the FM- xy region for $D_z = 0.6$ is almost unchanged from that at $D_z = 0$, but the magnitude of $\mathcal{O}_{\text{FM}-xy}$ itself decreases. Although the magnetization in the FM- xy phase does not point along the z axis, its wave function is composed of linear combinations of $|\uparrow\rangle$ and $|\downarrow\rangle$. Therefore, as the weight of the $|0\rangle$ component increases with D_z , the stability of the FM- xy order is reduced. For sufficiently large positive D_z , the system is expected to evolve into a paramagnetic state with short-range FM- xy correlations. For $D_z = -0.6$, the maximum value of $\mathcal{O}_{\text{FM}-xy}$ remains close to unity, but the FM- xy region is significantly reduced. This reduction originates not from the destabilization of the FM- xy order itself, but rather from the expansion of the FM- z phase into the $\phi/\pi > 1$ region. In all cases, the transition between the FM- z and FM- xy phases is of the first order.

5. Kitaev spin-liquid states

Figure 9 shows the dimer order parameter as a function of ϕ/π for several values of D_z near (a) the AFM-KSL region ($\phi/\pi \approx 0.5$) and (b) the FM-KSL region ($\phi/\pi \approx 1.5$). Both KSL regions exhibit qualitatively similar D_z dependence: each expands as D_z is increased from $D_z = 0$ and shrinks as D_z is decreased. This trend is consistent with the previous study [44]. The underlying reason is that the positive D_z suppresses all types of magnetic order, while the negative D_z strongly enhances the Néel- z and FM- z phases. For $D_z > 0$, however, a crossover likely occurs between the KSL and paramagnetic states. Therefore, D_z does not directly affect the intrinsic stability of the KSL itself but rather controls the relative stability of the surrounding magnetically ordered phases. This interpretation is further supported by the observation that the magnitude of $\mathcal{O}_{\text{dim}}$ at $\phi/\pi = 0.5$ and 1.5 remains nearly unchanged with varying D_z .

To further characterize the KSL regions, we also analyze the entanglement entropy for representative points in both the AFM-KSL and FM-KSL regimes. For periodic chains, we estimated an effective central charge using [57,58]

$$c = \frac{3[S_L(\frac{L}{2}) - S_L(\frac{L}{4})]}{\ln[\cos(\frac{8\pi}{L})]}. \quad (21)$$

FIG. 10. Ground-state phase diagram in the ϕ - D_z plane.

In both the AFM-KSL and FM-KSL regimes, the entanglement entropy does not exhibit the logarithmic growth characteristic of a critical 1D system, and the extracted effective central charge is ($c \simeq 0$) within our numerical accuracy. This result indicates that these Kitaev-dominated regimes are not gapless conformal phases with finite central charge, but are instead consistent with short-range-correlated non-magnetic states. Therefore, the term “KSL-like” used here should be understood as referring to Kitaev-dominated disordered regimes without conventional magnetic long-range order, rather than to gapless spin liquids.

We also examine the entanglement spectrum at representative points in the Kitaev-dominated regimes, including the pure Kitaev point. In the present finite-size OBC and PBC calculations, we do not observe a robust entanglement-spectrum degeneracy in these regimes. However, this absence should not be interpreted as evidence against possible topological structure in the thermodynamic limit. As discussed above for the Haldane phase, the same finite-size OBC setup does not yield a clean entanglement-spectrum degeneracy even in a regime where such a degeneracy is expected in the thermodynamic or infinite-MPS limit. Thus, the entanglement spectrum is used here only as a finite-size observation, not as a primary diagnostic of the Kitaev-dominated regimes. Our characterization of these regimes relies instead on the absence of magnetic long-range order, short-range spin correlations, Kitaev-bond/dimer correlations, and the entanglement-entropy analysis yielding an effective central charge $c \simeq 0$.

V. DISCUSSION

All the above discussions/explanations regarding various phases have been summarized to map out the ground-state phase diagram in the $\phi/\pi - D_z$ plane, as shown in Fig. 10. In general, as D_z increases to positive values, the KSL regions expand while the magnetic orders are suppressed. In contrast, when D_z becomes more negative, the FM-z and Néel-z regions are enlarged significantly.

Several phase boundaries come close to one another near $(\phi/\pi, D_z) \simeq (0.5, -1)$. This should not be regarded as an exactly solvable or symmetry-enforced point. At $\phi/\pi = 0.5$, the model is the pure antiferromagnetic Kitaev chain, while

negative D_z favors the $|S^z| = 1$ states and enhances Ising-like magnetic tendencies. The apparent meeting of the neighboring phases is therefore a numerically determined feature caused by the rapid suppression of the Kitaev-dominated disordered region.

Let us now compare our results with those of the spin-1/2 KH chain [39–41]. Since the D_z term has no physical meaning for spin-1/2, we focus on the case of $D_z = 0$. Although there are quantitative differences in the transition points, the Néel-xy, LLRR1, FM-z, FM-xy, LLRR2, and Néel-z phases exhibit essentially the same characteristics in both spin-1 and spin-1/2 systems. The major qualitative difference emerges around the Heisenberg limit ($K = 0$), where the TLL phase in the spin-1/2 system is replaced by the Haldane phase in the spin-1 case. Moreover, we have clarified that the AFM-KSL and FM-KSL phases in the spin-1 KH chain occupy finite parameter regions, whereas in the spin-1/2 case it remains unclear whether the KSL exists only at the two isolated points $\phi/\pi = 0.5$ and 1.5 or extends over finite ranges.

It is instructive to compare our phase diagram with that reported in Ref. [44], which investigated the effect of D_z in the spin-1 KH chain in the vicinity of the AFM-KSL regime (i.e., within a restricted range of J and $K > 0$). While the overall connectivity of the robust magnetically ordered phases is consistent, the main differences appear in the magnetically disordered/critical regimes, where phase identification is more sensitive to the diagnostics and to thermodynamic-limit extrapolations. In our phase diagram, the most notable discrepancies are: (i) between the Haldane and AFM-KSL regimes, we find a sizable intervening Néel-xy region; (ii) near the Heisenberg limit ($\phi \simeq 0$), the Haldane phase terminates already at relatively small negative D_z and gives way to the Néel-z phase; (iii) the LLRR1 regime does not develop true LRO, but remains magnetically SRO or critical; and (iv) the phase labeled “Dimer” in Ref. [44] is not treated as a separate phase in our classification. Rather, the corresponding region is included in the Kitaev-dominated disordered sector, where the system has short-range Kitaev-bond/dimer correlations but no conventional magnetic long-range order. Thus, part of the difference from Ref. [44] reflects not only shifted phase boundaries but also a difference in the diagnostic criteria and terminology used to classify the nonmagnetic Kitaev-dominated region. Regarding point (ii), we find that at $\phi = 0$ the transition to the Néel-z phase occurs at $D_z \simeq -0.5$, which is in good agreement with the estimate reported in Ref. [56]. A direct graphical comparison over the full ϕ - D_z plane, including a representation in the parametrization of Ref. [44], is provided in Appendix C (Figs. 13 and 14).

It would also be interesting to compare our results with those for the 2D spin-1 KH model on the honeycomb lattice [26,34], where the effect of D_z has also been examined. In the 2D case, a large negative D_z enhances Ising anisotropy and consequently stabilizes states corresponding to the Néel-z and FM-z phases, similar to the 1D case. However, for large positive D_z , the KSL region becomes narrower rather than broader. One of the primary reasons for this contrast is that in the honeycomb lattice, positive D_z promotes the formation of magnetic vortex states with enlarged magnetic unit cells, which tend to invade and destabilize the KSL region.

VI. SUMMARY

Using the DMRG method, we have determined the ground-state phase diagram of the spin-1 KH chain with uniaxial SIA D_z , by combining energy-curvature diagnostics on periodic clusters with order-parameter and correlation analyses on larger open-chain systems.

The resulting ϕ - D_z phase diagram hosts magnetically ordered FM- z , FM- xy , LLRR2, and Néel- z phases; magnetically disordered/critical Néel- xy and LLRR1 regimes; two Kitaev spin-liquid-like regions, denoted as AFM-KSL and FM-KSL; and a topological Haldane phase near the Heisenberg limit. Our calculations indicate that the AFM- and FM-KSL regimes acquire finite parameter widths in the spin-1 model. Entanglement-entropy analysis further shows that the effective central charge is ($c \simeq 0$) in both Kitaev-dominated regions, indicating that they are short-range-correlated spin-liquid-like regimes rather than gapless conformal phases. We also clarify that LLRR1 and LLRR2, despite exhibiting similar four-site spin patterns, differ fundamentally in that only LLRR2 develops true LRO.

SIA provides an efficient knob for tuning the competition among frustration, quantum fluctuations, and topology: positive D_z suppresses magnetic order and broadens the KSL-like and other magnetically disordered sectors, whereas negative D_z stabilizes Ising-like Néel- z and FM- z orders. At $D_z = 0$, we identify an exactly solvable point at $\tan \phi = -2(\phi/\pi \simeq 1.6476)$, which enforces a first-order boundary between the Néel- z and LLRR2 phases. We further compare the present phase diagram with those of the spin-1/2 KH chain and the spin-1 honeycomb KH model, thereby highlighting the distinct roles of dimensionality and SIA in Kitaev-type magnets.

Finally, comparison with the spin-1/2 KH chain shows qualitative agreement for most phases but a key replacement of the TLL at $K = 0$ by the Haldane phase in the spin-1 case; it also highlights that finite KSL widths are supported in spin-1, while their extent in spin-1/2 remains unsettled. In contrast, on the spin-1 honeycomb lattice, large positive D_z favors vortex states with enlarged magnetic unit cells that encroach upon and narrow the KSL sector, underscoring the crucial role of dimensionality and anisotropy in Kitaev-type magnets.

ACKNOWLEDGMENTS

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DATA AVAILABILITY

The data that support the findings of this article are openly available [60].

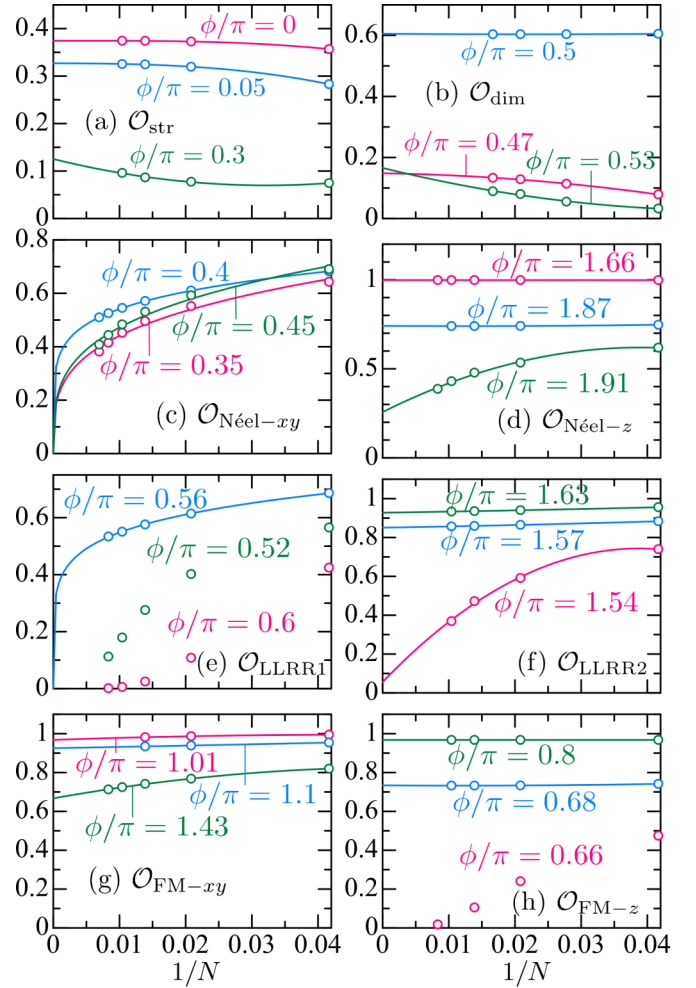


FIG. 11. Finite-size scaling of the various order parameters at representative ϕ/π values of corresponding phases at $D_z = 0$.

APPENDIX A: FINITE-SIZE SCALING FOR THE ORDER PARAMETERS

In this appendix, we present representative examples of the finite-size scaling analyses used to obtain the thermodynamic-limit values of the order parameters. Figure 11 shows the size dependence of the order parameters for typical points in each phase at $D_z = 0$, computed on open chains with lengths ranging from $N = 24$ up to $N = 144$.

To extrapolate $\mathcal{O}(N)$ to the thermodynamic limit, we employ two types of fitting functions depending on the convergence behavior. For the LLRR1 and Néel- xy phases, where the order parameters approach their asymptotic values relatively slowly with increasing N , we use a power-law form,

$$\mathcal{O}(N) = \frac{a}{N^b} + c. \quad (\text{A1})$$

For the other phases, the finite-size corrections are well described by a second-order polynomial in $1/N$,

$$\mathcal{O}(N) = \frac{a}{N^2} + \frac{b}{N} + c. \quad (\text{A2})$$

In all cases, the extrapolated value c is taken as the order parameter in the thermodynamic limit.

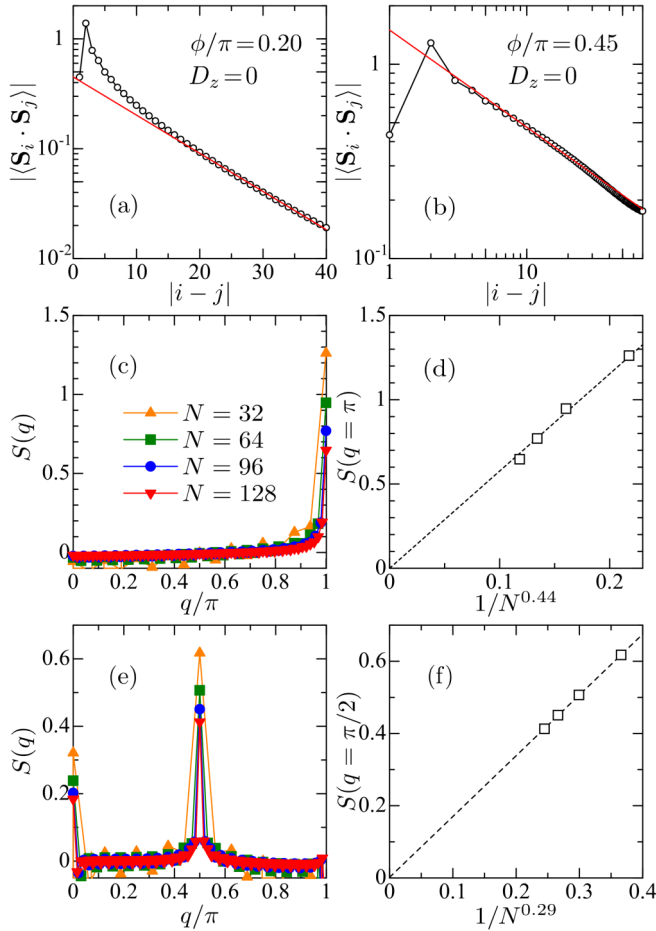


FIG. 12. Spin-spin correlation function $|\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle|$ as a function of the distance $r = |i - j|$ for representative parameters in the (a) Haldane and (b) Néel-xy regimes. The solid lines show fits to the long-distance behavior using an exponential decay in (a) and a power-law decay in (b). (c) Spin structure factor $S(q)$ in the Néel-xy regime at $\phi/\pi = 0.45$ and $D_z = 0$ for $N = 32, 64, 96$, and 128 . The dominant peak appears at $q = \pi$. (d) Finite-size scaling of the peak intensity $S(\pi)$ as a function of $1/N^{0.44}$. Since $S(q)$ is normalized by the system size in its definition, the extrapolation of $S(\pi)$ to zero indicates the absence of dipolar long-range order. (e) Spin structure factor $S(q)$ in the LLRR1 regime at $\phi/\pi = 0.56$ and $D_z = 0$ for $N = 32, 64, 96$, and 128 . The dominant peak appears at $q = \pi/2$. (f) Finite-size scaling of the peak intensity $S(\pi/2)$ as a function of $1/N^{0.29}$. The extrapolated value vanishes in the thermodynamic limit.

APPENDIX B: SPIN CORRELATIONS AND STRUCTURE FACTORS IN THE HALDANE, NÉEL-xy, AND LLRR1 REGIMES

As discussed in the main text, the Haldane phase is a gapped valence-bond-solid state. Consequently, the spin-spin correlation function decays exponentially with distance. By contrast, the adjacent Néel-xy regime is characterized by gapless TLL-like behavior, for which spin correlations exhibit a power-law decay. Figures 12(a) and 12(b) display $|\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle|$ as a function of the distance $r = |i - j|$ for representative points in these two regimes. As expected, we clearly observe an exponential decay in the Haldane phase and a power-law decay in the Néel-xy regime.

In the Néel-xy regime, the long-distance tail is well fitted by $|\langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle| \propto r^{-0.44}$. This slow decay is consistent with the slow convergence with system size observed for the pinning-field-induced order parameter $\mathcal{O}_{\text{Néel-xy}}$ in the finite-size scaling analyses.

We do not attempt a quantitative extraction of the correlation length ξ very close to the Haldane–Néel-xy boundary. Although the spin correlations in the Haldane phase are exponential away from the transition, the continuous nature of the transition leads to a strong enhancement of long-distance correlations near the boundary. In finite open chains, these correlations are further affected by boundary-induced Friedel oscillations even without pinning fields. Consequently, a simple exponential fit of the real-space correlations near the transition does not yield a sufficiently stable estimate of ξ . We therefore use the qualitative change from exponential decay in the Haldane phase to algebraic decay in the Néel-xy regime, together with the finite-size scaling of the string order parameter, to locate the boundary.

To further characterize the dominant correlations in the Néel-xy and LLRR1 regimes, we compute a central-correlation estimate of the spin structure factor normalized by the system size,

$$S(q) = \frac{1}{N} \sum_{r=0}^{N/2} \cos(qr) C(r), \quad (\text{B1})$$

where

$$C(r) = \langle \mathbf{S}_{i_r} \cdot \mathbf{S}_{j_r} \rangle, \quad j_r - i_r = r. \quad (\text{B2})$$

For each distance r , the pair of sites (i_r, j_r) is chosen such that its midpoint is located closest to the center of the open chain. This choice minimizes boundary effects in the real-space correlations. Since $S(q)$ is normalized by the system size in its definition, a finite extrapolated value of $S(q_{\text{peak}})$ would indicate dipolar long-range order, whereas $S(q_{\text{peak}}) \rightarrow 0$ indicates the absence of such order.

Figures 12(c) and 12(e) show $S(q)$ for representative points in the Néel-xy and LLRR1 regimes, respectively. In the Néel-xy regime at $\phi/\pi = 0.45$ and $D_z = 0$, $S(q)$ has a dominant peak at $q = \pi$. In the LLRR1 regime at $\phi/\pi = 0.56$ and $D_z = 0$, the dominant peak appears at $q = \pi/2$, reflecting the four-site modulation.

To examine whether these peaks correspond to true dipolar long-range order, we plot the peak intensities as a function of system size in Figs. 12(d) and 12(f). The Néel-xy peak intensity $S(\pi)$ decreases approximately linearly as a function of $1/N^{0.44}$, while the LLRR1 peak intensity $S(\pi/2)$ decreases approximately linearly as a function of $1/N^{0.29}$. In both cases, the peak intensity extrapolates to zero in the thermodynamic limit. Therefore, these regimes have dominant quasi-long-range correlations at the corresponding wave vectors, but do not exhibit true dipolar long-range order.

The exponents used in the finite-size scaling of the normalized peak intensities have a simple interpretation. If the dominant real-space spin correlation behaves as $C(r) \sim \cos(q_{\text{peak}} r) r^{-\eta}$, then $\sum_r \cos(q_{\text{peak}} r) C(r) \sim N^{1-\eta}$ for $\eta < 1$. Since the structure factor defined in Eq. (B1) is normalized by $1/N$, the peak intensity scales as $S(q_{\text{peak}}) \sim N^{-\eta}$. The fits in Figs. 12(d) and 12(f) therefore correspond to effective

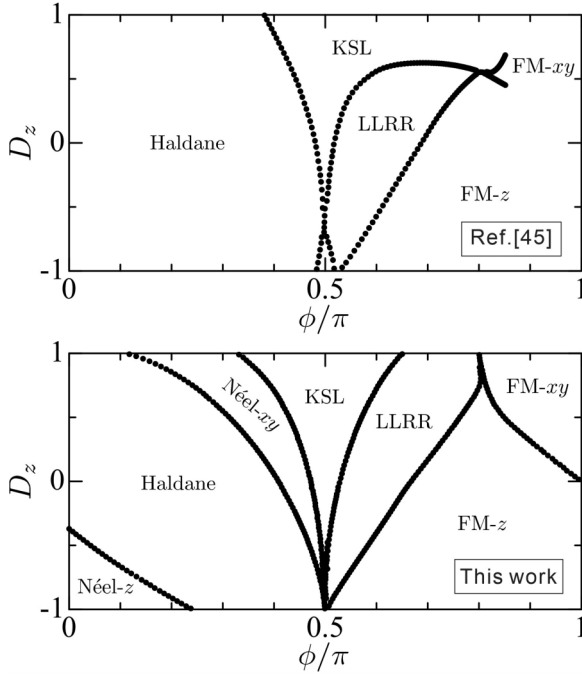


FIG. 13. Comparison between our phase diagram and that of Ref. [44] in our parametrization. The two diagrams are shown side by side in the ϕ/π - D_z plane to facilitate a direct visual comparison of the location and connectivity of the phases.

decay exponents $\eta \simeq 0.44$ for the Néel-xy regime and $\eta \simeq 0.29$ for the LLRR1 regime, respectively. These small exponents indicate very slowly decaying algebraic correlations over the accessible system sizes. At the same time, the normalized peak intensities extrapolate to zero, supporting the absence of true dipolar long-range order in the thermodynamic limit.

APPENDIX C: COMPARISON WITH PREVIOUS PHASE DIAGRAMS

For completeness, we compare our phase diagram with that reported in Ref. [44]. Figure 13 shows a direct side-by-side comparison using our parametrization in the ϕ/π - D_z plane, while Fig. 14 presents the same comparison after converting to the notation employed in Ref. [44]. Overall, we find good agreement for the main magnetically ordered regions and their overall connectivity. The most notable differences occur in the magnetically disordered/critical regimes, where phase identification is more subtle and sensitive to the diagnostics used. In particular, at $D_z = 0$ and for $J > 0$, Ref. [44] assigns a broad parameter interval to the Haldane phase, whereas our analysis based on the thermodynamic-limit behavior of order parameters and correlation functions resolves sizable portions of this region into the Néel-xy phase and the LLRR1 regime. Relatedly, we explicitly distinguish LLRR1 and LLRR2: although they exhibit similar local spin patterns, we find that LLRR2 develops true LRO, while LLRR1 does not show a finite order parameter in the thermodynamic limit. These refinements lead to a reduced extent of the Haldane region and modified boundaries near the adjacent critical regimes, while leaving the robust ordered phases essentially unchanged.

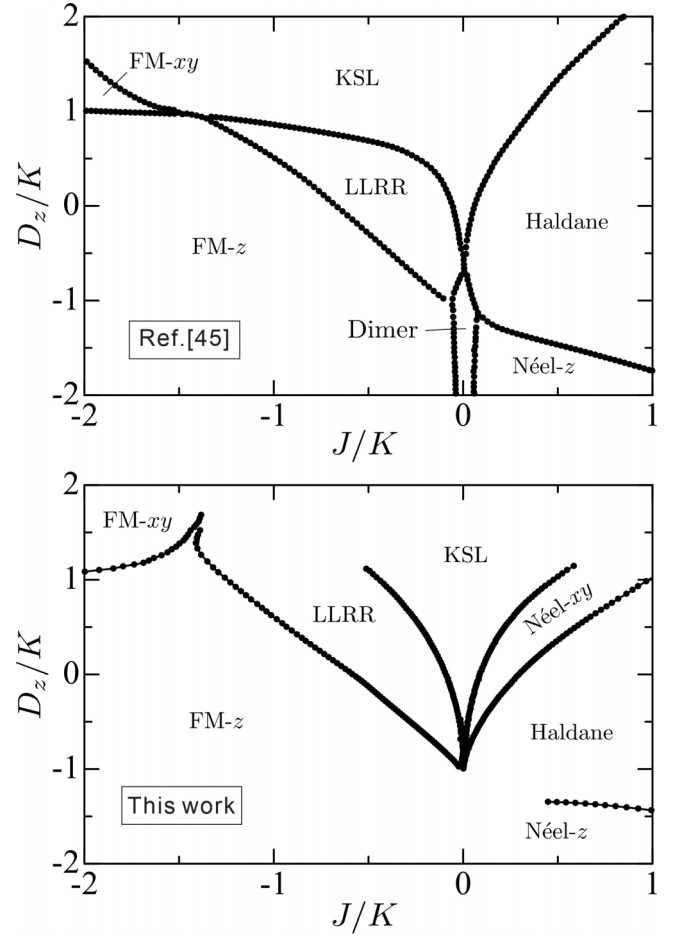


FIG. 14. Same comparison as in Fig. 13, but displayed in the notation used in Ref. [44]. Here, we convert our parameters to the corresponding ratios employed in Ref. [44] (e.g., J/K and D_z/K), enabling a one-to-one comparison with their phase boundaries.

APPENDIX D: QUADRUPOLEAR CORRELATIONS

In spin-1 systems, magnetically disordered phases may still exhibit quadrupolar, or spin-nematic correlations. To examine this possibility, we calculate connected quadrupolar correlation functions in representative magnetically disordered regimes, with particular attention to the LLRR1 region.

We define the five local quadrupolar operators as

$$Q_i^{x^2-y^2} = (S_i^x)^2 - (S_i^y)^2, \quad (D1)$$

$$Q_i^{3z^2-r^2} = \frac{1}{\sqrt{3}}[2(S_i^z)^2 - (S_i^x)^2 - (S_i^y)^2], \quad (D2)$$

$$Q_i^{xy} = S_i^x S_i^y + S_i^y S_i^x, \quad (D3)$$

$$Q_i^{yz} = S_i^y S_i^z + S_i^z S_i^y, \quad (D4)$$

$$Q_i^{zx} = S_i^z S_i^x + S_i^x S_i^z. \quad (D5)$$

The connected quadrupolar correlation function is then defined as

$$C_Q^a(r) = \langle Q_i^a Q_j^a \rangle - \langle Q_i^a \rangle \langle Q_j^a \rangle, \quad r = |i - j|, \quad (D6)$$

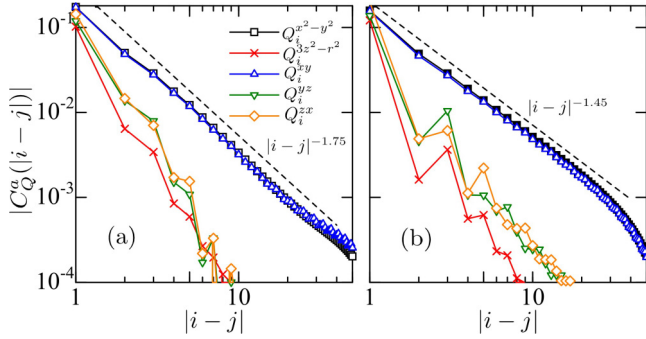


FIG. 15. Distance dependence of the connected quadrupolar correlation functions at $\phi/\pi = 0.6$. The five quadrupolar components $Q^{x^2-y^2}$, $Q^{3z^2-r^2}$, Q^{xy} , Q^{yz} , and Q^{zx} are defined in Appendix D. All components decay algebraically. The slowest decay is found in the $Q^{x^2-y^2}$ and Q^{xy} channels. At $D_z = 0$, the dominant correlations decay approximately as $r^{-1.75}$, while at $D_z = 0.3$ the decay becomes slightly slower, approximately as $r^{-1.45}$. This indicates that positive D_z enhances quadrupolar correlations, but does not produce quadrupolar long-range order.

where

$$a \in \{x^2 - y^2, 3z^2 - r^2, xy, yz, zx\}. \quad (D7)$$

The subtraction of the disconnected part is important because the single-ion anisotropy can explicitly induce a local quadrupolar polarization, which should be distinguished from spontaneous quadrupolar long-range order. For open chains, the pair of sites (i, j) is chosen so that the midpoint of the two sites is located as close as possible to the center of the system.

Figure 15 shows the distance dependence of the connected quadrupolar correlations at $\phi/\pi = 0.6$. All components decay algebraically and do not approach a finite constant at long distances. Among them, the $Q^{x^2-y^2}$ and Q^{xy} components show the slowest decay and have comparable amplitudes. At $D_z = 0$, the dominant quadrupolar correlations decay approximately as $r^{-1.75}$. For positive SIA, e.g., at $D_z = 0.3$, the decay becomes slightly slower, approximately as $r^{-1.45}$. Thus, positive D_z enhances quadrupolar correlations, as expected for a spin-1 system. Nevertheless, since the quadrupolar correlations still decay to zero at long distances, we find no evidence for quadrupolar long-range order in this region.

TABLE I. Convergence of the DMRG calculations with respect to the kept bond dimension m . We show representative results for the $N = 128$ open chain and the $N = 24$ periodic chain at $\phi/\pi = 0.6$ and $D_z = 0$. Here, w_{disc} denotes the discarded weight in the final sweep, and E_0/N is the ground-state energy per site.

Boundary condition	m	w_{disc}	E_0/N
OBC, $N = 128$	2000	2.584×10^{-7}	-0.58684647240
OBC, $N = 128$	3000	3.835×10^{-8}	-0.58684700091
OBC, $N = 128$	4000	8.073×10^{-9}	-0.58684706912
PBC, $N = 24$	2000	7.381×10^{-8}	-0.59051825032
PBC, $N = 24$	3000	7.034×10^{-9}	-0.59051830038
PBC, $N = 24$	4000	1.133×10^{-9}	-0.59051830460

TABLE II. Check of the spatial uniformity of the converged $N = 24$ PBC wave function at $\phi/\pi = 0.6$ and $D_z = 0$. We list the minimum and maximum values of $C_r(i) = \langle \mathbf{S}_i \cdot \mathbf{S}_{i+r} \rangle$ around the ring, together with $\Delta C_r = C_r^{\text{max}} - C_r^{\text{min}}$. For $N = 24$, distances up to $r = 12$ are independent.

r	C_r^{min}	C_r^{max}	ΔC_r
1	0.2042692644	0.2042695219	2.57×10^{-7}
2	-0.8190324895	-0.8190322752	2.14×10^{-7}
3	0.0312300047	0.0312304450	4.40×10^{-7}
4	0.6825206950	0.6825248936	4.20×10^{-6}
5	-0.0017387438	-0.0017335765	5.17×10^{-6}
6	-0.6163161388	-0.6163136110	2.53×10^{-6}
7	0.0064157845	0.0064189301	3.15×10^{-6}
8	0.5755349436	0.5755442389	9.29×10^{-6}
9	-0.0005571518	-0.0005504494	6.70×10^{-6}
10	-0.5593058128	-0.5592943417	1.15×10^{-5}
11	0.0020505887	0.0020551699	4.58×10^{-6}
12	0.5508570569	0.5508702837	1.32×10^{-5}

APPENDIX E: CONVERGENCE CHECKS AND DEPENDENCE ON THE PINNING FIELD

To quantify the convergence of the DMRG calculations, we examine the dependence of the ground-state energy and

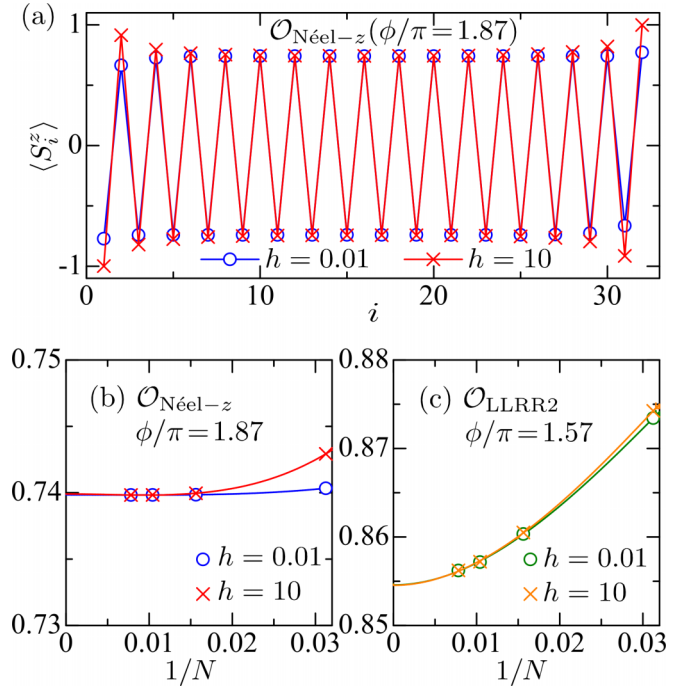


FIG. 16. Representative checks of the dependence on the boundary pinning field. (a) Spatial profile of the local moment $\langle S_i^z \rangle$ for an $N = 32$ open chain at $\phi/\pi = 1.87$ for two pinning-field strengths, $h = 0.01$ and $h = 10$. Although the edge moments depend somewhat on h , the values in the central region are nearly identical. (b) Finite-size extrapolation of the Néel- z order parameter $O_{\text{Néel-}z}$ at $\phi/\pi = 1.87$ for $h = 0.01$ and $h = 10$. (c) Finite-size extrapolation of the LLRR2 order parameter O_{LLRR2} at $\phi/\pi = 1.57$ for $h = 0.01$ and $h = 10$. In (b) and (c), the solid lines are fits to $O(N) = O_\infty + a/N^2 + b/N^3$.

discarded weight on the kept bond dimension m . As a representative and conservative test, we choose the parameter point $\phi/\pi = 0.6$ and $D_z = 0$, where the numerical convergence is relatively demanding among the parameter sets studied in this work.

Table I shows the results for both the $N = 128$ open chain and the $N = 24$ periodic chain at $m = 2000, 3000$, and 4000 . Here, w_{disc} denotes the discarded weight in the final sweep, and E_0/N is the ground-state energy per site. The weak dependence of E_0/N on m , together with the small discarded weight, confirms that the bond dimensions used in the main calculations are sufficient for identifying the phase boundaries and evaluating the order parameters.

We also checked the spatial uniformity of the converged $N = 24$ PBC wave function at the same parameter point. The local moments are negligibly small: $|\langle S_i^z \rangle| < 2 \times 10^{-10}$ for all sites, while $|\langle S_i^x \rangle|$ and $|\langle S_i^y \rangle|$ are below the numerical precision (of order 10^{-16}). In addition, Table II shows the minimum and maximum values of the spin-spin correlation function $C_r(i) = \langle \mathbf{S}_i \cdot \mathbf{S}_{i+r} \rangle$ around the ring for distances $r = 1, \dots, 12$. The variation $\Delta C_r = \max_i C_r(i) - \min_i C_r(i)$ is very small for all distances, confirming that the converged PBC wave function respects the expected spatial periodicity to high numerical accuracy.

We next examine the dependence of the OBC results on the strength of the boundary pinning field. This check is important because the pinning field is introduced only to select a representative symmetry-broken configuration and should not affect the extrapolated bulk order parameters. Representative results are shown in Fig. 16.

Figure 16(a) compares the spatial profile of the local moment $\langle S_i^z \rangle$ for an $N = 32$ open chain for two strongly different pinning-field strengths, $h = 0.01$ and $h = 10$. While the local moments near the edges are somewhat affected by the pinning field, the values in the central region are almost identical. This confirms that the pinning field mainly serves to select one of the symmetry-broken configurations and does not significantly affect the bulk order parameter.

To further confirm this point, we compare the finite-size extrapolations of representative order parameters for two ordered phases using the fitting form $O(N) = O_\infty + \frac{a}{N^2} + \frac{b}{N^3}$. Figure 16(b) shows the extrapolation of $O_{\text{Néel-z}}$ at $\phi/\pi = 1.87$, yielding $O_{\text{Néel-z}}^\infty = 0.739841632$ for $h = 0.01$ and 0.739905865 for $h = 10$. Figure 16(c) shows the extrapolation of O_{LLRR2} at $\phi/\pi = 1.57$. The extrapolated values are $O_{\text{LLRR2}}^\infty = 0.854576687$ for $h = 0.01$ and 0.854537234 for $h = 10$. The excellent agreement between the two pinning-field strengths demonstrates that the thermodynamic bulk order parameters are essentially independent of the choice of h .

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