



Ground-state phase diagram of a spin- $\frac{1}{2}$ frustrated ferromagnetic XXZ chain: Haldane dimer phase and gapped/gapless chiral phases

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The ground-state phase diagram of a spin- $\frac{1}{2}$ XXZ chain with competing ferromagnetic nearest-neighbor ($J_1 < 0$) and antiferromagnetic second-neighbor ($J_2 > 0$) exchange couplings is studied by means of the infinite time evolving block decimation algorithm and effective field theories. For the SU(2)-symmetric (Heisenberg) case, we show that the nonmagnetic phase in the range $-4 < J_1/J_2 < 0$ has a small but finite ferromagnetic dimer order. We argue that this spontaneous dimer order is associated with effective spin-1 degrees of freedom on dimerized bonds, which collectively form a valence bond solid state as in the spin-1 antiferromagnetic Heisenberg chain (the Haldane spin chain). We thus call this phase the Haldane dimer phase. With easy-plane anisotropy, the model exhibits a variety of phases including the vector chiral phase with gapless excitations and the even-parity dimer and Néel phases with gapped excitations, in addition to the Haldane dimer phase. Furthermore, we show the existence of gapped phases with coexisting orders in narrow regions that intervene between the gapless chiral phase and any one of Haldane dimer, even-parity dimer, and Néel phases. Possible implications for quasi-one-dimensional edge-sharing cuprates are discussed.

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I. INTRODUCTION

The search for novel quantum states in frustrated magnets has been a subject of intensive theoretical and experimental research. One-dimensional (1D) systems offer unique laboratories for this search, as strong fluctuations enhance the tendency toward unconventional quantum states.¹ Among them, the 1D XXZ model with competing nearest-neighbor J_1 and second-neighbor J_2 interactions, defined by the Hamiltonian

$$H = \sum_{n=1}^2 \sum_{\ell} J_n (S_{\ell}^x S_{\ell+n}^x + S_{\ell}^y S_{\ell+n}^y + \Delta S_{\ell}^z S_{\ell+n}^z), \quad (1)$$

provides a paradigmatic example expected to host rich variety of physics. Here, $\mathbf{S}_{\ell} = (S_{\ell}^x, S_{\ell}^y, S_{\ell}^z)$ represents the spin-1/2 operator at the site $\ell \in \mathbb{Z}$ and Δ parametrizes the XXZ exchange anisotropy. The model has frustration as far as J_2 is antiferromagnetic, irrespective of the sign of J_1 .

Early theoretical studies on the model (1) mostly considered the case when both J_1 and J_2 are antiferromagnetic.²⁻⁷ However, interest is now growing in the case of ferromagnetic $J_1 < 0$ and antiferromagnetic $J_2 > 0$ because of its relevance to quasi-1D edge-sharing cuprates. Among such cuprates, LiCu₂O₂ (Refs. 8 and 9), LiCuVO₄ (Refs. 10 and 11), and PbCuSO₄(OH)₂ (Ref. 12), for example, exhibit multiferroic behaviors,^{13,14} i.e., spiral magnetic orders and concomitant ferroelectric polarization at low temperatures. The negative sign of J_1 indeed plays a key role in stabilizing the vector chiral order responsible for these phenomena.¹⁵ By contrast, Rb₂Cu₂Mo₃O₁₂ (Ref. 16) shows no sign of magnetic order down to very low temperatures and may be considered as a candidate system for a spin liquid or a valence bond solid.

In this paper, we study the ground-state properties of the spin-1/2 frustrated ferromagnetic XXZ chain (1) with $J_1 < 0$

and $J_2 > 0$, by means of the infinite time evolving block decimation algorithm (iTEBD)¹⁷ and effective field theories based on the bosonization methods. Previous works on the case with easy-plane anisotropy $0 \leq \Delta \leq 1$ have discussed the competition among the vector chiral phase with gapless excitations and the dimer and Néel phases with gapped excitations.^{6,15,18-25} The main goal of this paper is to present a conclusive phase diagram of the model (1), which is shown in Fig. 1, through detailed analyses that extends our previous works.^{15,24,25} Firstly, we uncover the nature of the nonmagnetic phase around the SU(2)-symmetric case $\Delta = 1$, which has long been controversial. We show that this phase has a dimer order associated with an emergent spin-1 degree of freedom on every other bond. We term this new phase the Haldane dimer phase. Secondly, we show the existence of narrow gapped phases that intervene between the gapless chiral phase and any one of gapped dimer and Néel phases. As weak interchain couplings are turned on, while the gapless chiral phase evolves into a spiral magnetic order, the Haldane dimer phase can be stabilized by a coupling with phonons due to the spin-Peierls mechanism. Our phase diagram may thus provide a useful starting point for understanding the competing phases in quasi-1D cuprates.

Let us briefly review previous results on the model (1) and summarize our new findings. While we are mainly concerned with the case of $J_1 < 0$ and $J_2 > 0$ in this paper, for comparison, we also review established results on the case of antiferromagnetic $J_1, J_2 > 0$ alongside.

In the classical limit $S \rightarrow \infty$, the ground-state phase diagram of Eq. (1) does not depend on Δ in the range $0 \leq \Delta \leq 1$. The ground state has ferromagnetic order for $J_1/J_2 < -4$ and antiferromagnetic (Néel) order for $J_1/J_2 > 4$. For $0 < |J_1|/J_2 < 4$, the ground state is in a spiral magnetic ordered phase in which the spins rotate by an incommensurate pitch angle $Q = \pm \arccos(-J_1/4J_2)$ along the spin chain.

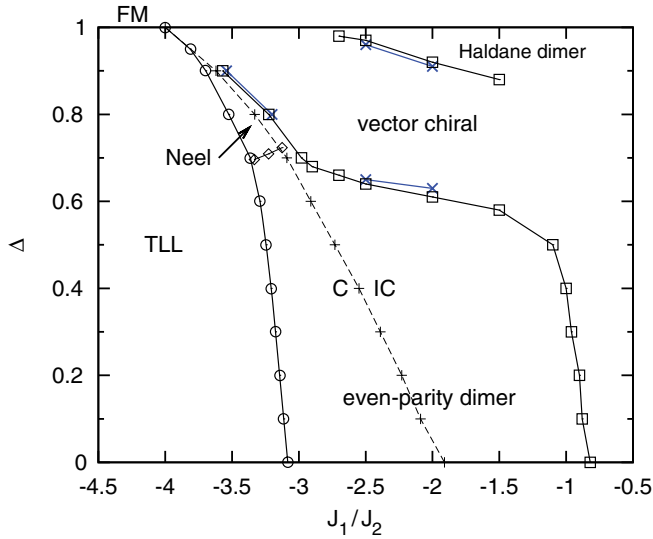


FIG. 1. (Color online) The ground-state phase diagram of the model (1) with $J_1 < 0$ and $J_2 > 0$. The vector chiral phase, which has a nonvanishing vector chirality (2), extends between the two boundaries with the “□” symbols. These boundaries are determined as in Figs. 2 and 3 (see the vertical solid lines in these figures). Around the highly degenerate point $(J_1/J_2, \Delta) = (-4, 1)$, these two boundaries could not be determined accurately, but we expect both of them to continue to this point. It was also difficult to draw the boundary around the right top corner of the phase diagram. The onsets of (Haldane and even-parity) dimer and Néel orders occur inside the vector chiral phase, as indicated by the “×” symbols (determined as in Figs. 14 and 15). Thus there are narrow intermediate phases (between the “□” and “×” symbols) where two kinds of orders coexist. The phase boundaries among the TLL, even-parity dimer, and Néel phases are determined in a previous work.²⁴ On the right of the “○” symbols, the even-parity dimer and Néel phases alternately appear when approaching the point $(J_1/J_2, \Delta) = (-4, 1)$: the first transition occurs at $\Delta \approx 0.7$ (“◇” symbols) and the second at $\Delta \approx 0.93$ (not shown).²⁴ On the line where $\Delta = 1$ and $J_1/J_2 < -4$, the ground state is ferromagnetic (FM). The “+” symbols inside the dimer and Néel phases indicate the Lifshitz line on which the short-range spin correlation changes its character from incommensurate (IC) to commensurate (C); see Fig. 16.

Except for the isotropic case $\Delta = 1$, the spiral plane is fixed in the xy plane, and the vector chirality

$$\kappa_{\ell, \ell+1}^z := \langle (\mathbf{S}_\ell \times \mathbf{S}_{\ell+1})^z \rangle \quad (2)$$

has a nonvanishing uniform value $\kappa_{\ell, \ell+1}^z = \pm \sin Q$ independent of ℓ . Here, $\langle \dots \rangle$ stands for average in the ground state (with long-range order, if any).

In the ground state of the quantum spin-1/2 model, a long-range magnetic order with broken $U(1)$ spin rotational symmetry is generally prohibited, unless the uniform magnetic susceptibility is divergent as in the case of ferromagnetism.²⁶ However, a long-range order (LRO) of the vector chirality $\kappa_{\ell, \ell+1}^z$ that breaks only the \mathbb{Z}_2 parity symmetry can survive quantum fluctuations in the case of $\Delta \neq 1$. Using the bosonization theory for $|J_1|/J_2 \ll 1$ and $0 \leq \Delta < 1$, Nersisyan *et al.*⁶ predicted the appearance of the vector chiral phase with gapless excitations (as reviewed in Sec. IV A2). This gapless

chiral phase shows the spatially uniform vector chirality $\kappa_{\ell, \ell+1}^z \neq 0$ and power-law decaying (incommensurate) spiral spin correlations; this phase may therefore be viewed as a quantum counterpart of the classical spiral phase. The gapless chiral phase competes with other quantum phases, in particular, valence bond solids driven by quantum fluctuations. In fact, for antiferromagnetic $J_1 > 0$, a dimerized phase, in which the singlet state $(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$ (written in the $\{S_\ell^z\}$ basis) is formed on dimerized bonds, appears in a large part of the classical spiral regime $0 < J_1/J_2 < 4$,²⁻⁵ and the gapless chiral phase appears only in a small region in the space spanned by J_1/J_2 and Δ .⁷

The phase diagram for the case of ferromagnetic $J_1 < 0$ and easy-plane anisotropy $0 \leq \Delta \leq 1$ is presented in Fig. 1. Early works^{18,19} mainly discussed the transition from the Tomonaga-Luttinger liquid (TLL) phase to a dimer phase with an even-parity unit²⁰ $|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle$ appearing for $0 < \Delta \lesssim 0.7$. Our recent works^{15,24} have uncovered a rich phase structure in an extended parameter space of J_1/J_2 and Δ . In Ref. 15, it was shown that the gapless chiral phase appears in a wide region, and survives up to the close vicinity of the isotropic case $\Delta = 1$ for $-4 < J_1/J_2 \lesssim -2.5$ (we also refer to Refs. 22 and 23 for related earlier works). This remarkable stability of the gapless chiral phase for $J_1 < 0$ indicates that the sign of J_1 plays a crucial role in stabilizing the vector chirality and the associated ferroelectric polarization in multiferroic cuprates.⁸⁻¹² In Ref. 24, the instability of the TLL phase toward gapped phases was analyzed using the effective sine-Gordon theory combined with numerical diagonalization. It was found that the even-parity dimer phase²⁷ discussed in Refs. 18–20 and a Néel ordered phase appear alternately as Δ is increased on the right side of the TLL phase in the phase diagram.

An important result of this paper is concerned with the nature of the nonmagnetic phase for $-4 < J_1/J_2 < 0$ around the $SU(2)$ -symmetric case $\Delta = 1$. Previous field-theoretical analyses^{6,21} have suggested that a dimer phase with a very small energy gap should appear in this region (as reviewed in Sec. III A). However, neither a dimer order nor an energy gap has been detected in previous numerical studies. Using the iTEBD, which allow us to treat infinite-size systems directly, we present the first numerical evidence of a finite dimer order parameter

$$D_{\ell, \ell+1, \ell+2} = \langle \mathbf{S}_\ell \cdot \mathbf{S}_{\ell+1} \rangle - \langle \mathbf{S}_{\ell+1} \cdot \mathbf{S}_{\ell+2} \rangle. \quad (3)$$

Remarkably, this dimer order is associated with ferromagnetic correlations $\langle \mathbf{S}_\ell \cdot \mathbf{S}_{\ell+1} \rangle > 0$ of alternating strengths, in contrast to antiferromagnetic correlations in singlet dimers for $J_1 > 0$. In this case, it is natural to interpret that effective spin-1 degrees of freedom emerge on the bonds with stronger ferromagnetic correlation, forming a valence bond solid state²⁸ as in the Haldane chain.²⁹ We thus call this new phase the Haldane dimer phase.

We also present detailed analyses of the anisotropic case $\Delta \neq 1$, extending our previous works.^{15,24} In particular, we analyze the transition from the gapless chiral phase to each of the Haldane dimer, even-parity dimer, and Néel phases, and identify narrow intermediate gapped phases where two kinds of orders coexist (the regions between “□” and “×” symbols in Fig. 1). Furthermore, we describe how the properties of

various phases can be captured in the language of the Abelian bosonization^{30,31} for $|J_1/J_2| \ll 1$, as summarized in Table I.

The rest of the paper is organized as follows. In Sec. II, we present the numerical results on the order parameters and half-chain entanglement entropy, which provide the most basic information for identifying symmetry-broken phases. In Sec. III, we discuss in detail the dimer phases in the SU(2)-symmetric case $\Delta = 1$ from both field-theoretical³⁰⁻³³ and numerical analyses. In Sec. IV, we discuss the case with the easy-plane anisotropy $0 \leq \Delta < 1$. In particular, we review the effective field theory for the gapless chiral phase,⁶ and, following Ref. 34, discuss its instability toward gapped chiral phases. The ranges of the gapped chiral phases are then determined numerically by analyzing the spin correlations. In Sec. V, we briefly describe how the quantum phases in the easy-axis case^{18,35,36} can be understood in the Abelian bosonization framework. In Sec. VI, we conclude the paper and discuss implications of our results for quasi-1D cuprates.

II. NUMERICAL ANALYSIS OF ORDER PARAMETERS

In this section, we present numerical results on several order parameters and half-chain entanglement entropy calculated by iTEBD. The vector chiral order parameter and the entanglement entropy are used to determine the boundaries of the region where the long-range vector chiral order exists (the “□” symbols in Fig. 1). The numerical results in this section also suggest the existence of the narrow intermediate phases (between “□” and “×” symbols) in which the vector chiral order coexists with the dimer or Néel order. The precise ranges of these intermediate phases, however, will be determined in Sec. IV B 2.

Before presenting the numerical results, let us briefly note characteristic features of our numerical method; for a more detailed account of the method, see Supplemental Material of Ref. 15. The iTEBD algorithm¹⁷ we employed is based on the periodic matrix product representation of many-body wave functions of an infinite system. It can directly address physical quantities in the thermodynamic limit, and is free from finite-size or boundary effects. The (variational) wave function is optimized to minimize the energy. The precision of the algorithm is controlled by the Schmidt rank χ , which gives the linear dimension of the matrices. We exploited the conservation of the total magnetization $\sum_\ell S_\ell^z = 0$ to achieve higher efficiency and precision of the calculations. When this algorithm is used in ordered phases, a variational state finally converges to a symmetry-broken state with an associated finite order parameter (if it is allowed by the periodicity of the matrix product state).³⁷ In our implementation, we used a period-4 structure for the variational matrix product state. In this setting, the vector chiral, dimer, and Néel order parameters analyzed in this section can all be calculated through local quantities. In order to allow a finite vector chiral order parameter, the initial state must contain complex elements as a “seed” for the symmetry breaking.³⁸

A. Vector chiral order

Figures 2 and 3 present our numerical results along the vertical line $J_1/J_2 = -2$ and the horizontal line $\Delta = 0.8$,

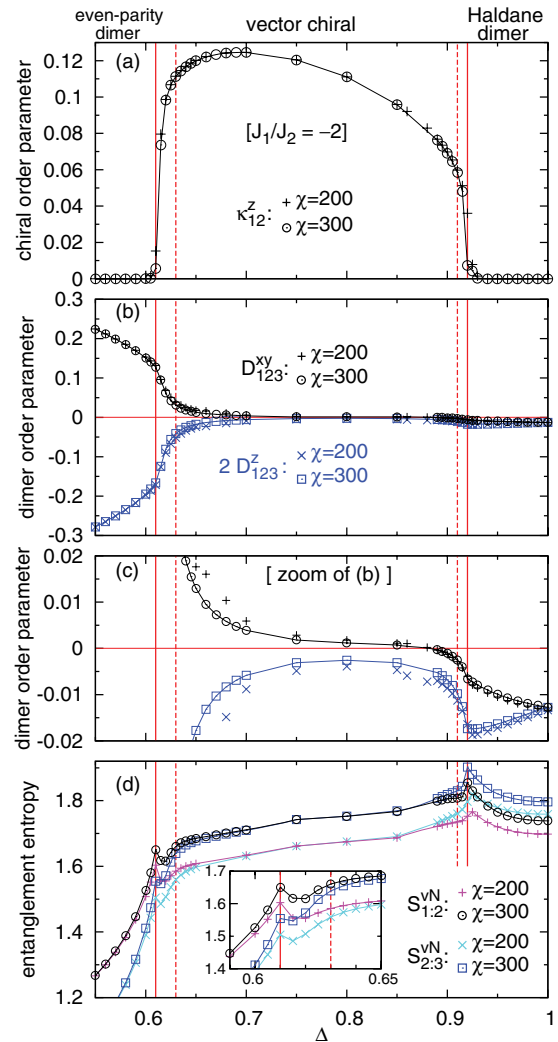


FIG. 2. (Color online) (a) Chiral and (b), (c) dimer order parameters and (d) half-chain entanglement entropy as functions of Δ for fixed $J_1/J_2 = -2$. These are calculated by the iTEBD with Schmidt ranks $\chi = 200$ and 300 . (c) is a zoom of (b). In (d), $S_{1,2}^{\text{vN}}$ and $S_{2,3}^{\text{vN}}$ are defined for the bipartitions of the system at the bonds (1,2) and (2,3), respectively. Solid vertical lines indicate the boundaries of the vector chiral phase, and are determined from the onsets of the vector chiral order parameter in (a) or more accurately from the peaks in the entanglement entropy in (d). Broken vertical lines indicate the transition points on which dimer orders set in. These points are difficult to locate within the analysis of dimer order parameters in (b) and (c) and are instead determined by the analysis of spin correlations in Fig. 14. Narrow intermediate phases exist between solid and broken vertical lines, where the vector chiral and dimer orders coexist. In the intermediate phase in $0.61 \lesssim \Delta \lesssim 0.63$, a dip in the entanglement entropy is seen in (d), as zoomed in the inset.

respectively, in the phase diagram (see Fig. 1). Let us first look at the vector chiral order parameter $\kappa_{12}^z = \langle (\mathbf{S}_1 \times \mathbf{S}_2)^z \rangle$ displayed in Figs. 2(a) and 3(a). This order parameter is always found to be spatially uniform along the spin chain in the present model, so we have fixed the site labels. By observing the rapid increase of κ_{12}^z , we find the onset of the vector chiral phase. It is natural to think that this rapid increase comes from the Ising nature of the transition with exponent $\beta = 1/8$ for

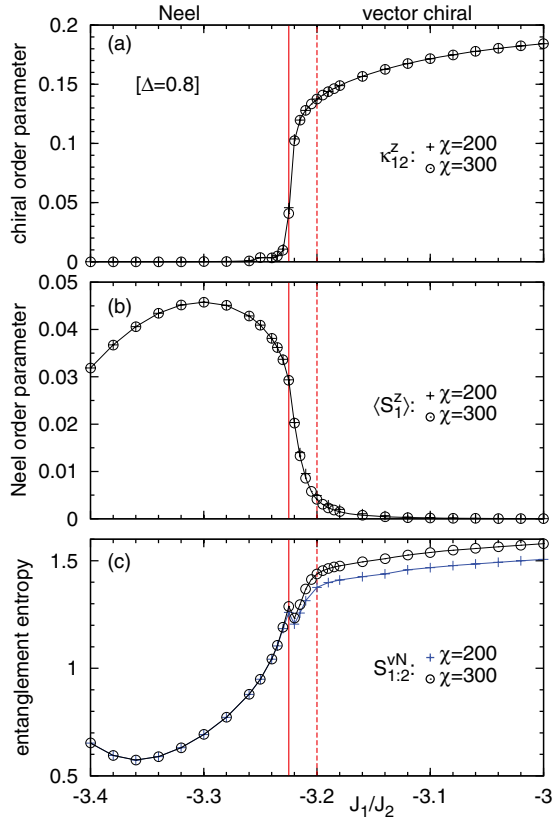


FIG. 3. (Color online) (a) Chiral and (b) Néel order parameters and (c) half-chain entanglement entropy as a function of J_1/J_2 for fixed $\Delta = 0.8$, calculated by the iTEBD. The solid and broken vertical lines indicate the onsets of the vector chiral and Néel orders, respectively. The former is determined by the peak position in the entanglement entropy in (c), while the latter is determined in Fig. 15. In the narrow intermediate phase in $-3.225 \lesssim J_1/J_2 \lesssim -3.200$, the vector chiral and Néel orders coexist.

the spontaneous order parameter, as previously demonstrated in the XY case $\Delta = 0$.³⁸ To determine the transition points more precisely, however, we use the half-chain entanglement entropy explained next.

The half-chain von Neumann (vN) entanglement entropy is defined as¹⁷

$$S^{\text{vN}} = - \sum_{\alpha=1}^{\chi} \lambda_{\alpha}^2 \ln \lambda_{\alpha}^2, \quad (4)$$

where $\{\lambda_{\alpha}\}$ is a set of Schmidt coefficients associated with the decomposition of the infinite system into the left and right halves and χ is the Schmidt rank. As the system approaches a critical point characterized by a conformal field theory with a central charge c , this quantity is known to diverge as^{39,40}

$$S^{\text{vN}} = \frac{c}{6} \ln \xi + s_1, \quad (5)$$

where ξ is the correlation length and s_1 is a nonuniversal constant. In an iTEBD calculation with a finite Schmidt rank χ , the divergence of S^{vN} at the critical point is replaced by the increasing function of χ ,⁴¹

$$S^{\text{vN}} = \frac{1}{\sqrt{12/c + 1}} \ln \chi + s'_1, \quad (6)$$

where s'_1 is another nonuniversal constant. The calculated entanglement entropy is shown in Figs. 2(d) and 3(c). In Fig. 2(d), we plot two entropies $S_{1:2}^{\text{vN}}$ and $S_{2:3}^{\text{vN}}$ associated with the bipartitions of the system at the bonds (1,2) and (2,3), since these bonds are inequivalent in the neighboring dimer phases. By finding peaks of S^{vN} , we can determine the boundaries of the vector chiral phase, more accurately than by using κ_{12}^z ; see the solid vertical lines in Figs. 2 and 3. In this way, we have determined the square symbols in Fig. 1. Although we could not extract c from the current data of S^{vN} using Eq. (6) (which is expected to be satisfied for larger χ), it is natural to expect that these critical points are characterized by the two-dimensional Ising universality class with $c = 1/2$ (we again note that the critical exponent $\beta = 1/8$ for this class was confirmed in the XY case³⁸).

In most part of the vector chiral phase, the entanglement entropy increases as a function of χ , indicating a critical nature. Indeed, in the effective field theory of Nersisyan *et al.*,⁶ the gapless chiral phase has $c = 1$, and the increase of S from the cases of $\chi = 200$ to 300 is roughly consistent with $\Delta S = 0.224 \ln(300/200) = 0.091$ expected from Eq. (6) for $c = 1$. Near the boundaries (solid vertical lines), the entanglement entropy shows dips, whose implications will be discussed later.

B. Dimer orders

Next we look at the xy and z components of dimer order parameters:

$$D_{\ell, \ell+1, \ell+2}^{xy} := \langle (S_{\ell+1}^x S_{\ell+2}^x + S_{\ell}^y S_{\ell+1}^y) - (S_{\ell+1}^x S_{\ell+2}^y + S_{\ell+1}^y S_{\ell+2}^x) \rangle, \quad (7a)$$

$$D_{\ell, \ell+1, \ell+2}^z := \langle S_{\ell}^z S_{\ell+1}^z - S_{\ell+1}^z S_{\ell+2}^z \rangle. \quad (7b)$$

The alternation of the sign of $D_{\ell, \ell+1, \ell+2}^{xy}$ or $D_{\ell, \ell+1, \ell+2}^z$ along the spin chain would indicate some sort of dimer ordering. We assign the site labels in such a way that $D_{123}^z < 0$. The two order parameters are plotted in Figs. 2(b) and 2(c). We find that D_{123}^{xy} and D_{123}^z are both finite and have mutually opposite signs for $\Delta \lesssim 0.65$. By contrast, the two order parameters have small finite values of the same sign for $\Delta \gtrsim 0.9$; in spite of the smallness, they are rather stable when the Schmidt rank χ is increased as seen in the zoomed plot in Fig. 2(c). These results indicate that the dimer phases in the two regions are of distinct types.

The nature of the dimer phase for $\Delta \lesssim 0.6$ can be easily understood as follows.^{20,24} In the XY limit $\Delta = 0$, the sign of J_1 in Eq. (1) can be reversed by performing the π rotations of spins around the z axis on every second sites. From the fact that the doubly degenerate ground states at $(J_1/J_2, \Delta) = (2, 0)$ are given by the products of singlet dimers, one finds, through the above π -rotation transformation, that the exact ground states at $(J_1/J_2, \Delta) = (-2, 0)$ are given by the dimer states whose unit is now replaced by $(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)/\sqrt{2}$. We note that this unit has the even parity with respect to the inversion about a bond center, in contrast to the odd parity of the singlet dimer at $J_1 > 0$. The direct product states of even-parity dimers show $D_{123}^{xy} = -2D_{123}^z = \pm 1/2$. The mutually opposite signs of D_{123}^{xy} and D_{123}^z and the approximate relation $D_{123}^{xy} \approx -2D_{123}^z$ found for $\Delta \lesssim 0.6$ in Fig. 2(b) indicate that the even-parity nature of the dimer unit persists in this region. We thus call this phase

the even-parity dimer phase.²⁷ It is distinct from the singlet dimer phase appearing for $J_1 > 0$, in which D_{123}^{xy} and D_{123}^z show the same sign.

In the region $\Delta \gtrsim 0.9$ in Fig. 2, D_{123}^{xy} and D_{123}^z are both negative as in the singlet dimer phase. However, forming nearest-neighbor singlet dimers is unlikely for ferromagnetic $J_1 < 0$. In Sec. III, we point out that the dimer order in this region is associated with ferromagnetic nearest-neighbor correlations $\langle S_\ell \cdot S_{\ell+1} \rangle > 0$ of alternating strengths along the chain, in marked contrast to an antiferromagnetic correlation in a singlet dimer. A more detailed comparison of the dimer phases for $J_1 < 0$ and $J_1 > 0$ in the isotropic case ($\Delta = 1$) will be presented in Sec. III.

In the region of a finite vector chiral order ($0.61 \lesssim \Delta \lesssim 0.92$) in Fig. 2, we find that the two dimer order parameters remain finite in the narrow regions between the solid and broken vertical lines. This indicates the existence of the chiral dimer phases (originally predicted in Ref. 34), in which the vector chiral and dimer orders coexist and there are four-fold degenerate ground states below an excitation gap. In the entanglement entropy, a dip is seen in the interval $0.61 \lesssim \Delta \lesssim 0.63$, which also supports the existence of an intermediate gapped phase. The peaks in the entanglement entropy indicated by the solid lines in Fig. 2(d) correspond to the Ising critical point between two gapped phases. Between the two broken lines in Fig. 2, the dimer order parameters diminish and the entanglement entropy increases as we increase the Schmidt rank χ ; these features are consistent with the gapless chiral phase. The precise determination of the phase boundaries between gapped and gapless chiral phases is difficult within the analysis of the order parameters and entanglement entropy in Fig. 2; it will be done instead by analyzing spin correlation functions in Fig. 14 in Sec. IV B2.

C. Néel order

The appearance of a Néel phase with spontaneous staggered magnetizations $\langle S_\ell^z \rangle \propto (-1)^\ell$ is discussed in detail in Ref. 24. In Fig. 3(b), this Néel order is detected in the region $J_1/J_2 \lesssim -3.2$ by measuring $\langle S_1^z \rangle$. As in the case of the dimer phases, even in the region where the vector chiral order is finite ($J_1/J_2 \gtrsim -3.225$), the Néel order parameter remains finite. This indicates the existence of a narrow chiral Néel phase, in which the vector chiral and Néel orders coexist. The ground states in this phase should be four-fold degenerate with a finite excitation gap. In Fig. 3(c), a dip in the entanglement entropy can be found in this region, consistent with the expected gapped excitation spectrum. The precise determination of the transition point will be done in Fig. 15 in Sec. IV B2.

III. ISOTROPIC CASE $\Delta = 1$

In this section, we present detailed analyses of the model (1) in the isotropic case $\Delta = 1$. While it is known that the singlet dimer phase appears for $0 < J_1/J_2 \lesssim 4.15$,^{2-5,42} the nature of the nonmagnetic ground state in $-4 < J_1/J_2 < 0$ has not been well understood. In Sec. III A, we summarize previous field-theoretical analyses^{6,21} for the weak-coupling limit $|J_1| \ll J_2$, which predicted the appearance of dimer orders for both signs

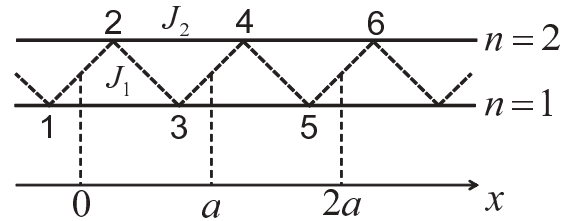


FIG. 4. Zigzag chain picture for the J_1 - J_2 chain model (1). The x axis indicates the coordinate for the continuum description.

of J_1 . At first glance, this result may seem bizarre since the singlet dimerization on the J_1 bonds, as formed in the case of antiferromagnetic $J_1 > 0$, is unlikely to occur in the case of ferromagnetic $J_1 < 0$. In Sec. III B, we present our numerical results and point out a remarkable difference between the $J_1 > 0$ and $J_1 < 0$ cases in the way how the system hosts the dimer order. This leads us to propose the picture of the “Haldane dimer phase” for the dimer phase with $J_1 < 0$. Although the ground-state wave functions are largely different between the Haldane and singlet dimer phases, we argue that the two phases in fact share a common hidden order.

A. Field-theoretical analyses

Here we summarize previous field-theoretical analyses^{6,21,43-45} for $|J_1| \ll J_2$. In this regime, the model (1) can be viewed as two antiferromagnetic Heisenberg spin chains which are weakly coupled by the zigzag interchain coupling J_1 as in Fig. 4. We apply the Abelian and non-Abelian bosonization techniques to describe the two chains separately, and then treat the interchain coupling J_1 as a weak perturbation.

1. Non-Abelian bosonization

We start from the non-Abelian bosonization³¹⁻³³ description of the isotropic model (1) with $\Delta = 1$ and present the renormalization group (RG) analysis to identify (marginally) relevant perturbations. In the limit $J_1/J_2 \rightarrow 0$, each isolated antiferromagnetic Heisenberg chain is described by the $SU(2)_1$ Wess-Zumino-Witten (WZW) theory, with the spin velocity $v = (\pi/2)J_2a$, perturbed by a marginally irrelevant backscattering term.^{31,32,42} The spin operators in the n th chain ($n = 1, 2$) can be decomposed as

$$S_{2j+n} \rightarrow a[\mathbf{M}_n(x_n) + (-1)^j \mathbf{N}_n(x_n)] \quad (8)$$

with $x_1(j) = (j - \frac{1}{4})a$ and $x_2(j) = (j + \frac{1}{4})a$, where a is the lattice spacing of each chain; see Fig. 4. The uniform and staggered components, \mathbf{M}_n and \mathbf{N}_n , have the scaling dimensions 1 and $1/2$, respectively. The former can be decomposed into chiral (right and left) components: $\mathbf{M}_n = \mathbf{M}_{nR} + \mathbf{M}_{nL}$. Another important operator is the (in-chain) staggered dimerization operator ϵ_n defined by

$$(-1)^j S_{2j+n} \cdot S_{2j+n+2} \rightarrow a\epsilon_n(x_n), \quad (9)$$

which has the scaling dimension $1/2$.

The interchain zigzag coupling J_1 produces at most marginal perturbations, in the RG sense, around the WZW fixed point; relevant perturbations such as $N_1 \cdot N_2$ are prohibited by the symmetry of the zigzag chain model. The

symmetry-allowed marginal perturbations are summarized as

$$H' = \int dx \sum_i g_i \mathcal{O}_i, \quad (10)$$

where i runs over the following five operators:²¹

$$\mathcal{O}_{\text{bs}} = \mathbf{M}_{1R} \cdot \mathbf{M}_{1L} + \mathbf{M}_{2R} \cdot \mathbf{M}_{2L}, \quad (11a)$$

$$\mathcal{O}_1 = \mathbf{M}_{1R} \cdot \mathbf{M}_{2L} + \mathbf{M}_{1L} \cdot \mathbf{M}_{2R}, \quad (11b)$$

$$\mathcal{O}_2 = \mathbf{M}_{1R} \cdot \mathbf{M}_{2R} + \mathbf{M}_{1L} \cdot \mathbf{M}_{2L}, \quad (11c)$$

$$\mathcal{O}_{\text{tw}} = \frac{a}{2} (N_1 \cdot \partial_x N_2 - N_2 \cdot \partial_x N_1), \quad (11d)$$

$$\mathcal{O}_{\text{dtw}} = \frac{a}{2} (\epsilon_1 \partial_x \epsilon_2 - \epsilon_2 \partial_x \epsilon_1). \quad (11e)$$

Here, \mathcal{O}_{bs} is the backscattering term present in isolated chains. The zigzag J_1 coupling produces the current-current interactions, \mathcal{O}_1 and \mathcal{O}_2 , and the twist operator \mathcal{O}_{tw} . The dimer twist operator \mathcal{O}_{dtw} is generated in the RG process as we see later. The bare coupling constants are given by

$$g_{\text{bs}}(0) = -0.23(2\pi v), \quad g_1(0) = g_2(0) = 2J_1 a, \quad (12)$$

$$g_{\text{tw}}(0) = J_1 a, \quad g_{\text{dtw}}(0) = 0, \quad (13)$$

where $g_{\text{bs}}(0)$ was estimated in Ref. 42. All the operators in Eq. (11) have the scaling dimensions 2, and their competition in the RG flow must be analyzed carefully by deriving the RG equations. We define the dimensionless coupling constants

$$G_i = \frac{g_i}{2\pi v} \quad (i = \text{bs}, 1, 2), \quad (14)$$

$$G_i = \frac{g_i}{2\pi v \lambda^2} \quad (i = \text{tw}, \text{dtw}), \quad (15)$$

where λ is a dimensionless constant of order unity. Using the operator product expansions in the WZW theory,^{33,47–50} the one-loop RG equations⁴⁶ are derived as^{6,21,44,45}

$$\dot{G}_{\text{bs}} = G_{\text{bs}}^2 + G_{\text{tw}}^2 - G_{\text{dtw}}^2, \quad (16a)$$

$$\dot{G}_1 = G_1^2 + G_{\text{tw}}^2 - G_{\text{tw}} G_{\text{dtw}}, \quad (16b)$$

$$\dot{G}_{\text{tw}} = -\frac{1}{2} G_{\text{bs}} G_{\text{tw}} + G_1 G_{\text{tw}} - \frac{1}{2} G_1 G_{\text{dtw}}, \quad (16c)$$

$$\dot{G}_{\text{dtw}} = \frac{3}{2} G_{\text{bs}} G_{\text{dtw}} - \frac{3}{2} G_1 G_{\text{tw}}, \quad (16d)$$

where the dot indicates the derivative ($\dot{G}_i = dG_i/dl$) with respect to the change of the cutoff: $a \rightarrow e^{dl} a$. See Appendix A for the derivation of Eq. (16). We have ignored G_2 since it does not affect the flow of the other coupling constants at the one-loop level.

Numerical solutions to the RG equations (16) are presented in Fig. 5. For both signs of J_1 , the three coupling constants G_1 , G_{tw} , and G_{dtw} finally grow to large values under the RG,^{6,21} they asymptotically have the simple ratio $G_1 : G_{\text{tw}} : G_{\text{dtw}} = 2 : 1 : (-1)$ or $2 : (-1) : 1$ for $J_1 > 0$ and $J_1 < 0$, respectively. Remarkably, G_1 finally grows with a *positive* sign for both signs of J_1 . For $J_1 < 0$, in particular, it is initially negative but changes sign before starting to grow in the RG process. By contrast, G_{tw} retains the same sign as its initial value. The properties of the fixed points governed by large $G_1 (> 0)$, G_{tw} , and G_{dtw} are nontrivial. In fact, while the non-Abelian formalism allows us to derive the RG equations in a manifestly SU(2)-invariant form, it is often not very useful for discussing the physical roles of (marginally) relevant perturbations. In the

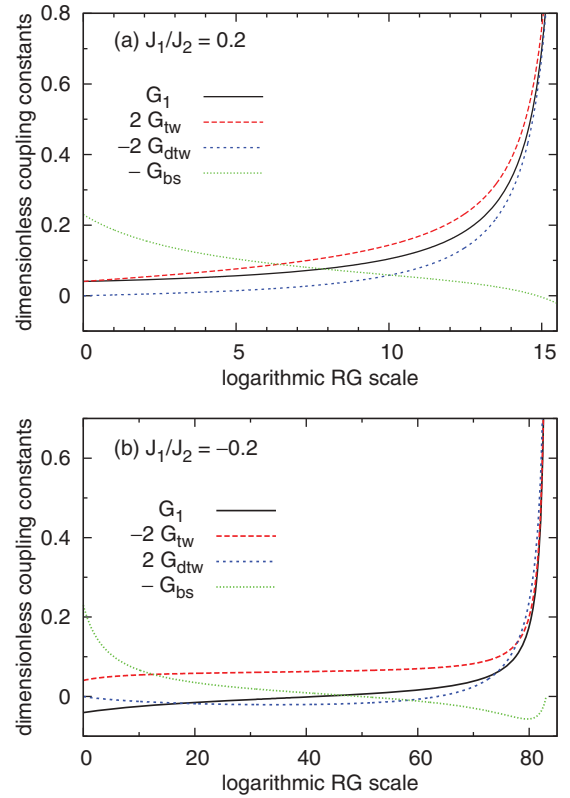


FIG. 5. (Color online) Numerical solutions to the one-loop RG equations (16) for (a) $J_1/J_2 = 0.2$ and (b) $J_1/J_2 = -0.2$. We set $\lambda = 1$ [see Eq. (14)]. It is found that the three coupling constants G_1 , G_{tw} , and G_{dtw} are most relevant and grow under the RG, with asymptotically a simple ratio $G_1 : G_{\text{tw}} : G_{\text{dtw}} = 2 : 1 : (-1)$ or $2 : (-1) : 1$ for $J_1 > 0$ and $J_1 < 0$, respectively. In the plots, factors ± 2 are multiplied to G_{tw} and G_{dtw} so that these ratios can be visually confirmed.

next section, we proceed to the Abelian bosonization analysis to show that the positive development of G_1 induces a gapped state with a finite dimer order parameter $D_{123} \neq 0$.

As seen in Figs. 5(a) and 5(b), the coupling constants grow much more slowly for $J_1 < 0$ than for $J_1 > 0$. This implies that for $J_1 < 0$, the energy gap associated with the dimer order should be much smaller and the spin correlation length ξ should be much larger. In fact, as argued by Itoi and Qin,²¹ the correlation length becomes of astronomical scale [e.g., $\xi/a \sim e^{83} \sim 10^{36}$ for the case of Fig. 5(b)]. Such a tiny gap or a large correlation length is very difficult to detect by any numerical investigation; the system effectively behaves like a gapless system even when the system size is macroscopically large. We stress, however, that this insight is based on the perturbative RG analysis for small $J_1/J_2 < 0$, and it is possible that the energy gap grows to an observable magnitude as we increase $|J_1|/J_2$. Our numerical result presented in Sec. III B indeed identifies a large but detectable correlation lengths around $J_1/J_2 = -2$.

2. Abelian bosonization

In this section, we use the Abelian bosonization formalism³⁰ to discuss the physical roles of the marginally relevant perturbations $G_1 (> 0)$, G_{tw} , and G_{dtw} identified in

the non-Abelian analysis. Although the Abelian formalism obscures the SU(2) symmetry of the model, it has the advantage of simplifying identification of various orders with the pattern of locking of bosonic fields, as illustrated in Table I.

Let us start from the two decoupled antiferromagnetic chains in the limit $J_1/J_2 \rightarrow 0$. We summarize the Abelian bosonization description^{30,31} of a single XXZ chain ($0 \leq \Delta \leq 1$), so that the same formulation can be used later in Sec. IV A. Each decoupled XXZ chain labeled by $n = 1, 2$ is described by a Gaussian Hamiltonian

$$H_n = \int dx \frac{v}{2} [K(\partial_x \theta_n)^2 + K^{-1}(\partial_x \phi_n)^2] \quad (17)$$

where the velocity v and the TLL parameter K are given by

$$v = \frac{\pi \sqrt{1 - \Delta^2}}{2 \arccos \Delta} J_2 a, \quad K = \frac{1}{1 - (1/\pi) \arccos \Delta}. \quad (18)$$

The bosonic fields ϕ_n and θ_n satisfy the commutation relation

$$[\phi_n(x), \theta_{n'}(x')] = i \delta_{nn'} Y(x - x'), \quad (19)$$

where $Y(x - x')$ is the step function

$$Y(x - x') = \begin{cases} 0 & (x < x'), \\ 1/2 & (x = x'), \\ 1 & (x > x'). \end{cases} \quad (20)$$

The spin and (in-chain) dimer operators are expressed in terms of the bosonic fields as

$$S_{2j+n}^z = \frac{a}{\sqrt{2\pi}} \partial_x \phi_n(x_n) + (-1)^j A_1 \cos[\sqrt{2\pi} \phi_n(x_n)] + \dots, \quad (21)$$

$$S_{2j+n}^+ = e^{i\sqrt{2\pi}\theta_n(x_n)} \{(-1)^j B_0 + B_1 \cos[\sqrt{2\pi} \phi_n(x_n)] + \dots\}, \quad (22)$$

$$(-1)^j \mathbf{S}_{2j+n} \cdot \mathbf{S}_{2j+n+2} = C \sin(\sqrt{2\pi} \phi_n) + \dots, \quad (23)$$

where A_1 , B_0 , B_1 (Refs. 51 and 52), and C (Ref. 53) are nonuniversal constants which depend on Δ .

We now focus on the case $\Delta = 1$ in which $K = 1$. To treat the coupled chains, it is useful to introduce the bosonic fields for symmetric (+) and antisymmetric (-) sectors:

$$\phi_{\pm} = \frac{1}{\sqrt{2}}(\phi_1 \pm \phi_2), \quad \theta_{\pm} = \frac{1}{\sqrt{2}}(\theta_1 \pm \theta_2). \quad (24)$$

The three perturbations found to grow in the non-Abelian analysis have the following expressions:^{6,44,54,55}

$$\begin{aligned} \mathcal{O}_1 &= -\frac{B_1^2}{2a^2} \cos(\sqrt{4\pi} \phi_+) \cos(\sqrt{4\pi} \phi_-) \\ &+ \frac{1}{8\pi} [(\partial_x \phi_+)^2 - (\partial_x \theta_+)^2 - (\partial_x \phi_-)^2 + (\partial_x \theta_-)^2], \end{aligned} \quad (25a)$$

$$\begin{aligned} \mathcal{O}_{\text{tw}} &= \frac{\sqrt{\pi} B_0^2}{a} (\partial_x \theta_+) \sin(\sqrt{4\pi} \theta_-) \\ &+ \frac{\sqrt{\pi} A_1^2}{2a} [(\partial_x \phi_+) \sin(\sqrt{4\pi} \phi_-) + (\partial_x \phi_-) \sin(\sqrt{4\pi} \phi_+)], \end{aligned} \quad (25b)$$

$$\mathcal{O}_{\text{dtw}} = \frac{\sqrt{\pi} C^2}{a} [(\partial_x \phi_+) \sin(\sqrt{4\pi} \phi_-) - (\partial_x \phi_-) \sin(\sqrt{4\pi} \phi_+)]. \quad (25c)$$

Furthermore, the \mathcal{O}_2 term, which is decoupled from the other terms in the RG equation (16), has the expression

$$\begin{aligned} \mathcal{O}_2 &= -\frac{B_1^2}{2a^2} \cos(\sqrt{4\pi} \phi_-) \cos(\sqrt{4\pi} \theta_-) \\ &+ \frac{1}{8\pi} [(\partial_x \phi_+)^2 + (\partial_x \theta_+)^2 - (\partial_x \phi_-)^2 - (\partial_x \theta_-)^2]. \end{aligned} \quad (26)$$

The second lines of Eqs. (25a) and (26) can be combined with the Gaussian Hamiltonians (17) of the decoupled chains, leading to

$$H_0 = \int dx \sum_{v=\pm} \frac{v_v}{2} [K_v (\partial_x \theta_v)^2 + K_v^{-1} (\partial_x \phi_v)^2] \quad (27)$$

with

$$\begin{aligned} K_{\pm} &= 1 \mp \frac{G_1}{2} + O(G_1^2, G_2^2), \\ v_{\pm} &= v \left[1 \pm \frac{G_2}{2} + O(G_1^2, G_2^2) \right]. \end{aligned} \quad (28)$$

Using the new Gaussian Hamiltonian H_0 , we can calculate the scaling dimension of the operators in Eq. (25). Specifically, the scaling dimension of $e^{i\sqrt{4\pi}\phi_{\pm}}$ and $e^{i\sqrt{4\pi}\theta_{\pm}}$ is given by K_{\pm} and K_{\pm}^{-1} , respectively. In the non-Abelian analysis, we have seen that G_1 grows to a positive value in the RG flow irrespective of the sign of J_1 . Assuming $G_1 > 0$, we find that the product of the two cosine operators in the first line of Eq. (25a) (with scaling dimension $2 - G_1$) is the most relevant term among those in Eq. (25). This term locks the bosonic fields at

$$(\sqrt{4\pi} \phi_+, \sqrt{4\pi} \phi_-) = (0, 0) \text{ or } (\pi, \pi). \quad (29)$$

These correspond respectively to finite positive or negative value of the dimer order parameter $D_{123} = \langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle - \langle \mathbf{S}_2 \cdot \mathbf{S}_3 \rangle$, since the (interchain) dimer operator is expressed as

$$\begin{aligned} \mathbf{S}_{2j+1} \cdot \mathbf{S}_{2j+2} - \mathbf{S}_{2j+2} \cdot \mathbf{S}_{2j+3} \\ &= 2a^2 \mathbf{N}_1 \cdot \mathbf{N}_2 + \dots \\ &\approx 2B_0^2 \cos(\sqrt{4\pi} \theta_-) + A_1^2 [\cos(\sqrt{4\pi} \phi_+) + \cos(\sqrt{4\pi} \phi_-)]. \end{aligned} \quad (30)$$

In the last expression, the first term and the rest come from the xy and z components of the spins, respectively. For the locking in Eq. (29), these components acquire both positive or both negative expectation values, in agreement with Fig. 2(c) and with the SU(2) symmetry of the model. It is worth noting that the locking positions of the two degenerate ground states in Eq. (29) are independent of the sign of J_1 in the isotropic case $\Delta = 1$. The second most relevant terms in Eq. (25) are $(\partial_x \theta_+) \sin(\sqrt{4\pi} \theta_-)$ and $(\partial_x \phi_-) \sin(\sqrt{4\pi} \phi_+)$ with scaling dimension $2 - G_1/2$. As explained in Sec. IV A, the former has the effect of inducing the incommensurability in spin correlations.⁶ Since a finite energy gap opens due to $G_1 > 0$ in the dimer phases, the incommensurate spin correlations are expected to remain short ranged.

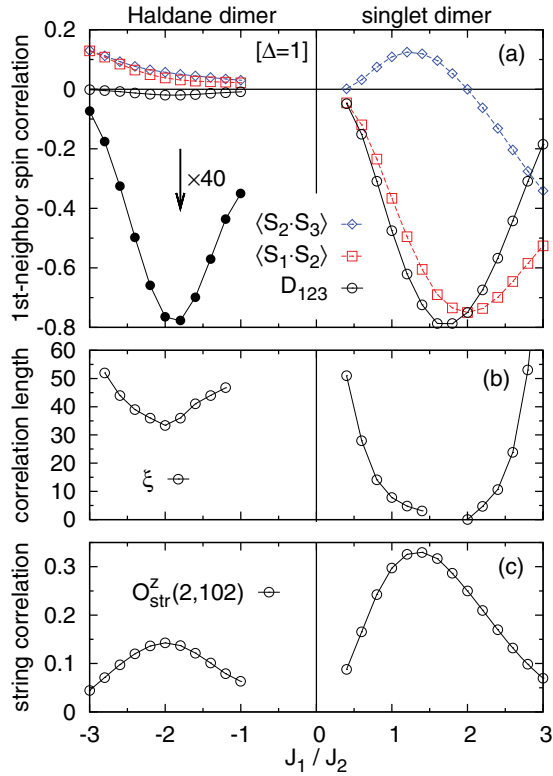


FIG. 6. (Color online) (a) Nearest-neighbor spin correlations $\langle S_j \cdot S_{j+1} \rangle$ and the dimer order parameter D_{123} , (b) the spin correlation length ξ , and (c) the string correlation (34) with $\ell = 2$ and $r = 50$, as a function of J_1/J_2 in the isotropic case $\Delta = 1$. In (a), D_{123} multiplied by 40 is also plotted for $J_1/J_2 < 0$ (filled circular symbols). In (b), ξ is too small to determine around $J_1/J_2 = 2$.

B. Numerical results and physical properties of dimer phases

In this section, we present numerical results on the model (1) in the isotropic case $\Delta = 1$, and discuss physical properties of the dimer phases for different signs of J_1 . In agreement with the field-theoretical results reviewed in the previous section, we find that the dimer order parameter D_{123} becomes finite for both signs of J_1 , and that there are doubly degenerate ground states with positive and negative D_{123} . While we propose different physical pictures for the dimer orders in the $J_1 > 0$ and $J_1 < 0$ cases (Sec. III B1), we also discuss a hidden order common to the two cases (Sec. III B3). In the following, our numerical results (based on iTEBD with $\chi = 300$) are presented for the ground state with $D_{123} < 0$.

1. Local spin correlations

In Fig. 6(a), we plot nearest-neighbor spin correlations $\langle S_\ell \cdot S_{\ell+1} \rangle$ (with $\ell = 1, 2$) and the dimer order parameter $D_{123} = \langle S_1 \cdot S_2 \rangle - \langle S_2 \cdot S_3 \rangle$ for $-3 \leq J_1/J_2 \leq 3$. While $D_{123} \neq 0$ can be confirmed for both $J_1 > 0$ and $J_1 < 0$, a notable difference between the two cases can be found in the signs of local spin correlations.

For $J_1 > 0$, one of the following inequalities is always satisfied:

$$\langle S_1 \cdot S_2 \rangle < -\langle S_2 \cdot S_3 \rangle < 0 \quad (0 < J_1/J_2 < 2), \quad (31a)$$

$$\langle S_1 \cdot S_2 \rangle < \langle S_2 \cdot S_3 \rangle \leq 0 \quad (2 \leq J_1/J_2 \lesssim 4.15). \quad (31b)$$

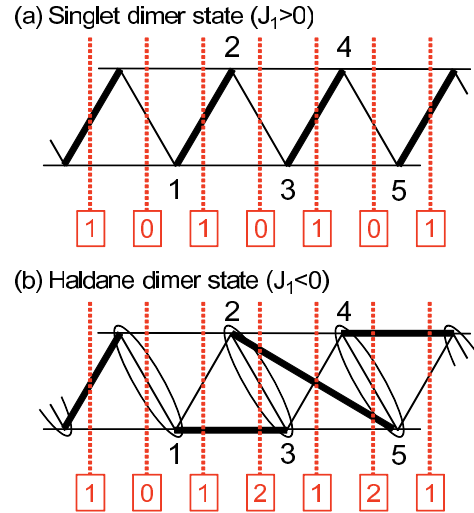


FIG. 7. (Color online) Sketches of (a) the singlet dimer state and (b) the Haldane dimer state. The thick lines indicate valence bonds. In (b), the encircled bonds indicate emergent spin-1's. From each of them, a valence bond emanate to each left and right; the wave function is given by a superposition of such valence bond covering states. Vertical cuts (dashed lines) are introduced to probe a hidden order; the number of valence bonds crossing with each cut is shown in the square. The alternation of odd and even numbers is found in both the states.

Namely, the system has a strong *antiferromagnetic* correlation on the bond (1,2) and a weaker correlation on (2,3). In this case, it is natural to assume that singlet dimers are formed on the bonds $(2j+1, 2j+2)$ ($j \in \mathbb{Z}$), and are weakly correlated with each other, as schematically shown in Fig. 7(a). Hence we call this phase the singlet dimer phase. In particular, the ground state is exactly given by a direct product of singlet dimers at the Majumdar-Ghosh point² $J_1/J_2 = 2$. In Fig. 6(a), we find that the weaker correlation $\langle S_2 \cdot S_3 \rangle$ changes the sign at this point.

By contrast, the following inequality is found to be satisfied when $-4 < J_1/J_2 < 0$:

$$0 < \langle S_1 \cdot S_2 \rangle < \langle S_2 \cdot S_3 \rangle. \quad (32)$$

Namely, strong and weak *ferromagnetic* nearest-neighbor correlations alternate along the chain. This observation led us to propose that there should be emergent spin-1 degrees of freedom on the bonds $(2j+2, 2j+3)$ ($j \in \mathbb{Z}$) that have stronger ferromagnetic correlation, as depicted by ellipses in Fig. 7(b). Since the total wave function is a spin singlet, such spin-1's are expected to form a valence bond solid state²⁸ as in the spin-1 Haldane chain.²⁹ Namely, from each encircled bond in Fig. 7(b), two valence bonds emanate, one to the left and one to the right; the total wave function is obtained by superposing such valence bond covering states. We thus call the dimer phase with $J_1 < 0$ the Haldane dimer phase. The emergence of the Haldane chain physics in this phase is also supported by the presence of a hidden nonlocal order analyzed in Sec. III B3.

In Sec. III A, it was argued that the marginal perturbation G_1 , which induces the dimer order, grows very slowly under

the RG for $J_1 < 0$ and that the energy gap associated with the dimer order can be extremely small.²¹ The result of Fig. 6(a) indicates that the dimer order parameter D_{123} grows to a numerically detectable magnitude for intermediate values of $|J_1|/J_2$ (≈ 2), although the obtained values are much smaller compared to the $J_1 > 0$ case (by a factor of around 1/40). The weakness of the effect of J_1 in inducing the dimer order and the associated energy gap for $J_1 < 0$ is also seen in the spin correlation length discussed next.

2. Spin correlation length

We determine the spin correlation length ξ in the dimer phases by using the method of Ref. 5. Except at the Lifshitz point $J_1/J_2 = 2$, the spin correlation function is expected to behave at long distances as^{5,56}

$$\langle \mathbf{S}_1 \cdot \mathbf{S}_{1+r} \rangle \approx A \cos(Qr) r^{-\frac{1}{2}} e^{-r/\xi}. \quad (33)$$

In the incommensurate regions $-4 < J_1/J_2 < 0$ and $0 < J_1/J_2 < 2$, the pitch angle Q changes continuously from 0 to π , as will be discussed in Sec. IV B3 (see Fig. 16). For $2 < J_1/J_2 \lesssim 4.15$, Q is fixed at $Q = \pi$. To determine ξ , we plot $r^{1/2} e^{r/\xi} \langle \mathbf{S}_1 \cdot \mathbf{S}_{1+r} \rangle$ as a function of r , and tune ξ such that the amplitude of oscillations becomes as constant as possible, as illustrated in Fig. 8. While the coefficient A in Eq. (33) is given by the oscillation amplitude in Fig. 8, it is not simple to determine Q that can fit these very rapid oscillations; instead, it will be determined by calculating the spin structure factor in Fig. 13.

The calculated ξ is plotted in Fig. 6(b). The data for $J_1 > 0$ are broadly in agreement with Ref. 5.⁵⁷ We find that the values of ξ are much larger for $J_1 < 0$ than for $J_1 > 0$, as anticipated from the magnitudes of the dimer order parameter in Fig. 6(a).

We use the above numerical data of the spin correlation length ξ to infer the magnitude of the spin gap Δ_s for $J_1 < 0$. In general the spin gap Δ_s should be inversely proportional to ξ , with the proportionality constant being the spin velocity. From the data of Ref. 5 for $J_1 > 0$, we extract an approximate relation $(\Delta_s/J_2)\xi \approx 2$. Applying the same relation to the $J_1 < 0$

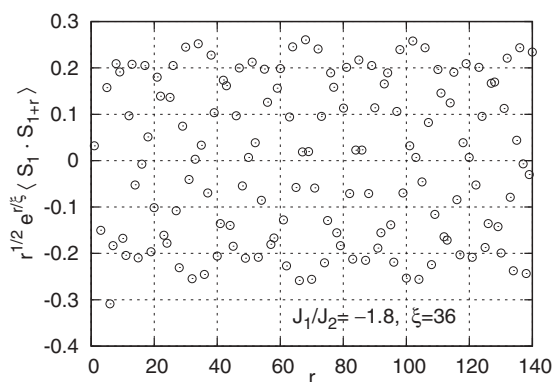


FIG. 8. Determination of the spin correlation length ξ , illustrated for $J_1/J_2 = -1.8$. Assuming the asymptotic behavior (33), we plot the function $r^{1/2} e^{r/\xi} \langle \mathbf{S}_1 \cdot \mathbf{S}_{1+r} \rangle$ and tune ξ such that the oscillation width of this function becomes as constant as possible as a function of r .⁵ While the oscillations arise from the cosine factor in Eq. (33), it is difficult to extract the pitch angle Q from this figure; instead, calculations in Sec. IV B3 give $Q/(2\pi) \approx 0.235$.

case, we estimate the spin gap Δ_s around $J_1/J_2 = -2$ to be roughly equal to $0.06J_2$. We note that this should be considered as a crude order of magnitude estimate.

3. Hidden order

The singlet and Haldane dimer phases have different (local) features of short-range correlations as expressed in Eqs. (31) and (32). In spite of this local difference, the two phases in fact share a common nonlocal order, as we now explain. Let us count the number of valence bonds crossing the vertical cuts (dashed lines) depicted in Fig. 7. We find that even and odd numbers alternate in the same way in the two phases, when we take the ground state with $D_{123} < 0$. The existence of such a hidden nonlocal order can be probed numerically by calculating the string correlation function⁵⁸⁻⁶³

$$O_{\text{str}}^z(\ell, \ell + 2r) := - \left\langle \left(S_\ell^z + S_{\ell+1}^z \right) \exp \left(i\pi \sum_{m=\ell+2}^{\ell+2r-1} S_m^z \right) \times \left(S_{\ell+2r}^z + S_{\ell+2r+1}^z \right) \right\rangle. \quad (34)$$

The intuition behind this expression is as follows. Consider a pair of spins $S_{\ell+2j}^z + S_{\ell+2j+1}^z$ on the bond $(\ell + 2j, \ell + 2j + 1)$ ($j \in \mathbb{Z}$), which the string correlation function (34) consists of. If an odd number of valence bonds cross any cut placed between the neighboring pairs, then the pattern of $S_{\ell+2j}^z + S_{\ell+2j+1}^z = -1, 0, +1$ shows a hidden antiferromagnetic order, namely, alternation of $+1$ and -1 after removing all 0's (see figures in Refs. 61 and 63). The correlation function (34) detects this hidden order and takes a nonvanishing value in the long-distance limit $r \rightarrow \infty$.

Figure 9 presents the numerical data of the string correlation functions (34) calculated with different starting points $\ell = 1, 2$ for the ground state with $D_{123} < 0$. We find that for both signs of J_1 , $O_{\text{str}}^z(2, 2 + 2r)$ remains finite in the long-distance limit while $O_{\text{str}}^z(1, 1 + 2r)$ decays to zero, in agreement with the even-odd structure in Fig. 7. We note that this behavior is also consistent with the bosonized expressions of the string

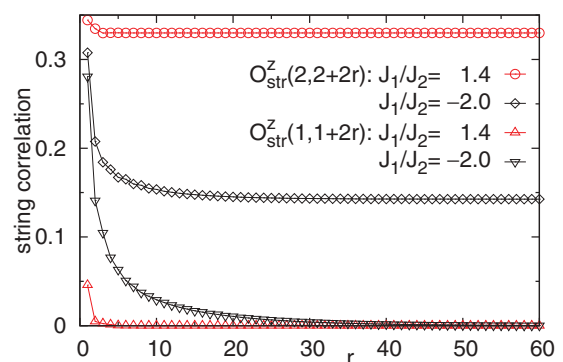


FIG. 9. (Color online) String correlation function (34) for $J_1/J_2 = 1.4$ and -2.0 in the isotropic case $\Delta = 1$. For both values of J_1/J_2 , $O_{\text{str}}^z(2, 2 + 2r)$ remains finite in the long-distance limit, while $O_{\text{str}}^z(1, 1 + 2r)$ decays to zero.

correlations:⁶⁴

$$O_{\text{str}}^z(1, 1 + 2r) \sim \langle \cos[\sqrt{\pi}\phi_+(x)] \cos[\sqrt{\pi}\phi_+(y)] \rangle, \quad (35)$$

$$O_{\text{str}}^z(2, 2 + 2r) \sim \langle \sin[\sqrt{\pi}\phi_+(x)] \sin[\sqrt{\pi}\phi_+(y)] \rangle, \quad (36)$$

(with x and y being the two endpoints of the string) and the field locking position $\sqrt{4\pi}\phi_+ = \pi$ for the ground state with $D_{123} < 0$ [see Eq. (29)]. The J_1/J_2 dependence of $O^z(2, 2 + 2r)$ for a long distance $r = 50$ is shown in Fig. 6(c). Although the dimer order parameter shows a large difference in magnitude between the $J_1 > 0$ and $J_1 < 0$ cases, the values of the string correlation are rather comparable between the two cases.

Another way of probing the hidden order is to find the degeneracy in the entanglement spectrum.⁶⁵ Using the Schmidt coefficients $\{\lambda_{m\alpha}\}$ calculated in iTEBD, we plot the spectra $\{-2 \ln \lambda_{m\alpha}\}$ in Fig. 10. Here, the spectra are classified by the z -component magnetization m in the right half of the system (this classification is done in the process of our calculations to exploit the $U(1)$ spin rotational symmetry for

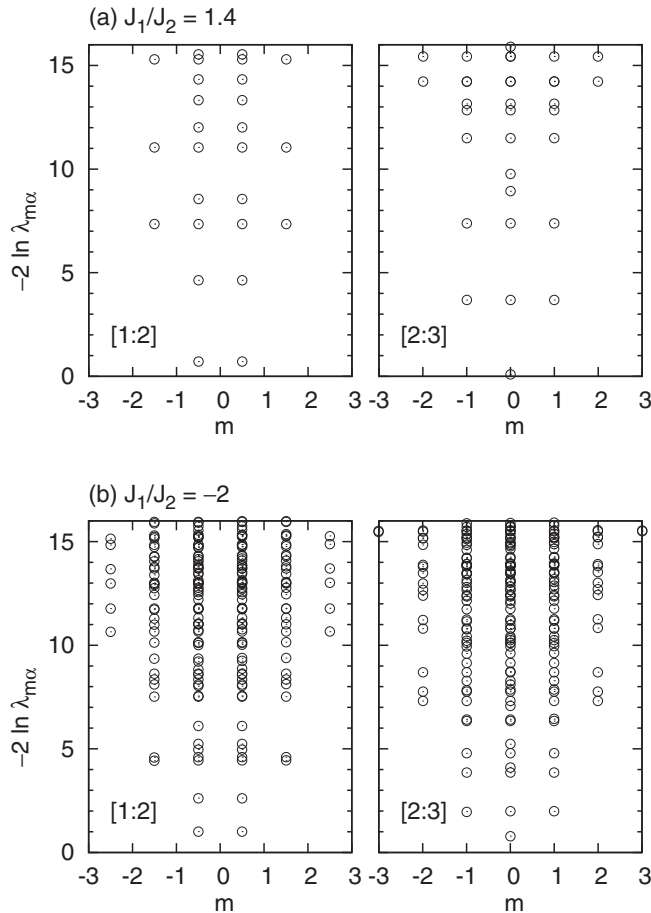


FIG. 10. Entanglement spectra $\{-2 \ln \lambda_{m\alpha}\}$ for (a) $J_1/J_2 = 1.4$ and (b) $J_1/J_2 = -2$. The left and right panels are for the bipartition of the system at the bonds (1,2) and (2,3), respectively. m refers to the magnetization in the right half of the system. The lower entanglement level corresponds to the more important weight in the total state. We note that as an example, the exact singlet dimer ground state of Ref. 2 shows $-2 \ln \lambda_{\pm \frac{1}{2}, 1} = \ln 2$ and $-2 \ln \lambda_{0,1} = 0$ for the two types of bipartition (with all the other levels at infinity).

better efficiency). For the bipartition of the system at the bond (1,2) (left panels), we find that the entanglement levels appear only for half-integer m and are all doubly degenerate due to the left-right symmetry around $m = 0$. By contrast, for the bipartition at (2,3) (right panels), the entanglement levels appear only for integer m , and nondegenerate levels are found for $m = 0$.⁶⁶ These features are found commonly for both signs of J_1 , and are consistent with the even-odd structure in Fig. 7.

In Fig. 7, we depicted short-range valence bonds only. However, the even-odd structure we discussed can be also defined in the presence of longer-range valence bonds. As the correlation length becomes longer, the weights of such longer-range valence bonds in the wave function would gradually grow while retaining the even-odd structure.⁶⁷ We expect that through this process, the Haldane dimer state of Fig. 7(b) smoothly changes into the exact resonating valence bond ground state at $J_1/J_2 = -4$ in which valence bonds are uniformly distributed over all distances.⁶⁸

4. Adiabatic connectivity to a ladder model

In order to gain further intuition about the two dimer phases, it is useful to introduce explicit bond alternation of the J_1 couplings in the Hamiltonian (1) (with $\Delta = 1$). Namely, we place inequivalent couplings J_1 and J'_1 on the bonds $(2j + 1, 2j + 2)$ and $(2j + 2, 2j + 3)$ ($j \in \mathbb{Z}$), respectively. Figure 11 displays an expected phase diagram for small J_1/J_2 and J'_1/J_2 . This phase diagram can be obtained^{45,63} by noticing that in the non-Abelian bosonization framework, the bond alternation induces the relevant term $(J_1 - J'_1)N_1 \cdot N_2$ with scaling dimension 1 in the Hamiltonian, which leads to the ground state where $D_{123} \sim \langle N_1 \cdot N_2 \rangle$ acquires a finite average with the same sign as that of $J'_1 - J_1$. The limit $J_1 \rightarrow 0$ or $J'_1 \rightarrow 0$ (the vertical or horizontal axis of Fig. 11) corresponds to a spin ladder model for which it is established that the rung singlet and Haldane phases appear for antiferromagnetic and ferromagnetic rung couplings, respectively.^{47,61,62,69} Therefore we expect that the Haldane dimer state with $D_{123} < 0$ in

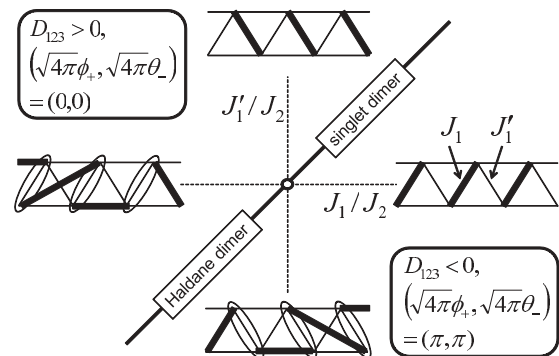


FIG. 11. Expected phase diagram of the zigzag ladder model with alternating nearest-neighbor couplings J_1 and J'_1 . $|J_1|/J_2$ and $|J'_1|/J_2$ are assumed to be small. The solid diagonal line $J_1 = J'_1$ corresponds to the original model (1) (with $\Delta = 1$), and represents the first-order phase transition line in the current model. The vertical and horizontal dashed lines correspond to a usual ladder model (no phase transition on these lines). In four insets of zigzag ladders, thick lines indicate valence bonds, and ovals indicate the formation of effective spin-1's.

Fig. 7(b) should be adiabatically connected to the Haldane state of a ladder model (the lower half of the vertical axis of Fig. 11) by gradually switching off the J_1 coupling. It is also possible to adiabatically change the ground state from the Haldane dimer state to the singlet dimer state (both with $D_{123} < 0$) by moving counterclockwise around the origin in Fig. 11, although the wave function may considerably change in this process. In the zigzag ladder model with $J_1 = J'_1$ (diagonal line), however, the singlet and Haldane dimer phases are separated by the origin (open circle in Fig. 11), at which the two chains are decoupled. We note that only on the $J_1 = J'_1$ line in Fig. 11, the model has the symmetry with respect to the translation $S_\ell \rightarrow S_{\ell+1}$, and the dimer order appears by spontaneously breaking this symmetry. It would thus be interesting to investigate under what kind of *translationally symmetric* perturbation the Haldane and singlet dimer phases can be adiabatically connected to each other while retaining the double degeneracy below a finite excitation gap.

IV. EASY-PLANE CASE $0 \leq \Delta < 1$

In this section, we consider the model (1) in the easy-plane case $0 \leq \Delta < 1$. In Sec. IV A, we present the Abelian bosonization formulation of the model for $|J_1|/J_2 \ll 1$ and explain how various phases in Fig. 1 are described in this framework. In particular, we review the effective theory for the gapless chiral phase⁶ and, following Ref. 34, discuss its instability towards gapped chiral phases due to a symmetry-allowed perturbation. Section IV B presents our numerical results. We compute the spin correlation functions in the gapless chiral phase and determine the phase boundaries to the gapped chiral phases.

A. Bosonization analyses

We consider the easy-plane XXZ Hamiltonian (1) in the regime $|J_1|/J_2 \ll 1$. Using the formulation described in

Sec. III A2, we obtain the effective Hamiltonian

$$H = \int dx \left\{ \sum_{v=\pm} \frac{v_v}{2} [K_v (\partial_x \theta_v)^2 + K_v^{-1} (\partial_x \phi_v)^2] - \gamma_1 \cos(\sqrt{4\pi} \phi_+) \cos(\sqrt{4\pi} \theta_-) + \gamma_{tw} (\partial_x \theta_+) \sin(\sqrt{4\pi} \theta_-) + \gamma_{tw}'' (\partial_x \phi_-) \sin(\sqrt{4\pi} \phi_+) + \dots \right\}. \quad (37)$$

The first line represents the Gaussian Hamiltonian while the other lines represent perturbations that can become relevant in the easy-plane case.^{6,22,44} As seen in Eq. (25), the γ_1 term is related to the G_1 term in the non-Abelian bosonization, while γ_{tw} and γ_{tw}'' correspond to G_{tw} . The coupling constants are obtained in lowest order in J_1 as

$$K_{\pm} = K \left(1 \mp \frac{K J_1 \Delta a}{2\pi v} \right), \quad v_{\pm} = v \left(1 \pm \frac{K J_1 \Delta a}{2\pi v} \right), \quad (38)$$

$$\gamma_1 = \frac{B_1^2 J_1}{a}, \quad \gamma_{tw} = \sqrt{\pi} J_1 B_0^2, \quad \gamma_{tw}'' = \frac{\sqrt{\pi}}{2} J_1 \Delta A_1^2, \quad (39)$$

where K and v are given by Eq. (18). We have discussed in Sec. III that, in the isotropic case $\Delta = 1$, γ_1 grows to large positive values for both signs of J_1 under the RG, and induces the singlet and Haldane dimer phases for $J_1 > 0$ and $J_1 < 0$, respectively. Below we explain how other phases in Fig. 1 are described using the effective Hamiltonian (37). The results are summarized in Table I.

1. Even-parity dimer phase

If $J_1 < 0$, the coupling constant γ_1 is negative at the bare level. Suppose that this term grows, keeping the negative sign under the RG. Then the bosonic fields are locked at

$$(\sqrt{4\pi} \phi_+, \sqrt{4\pi} \theta_-) = (0, \pi) \text{ or } (\pi, 0). \quad (40)$$

In either case, it follows from Eq. (30) that the xy and z components of the dimer order parameter, D_{123}^{xy} and D_{123}^z , become finite and have mutually opposite signs ($D_{123}^{xy} D_{123}^z < 0$). This situation corresponds to the even-parity dimer phase

TABLE I. Summary of the Abelian bosonization description of the phases for small $|J_1|/J_2$. Both the easy-plane (see Sec. IV) and easy-axis (see Sec. V) cases are presented. We note that the (chiral) even-parity dimer and chiral Néel phases appear for rather large $|J_1|/J_2$ in Fig. 1 although their essential features can be captured in the Abelian bosonization framework.

Phase	Relevant perturbations	Field-locking positions	Order parameters
Singlet/Haldane dimer	$\gamma_1 > 0$	$(\sqrt{4\pi} \phi_+, \sqrt{4\pi} \theta_-) = (0, 0), (\pi, \pi)$	$D_{123}^{xy} D_{123}^z > 0$
Even-parity dimer	$\gamma_1 < 0$	$(\sqrt{4\pi} \phi_+, \sqrt{4\pi} \theta_-) = (0, \pi), (\pi, 0)$	$D_{123}^{xy} D_{123}^z < 0$
Gapless chiral	$\gamma_{tw} \sim J_1 \neq 0$	$\sqrt{4\pi} \theta_- = -\frac{\pi}{2} \text{sgn}(J_1 (\partial_x \theta_+))$	$\kappa_{12}^z \neq 0$
Chiral singlet/Haldane dimer	$\gamma_{tw} \sim J_1, \gamma_{nd} < 0, \gamma_1 > 0$	$(\sqrt{4\pi} \phi_+, \sqrt{4\pi} \theta_-) = \begin{cases} (0, \pm \frac{\pi}{2}) \rightarrow (0, 0) \\ (\pi, \pm \frac{\pi}{2}) \rightarrow (\pi, \pm \pi) \end{cases}$	$\kappa_{12}^z \neq 0, D_{123}^{xy} D_{123}^z > 0$
Chiral even-parity dimer	$\gamma_{tw} < 0, \gamma_{nd} < 0, \gamma_1 < 0$	$(\sqrt{4\pi} \phi_+, \sqrt{4\pi} \theta_-) = \begin{cases} (0, \pm \frac{\pi}{2}) \rightarrow (0, \pm \pi) \\ (\pi, \pm \frac{\pi}{2}) \rightarrow (\pi, 0) \end{cases}$	$\kappa_{12}^z \neq 0, D_{123}^{xy} D_{123}^z < 0$
Chiral Néel	$\gamma_{tw} < 0, \gamma_{nd} > 0, \gamma_{tw}'' \neq 0$	$\sqrt{4\pi} \phi_+ = \pm \pi/2, \sqrt{4\pi} \theta_- = \pm \pi/2$	$\kappa_{12}^z \neq 0, \langle S_\ell^z \rangle \propto (-1)^\ell$
uudd	$\gamma_{bs} < 0$	$\sqrt{2\pi} \phi_1 = 0, \pi, \sqrt{2\pi} \phi_2 = 0, \pi$	$\langle S_{2j+1}^z \rangle = \pm \langle S_{2j}^z \rangle \propto (-1)^j$
Partially polarized	$\gamma_{tw}' < 0$	$\sqrt{4\pi} \phi_- = \frac{\pi}{2} \text{sgn}(\partial_x \phi_+)$	$\langle S_\ell^z \rangle \neq 0$

appearing at strong easy-plane anisotropy ($\Delta \lesssim 0.6$); see Fig. 2(b).

2. Gapless chiral phase

As shown by Nersisyan *et al.*,⁶ the gapless chiral phase appears when γ_{tw} grows under the RG. To discuss the effect of the γ_{tw} term, it is useful to perform the mean-field decoupling⁶

$$(\partial_x \theta_+) \sin(\sqrt{4\pi} \theta_-) \rightarrow \langle \partial_x \theta_+ \rangle \sin(\sqrt{4\pi} \theta_-) + (\partial_x \theta_+) \langle \sin(\sqrt{4\pi} \theta_-) \rangle. \quad (41)$$

Then the Hamiltonian (37) separates into “+” and “−” sectors:

$$H = H_+ + H_- \quad (42)$$

with

$$H_+ = \int dx \frac{v_+}{2} [K_+ (\partial_x \tilde{\theta}_+)^2 + K_+^{-1} (\partial_x \phi_+)^2], \quad (43)$$

$$H_- = \int dx \left\{ \frac{v_-}{2} [K_- (\partial_x \theta_-)^2 + K_-^{-1} (\partial_x \phi_-)^2] + \gamma_{\text{tw}} \langle \partial_x \theta_+ \rangle \sin(\sqrt{4\pi} \theta_-) \right\}. \quad (44)$$

Here we have introduced

$$\tilde{\theta}_+ := \theta_+ - qx, \quad q := -\frac{\gamma_{\text{tw}} \langle \sin(\sqrt{4\pi} \theta_-) \rangle}{v_+ K_+}. \quad (45)$$

While H_+ is a Gaussian Hamiltonian of free bosons ($\phi_+, \tilde{\theta}_+$), H_- is a sine-Gordon Hamiltonian in which the relevant sine potential generates a finite energy gap for the θ_- field. Since $\langle \partial_x \tilde{\theta}_+ \rangle = 0$ from H_+ , $\langle \partial_x \theta_+ \rangle = q$. The coefficient of the sine potential in H_- is thus given by $\gamma_{\text{tw}} q$, and the field θ_- is locked at distinct positions depending on the sign of this coefficient:

$$\langle \sqrt{4\pi} \theta_- \rangle = -\frac{\pi}{2} \text{sgn}(\gamma_{\text{tw}} q). \quad (46)$$

Correspondingly, the sine term acquires a finite expectation value:

$$\langle \sin(\sqrt{4\pi} \theta_-) \rangle = -c_1 \text{sgn}(\gamma_{\text{tw}} q), \quad (47)$$

where c_1 is a positive constant. Equations (45) and (47) can be solved self-consistently⁷⁰ by inserting the exact solution of the sine-Gordon model into Eq. (47), yielding two solutions, one positive and one negative q . It should be understood that the mean-field parameters c_1 and q used in the following calculation of correlation functions are determined self-consistently.

First, the nonvanishing value of the mean-field parameter in Eq. (47) directly leads to a finite vector chiral order parameter (2):

$$\kappa_{\ell, \ell+1}^z = -B_0^2 \langle \sin(\sqrt{4\pi} \theta_-) \rangle = B_0^2 c_1 \text{sgn}(\gamma_{\text{tw}} q). \quad (48)$$

Therefore the two mean-field solutions correspond to the ground states with positive and negative $\kappa_{\ell, \ell+1}^z$. Let us take the ground state with $\kappa_{\ell, \ell+1}^z > 0$ (i.e., $\gamma_{\text{tw}} q > 0$) and discuss the expressions of the spin operators. We focus on gapless degrees of freedom, and ignore the fluctuations of θ_- around its average (46). Then we find

$$\sqrt{2\pi} \theta_{1,2} = \sqrt{\pi} (\theta_+ \pm \theta_-) = \sqrt{\pi} \tilde{\theta}_+ + \sqrt{\pi} q x_{1,2} \mp \frac{\pi}{4}, \quad (49)$$

which are combined into

$$\sqrt{2\pi} \theta_n(x_n) = \sqrt{\pi} \tilde{\theta}_+(x_n) + \sqrt{\pi} q x_n + \frac{\pi}{2} \left(n - \frac{3}{2} \right). \quad (50)$$

The in-plane component of the spins are then expressed as

$$\begin{aligned} S_{2j+n}^+ &\approx B_0 (-1)^j e^{i\sqrt{2\pi} \theta_n(x_n)} \\ &= B_0 \exp \left\{ i \left[\sqrt{\pi} (\tilde{\theta}_+ + qx_n) + \frac{\pi}{2} \left(2j + n - \frac{3}{2} \right) \right] \right\}. \end{aligned} \quad (51)$$

Introducing $\ell = 2j + n$ and $x(\ell) = x_n(j) = (a/2)(\ell - 3/2)$, we obtain

$$S_\ell^+ \approx B_0 e^{i[\sqrt{\pi} \tilde{\theta}_+(x) + Q(\ell - 3/2)]}, \quad (52)$$

with

$$Q = \frac{\pi + \sqrt{\pi} qa}{2}. \quad (53)$$

As for the z component of the spins, we simply ignore the ϕ_- part of the expression:

$$S_\ell^z \approx \frac{a}{\sqrt{4\pi}} \partial_x \phi_+. \quad (54)$$

Spin correlation functions are then calculated as^{6,71}

$$\langle S_\ell^+ S_{\ell'}^- \rangle = A \frac{e^{-iQ(\ell' - \ell)}}{|\ell' - \ell|^{1/(2K_+)}} + \dots, \quad (55)$$

$$\langle S_\ell^z S_{\ell'}^z \rangle = -\frac{K_+}{2\pi^2 |\ell' - \ell|^2} + \dots \quad (56)$$

with $A = B_0^2 2^{1/(2K_+)}$. The finite vector chiral order parameter $\kappa_{\ell, \ell+1}^z$ in Eq. (48) and the quasi-long-range in-plane spiral correlation with an incommensurate pitch angle Q in Eq. (55) are two major features of the gapless chiral phase.

3. Gapped chiral phases

Following Lecheminant *et al.*,³⁴ we consider the following symmetry-allowed perturbation to the effective theory of the gapless chiral phase:

$$\gamma_{\text{nd}} \int dx \cos(2\sqrt{4\pi} \phi_+), \quad (57)$$

with which the “+” sector of the Hamiltonian becomes a sine-Gordon model. The scaling dimension of this perturbation is $4K_+$. If the γ_{nd} term becomes relevant ($4K_+ < 2$), a Berezinskii-Kosterlitz-Thouless (BKT) transition takes place and as a result, the bosonic field ϕ_+ is locked at distinct positions dependent on the sign of γ_{nd} . This leads to gapped chiral phases in which the chiral order coexist with either the dimer or the Néel order, depending on the sign of γ_{nd} .

First, when $\gamma_{\text{nd}} < 0$, $\sqrt{4\pi} \phi_+$ is locked at

$$\sqrt{4\pi} \phi_+ = 0 \text{ or } \pi, \quad (58)$$

which produces a finite value of the z component of the dimer order parameter, D_{123}^z , as seen in Eq. (30). We have thus obtained the “chiral dimer phase” in which the vector chiral and dimer orders coexist.³⁴ Once ϕ_+ is locked as in Eq. (58), the locking position of $\sqrt{4\pi} \theta_-$ is affected by the γ_1 term in Eq. (37) and changed from $\pm\pi/2$ of the gapless chiral phase [see Eq. (46)], so that the xy component of the dimer

order parameter, D_{123}^{xy} , also becomes finite, in agreement with Fig. 2. Specifically, for positive γ_1 , the field-locking positions of the four degenerate ground states change smoothly with the strength of γ_1 as

$$(\sqrt{4\pi}\phi_+, \sqrt{4\pi}\theta_-) = \begin{cases} (0, \pm\frac{\pi}{2}) \longrightarrow (0, 0), \\ (\pi, \pm\frac{\pi}{2}) \longrightarrow (\pi, \pm\pi) \equiv (\pi, \pi), \end{cases} \quad (59)$$

finally resulting in the two degenerate ground states of either the Haldane dimer or the singlet dimer phase as specified by Eq. (29). For negative γ_1 , the field-locking positions change as

$$(\sqrt{4\pi}\phi_+, \sqrt{4\pi}\theta_-) = \begin{cases} (0, \pm\frac{\pi}{2}) \longrightarrow (0, \pm\pi) \equiv (0, \pi), \\ (\pi, \pm\frac{\pi}{2}) \longrightarrow (\pi, 0), \end{cases} \quad (60)$$

resulting in the two degenerate ground states of the even-parity dimer phase as indicated by Eq. (40).

Second, when $\gamma_{nd} > 0$, ϕ_+ is locked at

$$\sqrt{4\pi}\phi_+ = \pm\frac{\pi}{2}. \quad (61)$$

This yields a finite Néel order parameter along the z direction, as we explain below. From Eqs. (21) and (24), the S_ℓ^z operator has the staggered component

$$(-1)^\ell S_\ell^z = \frac{a}{\sqrt{4\pi}} \partial_x \phi_- + \dots, \quad (62)$$

which, at first sight, looks insensitive to the locking of ϕ_+ . However, after the locking (61), the γ_{tw}'' term in Eq. (37) reduces to the operator $\pm\gamma_{tw}'' \partial_x \phi_-$, which can be absorbed into the Gaussian part of H_- in Eq. (44) by redefining ϕ_- (so that $\partial_x \phi_-$ is shifted by a constant). Consequently, Eq. (62) acquires a nonvanishing expectation value

$$(-1)^\ell \langle S_\ell^z \rangle = -\frac{K_+ a}{\sqrt{4\pi} v_+} \gamma_{tw}'' \langle \sin(\sqrt{4\pi}\phi_+) \rangle + \dots \quad (63)$$

We have therefore obtained the ‘‘chiral Néel phase’’ in which the vector chiral and Néel orders coexist.

At the BKT transition point $K_+ = 1/2$, the sine-Gordon theory for the ‘‘+’’ sector predicts the appearance of a multiplicative logarithmic correction to the correlation functions:^{30,42,72,73}

$$\langle S_\ell^+ S_{\ell'}^- \rangle = A \frac{e^{-iQ(\ell'-\ell)}}{|\ell'-\ell|} \ln^{1/2}(|\ell'-\ell|/a) + \dots \quad (64)$$

This logarithmic correction is utilized to locate the BKT phase transition point numerically in the next section.

B. Numerical results

In this section, we present our numerical iTEBD results (with the Schmidt rank $\chi = 300$) on the spin correlation functions in the easy-plane case $0 \leq \Delta < 1$.

1. Spin correlations in the gapless chiral phase

We first discuss the numerical results for the gapless chiral phase, where we choose the ground state with $\kappa_{12} > 0$. Figure 12 shows the in-plane spin correlation function $|\langle S_{1+r}^+ S_{1+r}^- \rangle|$ at $\Delta = 0.8$ for various values of J_1/J_2 in the gapless chiral phase. The data for $|J_1|/J_2 \gtrsim 2$ follow straight

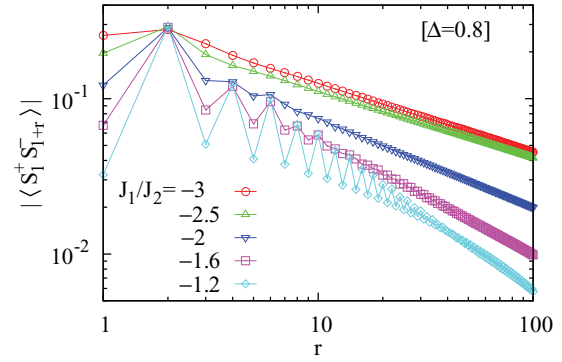


FIG. 12. (Color online) In-plane spin correlation function $|\langle S_{1+r}^+ S_{1+r}^- \rangle|$ for fixed $\Delta = 0.8$ and various values of J_1/J_2 in the gapless chiral phase. Logarithmic scales are used in both axes.

lines in logarithmic scales, in agreement with the power-law behavior in Eq. (55). By contrast, the data for $J_1/J_2 = -1.6$ and -1.2 show some oscillations at short distances although the overall behaviors are linear as expected from Eq. (55) (we suspect that the downward bending at large r for $J_1/J_2 = -1.2$ is due to a finite Schmidt rank $\chi = 300$ and is not a genuine behavior).

The origin of the oscillations can be found in the spin structure factors shown in Fig. 13. For L consecutive spins at the sites $\ell = 1, 2, \dots, L$ in a translationally invariant infinite

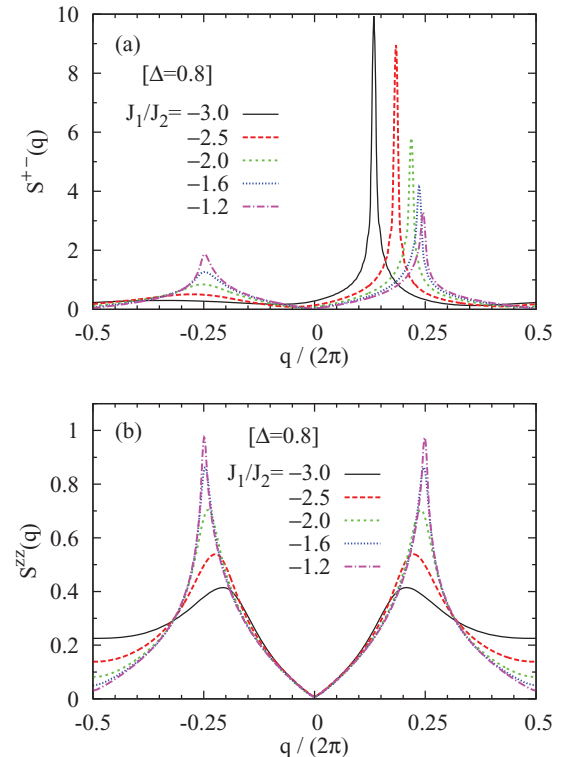


FIG. 13. (Color online) Equal-time spin structure factors [see Eq. (66)], (a) $S^{+-}(q)$ and (b) $S^{zz}(q)$, in the gapless chiral phase. Calculations were done for the same parameter points as in Fig. 12, and we set $L = 100$.

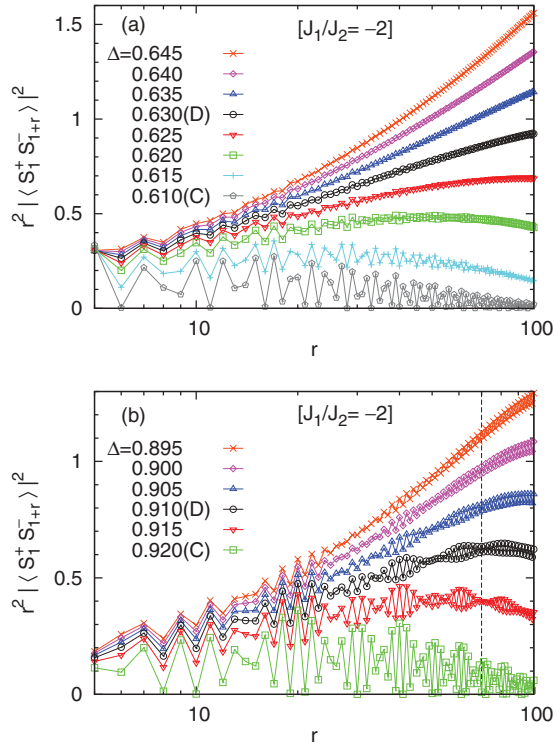


FIG. 14. (Color online) In-plane spin correlation function, calculated for fixed $J_1/J_2 = -2$ and various values of Δ around the transition points shown in Fig. 2. The symbols “C” and “D” indicate our estimates of the transition points (with a precision of 0.005) for the onsets of the vector chiral and dimer orders, respectively. Logarithmic scale is used for the horizontal axis. At the BKT transition related to the onset of the dimer order, the plotted function is expected to become linear in the long-distance limit, which we use to determine the “D” points. In (b), all the curves are slightly bent downward around $r = 70$ (broken vertical line) due to the finiteness of the Schmidt rank $\chi (= 300)$ in iTEBD, so we use the range $r \lesssim 70$ for our analysis.

system treated by iTEBD, we introduce

$$S_q^\alpha = \frac{1}{\sqrt{L}} \sum_{\ell=1}^L S_\ell^\alpha e^{-iq\ell} \quad (65)$$

and define the equal-time spin structure factors as

$$S^{\alpha\beta}(q) = \langle S_q^\alpha S_{-q}^\beta \rangle \text{ with } (\alpha, \beta) = (+, -), (z, z). \quad (66)$$

In Fig. 13(a), $S^{+-}(q)$ shows sharp peaks at incommensurate wave number $q = Q > 0$, which become sharper and higher for large $|J_1|/J_2$. This feature is consistent with Eq. (55), provided that K_+ becomes larger with increasing $|J_1|/J_2$; see Eq. (38). These peaks are expected to diverge as $L \rightarrow \infty$ in the gapless chiral phase. For small $|J_1|/J_2$, a second peak around $q = -Q < 0$ develops, which indicates the ellipticity of the spiral correlations and is the origin of the oscillating behavior in Fig. 13. The appearance of the second peak can be understood by observing that $S^{+-}(q)$ should gradually become left-right symmetric as the vector chiral order parameter κ^z decreases.²² In Fig. 13(b), $S^{zz}(q)$ shows linear behaviors around $q = 0$ as expected from the Fourier transform of Eq. (56): $S^{zz}(q) = K_+ |q|/2\pi$ for $|q| \ll 1$. In addition, it shows finite peaks at incommensurate q . Although the explanation of

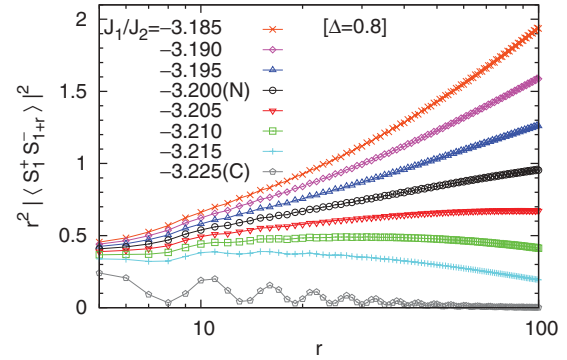


FIG. 15. (Color online) In-plane spin correlation, calculated for fixed $\Delta = 0.8$ and various values of J_1/J_2 around the transition points shown in Fig. 3. The symbols “C” and “N” indicate our estimates of the transition points (with a precision of 0.005) for the onsets of the vector chiral and Néel orders, respectively.

these peaks is beyond the scope of the effective theory, their occurrence is rather natural for $\Delta = 0.8$, since the xy and z components should show similar behaviors as the system approaches the isotropic limit $\Delta = 1$.

2. Transitions to the gapped chiral phases

Next we analyze how the spin correlation changes at the transition from the gapless chiral phase to the gapped dimer or Néel phase. The existence of the intermediate gapped chiral phases where two kinds of orders coexist is anticipated from the analyses of the order parameters and entanglement entropy in Figs. 2 and 3 and from the bosonization analysis of Sec. IV A3. The in-plane spin correlation function is expected to show a multiplicative logarithmic correction in Eq. (64) at the BKT transition point from the gapless to gapped chiral phases. Therefore, in Figs. 14 and 15, we plot $r^2 |\langle S_1^+ S_{1+r}^- \rangle|^2$, which is expected to become a linear function of $\ln r$ at the BKT transition point. In Figs. 14(a) and 14(b), the symbols “C” indicate the Ising transition points (determined in Fig. 2) at which the inversion symmetry is spontaneously broken and the vector chiral order appears. Finding the linear behavior of the plotted functions, we determine the BKT transition points as indicated by the symbols “D.” Narrow but finite ranges of intermediate phases between “C” and “D” are found in the intervals $0.61 \lesssim \Delta \lesssim 0.63$ and $0.91 \lesssim \Delta \lesssim 0.92$, which we identify with the “chiral (even-parity and Haldane) dimer phases.” Similarly, we determine the range of the “chiral Néel phase” in Fig. 15. In this way, we have determined the “ \times ” symbols in Fig. 1. Since the method of determining the BKT point from the logarithmic correction to spin correlation, as employed here, has not been discussed in literature (as far as we know), we demonstrate its validity using a simpler example in Appendix B.

3. Pitch angle

Finally, we determine the pitch angle Q of the incommensurate spin correlations in the vector chiral and gapped phases. It is determined from the maximum position of the in-plane structure factor $S^{+-}(q)$ (as in Ref. 74). The data of Q so obtained as a function of J_1/J_2 are shown for different values of Δ in Fig. 16. The Lifshitz points, at which the

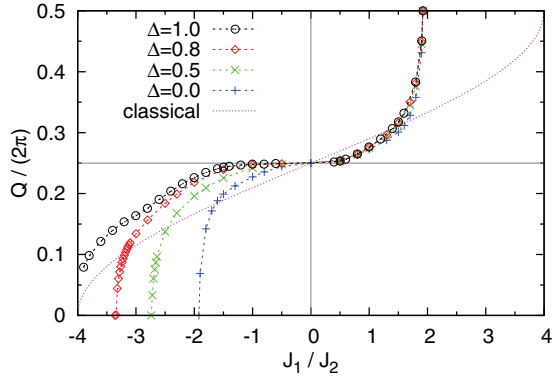


FIG. 16. (Color online) Pitch angle Q as a function of J_1/J_2 for different values of Δ . This angle is determined by finding the peak in the in-plane structure factor $S^+(q)$ as shown in Fig. 13(a). The classical value $Q = \arccos(-\frac{J_1}{J_2})$, which is independent of Δ , is plotted together for comparison.

in-plane spin correlation function changes its character from incommensurate to commensurate ($Q = 0$ or π), occur inside the singlet dimer phase for $J_1 > 0$ and inside the even-parity dimer or Néel phase for $J_1 < 0$. For $J_1 > 0$ and all values of Δ , the determined Lifshitz points are very close to the point $J_1/J_2 = 2$ with the exact singlet dimer ground states. According to the argument of Ref. 56, the Lifshitz points should be in fact located exactly at $J_1/J_2 = 2$. The small discrepancy comes from the difference in the definition of Q ; in Ref. 56, it is defined in terms of the asymptotic behavior of the correlation function in the long-distance limit. For $J_1 < 0$, the determined Lifshitz line is drawn by broken lines in Fig. 1; it starts from the highly degenerate point^{68,74} $(J_1/J_2, \Delta) = (-4, 1)$ and ends near the point $(J_1/J_2, \Delta) = (-2, 0)$ with the exact even-parity dimer ground states.

V. EASY-AXIS CASE $\Delta > 1$

To complete our analysis of the XXZ chain model (1) with $J_1 < 0$ and $J_2 > 0$, let us shortly discuss the case with easy-axis anisotropy $\Delta > 1$. In this case, Igarashi³⁵ and Tonegawa *et al.*¹⁸ have found the following three phases. For $J_1/J_2 \lesssim -4$, the ground state is fully polarized (ferromagnetic) along the z direction. For small $|J_1|/J_2$ and large Δ , the ground state is antiferromagnetic, having a period-4 structure $\uparrow\uparrow\downarrow\downarrow \dots$ (uudd). Between the fully polarized and uudd phases intervenes the partially polarized phase, in which the spontaneous ferromagnetic moment along the z direction changes continuously as a function of J_1/J_2 and Δ . We note that the uudd phase was also found in the model with antiferromagnetic $J_{1,2} > 0$.³⁶ Here, we describe the uudd and partially polarized phases in terms of the Abelian bosonization formulation for $|J_1|/J_2 \ll 1$ and $0 < \Delta - 1 \ll 1$.

A. uudd phase

We start from the decoupled isotropic Heisenberg chains with $J_2 > 0$. The in-chain easy-axis anisotropy $J_2(\Delta - 1) \sum_{j,n} S_{2j+n}^z S_{2j+n+2}^z$ (with $\Delta > 1$) adds to the Hamiltonian the backscattering terms

$$\gamma_{\text{bs}} [\cos(2\sqrt{2\pi}\phi_1) + \cos(2\sqrt{2\pi}\phi_2)] \quad (67)$$

with $\gamma_{\text{bs}} < 0$. If this term grows dominantly under the RG, the fields are locked at

$$(\sqrt{2\pi}\phi_1, \sqrt{2\pi}\phi_2) = (0, 0), (0, \pi), (\pi, 0), \text{ or } (\pi, \pi). \quad (68)$$

These fourfold degenerate ground states correspond to the period-4 uudd structures with

$$\langle S_{2j+1}^z \rangle = c_2(-1)^j, \quad \langle S_{2j+2}^z \rangle = \pm c_2(-1)^j, \quad (69)$$

where c_2 is a nonzero constant [see Eq. (21)].

B. Partially polarized phase

The partially polarized phase found numerically¹⁸ can be understood from the mean-field treatment of the operator $(\partial_x \phi_+) \sin(\sqrt{4\pi}\phi_-)$,⁵⁴ which is contained in \mathcal{O}_{tw} in Eq. (25b). Here we review the formulation of Zarea *et al.*,⁵⁴ and then discuss the behaviors of correlation functions, which were not discussed in detail in previous studies.^{18,35,54}

We start from the effective Hamiltonian⁵⁴

$$H = \int dx \left\{ \sum_{v=\pm} \frac{v_v}{2} [K_v(\partial_x \theta_v)^2 + K_v^{-1}(\partial_x \phi_v)^2] + \gamma'_{\text{tw}} (\partial_x \phi_+) \sin(\sqrt{4\pi}\phi_-) \right\} \quad (70)$$

with $\gamma'_{\text{tw}} < 0$. The mean-field decoupling similar to the one used in Sec. IV A2 yields the effective Hamiltonian $H = H_+ + H_-$, where

$$H_+ = \int dx \frac{v_+}{2} [K_+(\partial_x \theta_+)^2 + K_+^{-1}(\partial_x \tilde{\phi}_+)^2], \quad (71)$$

$$H_- = \int dx \left\{ \frac{v_-}{2} [K_-(\partial_x \theta_-)^2 + K_-^{-1}(\partial_x \phi_-)^2] + \gamma'_{\text{tw}} \mu \sin(\sqrt{4\pi}\phi_-) \right\}. \quad (72)$$

Here we have introduced

$$\tilde{\phi}_+(x) = \phi_+(x) - \mu x, \quad (73)$$

with

$$\mu = -\frac{K_+ \gamma'_{\text{tw}} \langle \sin(\sqrt{4\pi}\phi_-) \rangle}{v_+} = \langle \partial_x \phi_+ \rangle. \quad (74)$$

There are two self-consistent solutions: $\mu = +|\mu|$, $-|\mu|$. A nonvanishing μ directly leads to the spontaneous magnetization

$$\langle S_\ell^z \rangle = \frac{a}{\sqrt{4\pi}} \langle \partial_x \phi_+ \rangle = \frac{a}{\sqrt{4\pi}} \mu \equiv M. \quad (75)$$

Furthermore, the sine potential in H_- locks the bosonic field at

$$\sqrt{4\pi}\phi_- = \frac{\pi}{2} \text{sgn}(\mu). \quad (76)$$

To see the physical consequence of the field locking in Eq. (76), we discuss spin correlation functions in the ground state. The transverse component of spin, S_ℓ^+ , contains the operator $e^{\pm\sqrt{\pi}\theta_-}$, which strongly fluctuates due to the locking of the dual field ϕ_- ; therefore the correlation function $\langle S_\ell^+ S_{\ell'}^- \rangle$ decays exponentially with the distance. Instead, the longitudinal correlation $\langle S_\ell^z S_{\ell'}^z \rangle$ and the bond nematic correlation^{71,75}

$\langle S_\ell^+ S_{\ell+1}^+ S_{\ell'}^- S_{\ell'+1}^- \rangle$ show power-law decays. Ignoring fluctuations of ϕ_- , we obtain the bosonized expressions for these operators as

$$S_\ell^z = M + \frac{a}{\sqrt{4\pi}} \tilde{\phi}_+ + A_1 \cos \left\{ \sqrt{\pi} \tilde{\phi}_+ + \pi \left[M - \frac{\text{sgn}(M)}{2} \right] \left(\ell - \frac{3}{2} \right) \right\} + \dots, \quad (77)$$

$$S_\ell^+ S_{\ell+1}^+ = (-1)^{\ell+1} B_0^2 e^{i\sqrt{4\pi}\theta_+} + 2B_0 B_1 e^{i\sqrt{4\pi}\theta_+} \cos \left[\frac{\pi}{2} \left(\frac{1}{2} - |M| \right) \right] \times \cos \left\{ \sqrt{\pi} \tilde{\phi}_+ + \pi \left[M + \frac{\text{sgn}(M)}{2} \right] (\ell - 1) \right\} + \dots, \quad (78)$$

from which the correlation functions are calculated as

$$\langle S_\ell^z S_{\ell'}^z \rangle = M^2 - \frac{K_+}{2\pi^2 |\ell' - \ell|^2} + B \frac{\cos \left[\pi \left(|M| - \frac{1}{2} \right) (\ell' - \ell) \right]}{|\ell' - \ell|^{K_+/2}} + \dots, \quad (79)$$

$$\langle S_\ell^+ S_{\ell+1}^+ S_{\ell'}^- S_{\ell'+1}^- \rangle = B' \frac{(-1)^{\ell'-\ell}}{|\ell' - \ell|^{2/K_+}} - B'' \frac{\cos \left[\pi \left(|M| + \frac{1}{2} \right) (\ell' - \ell) \right]}{|\ell' - \ell|^{2/K_+ + K_+/2}} + \dots, \quad (80)$$

with $B \propto A_1^2$, $B' \propto B_0^4$, and $B'' \propto B_0^2 B_1^2$. We note that the TLL phases with similar power-law correlations, called the nematic and SDW₂ phases, have also been discussed for the model (1) in a magnetic field, for both ferromagnetic^{71,75–77} and antiferromagnetic^{78,79} J_1 . For small $|J_1|/J_2$ and $\Delta = 1$, K_+ is close to unity, and the longitudinal (spin-density-wave; SDW) correlation decays more slowly than the nematic correlation. The TLL phase with a dominant SDW correlation and short-ranged transverse spin correlation is called the SDW₂ state in Refs. 71 and 79. It is natural to assume that the partially polarized phase at $\Delta > 1$ in zero magnetic field is continuously connected to the SDW₂ phase in a finite magnetic field.^{71,75,76} With interchain couplings, the dominant quasi-long-range SDW correlation is expected to evolve into a true long-range order.⁸⁰ Since K_+ changes continuously in the TLL phases, it is also possible that the system crosses over to a region with the dominant nematic correlation ($K_+ > 2$). It is known that such a region does appear at high-magnetic fields.^{71,75,76}

VI. CONCLUSIONS

In this paper, we have studied the ground-state properties of the one-dimensional spin-1/2 frustrated ferromagnetic XXZ model (1). In the isotropic case $\Delta = 1$, the nonmagnetic phase in the region $-4 < J_1/J_2 < 0$ was characterized as the Haldane dimer phase, in which the ground state has spontaneous ferromagnetic dimerization and nonlocal string order. We argued that the dimer order is associated with an emergent spin-1 degree of freedom on every other bond. In the easy-plane case $0 \leq \Delta < 1$, the model displays a rich

phase diagram as in Fig. 1. Our previous works have revealed the appearance of the gapless chiral phase in a wide region for $-4 < J_1/J_2 < 0$ ¹⁵ and the unusual alternate appearance of the Néel and even-parity dimer phases.²⁴ In this paper, we have newly discovered narrow intermediate gapped phases in which the vector chiral order coexists with the dimer or Néel order. We described how the properties of the various phases can be captured for $|J_1|/J_2 \ll 1$ and general anisotropy $\Delta \geq 0$ by the Abelian bosonization formalism, as summarized in Table I (by continuity, the same qualitative description can be extended to larger $|J_1|/J_2$).

The Haldane dimer phase we found for $\Delta = 1$ has only a very small excitation gap and, with a weak easy-plane anisotropy, is easily replaced by the gapless chiral phase. With small interchain couplings, the gapless chiral phase would evolve into a genuine spiral long-range-order. Therefore the stable appearance of the gapless chiral phase up to the close vicinity of the isotropic case $\Delta = 1$ naturally explains why many quasi-one-dimensional cuprates with ferromagnetic $J_1 < 0$ show the spiral magnetism and the associated multiferroicity.¹⁵ By contrast, it is also expected that the small excitation gap ($\lesssim 0.06 J_2$; see Sec. III B 2) in the Haldane dimer phase can be enhanced by a coupling with phonons, due to the spin-Peierls mechanism as is known in the antiferromagnetic J_1 - J_2 chain compound CuGeO₃.⁸¹ It will be interesting to explore a spin-Peierls transition to the Haldane dimer phase in quasi-1D edge-sharing cuprates without a spiral magnetic order. The present study also raises the possibility of observing the chiral Haldane dimer state, which shows no magnetic order but a spontaneous electric polarization due to a vector chiral order of spins.

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APPENDIX A: DERIVATION OF THE RENORMALIZATION GROUP EQUATIONS (16)

Here we briefly explain how the RG equations (16) are derived by using the perturbative RG method⁴⁶ and the operator product expansions (OPE) in the $SU(2)_1$ WZW theory. We first discuss the OPEs in the decoupled spin chains, each described by the $SU(2)_1$ WZW theory. We drop the chain subscript $n = 1, 2$. The OPEs of the uniform spin components $M_{R/L}$ obey the well-known $SU(2)$ current algebra:^{31,33,47–49}

$$M_{R/L}^a(x, \tau) M_{R/L}^b(\mathbf{0}) = \frac{\delta^{ab}}{8\pi^2 z_{R/L}^2} + \frac{i \varepsilon^{abc} M_{R/L}^c(\mathbf{0})}{2\pi z_{R/L}} \quad (A1)$$

with $z_{R/L} = v\tau \mp ix$. Here, ε^{abc} is the fully antisymmetric tensor with $\varepsilon^{123} = 1$, and summation over repeated indices are assumed throughout the appendix. The OPEs present the singular terms that appear when two operators at the points (x, τ) and $\mathbf{0} = (0, 0)$ are brought close together.

The OPEs of the uniform components $M_{R/L}^a$ with the staggered components N^a and the dimerization ϵ are given by⁴⁹

$$M_{R/L}^a(x, \tau)N^b(\mathbf{0}) = \frac{i}{4\pi z_{R/L}} [\varepsilon^{abc} N^c(\mathbf{0}) \pm \delta^{ab} \epsilon(\mathbf{0})], \quad (\text{A2})$$

$$M_{R/L}^a(x, \tau)\epsilon(\mathbf{0}) = \frac{\mp i N^a(\mathbf{0})}{4\pi z_{R/L}}. \quad (\text{A3})$$

These equations imply that $M_{R/L}$ induce mixing of N and ϵ .

Similar to Eqs. (A2) and (A3), the OPEs among N and ϵ can be derived^{33,49} by taking advantage of the well-known spin-charge separation in 1D spin-1/2 Dirac fermions; with bosonization, the charge and spin sectors of Dirac fermions are described by a free scalar boson and the $SU(2)_1$ WZW theory, respectively. The use of fermionic fields simplifies the calculations of OPEs in the WZW theory. For illustration, here we derive the OPE of two ϵ 's. We take the same conventions as used in the Appendix of Ref. 49, and introduce the right- and left-moving fermionic fields $\Psi_{R/L,s}$ ($s = \uparrow, \downarrow$), which obey the OPEs

$$\Psi_{R/L,s}(x, \tau)\Psi_{R/L,s'}^\dagger(\mathbf{0}) = \frac{\delta_{ss'}}{2\pi z_{R/L}}. \quad (\text{A4})$$

We define the fermionic staggered dimerization operator as

$$\epsilon_F = \frac{i}{2}(\Psi_{R_s}^\dagger \Psi_{L_s} - \Psi_{L_s}^\dagger \Psi_{R_s}). \quad (\text{A5})$$

Using bosonization, one can show that ϵ_F is related to ϵ as

$$\epsilon_F = \epsilon \cos(\sqrt{2\pi}\phi_\rho), \quad (\text{A6})$$

where ϕ_ρ is the bosonic field of the charge sector. We now assume that the charge sector is in the gapped Mott phase where ϕ_ρ is locked ($\langle \phi_\rho \rangle = 0$) as in the Hubbard chain at half-filling. This allows us to identify ϵ_F with $\lambda\epsilon$, where $\lambda = \langle \cos(\sqrt{2\pi}\phi_\rho) \rangle$ is a dimensionless constant of order unity. The OPE of two ϵ 's is then obtained from the OPE of two ϵ_F 's.

Performing all possible contractions of four fermion fields (see Appendix A of Ref. 82), the OPE of two ϵ_F 's is calculated as

$$\begin{aligned} \epsilon_F(x, \tau)\epsilon_F(\mathbf{0}) &= \frac{1}{4}\Psi_{R_s}^\dagger(x, \tau)\Psi_{L_s}(x, \tau)\Psi_{L_{s'}}^\dagger(\mathbf{0})\Psi_{R_{s'}}(\mathbf{0}) \\ &\quad + (R \leftrightarrow L) \\ &= \frac{1}{4\pi z_R z_L} + \frac{1}{4\pi} \left[\frac{\rho_R(\mathbf{0})}{z_L} - \frac{\rho_L(\mathbf{0})}{z_R} \right] \\ &\quad + \frac{1}{2}\Psi_{R_s}^\dagger(\mathbf{0})\Psi_{L_s}(\mathbf{0})\Psi_{L_{s'}}^\dagger(\mathbf{0})\Psi_{R_{s'}}(\mathbf{0}) \end{aligned}$$

with $\rho_{R/L} = \Psi_{R/L,s}^\dagger \Psi_{R/L,s}$. The last term is related to the backscattering term:

$$\Psi_{R_s}^\dagger \Psi_{L_s} \Psi_{L_{s'}}^\dagger \Psi_{R_{s'}} = -2\mathbf{M}_R \cdot \mathbf{M}_L - \frac{1}{2}\rho_R \rho_L, \quad (\text{A7})$$

where the uniform components of the fermionic spin density are defined as

$$M_R^a = \frac{1}{2}\Psi_{R_s}^\dagger \sigma_{ss'}^a \Psi_{R_{s'}}, \quad M_L^a = \frac{1}{2}\Psi_{L_s}^\dagger \sigma_{ss'}^a \Psi_{L_{s'}}. \quad (\text{A8})$$

After gapping out the charge sector, we can neglect the fluctuations of $\rho_{R/L}$. Thus we obtain

$$\epsilon(x, \tau)\epsilon(\mathbf{0}) = \frac{1}{4\pi^2 \lambda^2 z_R z_L} - \frac{1}{\lambda^2} \mathbf{M}_R(\mathbf{0}) \cdot \mathbf{M}_L(\mathbf{0}). \quad (\text{A9})$$

Similar calculations yield

$$\begin{aligned} N^a(x, \tau)N^b(\mathbf{0}) &= \frac{\delta^{ab}}{4\pi^2 \lambda^2 z_R z_L} \\ &\quad + \frac{i\varepsilon^{abc}}{2\pi \lambda^2} \left[\frac{M_R^c(\mathbf{0})}{z_L} + \frac{M_L^c(\mathbf{0})}{z_R} \right] \\ &\quad + \frac{1}{\lambda^2} \mathcal{O}_{NN}^{ab}(\mathbf{0}), \end{aligned} \quad (\text{A10})$$

$$N^a(x, \tau)\epsilon(\mathbf{0}) = \frac{-i}{2\pi \lambda^2} \left[\frac{M_R^a(\mathbf{0})}{z_L} - \frac{M_L^a(\mathbf{0})}{z_R} \right] \quad (\text{A11})$$

where \mathcal{O}_{NN}^{ab} in Eq. (A10) is expressed in terms of fermionic fields as

$$\mathcal{O}_{NN}^{ab} = \frac{1}{2}\sigma_{s_1 s_2}^a \sigma_{s_3 s_4}^b \Psi_{R_{s_1}}^\dagger \Psi_{L_{s_2}} \Psi_{L_{s_3}}^\dagger \Psi_{R_{s_4}}. \quad (\text{A12})$$

For the current purpose, we only need the trace (in the spin direction indices) of this term, which gives the backscattering term: $\mathcal{O}_{NN}^{aa} = \mathbf{M}_R \cdot \mathbf{M}_L - \frac{3}{4}\rho_R \rho_L$.

In the limit of weak interchain coupling $|J_1| \ll J_2$, the OPEs of the perturbation operators in Eq. (11) are readily obtained from the OPEs of operators in each decoupled chain described above. Given the OPEs, one can write down the corresponding one-loop RG equations.⁴⁶ For example, if the OPE of marginal operators \mathcal{O}_a and \mathcal{O}_b have the form

$$\mathcal{O}_a \mathcal{O}_b = \frac{\lambda_{ab}^c}{(2\pi)^2 z_R z_L} \mathcal{O}_c + \dots, \quad (\text{A13})$$

where λ_{ab}^c are dimensionless constants, then the one-loop RG equation for the perturbation $g_c \mathcal{O}_c$ has the contribution

$$\frac{dg_c}{dl} = -\frac{g_a g_b \lambda_{ab}^c}{4\pi v} + \dots. \quad (\text{A14})$$

APPENDIX B: TLL-DIMER TRANSITION

In Sec. IV B, we determined the BKT transition points between gapless and gapped chiral phases by observing the logarithmic correction in the spin correlation function (see Figs. 14 and 15). Here we test the validity of the method with a simpler example. We consider the antiferromagnetic XY model with $J_1, J_2 > 0$ and $\Delta = 0$. For large $J_1/J_2 (\gtrsim 3)$, the system is in a TLL phase in which the transverse spin correlation function behaves as³⁰

$$\langle S_\ell^x S_{\ell'}^x \rangle = \frac{A_0^x (-1)^{\ell' - \ell}}{|\ell' - \ell|^\eta} - \frac{A_1^x}{|\ell' - \ell|^{\eta+1/\eta}} + \dots. \quad (\text{B1})$$

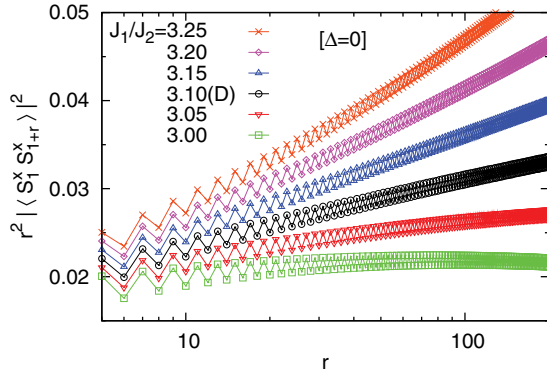


FIG. 17. (Color online) Plots of $r^2 |\langle S_1^x S_{1+r}^x \rangle|^2$ for fixed $\Delta = 0$ and various values of J_1/J_2 around the TLL-dimer transition point studied in Ref. 4. A logarithmic scale is used for the horizontal axis. The symbol “D” indicates the estimate of the transition point within the current analysis (with a precision of 0.05), which agrees reasonably well with the previous accurate estimate⁴ $J_2/J_1 \approx 3.0893$.

Here, A_0^x and A_1^x are nonuniversal constants. The decay exponent η gradually increases as J_1/J_2 is decreased. At $\eta = 1$, a BKT transition from the TLL to the singlet dimer phase occurs. At the transition point, a multiplicative logarithmic correction appears in the spin correlation function:^{30,42,72,73}

$$\langle S_\ell^x S_{\ell'}^x \rangle = \frac{A_0^x (-1)^{\ell' - \ell}}{|\ell' - \ell|} \ln^{\frac{1}{2}}(|\ell' - \ell|/a) + \dots \quad (\text{B2})$$

In Fig. 17, we plot the function $r^2 |\langle S_1^x S_{1+r}^x \rangle|^2$ for various J_1/J_2 around the BKT transition point. From the linear behavior as a function of $\ln r$, we locate the BKT transition point. In this figure, the data points of $J_1/J_2 = 3.10$ and 3.15 exhibit almost linear behavior. It is not easy to decide which one of the two curves is closer to the perfect linear dependence. Here we choose the one with smaller correlations since the iTEBD method tends to underestimate correlations at large r . The determined point $J_1/J_2 = 3.10$ agrees reasonably well with the previous accurate estimate⁴ $J_2/J_1 \approx 3.0893$.

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- $$\begin{aligned} e^{i\sqrt{2\pi}\theta_n(x)} e^{\pm i\sqrt{2\pi}\phi_n(x)} &= e^{\pm i\sqrt{2\pi}\phi_n(x)} e^{i\sqrt{2\pi}\theta_n(x)} e^{\mp 2\pi[\theta_n(x), \phi_n(x)]} \\ &= -e^{\pm i\sqrt{2\pi}\phi_n(x)} e^{i\sqrt{2\pi}\theta_n(x)}, \end{aligned}$$
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