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

Shunsuke Furukawa,† Masahiro Sato,‡ Shigeki Onoda,§ and Akira Furusaki

†Department of Physics, University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-0033, Japan
‡Department of Physics and Mathematics, Aoyama Gakuin University, Sagamihara, Kanagawa 252-5258, Japan
§Condensed Matter Theory Laboratory, RIKEN, Wako, Saitama 351-0198, Japan

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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. Among them, the 1D XXZ model with competing nearest-neighbor $J_1$ and second-neighbor $J_2$ interactions, defined by the Hamiltonian

$$H = \sum_{n=1}^{2} \sum_{\ell} J_n \left(S^x_{\ell+n} S^x_{\ell+n} + S^y_{\ell+n} S^y_{\ell+n} + \Delta S^z_{\ell+n} S^z_{\ell+n}\right),$$

provides a paradigmatic example expected to host rich variety of physics. Here $S_\ell = (S^x_\ell, S^y_\ell, S^z_\ell)$ represents the spin-$\frac{1}{2}$ operator at the site $\ell \in \mathbb{Z}$ and $\Delta$ 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 mostly considered the case when both $J_1$ and $J_2$ are antiferromagnetic. 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, LiCu$_2$O$_2$, LiCuVO$_4$ (Refs. [1,2]), and PbCuSO$_4$(OH)$_2$ (Ref. [2]), for example, exhibit multiferroic behaviors, 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. By contrast, Rb$_2$Cu$_2$Mo$_3$O$_7$ (Ref. [3]) 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-$\frac{1}{2}$ frustrated ferromagnetic XXZ chain (1) with $J_1 < 0$ and $J_2 > 0$, by means of the infinite time evolving block decimation algorithm (iTEBD) 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 even-parity dimer and Néel phases with gapped excitations (Refs. [4,5,6,7]). 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 (Refs. [5,6,7]). 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 inter-chain 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 $S \to \infty$, the ground state phase...
parity dimer and Néel phases alternately appear when \( \Delta \) occurs at \( T_{\text{LL}} \), even-parity dimer, and Néel phases are determined in a two kinds of orders coexist. The phase boundaries among the

\[
\cos(\theta_{\text{even-parity dimer}}) = \frac{J_1}{\sqrt{J_1^2 + J_2^2}}
\]

and ∆. 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 ∆ = 1 for \( -4 < J_1/J_2 \leq -2.5 \) (we also refer to Refs. 22, 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. 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 phase discussed in Refs. 22, 23 and a Néel ordered phase appear alternately as ∆ 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 ∆ = 1. Previous field-theoretical analyses has 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

\[
D_{\ell,\ell+1,\ell+2} = \langle S_{\ell} \cdot S_{\ell+1} \rangle - \langle S_{\ell+1} \cdot S_{\ell+2} \rangle.
\]
Remarkably, this dimer order is associated with ferromagnetic correlations \( \langle S_i \cdot S_{i+1} \rangle > 0 \) 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 state as in the Haldane chain. 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. 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. In this section, we present numerical results on several order parameters and half-chain entanglement entropy, which provide the most basic information for identifying symmetry-broken phases. In Sec. II, we discuss in detail the dimer phases in the SU(2)-symmetric case \( \Delta = 1 \) from both field-theoretical and numerical analyses. In Sec. VI, 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 and, following Ref. [28], discuss its instability towards 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 \( \Delta = 0 \) can be understood in the Abelian bosonization framework. In Sec. VII, 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. VI.

Before presenting the numerical results, let us briefly note characteristic features of our numerical method; for a more detailed account of the method, see Supplementary Material of Ref. [28]. The iTEBD algorithm 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 \( \chi \), which gives the linear dimension of the matrices. We exploited the conservation of the total magnetization \( \sum_i S^z_i = 0 \) 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). 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.

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 \( \Delta = 0.8 \), respectively, in the phase diagram (Fig. 1). Let us first look at the vector chiral order parameter \( \kappa_{12} = \langle (S_1 \times S_2)^z \rangle \) 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 \( \kappa_{12} \), 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 the spontaneous order parameter, as previously demonstrated in the XY case \( \Delta = 0 \). 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 as

\[
S_{vN}^{vN} = -\sum_{\alpha=1}^{\chi} \lambda_\alpha^2 \ln \lambda_\alpha^2, \tag{4}
\]

where \( \{\lambda_\alpha\} \) is a set of Schmidt coefficients associated with the decomposition of the infinite system into the left and right halves and \( \chi \) 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

\[
S_{vN}^{vN} = \frac{c}{6} \ln \xi + s_1, \tag{5}
\]

where \( \xi \) is the correlation length and \( s_1 \) is a non-universal constant. In an iTEBD calculation with a finite Schmidt
FIG. 2: (Color online) (a) Chiral and (b,c) dimer order parameters and (d) half-chain entanglement entropy as functions of $\Delta$ for fixed $J_1/J_2 = -2$. These are calculated by the iTEBD with Schmidt ranks $\chi = 200$ and 300. Panel (c) is a zoom of panel (b). In panel (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 panel (a) or more accurately from the peaks in the entanglement entropy in panel (d). Broken vertical lines indicate the transition points on which dimer orders set in. In the intermediate phase in $0.61 \lesssim \Delta \lesssim 0.63$, a dip in the entanglement entropy is seen in panel (d), as zoomed in the inset.

FIG. 3: (Color online) (a) Chiral and (b) Neel 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 Neel orders, respectively. The former is determined by the peak position in the entanglement entropy in panel (c), while the latter is determined in Fig. 14. In the narrow intermediate phase in $-3.225 \lesssim J_1/J_2 \lesssim -3.200$, the vector chiral and Neel orders coexist.

rank $\chi$, the divergence of $S^{\text{vN}}$ at the critical point is replaced by the increasing function of $\chi$

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

where $s'_1$ is another non-universal 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 $S^{\text{vN}}$, we can determine the boundaries of the vector chiral phase, more accurately than by using $\kappa_{12}^z$; 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 $S^{\text{vN}}$ using Eq. (6) (which...
is expected to be satisfied for larger $\chi$, 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 case \textsuperscript{34}).

In most part of the vector chiral phase, the entanglement entropy increases as a function of $\chi$, indicating a critical nature. Indeed, in the effective field theory of Nersesyan \textit{et al.} \textsuperscript{27} 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,

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

$$
D_{\ell,\ell+1,\ell+2}^{z} := (S_{\ell}^z S_{\ell+1}^z - S_{\ell}^{z} S_{\ell+1}^{z}.
$$

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 $D_{123}^{xy} < 0$. The two order parameters are plotted in Figs. 2(b,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 $\chi$ 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: In the $\overline{XY}$ limit $\Delta = 0$, the sign of $J_1$ in Eq. (6) can be reversed by performing the $\pi$ 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, taking the above $\pi$-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 $(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)/\sqrt{2}$ (written in the $\{S_{\ell}^z\}$ basis). 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. 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 the $D_{123}^{xy}$ 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. IV, we point out that the dimer order in this region is associated with ferromagnetic nearest-neighbor correlations $\langle S_{\ell} S_{\ell+1}\rangle > 0$ 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. IV.

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. \textsuperscript{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 $\chi$; 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 B 3.

### C. Néel order

The appearance of a Néel phase with spontaneous staggered magnetizations $(S_{\ell}^z) \propto (-1)^{\ell}$ is discussed in detail in Ref. \textsuperscript{27}. In Fig. 2(b), this Néel order is detected in the region $J_1/J_2 \lesssim -3.2$ by measuring $\langle S_{\ell}^z\rangle$. 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. 2(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 B 3.
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 \( 0 < J_1/J_2 \lesssim 4.15 \), 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 for the weak-coupling limit \( |J_1| \ll J_2 \), which predicted the appearance of dimer orders for both signs 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 bosonization\(^{15,23}\) 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 (11c). The spin operators in the \( n \)-th chain \( (n = 1, 2) \) can be decomposed as

\[
S_{2j+n} \rightarrow a[M_n(x_n) + (-1)^jN_n(x_n)]
\]

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

\[
(-1)^jS_{2j+n} \cdot S_{2j+n+2} \rightarrow a\epsilon_n(x_n),
\]

which has the scaling dimension 1/2.

The inter-chain 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

\[
H' = \int dx \sum_i g_i O_i,
\]

where \( i \) runs over the following five operators\(^{23}\)

\[
O_{bs} = M_{1R} \cdot M_{1L} + M_{2R} \cdot M_{2L},
\]

\[
O_1 = M_{1R} \cdot M_{2L} + M_{1L} \cdot M_{2R},
\]

\[
O_2 = M_{1R} \cdot M_{2R} + M_{1L} \cdot M_{2L},
\]

\[
O_{tw} = \frac{a}{2}(N_1 \cdot \partial_x N_2 - N_2 \cdot \partial_x N_1),
\]

\[
O_{dtw} = \frac{a}{2}(\epsilon_1 \partial_x \epsilon_2 - \epsilon_2 \partial_x \epsilon_1).
\]

Here \( O_{bs} \) is the backscattering term present in isolated chains. The zigzag \( J_1 \) coupling produces the current-current interactions, \( O_1 \) and \( O_2 \), and the twist operator \( O_{tw} \). The dimer twist operator \( O_{dtw} \) is generated in the RG process as we see later. The bare coupling constants are given by

\[
g_{bs}(0) = -0.23(2\pi v), \quad g_1(0) = g_2(0) = 2J_1a,
\]

\[
g_{tw}(0) = J_1a, \quad g_{dtw}(0) = 0,
\]

where \( g_{bs}(0) \) was estimated in Ref. \(^{23}\). All the operators in Eq. (10) 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

\[
G_i = \frac{g_i}{2\pi v \lambda^2} (i = bs, 1, 2),
\]

\[
G_i = \frac{g_i}{2\pi v \lambda^2} (i = tw, dtw),
\]

FIG. 4: Zigzag chain picture for the \( J_1-J_2 \) chain model (1). The \( x \) axis indicates the coordinate for the continuum description.
Numerical solutions to the RG equations (16) are presented in Fig. 5. For both signs of \( J_1 \), the three coupling constants \( G_1 \), \( G_{\text{tw}} \), and \( G_{\text{dtw}} \) finally grow to large values under the RG, 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, \( G_{\text{tw}} \) retains the same sign as its initial value. The properties of the fixed points governed by large \( G_1 (> 0) \), \( G_{\text{tw}} \), and \( G_{\text{dtw}} \) are non-trivial. 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 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 Fig. 5(a) and (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 \( \xi \) should be much larger. In fact, as argued by Itoi and Qin, the correlation length becomes of astronomical scale [e.g., \( \xi/a \approx 10^{83} \sim 10^{86} \) 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 formalism to discuss the physical roles of the marginally relevant perturbations \( G_1 (> 0) \), \( G_{\text{tw}} \), and \( G_{\text{dtw}} \) 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 1.

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

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

(17)

where the velocity \( v \) and the TLL parameter \( K \) are given.
The bosonic fields $\phi_n$ and $\theta_n$ satisfy the commutation relation
\[ [\phi_n(x), \theta_{n'}(x')] = i\delta_{nn'} Y(x-x'), \]
where $Y(x-x')$ is the step function
\[ Y(x-x') = \begin{cases} 0 & (x < x'), \\ 1/2 & (x = x'), \\ 1 & (x > x'). \end{cases} \]

The spin and (in-chain) dimer operators are expressed in terms of the bosonic fields as
\[ S_{2j+n} = \frac{a}{\sqrt{2}\pi} \partial_x \phi_n(x_n) + (-1)^j A_1 \cos[2\pi \phi_n(x_n)] + \ldots, \]
\[ S_{2j+n}^+ = e^{i\sqrt{4\pi} \phi_n(x_n)} \{ (-1)^j B_0 \\ + B_1 \cos[2\pi \phi_n(x_n)] + \ldots \}, \]

where $A_1, B_0, B_1$ (Refs. [21,22], and $C$ (Ref. [23]) are non-universal constants which depend on $\Delta$.

We now focus on the case $\Delta = 1$, at which $K = 1$. To treat the coupled chains, it is useful to introduce the bosonic fields for symmetric (+) and antisymmetric (−) sectors:
\[ \phi_\pm = \frac{1}{\sqrt{2}} (\phi_1 \pm \phi_2), \quad \theta_\pm = \frac{1}{\sqrt{2}} (\theta_1 \pm \theta_2). \]

The three perturbations found to grow in the non-Abelian analysis have the following expressions:

\[ \mathcal{O}_1 = -\frac{B_1^2}{2a^2} \cos(\sqrt{4\pi} \phi_+) \cos(\sqrt{4\pi} \theta_-) \\ + \frac{1}{8\pi} \left[ (\partial_x \phi_+)^2 - (\partial_x \theta_+)^2 - (\partial_x \phi_-)^2 + (\partial_x \theta_-)^2 \right], \] (25a)

\[ \mathcal{O}_{tw} = \sqrt{\pi} B_0^2 \left( \partial_x \theta_+ \sin(4\pi \theta_-) \\ + \frac{\sqrt{\pi} A_1}{2a} \left[ (\partial_x \phi_+) \sin(4\pi \phi_-) \\ + (\partial_x \phi_-) \sin(4\pi \phi_+) \right] \right), \] (25b)

\[ \mathcal{O}_{dtw} = \sqrt{\pi} C^2 \left[ (\partial_x \phi_+) \sin(4\pi \phi_-) \\ - (\partial_x \phi_-) \sin(4\pi \phi_+) \right]. \] (25c)

Furthermore, the $\mathcal{O}_2$ term, which is decoupled from the other terms in the RG equation (18), has the expression
\[ \mathcal{O}_2 = -\frac{B_1^2}{2a^2} \cos(\sqrt{4\pi} \phi_+) \cos(\sqrt{4\pi} \theta_-) \\ + \frac{1}{8\pi} \left[ (\partial_x \phi_+)^2 + (\partial_x \theta_+)^2 - (\partial_x \phi_-)^2 - (\partial_x \theta_-)^2 \right]. \] (26)

The second lines of Eq. (25a) and Eq. (24) can be combined with the Gaussian Hamiltonians (17) of the decoupled chains, leading to
\[ H_0 = \int dx \sum_{\nu = \pm} \left( K_\nu (\partial_x \nu)^2 + K_\nu^{-1} (\partial_x \nu)^2 \right) \] (27)

with
\[ K_\pm = 1 \mp \frac{G_1}{2} + O(G_1^2, G_2^2), \]
\[ v_\pm = v \left[ 1 \pm \frac{G_2}{2} + O(G_1^2, G_2^2) \right]. \] (28)

Using the new Gaussian Hamiltonian $H_0$, we can calculate the scaling dimension of the operators in Eq. (23). 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 $K_\mp$, 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. (25a). This term locks the bosonic fields at
\[ (\sqrt{4\pi} \phi_+, \sqrt{4\pi} \theta_-) = (0, 0) \text{ or } (\pi, \pi). \] (29)

These correspond respectively to finite positive or negative value of the dimer order parameter $D_{123} = (S_1 \cdot S_2 - S_2 \cdot S_3)$, since the (inter-chain) dimer operator is expressed as
\[ S_{2j+1} \cdot S_{2j+2} = S_{2j+1} \cdot S_{2j+2} - S_{2j+2} \cdot S_{2j+3} = 2a^2 N_1 \cdot N_2 + \ldots \approx 2B_0^2 \cos(4\pi \theta_-) + A_1^2 \left[ \cos(4\pi \phi_+) + \cos(4\pi \phi_-) \right]. \] (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. (25a), 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. (24) are independent of the sign of $J_1$ in the isotropic case $\Delta = 1$. The second most relevant terms in Eq. (25a) are $(\partial_x \phi_-) \sin(\sqrt{4\pi} \theta_-)$ and $(\partial_x \phi_+) \sin(\sqrt{4\pi} \phi_-)$ with scaling dimension $2 - G_1/2$. As explained in Sec. V, we assume that the former has the effect of inducing the incommensurability in spin correlations. 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.
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 B 1), we also discuss a hidden order common to the two cases (Sec. III B 3). 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 $\langle S_j \cdot S_{j+1} \rangle$ (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:

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

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

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. 6(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 point 

\[
\frac{J_1}{J_2} = 2. \quad \text{In Fig. 6(a) we find that the weaker correlation (S$_2 \cdot $S$_3$) changes the sign at this point.}
\]

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. 6(b). Since the total wave function is a spin singlet, such spin-1’s are expected to form a valence bond solid state as in the spin-1 Haldane chain. Namely, from each encircled bond in Fig. 6(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 non-local order analyzed in Sec. III B 3.

The result of Fig. 6(a) indicates that the dimer order parameter $D_{123}$ grows to a numerically detectable magnitude for intermediate values of $|J_1| / J_2$ ($\approx 2$), although the obtained values are much 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.
In the incommensurate regions $-\pi < J_1/J_2 < 0$ and $0 < J_1/J_2 < 2$, the pitch angle $Q$ changes continuously from 0 to $\pi$, as will be discussed in Sec. IV B 3 (see Fig. 10). For $2 < J_1/J_2 \lesssim 4.15$, $Q$ is fixed at $Q = \pi$. To determine $\xi$, we plot $r^{1/2} e^{i \xi} (S_1 \cdot S_{1+r})$ as a function of $r$, and tune $\xi$ 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 $Q$ which can fit these very rapid oscillations; instead it will be determined by calculating the spin structure factor in Fig. 13.

The calculated $\xi$ is plotted in Fig. 8(b). The data for $J_1 > 0$ are broadly in agreement with Ref. [5]. We find that the values of $\xi$ are much larger for $J_1 < 0$ than for $J_1 > 0$, as anticipated from the magnitudes of the dimer order parameter in Fig. 13.

2. Spin correlation length

We determine the spin correlation length $\xi$ 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

$$\langle S_1 \cdot S_{1+r} \rangle \approx A \cos(Q r) r^{-\frac{1}{2}} e^{-r/\xi}. \quad (33)$$

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 $\pi$, as will be discussed in Sec. IV B 3 (see Fig. 10). For $2 < J_1/J_2 \lesssim 4.15$, $Q$ is fixed at $Q = \pi$. To determine $\xi$, we plot $r^{1/2} e^{i \xi} (S_1 \cdot S_{1+r})$ as a function of $r$, and tune $\xi$ 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 $Q$ which can fit these very rapid oscillations; instead it will be determined by calculating the spin structure factor in Fig. 13.

The calculated $\xi$ is plotted in Fig. 8(b). The data for $J_1 > 0$ are broadly in agreement with Ref. [5]. We find that the values of $\xi$ are much larger for $J_1 < 0$ than for $J_1 > 0$, as anticipated from the magnitudes of the dimer order parameter in Fig. 13.

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 non-local order, when we take the ground state with $D_{123} < 0$. The existence of such a hidden non-local order can be probed numerically by calculating the string correlation function

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

We use the above numerical data of the spin correlation length $\xi$, illustrated for $J_1/J_2 = -1.8$. Assuming the asymptotic behavior $e^{-r/\xi}$, we plot the function $r^{1/2} e^{i \xi} (S_1 \cdot S_{1+r})$, and tune $\xi$ such that the oscillation width of this function becomes as constant as possible as a function of $r$. While the oscillations arise from the cosine factor in (33), it is difficult to extract the pitch angle $Q$ from this figure; instead, calculations in Sec. IV B 3 give $Q/(2\pi) \approx 0.235$. 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 non-local order can be probed numerically by calculating the string correlation function

$$O_{str}(\ell, \ell + 2r) := -\left( S_\ell^z + S_{\ell+1}^z \right) \exp\left( i \pi \sum_{m=\ell+2}^{\ell+2r-1} S_m^z \right) \times \left( S_{\ell+2r}^z + S_{\ell+2r+1}^z \right). \quad (34)$$
We note that this behavior is also consistent with the even-odd structure in Fig. 7. OJ find that for both signs of \( J \) the correlation function (34) detects this 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) remains finite in the long-distance limit while \( O^r(1, 1 + 2r) \) decays to zero.

The intuition behind this expression is as follows. Consider a pair of spins \( S_{\ell + 2j}^r + S_{\ell + 2j + 1}^r \) on the bond \( (\ell + 2j, \ell + 2j + 1) \) \( (j \in \mathbb{Z}) \), which the string correlation function \( O^r \) consists of. If an odd number of valence bonds cross any cut placed between the neighboring pairs, then the pattern of \( S_{\ell + 2j}^r + S_{\ell + 2j + 1}^r \) is −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 non-vanishing value in the long-distance limit \( r \to \infty \).

Figure 9 presents the numerical data of the string correlation functions \( O^r \) calculated with different starting points \( \ell = 1, 2 \) for the ground state with \( D_{123} < 0 \). We find that for both signs of \( J \), \( O^r(2, 2 + 2r) \) remains finite in the long-distance limit while \( O^r(1, 1 + 2r) \) 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 correlation (44)

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

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

(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. (35)]. The \( J_1 / J_2 \)-dependence of \( O^2(2, 2 + 2r) \) for a long distance \( r = 50 \) is shown in Fig. 9(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. Using the Schmidt coefficients \( \{ \lambda_{\alpha\beta} \} \) calculated in iTEBD, we plot the spectra \( \{ -2 \ln \lambda_{\alpha\beta} \} \) 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 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 non-degenerate levels are found for \( m = 0 \). These features are found commonly for both signs of \( J \), and are consistent with the even-odd structure in Fig. 7.

In Fig. 9 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

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

**FIG. 10:** (Color online) Entanglement spectra \( \{ -2 \ln \lambda_{\alpha\beta} \} \) 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. 6 shows \( -2 \ln \lambda_{\pm 1/2} = \ln 2 \) and \( -2 \ln \lambda_{0} = 0 \) for the two types of bipartition (with all the other levels at infinity).
longer-range valence bonds in the wave function would gradually grow while retaining the even-odd structure. 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.

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 (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 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 $J_1 \to 0$ or $J_1' \to 0$ (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. Therefore, we expect that the Haldane dimer state with $D_{123} < 0$ in Fig. 11(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 $S_i \to S_i + 1$, 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 phase and, following Ref. 33, 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 A 1, we obtain the effective Hamiltonian

$$H = \int dx \left\{ \sum_{\nu = \pm} \frac{v_{\nu}}{2} \left[ K_\nu (\partial_x \theta_{\nu})^2 + K^{-1}_\nu (\partial_x \phi_{\nu})^2 \right] \right. $$

$$\left. - \gamma_1 \cos(\sqrt{4\pi} \phi_{+}) \cos(\sqrt{4\pi} \theta_{-}) + \gamma_1 \cos(\sqrt{4\pi} \phi_{-}) \sin(\sqrt{4\pi} \theta_{+}) + \gamma_2 \gamma''_1 \cos(\sqrt{4\pi} \phi_{+}) \sin(\sqrt{4\pi} \phi_{-}) + \ldots \right\}. \quad (37)$$

The first line represents the Gaussian Hamiltonian while the other lines represent perturbations which can become relevant in the easy-plane case. As seen in Eq. (29), the $\gamma_1$ term is related to the $G_1$ term in the non-Abelian bosonization, while $\gamma_2$ and $\gamma''_1$ correspond to $G_{1w}$. The
coupling constants are obtained in lowest order in $J_1$ as

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

(38)

$$\gamma_1 = \frac{B_{1}^2 J_1}{a} , \quad \gamma_{tw} = \sqrt{\pi} J_1 B_{1}^2 , \quad \gamma_{tw}'' = \frac{\sqrt{\pi}}{2} J_1 \Delta A_{1}^2 ,$$

(39)

where $K$ and $v$ are given by Eq. (35). We have discussed in Sec. 111 that, in the isotropic case $\Delta = 1$, $\gamma_1$ 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. 111 are described using the effective Hamiltonian [(57)]. The results are summarized in Table 111.

1. Even-parity dimer phase

If $J_1 < 0$, the coupling constant $\gamma_1$ 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

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

(40)

In either case, it follows from Eq. (30) that the $xy$ and $z$ components of the dimer order parameter, $\bar{D}_{123}^x$ and $\bar{D}_{123}^z$, become finite and have mutually opposite signs ($\bar{D}_{123}^x \bar{D}_{123}^z < 0$). This situation corresponds to the even-parity dimer phase appearing at strong easy-plane anisotropy ($\Delta \lesssim 0.6$); see Fig. 2(b).

2. Gapless chiral phase

As shown by Nersesyan et al. [(57)] the gapless chiral phase appears when $\gamma_{tw}$ grows under the RG. To discuss the effect of the $\gamma_{tw}$ term, it is useful to perform the mean-field decoupling

$$(\partial_2 \theta_+) \sin(\sqrt{4 \pi \theta_-}) \to \langle \partial_2 \theta_+ \rangle \sin(\sqrt{4 \pi \theta_-}) + \langle \partial_2 \theta_+ \rangle \sin(\sqrt{4 \pi \theta_-}).$$

(41)

Then the Hamiltonian [(57)] separates into “+” and “−” sectors:

$$H = H_+ + H_-$$

(42)

with

$$H_+ = \int dx \frac{v_+}{2} \left[ K_+ (\partial_2 \theta_+)^2 + K_+^{-1} (\partial_2 \phi_+)^2 \right] ,$$

(43)

$$H_- = \int dx \left( \frac{v_-}{2} \left[ K_- (\partial_2 \theta_+)^2 + K_-^{-1} (\partial_2 \phi_+)^2 \right] + \gamma_{tw} \langle \partial_2 \phi_+ \rangle \sin(\sqrt{4 \pi \theta_-}) \right) .$$

(44)

Here we have introduced

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

(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 $\theta_-$ field. Since $\langle \partial_2 \theta_+ \rangle = 0$ from $H_+$, $\langle \partial_2 \phi_+ \rangle = a$. The coefficient of the sine potential in $H_-$ is thus given by $\gamma_{tw} q$, and the field $\theta_-$ is locked at distinct positions depending on the sign of this coefficient:

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

(46)

Correspondingly, the sine term acquires a finite expectation value:

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

(47)

where $c_1$ is a positive constant. Equations (43) and (47) can be solved self-consistently 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 selfconsistently.

First, the non-vanishing value of the mean-field parameter in Eq. (17) directly leads to a finite vector chiral order parameter [(2)]:

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

(48)

Therefore the two mean-field solutions correspond to the ground states with positive and negative $\kappa_{\ell,\ell+1}$. Let us take the ground state with $\kappa_{\ell,\ell+1} > 0$ (i.e., $\gamma_{tw} q > 0$) and discuss the expressions of the spin operators. We focus on gapless degrees of freedom, and ignore the fluctuations of $\theta_-$ around its average [(44)]. Then we find

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

(49)

which are combined into

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

(50)

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

$$S^\pi_{2j+n} \approx B_0 (1)^j e^{i \sqrt{2 \pi \theta_n(x_n)}}$$

$$= B_0 \exp \left( i \left[ \sqrt{\pi} (\tilde{\theta}_+ + qx_n) + \frac{\pi}{2} \left( 2j + n - \frac{3}{2} \right) \right] \right) .$$

(51)

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

$$S^\pi_\ell \approx B_0 e^{i \sqrt{\pi} \tilde{\theta}_+ + Q(\ell-3/2)} ,$$

(52)

with

$$Q = \frac{\pi + \sqrt{\pi} qa}{2} .$$

(53)
TABLE I: Summary of the Abelian bosonization description of the phases for small $|J_1|/J_2$. Both the easy-plane (Sec. [5]) and easy-axis (Sec. [5]) 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. 4, although their essential features can be captured in the Abelian bosonization framework.

| Phase | Relevant perturbations | Field-locking positions | Order parameters |
|-------|-----------------------|-------------------------|-----------------|
| Singlet/Haldane dimer | $\gamma_1 > 0$ | $\sqrt{4\pi\phi_+}, \sqrt{4\pi\theta_-} = (0, 0)$ | $D_{123}^y D_{123}^z > 0$ |
| Even-parity dimer | $\gamma_1 < 0$ | $\sqrt{4\pi\phi_+}, \sqrt{4\pi\theta_-} = (0, 0)$ | $D_{123}^y D_{123}^z < 0$ |
| Gapless chiral | $\gamma_{tw} \sim J_1 \neq 0$ | $\sqrt{4\pi\theta_-} = -\frac{\pi}{2} \text{sgn}(J_1 \langle \partial_x \theta_+ \rangle)$ | $\kappa_{\text{tw}} \neq 0$ |
| Chiral singlet/Haldane dimer | $\gamma_{tw} \sim J_1$, $\gamma_{nd} < 0$, $\gamma_1 > 0$ | $\left\{ \begin{array}{ccc} (0, \pm \frac{\pi}{2}) & \rightarrow & (0, 0), \\ (\pi, \pm \frac{\pi}{2}) & \rightarrow & (\pi, \mp \pi) \end{array} \right.$ | $D_{123}^y D_{123}^z \neq 0$, $D_{123}^z \neq 0$ |
| Chiral even-parity dimer | $\gamma_{tw} < 0$, $\gamma_{nd} < 0$, $\gamma_1 < 0$ | $\left\{ \begin{array}{ccc} (0, \pm \frac{\pi}{2}) & \rightarrow & (0, \pm \pi), \\ (\pi, \pm \frac{\pi}{2}) & \rightarrow & (\pi, 0) \end{array} \right.$ | $D_{123}^y D_{123}^z < 0$ |
| Chiral Néel | $\gamma_{tw} < 0$, $\gamma_{nd} > 0$, $\gamma''_{nd} \neq 0$ | $\sqrt{4\pi\phi_+} = \pm \pi/2, \sqrt{4\pi\theta_-} = \mp \pi/2$ | $\langle S^z_{j+1} \rangle = \pm \langle S^z_j \rangle \propto (-1)^j$ |
| Partially polarized | $\gamma''_{tw} < 0$ | $\sqrt{4\pi\phi_-} = \frac{\pi}{4} \text{sgn}(\partial_x \phi_+)$ | $\langle S^z_j \rangle \neq 0$ |

As for the $z$ component of the spins, we simply ignore the $\phi_-$ part of the expression:

$$S^z_{\ell} \approx \frac{a}{\sqrt{4\pi}} \partial_z \phi_+.$$  (54)

Spin correlation functions are then calculated as

$$\langle S^z_{\ell} S^z_{-\ell} \rangle = \left\{ \begin{array}{ccc} (0, \pm \frac{\pi}{2}) & \rightarrow & (0, 0), \\ (\pi, \pm \frac{\pi}{2}) & \rightarrow & (\pi, \mp \pi) \end{array} \right.$$

(55)

$$\langle S^z_{\ell} S^z_{-\ell} \rangle = \begin{cases} 2 \pi \theta_0, & \sqrt{4\pi\phi_+} = 0, \sqrt{4\pi\phi_2} = 0, \pi \\text{sgn}(\partial_x \phi_+) \\
\frac{K}{2\pi^2 |l^2 - l'|^2} + \ldots \end{cases}$$

(56)

with $A = B^2_0 2^{3/2} K_+$. The finite vector chiral order parameter $\kappa_{\ell', \ell+1}$ in Eq. (58) and the quasi-long-range in-plane spiral correlation with an incommensurate pitch angle $Q$ in Eq. (54) are two major features of the gapless chiral phase.

3. Gapped chiral phases

Following Lecheminant et al. [25] we consider the following symmetry-allowed perturbation to the effective theory of the gapless chiral phase:

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

(57)

with which the “+” sector of the Hamiltonian becomes a sine-Gordon model. The scaling dimension of this perturbation is $4K_+$. If the $\gamma_{nd}$ term becomes relevant ($4K_+ < 2$), a Berezinskii-Kosterlitz-Thouless (BKT) transition takes place and as a result, the bosonic field $\phi_+$ is locked at distinct positions dependent on the sign of $\gamma_{nd}$. 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 $\gamma_{nd}$.

First, when $\gamma_{nd} < 0$, $\sqrt{4\pi\phi_+}$ is locked at $\sqrt{4\pi\phi_+} = 0$ or $\pi$. which produces a finite value of the $z$-component of the dimer order parameter, $D_{123}^z$, as seen in Eq. (59). We have thus obtained the “chiral dimer phase,” in which the vector chiral and dimer orders coexist. Once $\phi_+$ is locked as in Eq. (58), the locking position of $\sqrt{4\pi\theta_-}$ is affected by the $\gamma_1$ term in Eq. (57) and changed from $\pm \pi/2$ of the gapless chiral phase [Eq. (56)], so that the $xy$-component of the dimer order parameter, $D_{123}^y$, also becomes finite, in agreement with Fig. 4. Specifically, for positive $\gamma_1$, the field-locking positions of the four degenerate ground states change smoothly with the strength of $\gamma_1$ as

$$\left\{ \begin{array}{ccc} (0, \pm \frac{\pi}{2}) & \rightarrow & (0, 0), \\ (\pi, \pm \frac{\pi}{2}) & \rightarrow & (\pi, \mp \pi) \end{array} \right.$$

(59)

finally resulting in the two degenerate ground states of either the Haldane dimer or the single dimer phase as specified by Eq. (25). For negative $\gamma_1$, the field-locking positions change as

$$\left\{ \begin{array}{ccc} (0, \pm \frac{\pi}{2}) & \rightarrow & (0, \pm \pi), \\ (\pi, \pm \frac{\pi}{2}) & \rightarrow & (\pi, 0) \end{array} \right.$$

(60)

resulting in the two degenerate ground states of the even-parity dimer phase as indicated by Eq. (48).

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

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

This yields a finite Néel order parameter along the $z$ direction, as we explain below. From Eqs. (21) and (23), the $S^z_{\ell}$ operator has the staggered component

$$(-1)^l S^z_{\ell} = \frac{a}{\sqrt{4\pi}} \partial_z \phi_- + \ldots,$$  (62)

which, at first sight, looks insensitive to the locking of $\phi_+$. However, after the locking (61), the $\gamma''_{tw}$ term in Eq. (57) 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 $\phi$ (so that $\partial_\phi H_-$ is shifted by a constant). Consequently, Eq. (62) acquires a nonvanishing expectation value

$$(-1)^f\langle S_y^f \rangle = -\frac{K_+a}{\sqrt{4\pi v_+}}\zeta''(\sin(\sqrt{4\pi\phi})) + \ldots \quad (63)$$

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.

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

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 $\langle S_\ell^+ S_{\ell+1}^- \rangle$ at $\Delta = 0.8$ for various values of $J_1/J_2$ in the gapless chiral phase. The data for $|J_1|/J_2 > 2$ follow straight 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. (57) (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 $\ell = 1, 2, \ldots, L$ in a translationally invariant infinite 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

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

In Fig. 13(a), $S^{+\pm}(q)$ 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. \( \text{(55)} \), provided that $K_+$ becomes larger with increasing $|J_1|/J_2$; see Eq. \( \text{(58)} \). These peaks are expected to diverge as $L \to \infty$ 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 $\kappa^z$ decreases. In Fig. 13(b), $S^{zz}(q)$ shows linear behaviors around $q = 0$ as expected from the Fourier transform of Eq. \( \text{(56)} \): $S^{zz}(q) = K_+ |q|/2\pi$ for $|q| \ll 1$. In addition, it shows finite peaks at incommensurate $q$. Although the explanation of 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 A 3. The in-plane spin correlation function is expected to show a multiplicative logarithmic correction in Eq. \( \text{(54)} \) at the BKT transition point from the gapless to gapped chiral phases. Therefore, in Figs. 14 and 15, we plot $r^2 |\langle S^z S^z \rangle|$, which is expected to become a linear function of $\ln r$ at the BKT transition point. In Figs. 14(a) and (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 “×” sym-
The data of dimer ground states. The Lifshitz points, at which the in-plane spin correlation function changes its character from incommensurate to commensurate (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 \(S^{+\prime}(q)\) (as in Ref. 74). The data of \(Q\) so obtained as a function of \(J_1/J_2\) are shown for different values of \(\Delta\) in Fig. 14. The Lifshitz points, at which the in-plane spin correlation function changes its character from incommensurate to commensurate \((Q = 0\) or \(\pi)\), 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 \(\Delta\), 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. 68, 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. 50, 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 \((J_1/J_2, \Delta) = (−4, 1)\) 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 \(6\) with \(J_1 < 0\) and \(J_2 > 0\), let us shortly discuss the case with easy-axis anisotropy \(\Delta > 1\). In this case, Igarashi and Tonegawa et al.\(14\) have found the following three phases. For \(J_1/J_2 < -4\), the ground state is fully polarized (ferromagnetic) along the z direction. For small \(|J_1|/J_2\) and large \(\Delta\), the ground state is antiferromagnetic, having a period-4 structure \(↑↑↓↓\ldots\) (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 \(\Delta\). We note that the uudd phase was also found in the model with antiferromagnetic \(J_{1,2} > 0\). \(6\) 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 \(J_2(\Delta - 1) \sum_{\nu,n} S^z_{2j+n} S^z_{2j+\nu+n+2}\), (with \(\Delta > 1\)) adds to the Hamiltonian the backscattering terms

\[
\gamma_{bs} \left[ \cos(2\sqrt{2\pi} \phi_1) + \cos(2\sqrt{2\pi} \phi_2) \right]
\]

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

\[
(\sqrt{2\pi} \phi_1, \sqrt{2\pi} \phi_2) = (0, 0), (0, \pi), (\pi, 0), \text{ or } (\pi, \pi).
\]

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

\[
\langle S^z_{2j+1} \rangle = c_2(-1)^j, \quad \langle S^z_{2j+2} \rangle = \pm c_2(-1)^j,
\]

where \(c_2\) is a non-zero constant [see Eq. (21)].

B. Partially polarized phase

The partially polarized phase found numerically\(13\) can be understood from the mean-field treatment of the operator \((\partial_+ \phi_+) \sin(\sqrt{4\pi} \phi_-)\) which is contained in \(\mathcal{O}_{tw}\) in Eq. (25a). Here we review the formulation of Zarea et al.\(12\) and then discuss the behaviors of correlation functions, which were not discussed in detail in previous studies.\(12\)

We start from the effective Hamiltonian

\[
H = \int dx \left\{ \sum_{\nu=\pm} \frac{v_\nu}{2} [K_{\nu}(\partial_x \theta_\nu)^2 + K^{-1}_\nu(\partial_x \phi_\nu)^2] + \gamma_{tw}'(\partial_x \phi_+) \sin(\sqrt{4\pi} \phi_-) \right\}
\]
with $\gamma_{\text{w}} < 0$. The mean-field decoupling similar to the one used in Sec. [IV A 2] yields the effective Hamiltonian $H = H_+ + H_-$, where

$$H_+ = \int dx \frac{\nu_+}{2} \left[ K_+ (\partial_x \phi_+)^2 + K_+^{-1} (\partial_x \phi_+)^2 \right],$$

$$H_- = \int dx \left\{ \nu_- \left[ K_- (\partial_x \phi_-)^2 + K_-^{-1} (\partial_x \phi_-)^2 \right] + \gamma'_{\text{w}} \mu \sin(\sqrt{4\pi} \phi_-) \right\},$$

Here we have introduced

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

with

$$\mu = -\frac{K_+ \gamma'_{\text{w}} \langle \sin(\sqrt{4\pi} \phi_-) \rangle}{\nu_+} = \langle \partial_x \phi_+ \rangle.$$ (73)

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

$$\langle S_i^z \rangle = \frac{a}{\sqrt{4\pi}} \langle \partial_x \phi_+ \rangle = \frac{a}{\sqrt{4\pi}} \mu \equiv M.$$ (74)

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

$$\sqrt{4\pi} \phi_- = \frac{\pi}{2} \text{sgn}(\mu).$$ (75)

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, $S_i^x$, contains the operator $e^{\pm \sqrt{4\pi} \phi_-}$, which strongly fluctuates due to the locking of the dual field $\phi_-$; therefore the correlation function $\langle S_i^x S_{\ell'}^x \rangle$ decays exponentially with the distance. Instead, the longitudinal correlation $\langle S_i^z S_{\ell'}^z \rangle$ and the bond nematic correlation $\langle S_i^+ S_{\ell+1}^- S_{\ell'}^- S_{\ell'+1}^+ \rangle$ show power-law decays. Ignoring fluctuations of $\phi_-$, we obtain the bosonized expressions for these operators as

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

$$S_{\ell+1}^+ = (-1)^{\ell+1} B_0^2 e^{i \sqrt{4\pi} \phi_+} + 2 B_0 B_1 e^{i \sqrt{4\pi} \phi_+} \cos \left[ \frac{\pi}{2} \left( \frac{1}{2} - |M| \right) \right] \times \cos \left[ \sqrt{\pi} \tilde{\phi}_+ + \pi \left( M + \frac{\text{sgn}(M)}{2} \right) \frac{\ell - 1}{2} \right] + \ldots.$$ (77)

with $B \propto A_1^2$, $B' \propto B_0^2$, and $B'' \propto B_0^2 B_1^2$. We note that the TLL phases with similar power-law correlations, called the nematic and SDW phases, have also been discussed for the model [1] in a magnetic field for both ferromagnetic and antiferromagnetic $J_1$. 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 shortest-range transverse spin correlation is called the SDW state in Refs. [71] and [72]. It is natural to assume that the partially polarized phase at $\Delta > 1$ in zero magnetic field is continuously connected to the SDW phase in a magnetic field. With inter-chain couplings, the dominant quasi-long-range SDW correlation is expected to evolve into a true long-range-order. 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.

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 nonzero 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 $0 < \Delta < 1$, 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 $-4 < J_1/J_2 < 0$ and the unusual alternate appearance of the Néel and even-parity dimer phases. 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 [1] (by continuity, the same qualitative description can be extended to larger
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 inter-chain 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.$^5$ By contrast, it is also expected that the small excitation gap ($\lesssim 0.06J_2$; 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 CuGeO$_3$. 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 ($^4$)

Here we briefly explain how the RG equations ($^4$) are derived by using the perturbative RG method 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 components $M^a_{R/L}$ obey the well-known SU(2) current algebra:

$$\tag{A1} M^a_{R/L}(x, \tau)M^b_{R/L}(0) = \frac{\delta^{ab}}{8\pi^2 z_{R/L}} + \frac{i\varepsilon^{abc}M^c_{R/L}(0)}{2\pi z_{R/L}} + \frac{i\varepsilon^{abc}M^c_{R/L}(0)}{2\pi z_{R/L}}$$

with $z_{R/L} = v_\tau \mp i\pi$. Here, $\varepsilon^{abc}$ 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 $(x, \tau)$ and $0 = (0, 0)$ are brought close together.

The OPEs of the uniform components $M^a_{R/L}$ with the staggered components $N^a$ and the dimerization $\epsilon$ are given by:

$$\tag{A2} M^a_{R/L}(x, \tau)N^b(0) = \frac{i}{4\pi z_{R/L}} \left[ \varepsilon^{abc}N^c(0) \right],$$

$$\tag{A3} M^a_{R/L}(x, \tau)\epsilon(0) = \frac{\mp iN^a(0)}{4\pi z_{R/L}}.$$  

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

Similar to Eqs. (A2) and (A3), the OPEs among $N$ and $\epsilon$ can be derived 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 $\epsilon$'s. We take the same conventions as used in the Appendix of Ref. [4] and introduce the right- and left-moving fermionic fields $\Psi_{R/L,s}(s = \uparrow, \downarrow)$, which obey the OPEs:

$$\tag{A4} \Psi_{R/L,s}(x, \tau)\Psi^\dagger_{R/L,s'}(0) = \frac{\delta_{ss'}}{2\pi z_{R/L}}.$$  

We define the fermionic staggered dimerization operator as:

$$\tag{A5} \epsilon_F = \frac{i}{2}(\Psi^\dagger_{Rs}\Psi_{Ls} - \Psi^\dagger_{Ls}\Psi_{Rs}).$$

Using bosonization, one can show that $\epsilon_F$ is related to $\epsilon$ as:

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

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

Performing all possible contractions of four fermion fields (see Appendix A of Ref. [23]), the OPE of two $\epsilon_F$'s is calculated as:

$$\tag{A7} \epsilon_F(x, \tau)\epsilon_F(0) = \frac{1}{4}\Psi^\dagger_{Rs}(x, \tau)\Psi^\dagger_{Ls}(x, \tau)\Psi_{Rs'}(0)\Psi_{Ls'}(0) + (R \leftrightarrow L)$$

$$\tag{A8} = \frac{1}{4\pi z_{R/L}} + \frac{1}{4\pi} \left( \frac{\rho_R(0)}{z_{R/L}} - \frac{\rho_L(0)}{z_{R/L}} \right)$$

$$\tag{A9} + \frac{1}{2}\Psi^\dagger_{Rs}(0)\Psi^\dagger_{Ls}(0)\Psi_{Ls'}(0)\Psi_{Rs'}(0).$$
with $\rho_{R/L} = \Psi_{R/L,s}^\dagger \Psi_{R/L,s}$. The last term is related to the backscattering term:

$$\Psi_{R,s}^\dagger \Psi_{L,s}\Psi_{L,s'}^\dagger \Psi_{R,s'} = -2M_R \cdot M_L - \frac{1}{2} \rho_{R/L},$$

(A7)

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

$$M_R^b = \frac{1}{2} \Psi_{R,s}^\dagger \sigma_{as}^b \Psi_{R,s'}, \quad M_L^b = \frac{1}{2} \Psi_{L,s}^\dagger \sigma_{as}^b \Psi_{L,s'}.$$  

(A8)

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

$$\epsilon(x, \tau) \epsilon(0) = \frac{1}{4\pi^2 \lambda^2 z_R z_L} - \frac{1}{\lambda^2} M_R(0) \cdot M_L(0).$$

(A9)

Similar calculations yield

$$N^a(x, \tau) N^b(0) = \frac{g^{ab}}{4\pi^2 \lambda^2 z_R z_L} + \frac{i \sigma^{abc}}{2\pi \lambda^2} \left[ \frac{M_R^c(0)}{z_L} \right] + \frac{1}{\lambda^2} \mathcal{O}_{NN}^{ab}(0),$$

(A10)

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

(A11)

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

$$\mathcal{O}_{NN}^{ab} = \frac{1}{2} \sigma_{s_1 s_2}^a \sigma_{s_3 s_4}^b \Psi_{R,s_1}^\dagger \Psi_{L,s_2}^\dagger \Psi_{L,s_3} \Psi_{R,s_4}.$$  

(A12)

For the current purpose, we only need the trace (in the spin direction indices) of this term, which gives the backscattering term: $\mathcal{O}_{NN}^{aa} = M_R \cdot M_L - \frac{1}{2} \rho_{R} \rho_{L}$.

In the limit of weak interchain coupling $|J_1| \ll J_2$, the OPEs of the perturbation operators in Eq. (A11) 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. For example, if the OPE of marginal operators $O_a$ and $O_b$ have the form

$$O_a O_b = \frac{\lambda_{ab}}{(2\pi)^2 z_R z_L} O_c + \ldots,$$

(A13)

where $\lambda_{ab}$ are dimensionless constants, then the one-loop RG equation for the perturbation $g_c O_c$ has the contribution

$$\frac{dg_c}{dl} = g_a g_b \lambda_{ab} \frac{\lambda_c}{4\pi^2 v} + \ldots$$

(A14)

FIG. 17: (Color online) Plots of $r^2 \langle S_{\ell}^x S_{\ell+r}^x \rangle^2$ for fixed $\Delta = 0$ and various values of $J_1/J_2$ around the TLL-dimer transition point studied in Ref. [2]. 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 estimate $J_2/J_1 \approx 3.0893$.

**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 (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 Tomonaga-Luttinger liquid (TLL) phase, in which the transverse spin correlation function behaves as

$$\langle S_{\ell}^x S_{\ell}^x \rangle = \frac{\tilde{A}_1^x (1 - \ell/a)^{1 - \eta}}{\sqrt{\eta^{1 + \eta}}} + \ldots$$

(B1)

Here $A_1^x$ and $A_1^z$ are non-universal constants. The decay exponent $\eta$ 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 $\langle S_{\ell}^x S_{\ell}^x \rangle$ and $\langle S_{\ell}^z S_{\ell}^z \rangle$.$[2][3][4][5]$

$$\langle S_{\ell}^x S_{\ell}^x \rangle = \frac{\tilde{A}_1^x (1 - \ell/a)^{1 - \eta}}{\sqrt{\eta^{1 + \eta}}} \ln^\frac{r}{(\ell' - \ell)} + \ldots$$

(B2)

In Fig. 17, we plot the function $r^2 \langle S_{\ell}^x S_{\ell+r}^x \rangle^2$ 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 estimate $J_2/J_1 \approx 3.0893$. 

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$$e^{\sqrt{2\pi\theta_n}(x)}e^{\pm\sqrt{2\pi\phi_n}(x)} = e^{\mp\sqrt{2\pi\phi_n}(x)}e^{\pm\sqrt{2\pi\theta_n}(x)}$$

$$\times e^{\sqrt{2\pi[\theta_n(x),\phi_n(x)]}} = -e^{\pm\sqrt{2\pi\phi_n}(x)}e^{\pm\sqrt{2\pi\theta_n}(x)}$$

where Eq. (22) and $Y(0) = 1/2$ are used.
In Ref. 5, the correlation length was defined in unit of two lattice spacings, and should be doubled when comparing with the current data.

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Because of the $SU(2)$ symmetry of the model, we can further confirm that all the entanglement levels are even- or odd-fold degenerate in left and right panels of Fig. 10, respectively.

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