We summarize our theoretical findings on the ground-state phase diagram of the spin-$\frac{1}{2}$ XXZ chain having competing nearest-neighbor ($J_1$) and antiferromagnetic next-nearest-neighbor ($J_2$) couplings. Our study is mainly concerned with the case of ferromagnetic $J_1$, and the case of antiferromagnetic $J_1$ is briefly reviewed for comparison. The phase diagram contains a rich variety of phases in the plane of $J_1/J_2$ versus the XXZ anisotropy $\Delta$: vector-chiral phases, Néel phases, several dimer phases, and Tomonaga-Luttinger liquid phases. We discuss the vector-chiral order that appears for a remarkably wide parameter space, successive Néel-dimer phase transitions, and an emergent nonlocal string order in a narrow region of ferromagnetic $J_1$ side.

Keywords: frustration, one-dimensional quantum magnets, infinite time evolving block decimation

1. Introduction

Frustrated spin systems have been a subject of interest because of their rich physics arising from competing interactions and quantum/thermal fluctuations. One-dimensional (1D) frustrated spin models provide one of the prototypical families to theoretically study unconventional orders with high accuracy. We here focus on the spin-$\frac{1}{2}$ XXZ chain with nearest-neighbor (NN) exchange coupling $J_1$ and next-nearest-neighbor (NNN) coupling $J_2$. The Hamiltonian is given by

$$H = \sum_{n=1}^{N} \sum_{j} J_1(n)(S^x_j S^x_{j+n} + S^y_j S^y_{j+n} + \Delta S^z_j S^z_{j+n}).$$

(1)

Here $\Delta$ is the XXZ anisotropy, and we will consider the easy-plane region $0 \leq \Delta \leq 1$. In the case of antiferromagnetic (AF) $J_2 > 0$, NN and NNN couplings are geometrically frustrated irrespective of the sign of $J_1$. This model has been studied in detail when $J_1$ and $J_2$ are both AF, and its ground-state and low-energy properties are now well understood. By contrast, relatively less is understood for the case of ferromagnetic (FM) $J_1$ and AF $J_2$ despite earlier studies. Recently, interest has been growing in this FM $J_1$ case because of its possible relevance.
to several quasi-1D edge-sharing cuprates [LiCu$_2$O$_2$ (Ref. 13), LiCuVO$_4$ (Ref. 14), Rb$_2$Cu$_2$Mo$_3$O$_2$ (Ref. 15), PbCuSO$_4$(OH)$_2$ (Ref. 16,17), etc.]. Some of these compounds exhibit multiferroic behavior in low-temperature spiral spin ordered phases, where the long-range order (LRO) of the vector spin chirality produces the electric polarization. Motivated by these developments, we have recently performed intensive studies on the ground-state phase diagram of the spin-$\frac{1}{2}$ $J_1$-$J_2$ chain (1) with FM $J_1 < 0$ and AF $J_2 > 0$. In particular, among various phases which we have successfully characterized, the emergent LRO of the vector spin chirality for ferromagnetic $J_1$ with a weak easy-plane anisotropy would be relevant to quasi-1D multiferroic cuprates, when interchain couplings are taken into account.

The effect of external magnetic field is another interesting direction of research for the frustrated $J_1$-$J_2$ spin chain systems. Recently, field-induced Tomonaga-Luttinger liquid (TLL) phases with spin multipolar quasi LRO have been theoretically investigated in the model (1), and it has been predicted that these multipolar phases show characteristic dynamical spin response which can be observed in NMR and neutron-scattering experiments. Throughout this paper, however, we restrict ourselves to the case at zero magnetic field. In the following sections, we review our recent results on the phase diagram and the characteristic features of the phases in the model (1). Including the parameter space of AF $J_1 > 0$, the phase diagram consists of at least six (and presumably more) kinds of distinct phases.

2. Competition between chiral and dimer orders

In this section, we consider the regime $-4 < J_1/J_2 < 4$ with $J_2 > 0$, where the classical ground state has an incommensurate spin spiral structure. This spiral state has a non-vanishing vector spin chirality $\kappa^z_j = \langle (S_j \times S_{j+1})^z \rangle \neq 0$. In the quantum case, a true spiral LRO with broken spin rotational symmetry is difficult to occur in 1+1 dimensions, but a vector chiral LRO is allowed for $\Delta \neq 1$ since it only breaks a discrete $\mathbb{Z}_2$ symmetry. As explained below, this vector chiral order competes with several kinds of dimer orders driven by quantum fluctuations.

The ground-state phase diagram is presented in Fig. 1. The AF-$J_1$ side has already been established by several theoretical works. A strong enough AF NNN interaction $J_2$ causes a Kosterlitz-Thouless (KT) transition from the TLL phase (connected to a single XXZ spin chain with the NN exchange coupling $J_1$) to a dimerized phase with spontaneously broken translational symmetry, in which the ground state is doubly degenerate. This dimer phase occupies a large part of the classical spiral regime $J_1/J_2 < 4$ of the AF-$J_1$ side. In fact, the ground state on the line $J_1/J_2 = 2$ and with $\Delta > -1/2$ (extension of the Majumder-Ghosh model at $\Delta = 1$) is given by a product state of singlet bonds, $|GS\rangle = \prod_{j=even}(|\uparrow\rangle_j |\downarrow\rangle_{j+1} + |\downarrow\rangle_j |\uparrow\rangle_{j+1})$ or $\prod_{j=odd}(|\uparrow\rangle_j |\downarrow\rangle_{j+1} - |\downarrow\rangle_j |\uparrow\rangle_{j+1})$, where $|\uparrow\rangle_j$ (|$\downarrow\rangle_j$) is the eigenstate of $S_j^z$ with the eigenvalue $+1/2$ ($-1/2$). For later convenience, we introduce the $xy$
Phase Diagram

Fig. 1. Ground-state phase diagram of the $J_1$-$J_2$ model (1) in the classically spiral regime $-4 \lesssim J_1/J_2 \lesssim 4$ with $J_2 > 0$. Strength of the vector chirality $\langle (S_j \times S_{j+1})^z \rangle$ calculated by iTEBD is also plotted with red color. The small Neél phase in the FM-$J_1$ side will be discussed in Sec. 3.

and $z$ components of dimer order parameters

$$D_{j}^{xy} = \langle S_j^x S_{j+1}^x + S_j^y S_{j+1}^y \rangle - \langle S_j^x S_j^x + S_j^y S_j^y \rangle,$$

$$D_{j}^z = \langle S_{j-1}^z S_j^z - S_j^z S_{j+1}^z \rangle.$$

For the above product state, we can easily show that (i) $\text{sign}(D_{j}^{xy}) = \text{sign}(D_{j}^z)$, and (ii) the energy density $\langle S_j \cdot S_{j+1} \rangle$ on the dimerized bond is negative. These properties persist in the whole region of the dimer phase in the AF-$J_1$ side. We call this phase the “singlet-dimer” phase. In this phase, there is a Lifshitz line across which the short-range spin correlation changes its character from commensurate to incommensurate (C and IC in Fig. 1).\textsuperscript{30}

In the weak $J_1$ region where $0 < J_1/J_2 \lesssim 0.8$, a vector-chiral phase appears\textsuperscript{7,8} in which the $\mathbb{Z}_2$ parity symmetry is spontaneously broken, and a nonvanishing and spatially uniform average of $\kappa_j^z = \langle (S_j \times S_{j+1})^z \rangle$ is found. In contrast to the dimer phase, the vector-chiral phase has a gapless excitation mode, and both the longitudinal and transverse spin correlation functions decay in a power-law fashion. In particular, the transverse spin correlator has an incommensurate oscillating factor.

Now, we turn to the FM-$J_1$ side, which has been investigated in our recent works\textsuperscript{21,23}. Phase boundaries are numerically determined by using infinite time evolving block decimation (iTEBD) method\textsuperscript{31} and numerical diagonalization. The phase diagram in Fig. 1 clearly shows that for $J_1 < 0$ the vector-chiral phase with $\kappa_j^z \neq 0$ appears for much broader parameter space than in the AF-$J_1$ case ($J_1 > 0$), and extends up to the vicinity of the SU(2) line $\Delta = 1$ for moderate values of $|J_1|/J_2$. This result naturally explains why quasi-1D $J_1$-$J_2$ magnets with FM $J_1$ coupling often show a spiral spin order at low temperatures,\textsuperscript{13,14} while with AF $J_1$ coupling no quasi-1D magnet with a spiral order is found so far. Namely, a chiral ordered state appearing for realistically small easy-plane anisotropy $1 - \Delta \ll 1$ in the FM-$J_1$ side can be easily promoted to a 3D spiral ordered state by the addition of weak interchain couplings, while a gapped dimer state in the AF-$J_1$ side will be
robust against weak 3D couplings.

On the FM-$J_1$ side, there appear two distinct types of dimer phases between which the vector-chiral phase intervene in Fig. 1. The wider dimer phase appearing for strong easy-plane anisotropy $0 \leq \Delta \lesssim 0.6$ can be easily understood as follows.\textsuperscript{10} In the XY limit $\Delta = 0$, the spin chain with an AF NN coupling $J_1 = J > 0$ can be mapped to the same spin chain with the opposite sign of NN coupling ($J_1 = -J < 0$) through $\pi$ rotation of spins around $S^z$ axis on every second site. By this transformation a singlet dimer $| \uparrow \downarrow \rangle - | \downarrow \uparrow \rangle$ on a bond is changed into a triplet state $| \uparrow \downarrow \rangle + | \downarrow \uparrow \rangle$. Therefore, the ground state at $(J_1/J_2, \Delta) = (-2, 0)$ is a product state of triplet bonds, $|GS\rangle = \prod_{j=\text{even}} | \uparrow \rangle_j | \downarrow \rangle_{j+1} + | \downarrow \rangle_j | \uparrow \rangle_{j+1}$. These states show $\text{sign}(D^{xy}_j) = -\text{sign}(D^z_j)$, and this property persists in the whole region of this dimer phase. We therefore call this phase the “triplet-dimer” phase. The singlet- and triplet-dimer phases can be distinguished by the signs of the dimer order parameters.

The nature of the other dimer phase around the SU(2) line $\Delta = 1$ has long been controversial. We have clarified some characteristic properties of this phase by applying unbiased iTEBD method. As shown in Fig. 2(a)(b) where dimer correlations are plotted for one of doubly degenerate ground states, the magnitude of dimer orders is quite tiny and $\text{sign}(D^{xy}_j) = \text{sign}(D^z_j)$ is realized. The latter property is the same as in the singlet-dimer phase. However, we have found that $\langle S_j \cdot S_{j+1} \rangle$ on a dimerized bond is positive, while it is negative in the singlet-dimer phase. This FM dimerization suggests that an effective spin-1 degree of freedom emerges on each of dimerized bonds. Therefore, we can expect a realization of a valence-bond-solid (VBS) state\textsuperscript{32} like in a spin-1 AF chain. In fact, the emergence of an effective spin-1 chain is very natural for FM $J_1$ coupling. To judge whether the dimer phase around $\Delta = 1$ can be well approximated by a VBS state, we calculate the string order parameter\textsuperscript{33,34}

$$O^\alpha_{\text{str}}(j - k) = -\left( (S_{2j}^\alpha + S_{2j+1}^\alpha) \exp \left[ i\pi \sum_{i=j+1}^{k-1} (S_{2i}^\alpha + S_{2i+1}^\alpha) \right] (S_{2k}^\alpha + S_{2k+1}^\alpha) \right) , \quad (4)$$

where we have assumed that bonds $(2l, 2l + 1)$ are dimerized. Figure 2(c) clearly shows that the string parameter is long-range ordered. By contrast, the string order parameter defined on the non-dimerized bonds $(2l - 1, 2l)$ is found to be short-ranged. We may expect that the dimer phase around $\Delta = 1$ should be adiabatically connected to a spin-1 AF chain if we introduce a strong FM bond alternation on $J_1$ bonds. (Note, however, that the dimerization is a spontaneous symmetry breaking in our model.) We thus call this phase the “Haldane-dimer” phase. Here, we leave the issue of whether this Haldane-dimer phase is adiabatically connected to the singlet-dimer phase or not for future studies.\textsuperscript{23}

Figure 2 suggests the presence of another type of dimer phase, in a narrow region of parameter space ($0.61 \lesssim \Delta \lesssim 0.65$ at $J_1/J_2 = -2$), which is characterized by coexisting dimer order $D^{xy}_j, D^z_j$ and vector chirality $\kappa_j^z$. Let us call this phase...
Phase Diagram

Fig. 2. (a) $\Delta$ dependence of dimer order parameters $D_{xy}^{\nu}$ and $D_{z}^{\nu}$ on $J_1/J_2 = -2$ line, calculated by iTEBD method with Schmidt rank $\chi = 200$ and 300. The chirality $\kappa_z^{\nu}$ is finite between two vertical lines at $\Delta \approx 0.61$ and $\Delta \approx 0.92$. Panel (b) is a zoom of panel (a). (c) String order parameter $O_{zstr}(r)$ at points $(J_1/J_2, \Delta) = (-2, 1)$ and $(-1.5, 1)$ of the dimer phase, calculated by iTEBD method.

the “chiral-dimer” phase. We note that evaluated dimer order parameters in Fig. 2 cannot be used to determine the phase boundary between the chiral-dimer and vector-chiral phases. Further calculations are ongoing to verify the existence and to determine the range of this phase. More detailed discussions on the chiral, Haldane-dimer and chiral-dimer phases will be given in Ref. 23.

3. Strong $|J_1|$ region: successive Néel-dimer transitions

In this section, we focus on the narrow region between the chiral and TLL phase around $-4 \lesssim J_1/J_2 \lesssim -3$. For such large negative $J_1/J_2$, a single $J_1$ chain with $J_2 = 0$, which is exactly solvable, becomes a useful starting point. The low-energy effective Hamiltonian for the $J_1$ chain is a free boson (i.e., TLL) model with a nonlinear (vertex) term:

$$
H_{\text{eff}} = \frac{v}{2} \left[ K \left( \partial_x \theta \right)^2 + \frac{1}{K} \left( \partial_x \phi \right)^2 \right] - \frac{v\lambda}{2\pi} \cos(\sqrt{16\pi} \phi),
$$

where $x = ja$ ($a$ is lattice spacing), $(\phi(x), \theta(x))$ is a pair of dual scalar fields, $K$ is the TLL parameter, $v$ is the spinon velocity, and $\lambda$ is the coupling constant of the perturbative vertex term. For the $J_1$ chain with $0 \leq \Delta < 1$, the TLL parameter is given by $K = \pi/(2 \cos^{-1} \Delta)$. Since $K > 1$ in this case, the $\lambda$ term (scaling dimension $4K$) is irrelevant in the renormalization-group sense, and a TLL phase is realized. Furthermore, the exact value of $\lambda$ is known\(^{35}\) and has an oscillating factor $-\sin(2\pi K)$ in the $J_1$ chain. Thus, $\lambda$ changes its sign and becomes zero when $2K = n$, namely,

$$
\Delta = \cos(\pi/n), \quad n = 3, 4, \cdots.
$$

When small $J_2$ is introduced, the parameters $K$, $v$, and $\lambda$ generally change, and finally the $\lambda$ term becomes relevant and the TLL phase is destabilized towards
gapped phases.\textsuperscript{4,5} This boundary is determined in Ref.\textsuperscript{12}, and is plotted by circular symbols interpolated by solid lines in Fig. 3(a). For the effective theory (5) it is known that, if the $\lambda$ term is relevant, then positive $\lambda$ induces a Néel order with finite $\langle S^z_j \rangle = -\langle S^z_{j+1} \rangle$, while negative $\lambda$ induces a dimer order with finite $(S^x_j S^x_{j+1} - S^z_j S^z_{j+1})$. Thus a point of $\lambda = 0$ separates the dimer and Néel phases in the region with $4K < 2$. Using the level spectroscopy method of Ref.\textsuperscript{5}, we have determined the curves of $\lambda = 0$, which start from the points of Eq. (6) and are plotted as “+” symbols interpolated by broken lines. Remarkably, all the curves continue even outside the TLL phase. It means that successive dimer-Néel transitions occur as $\Delta$ is increased in the narrow region between TLL and chiral phases. In particular, the emergence of Néel order along $S^z$ axis is nontrivial since it seems unfavored by both FM $J_1$ and AF $J_2$ couplings in the classical-spin picture.

The above argument has been based on the effective theory (5). Using unbiased iTEBD, we have also directly calculated the dimer and Néel order parameters along the Lifshitz line, where the order parameters are relatively large; see Fig. 3(b). We find that the transition points determined in Fig. 3(a) and (b) are consistent.

### 4. Summary

In this paper, we have discussed the ground-state properties of a spin-1/2 $J_1$-$J_2$ chain (1) with easy-plane anisotropy, especially, for the FM-$J_1$ case. The ground-state phase diagram contains very rich physics: vector-chiral phase, four kinds of dimerized phases (singlet, triplet, Haldane and chiral dimers), Néel phases and TLL. Important findings in our recent studies on the FM-$J_1$ case include (i) remarkable stability of the vector-chiral phase even near $\Delta = 1$,\textsuperscript{21} (ii) a finite string order of the Haldane-dimer phase,\textsuperscript{23} and (iii) successive Néel-dimer transitions.\textsuperscript{22} Furthermore, our numerical result suggests the possible coexistence of chirality and dimeriza-
tion in the narrow chiral-dimer phase. More detailed properties of vector-chiral, Haldane-dimer, and chiral-dimer phases in FM- side will be discussed elsewhere.

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