

# Ground-state phase diagrams of frustrated spin- $S$ XXZ chains: Chiral ordered phases

T. Hikihara,<sup>1</sup> M. Kaburagi,<sup>2,3</sup> and H. Kawamura<sup>1</sup>

<sup>1</sup>*Department of Earth and Space Science, Graduate School of Science, Osaka University, Toyonaka, Osaka 560-0043, Japan*

<sup>2</sup>*Faculty of Cross-Cultural Studies, Kobe University, Tsurukabuto, Nada, Kobe 657-8501, Japan*

<sup>3</sup>*Graduate School of Science and Technology, Kobe University, Rokkodai, Kobe 657-8501, Japan*

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The ground-state phase diagram of the frustrated spin- $S$  XXZ chain with the competing nearest- and next-nearest-neighbor antiferromagnetic couplings is studied numerically by using the density-matrix renormalization-group method for the cases of  $S = 1/2$ ,  $3/2$ , and  $2$ . We are particularly interested in the possible gapless and gapped chiral phases, in which the chirality  $\kappa_l = S_l^x S_{l+1}^y - S_l^y S_{l+1}^x$  exhibits a finite long-range order whereas the spin correlation decays either algebraically or exponentially. We show that the gapless chiral phase appears in a broad region of the phase diagram for general  $S$ . By contrast, the gapped chiral phase is found for integer  $S$  in a narrow region of the phase diagram, while it has not been identified for half-odd integer  $S$  within our numerical accuracy. By combining the results with our previous result for  $S = 1$ , we discuss the  $S$  dependence of the phase diagram. The prediction from a bosonization analysis on the decay exponent of the spin correlation is verified.

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## I. INTRODUCTION

The study of frustrated quantum spin chains has been the subject of much interest for many years. This is mainly because these systems exhibit a wide variety of exotic phases accompanied with various types of spontaneous symmetry breaking due to the interplay between frustration and quantum fluctuations. Among them, one of the simplest model may be the quantum spin chain with the antiferromagnetic (AF) nearest-neighbor coupling  $J_1$  and the frustrating AF next-nearest-neighbor coupling  $J_2$ . The model Hamiltonian has the form

$$\mathcal{H} = \sum_{\rho=1}^2 \left\{ J_{\rho} \sum_l (S_l^x S_{l+\rho}^x + S_l^y S_{l+\rho}^y + \Delta S_l^z S_{l+\rho}^z) \right\}, \quad (1)$$

where  $\vec{S}_l$  is the spin- $S$  operator at site  $l$  and  $\Delta$  is the exchange anisotropy. Throughout this paper, we consider the case of  $0 \leq \Delta \leq 1$  and  $j \equiv J_2/J_1 > 0$ .

In the classical limit  $S \rightarrow \infty$ , the spin chain (1) exhibits a magnetic long-range order (LRO) in the ground state characterized by a certain wave number  $q$ . The order parameter is defined by

$$\vec{m}(q) = \frac{1}{LS} \sum_l \vec{S}_l e^{iql}, \quad (2)$$

where  $L$  is the total number of spins. The LRO is of the Néel type ( $q = \pi$ ) when the frustration is smaller than a critical value,  $j \leq 1/4$ , whereas it becomes of helical-type for  $j > 1/4$  with a wave number  $q = \cos^{-1}(-1/4j)$ . Both the time-reversal and parity symmetries are broken in this helical-ordered phase. In the XY-like case ( $0 \leq \Delta < 1$ ), the helical-ordered state possesses a twofold discrete chiral degeneracy characterized by the right- and left-handed chirality, in addition to a continuous degeneracy associated with the original  $U(1)$  symmetry of the XY spin. The chiral order parameter is defined by<sup>1</sup>

$$O_{\kappa} = \frac{1}{LS^2} \sum_l \kappa_l, \quad (3)$$

$$\kappa_l = S_l^x S_{l+1}^y - S_l^y S_{l+1}^x = [\vec{S}_l \times \vec{S}_{l+1}]_z.$$

Note that this vector chirality  $\kappa_l$  is distinct from the scalar chirality often discussed in the literature<sup>2</sup> defined by  $\chi_l = \vec{S}_{l-1} \cdot \vec{S}_l \times \vec{S}_{l+1}$ : The chirality  $O_{\kappa}$  changes its sign under the parity operation but is invariant under the time-reversal operation, while the scalar chirality changes its sign under the both operations.

In the quantum case  $S < \infty$ , it seems well established that no magnetic LRO emerges at least for  $0 \leq \Delta \leq 1$  in contrast to the classical limit. The magnetic LRO (2) is destroyed by quantum fluctuations. We note that the absence of magnetic LRO in the quantum spin chain (1) is proved rigorously for the XY ( $\Delta = 0$ ) and the Heisenberg ( $\Delta = 1$ ) cases.<sup>3</sup> By contrast, no theorem prohibiting the spontaneous breaking of the parity symmetry has been known. Accordingly, there remains a possibility of the appearance of a ‘‘chiral’’ ordered phase in which only the chirality (3) exhibits a LRO without the magnetic helical LRO (2). This phase breaks only the parity symmetry spontaneously with preserving both the time-reversal and translational symmetries.

For the  $S = 1/2$  chain, Nersisyan *et al.* predicted, using the bosonization technique combined with a mean-field analysis, that in the XY case ( $\Delta = 0$ ) the system might exhibit a chiral-ordered phase with gapless excitations for large  $j$ .<sup>4</sup> This gapless chiral phase, however, has not been identified in our previous numerical work in which the Binder parameter of the chirality was calculated numerically for the  $S = 1/2$  XY chain with up to  $L = 20$  sites using the exact-diagonalization (ED) method.<sup>5</sup> Although Aligia *et al.*<sup>6</sup> pointed out that the system size  $L = 20$  might be insufficient to deal with the chirality in the large- $j$  region where the gapless chiral phase was expected, the question whether the chiral phase is realized in the  $S = 1/2$  case has not been clarified so far.

Meanwhile, the situation seems less controversial in the  $S=1$  case. In the previous works, we determined the ground-state phase diagram of the  $S=1$   $XXZ$  chain by means of both the ED and the density-matrix renormalization-group (DMRG) calculations, and showed that the gapless chiral phase appeared in a broad region of the  $j$ - $\Delta$  plane.<sup>5,7</sup> This observation was supported by the recent field-theoretical analysis by Kolezhuk,<sup>8</sup> in which he obtained the gapless chiral phase not only for  $S=1$  but also for general integer  $S$ . Lecheminant *et al.* extended the bosonization analysis by Nersesyan *et al.* to general  $S$  and concluded the appearance of the gapless chiral phase.<sup>9</sup>

An interesting observation that was first revealed by our numerical study of the  $S=1$  chain is that there exist two different types of chiral phases.<sup>5,7</sup> In one of them, the gapless chiral phase, the chiral LRO exists while the string and spin correlations decay algebraically suggesting gapless excitations. In the other, called the gapped chiral phase or the ‘‘chiral Haldane’’ phase, the chiral and string LRO’s coexist and the spin correlation decays exponentially suggesting a finite energy gap. The chiral Haldane phase exists in a very narrow but finite region between the Haldane and the gapless chiral phases. For example, in the pure- $XY$  case ( $\Delta=0$ ), the system undergoes two successive transitions with increasing  $j$ , first at  $j=j_{c1}^{(1)}\approx 0.473$  from the Haldane phase to the chiral Haldane phase, and then at  $j=j_{c2}^{(1)}\approx 0.490$  from the chiral Haldane phase to the gapless chiral phase. The next question that arises naturally is whether the gapped chiral phase is even realized for general  $S\neq 1$ , or it is specific to  $S=1$ . In Ref. 8, Kolezhuk suggested that the gapped chiral phase existed also for general integer  $S$ , although the method used was not applicable to half-odd integer  $S$ . Lecheminant *et al.* showed within the bosonization analysis that the gapless chiral phase realized at larger  $j$  might undergo a transition into the gapped chiral phase with decreasing  $j$  for any  $S$  including both integer and half-odd integer  $S$ .<sup>9</sup> However, both of these analyses were based on some approximations, and the question whether the gapped chiral phase exists for general  $S\neq 1$  still remains open.

The aim of this paper is to examine whether the gapless and gapped chiral phases exist in the frustrated  $XXZ$  chain (1) for general  $S$ . Furthermore, we wish to clarify how the chiral-ordered phases change their character as the spin quantum number  $S$  increases, to be connected to the helical-ordered phase realized in the classical limit  $S\rightarrow\infty$ . For these purposes, we numerically determine the ground-state phase diagrams of the spin chain (1) in the cases of  $S=1/2$ ,  $3/2$ , and  $2$ . The method used is the same as that in our previous work.<sup>7</sup> Using the DMRG method, we calculate appropriate correlation functions associated with the order parameters characterizing each phase, and analyze their long-distance behaviors. A preliminary account of our result for the  $S=1/2$  chain has been given in Ref. 10. By combining the obtained results with those of the  $S=1$  chain determined previously,<sup>7</sup> we find that the gapless chiral phase appears in the cases of general  $S\geq 1/2$ . By contrast, the gapped chiral phase has been identified only in the cases of integer  $S$  ( $S=1$  and  $2$ ): It has not been identified within our present

numerical accuracy in the cases of half-odd integer  $S$  ( $S=1/2$  and  $3/2$ ). It also turns out that the region of the gapless chiral phase becomes broader as  $S$  becomes larger, smoothly converging to the region of the helical-ordered phase in the  $S\rightarrow\infty$  limit realized at  $j\geq 1/4$ .

The plan of this paper is as follows. In Sec. II, we explain the method used in this paper. Various correlation functions associated with each order parameter are introduced. We show the results of our DMRG calculation in Sec. III. The phase diagrams obtained for  $S=1/2$ ,  $3/2$ , and  $2$  are presented in Secs. III A, III B, and III C, respectively. By combining the results with the  $S=1$  phase diagram determined previously,<sup>7</sup> we discuss the  $S$  dependence of the phase diagram in Sec. IV. We also compare our result on the decay exponent of the spin correlation with the prediction from the bosonization studies.<sup>4,9</sup> Finally, our results are summarized in Sec. V.

## II. CORRELATION FUNCTIONS AND NUMERICAL METHOD

In this section, we introduce various correlation functions and explain our numerical method.

For half-odd integer  $S$ , it has been known via previous studies that there exist two distinct phases, the spin fluid (SF) and the dimer phases.<sup>11</sup> The SF phase is characterized by gapless excitations above the singlet ground state and an algebraic decay of spin correlations. By contrast, the dimer phase is characterized by a finite energy gap above the doubly degenerate ground states and an exponential decay of spin correlations. In the dimer phase, both the parity and translational symmetries are broken spontaneously. The order parameter characterizing the dimer phase is given as

$$O_{\text{dim}}^{\alpha} = \frac{1}{LS^2} \sum_l \tau_l^{\alpha} \quad (\alpha=x, z) \quad (4)$$

$$\tau_l^{\alpha} = (-1)^l S_l^{\alpha} S_{l+1}^{\alpha}.$$

For the  $S=1/2$  and  $S=3/2$  open chains, we calculate the chiral-, dimer-, and spin-correlation functions defined by

$$C_{\kappa}(r) = \frac{1}{S^4} \langle \kappa_{l_0-r/2} \kappa_{l_0+r/2} \rangle, \quad (5)$$

$$C_{\text{dim}}^x(r) = \frac{1}{S^4} \langle S_{l_0-r/2}^x S_{l_0-r/2+1}^x \times (S_{l_0+r/2}^x S_{l_0+r/2+1}^x - S_{l_0+r/2+1}^x S_{l_0+r/2+2}^x) \rangle, \quad (6)$$

$$C_s^{\alpha}(r) = \frac{1}{S^2} \langle S_{l_0-r/2}^{\alpha} S_{l_0+r/2}^{\alpha} \rangle \quad (\alpha=x, z), \quad (7)$$

which are associated with the order parameters (3), (4), and (2), respectively. The site number  $l_0$  represents the center position of the open chains, i.e.,  $l_0=L/2$  for even  $r$  and  $l_0=(L+1)/2$  for odd  $r$ . We note that the number of site  $L$  is

set to be even. The notation  $\langle \cdots \rangle$  represents the expectation value at the lowest energy state in the subspace of  $S_{total}^z = 0$ .

For integer  $S$ , on the other hand, it has been known that there generally exist the SF and the Haldane phases,<sup>12</sup> except for the  $S=1$  case where only the Haldane phase appears for  $\Delta \geq 0$ .<sup>7,9</sup> The Haldane phase, in which the spin correlation decays exponentially with a finite energy gap above the singlet ground state, is characterized by the generalized string order parameter<sup>13,14</sup>

$$O_{\text{str}} = \frac{1}{LS} \sum_l \exp\left(\sum_{k=1}^{l-1} i \frac{\pi}{S} S_k^z\right) S_l^z. \quad (8)$$

In the  $S=1$  case, it has also been found that there exists the ‘‘double-Haldane’’ phase in the region of larger  $j$ ,<sup>7,15</sup> although its existence has not been clear in the cases of  $S \geq 2$ .<sup>16</sup> In order to identify these possible Haldane and double-Haldane phases in the  $S=2$  open chain, we calculate the generalized-string-correlation function,

$$C_{\text{str}}(r) = \frac{1}{S^2} \left\langle S_{l_0-r/2}^z \exp\left(\sum_{k=l_0-r/2}^{l_0+r/2-1} i \frac{\pi}{2} S_k^z\right) S_{l_0+r/2}^z \right\rangle, \quad (9)$$

in addition to the chiral-correlation function  $C_\kappa(r)$  and the spin-correlation function  $C_s^\alpha(r)$  introduced above.

We calculate those correlation functions for various fixed values of  $\Delta$  ( $j$ ) with varying  $j$  ( $\Delta$ ), and estimate the transition point  $j_c$  ( $\Delta_c$ ) by examining the  $r$  dependence of the correlation functions at long distances. We employ the infinite-system DMRG algorithm proposed by White.<sup>17</sup> In the calculation of the  $S=2$  chain, in particular, the accelerated algorithm proposed by Nishino and Okunishi is used.<sup>18</sup> The number of kept states  $m$  is up to  $m=450$ ,  $m=260$ , and  $m=260$  for the  $S=1/2$ ,  $3/2$ , and  $2$  cases, respectively. Convergence of the data with respect to  $m$  is checked by consecutively increasing  $m$ . The truncation error of the DMRG calculation increases dramatically as  $j$  becomes larger. Accordingly, in the calculation of larger  $j$ , we need to keep more and more states in order to achieve the  $m$  convergence of the data. Due to this difficulty, our calculation is limited to rather small  $j$ , i.e.,  $j \leq 1.6$  for  $S=1/2$  and  $j \leq 1$  for  $S=3/2$  and  $2$ . In the infinite-system DMRG algorithm, the system size is increased by two at each DMRG step and the calculation is continued until the  $L$  convergence of the data has been attained. We have performed the calculation of typically 1000 DMRG steps (corresponding to the system with  $L=2000$  sites) by confirming the  $L$  convergence. We can thereby safely avoid the finite-size effect arising from the incommensurate character of the spin correlation as pointed out by Aligia *et al.*<sup>6</sup>

### III. NUMERICAL RESULTS

#### A. Spin-1/2 case

We begin with the  $S=1/2$  case. The frustrated XXZ spin chain (1) for  $S=1/2$  has been studied extensively so far. We first review the known properties of the ground-state phase diagram. With increasing  $j$ , the system undergoes a

Kosterlitz-Thouless (KT) phase transition from the SF phase to the dimer phase at  $j=j_d^{(1/2)}$ .<sup>19,20</sup> The critical value  $j_d^{(1/2)}$  has been estimated accurately for  $0 \leq \Delta \leq 1$ : It runs from  $j_d^{(1/2)}(\Delta=0) \approx 0.33$  in the XY case to  $j_d^{(1/2)}(\Delta=1) \approx 0.2411$  in the Heisenberg case as  $\Delta$  increases.<sup>20</sup> Furthermore, the phase diagram is divided into two regions according to the nature of the short-range spin correlation. The structure factor  $S(q)$  has a maximum at  $q=\pi$  for  $j < j_L^{(1/2)}$  whereas the maximum of  $S(q)$  occurs at an incommensurate position  $q < \pi$  for  $j > j_L^{(1/2)}$ . The Lifshitz point  $j_L^{(1/2)}$  in the Heisenberg case ( $\Delta=1$ ) has been estimated to be  $j_L^{(1/2)} \approx 0.52$ .<sup>21</sup> Meanwhile, the phase diagram in the large- $j$  region remains largely unclear. In particular, as already mentioned in Sec. I, the question whether the chiral phase ever exists for larger  $j$  still remains controversial.

Now, we show our numerical results on the dimer-chiral transition. Our results for the pure-XY case ( $\Delta=0$ ) have been presented in Ref. 10. Here, we consider the general case of  $\Delta > 0$ . As an example, the calculated chiral-, dimer-, and spin-correlation functions are shown in Figs. 1(a)–1(c) on log-log plots for  $j=1.4$  and for several typical values of  $\Delta$ . As can clearly be seen from Fig. 1 (a), the chiral-correlation function  $C_\kappa(r)$  for  $\Delta < \Delta_{c1}^{(1/2)} \approx 0.06$  is bent upward at larger  $r$  suggesting a finite chiral LRO, while  $C_\kappa(r)$  for  $\Delta > \Delta_{c1}^{(1/2)}$  is bent downward suggesting an exponential decay of chiral correlations. Although the data around the transition point suffer from the truncation error inherent to the DMRG calculation, we can estimate the transition point as  $\Delta_{c1}^{(1/2)} = 0.06_{-0.01}^{+0.03}$  by taking account of the  $m$  dependence of the data shown in the figure. Thus, we conclude that the chiral-ordered phase appears in the  $S=1/2$  chain with the XY-like anisotropy. The result is consistent with our finding in the pure-XY chain ( $\Delta=0$ ),<sup>10</sup> and with the prediction of the bosonization study.<sup>4</sup>

Meanwhile, as shown in Fig. 1(b), the dimer-correlation function  $C_{\text{dim}}^x(r)$  for  $\Delta > \Delta_{c2}^{(1/2)} \approx 0.06$  is bent upward for larger  $r$  suggesting a finite dimer LRO, whereas it is bent downward for  $\Delta < \Delta_{c2}^{(1/2)}$ . We estimate the dimer-transition point  $\Delta_{c2}^{(1/2)}$  to be  $\Delta_{c2}^{(1/2)} = 0.06 \pm 0.01$ . We note that, contrary to the chiral-correlation function, the  $m$  convergence of  $C_{\text{dim}}^x(r)$  has almost been attained at  $m=450$ . Figure 1(c) shows the spin-correlation function  $C_s^x(r)$  divided by the leading oscillating factor  $\cos(Qr)$ , where  $Q$  is the wave number characterizing the incommensurability of  $C_s^x(r)$  in real space. Here, the  $m$  convergence of the data has also almost been attained. Although the plots are largely scattered, which might be attributed to the possible influence of correction terms characterized by wave numbers  $Q' \neq Q$ , it is still clearly visible in the figure that the spin correlation is bent downward for  $\Delta > \Delta_{c2}^{(1/2)}$  suggesting an exponential decay, while it exhibits a linear behavior for  $\Delta < \Delta_{c2}^{(1/2)}$  suggesting a power-law decay. From these behaviors of the dimer and spin correlations, we conclude that, as  $\Delta$  decreases, the system exhibits a transition from the gapped phase with the dimer LRO ( $\Delta > \Delta_{c2}^{(1/2)}$ ) to the gapless phase without the dimer LRO ( $\Delta < \Delta_{c2}^{(1/2)}$ ). The behaviors of the chiral, dimer, and spin correlations mentioned above are essentially the same as those for  $\Delta=0$ .<sup>10</sup>

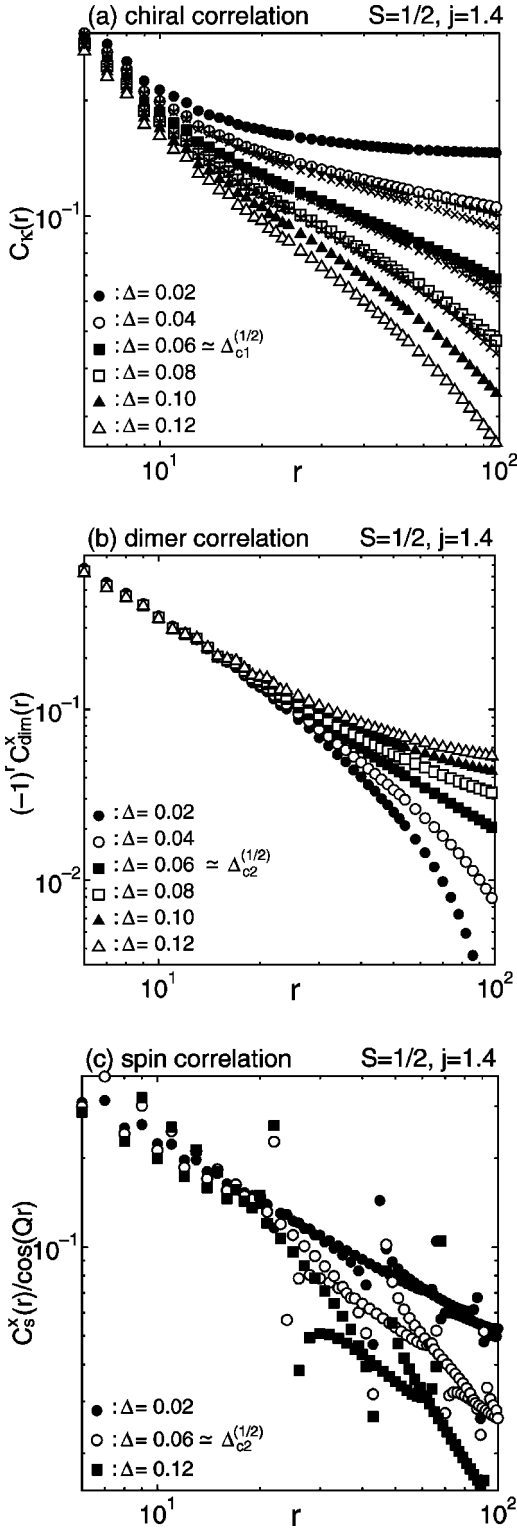


FIG. 1. Various correlation functions of the  $S=1/2$  chain for  $j=1.4$  and for several typical values of  $\Delta$  around the dimer-chiral transition: (a) chiral-correlation function  $C_\kappa(r)$ ; (b) dimer-correlation function  $(-1)^r C_{\text{dim}}^x(r)$ ; (c) spin-correlation function  $C_s^x(r)$  divided by the oscillating factor  $\cos(Qr)$ . The number of kept states is  $m=450$ . To illustrate the  $m$  dependence, we also indicate by crosses the data with  $m=400$  and  $350$  for  $\Delta=0.04, 0.06$ , and  $0.08$  in (a) where the  $m$  dependence is relatively large. In other cases, the truncation errors are smaller than the symbols.

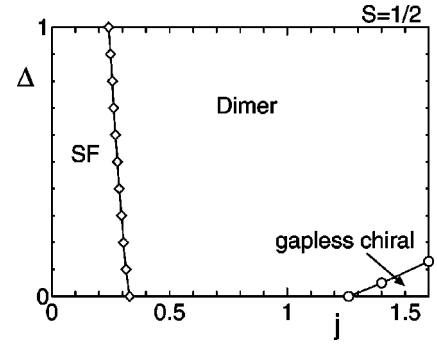


FIG. 2. The ground-state phase diagram of the  $S=1/2$  chain, where  $j$  and  $\Delta$  denote the ratio  $J_2/J_1$  and the exchange anisotropy, respectively, defined in Eq. (1). The diamonds and circles represent the transition points  $j_d^{(1/2)}$  and  $j_{c1}^{(1/2)}$ .

The remaining problem is the relation between  $\Delta_{c1}^{(1/2)}$  and  $\Delta_{c2}^{(1/2)}$ . Two possibilities seem to be allowed from our data, i.e., (i)  $\Delta_{c1}^{(1/2)} = \Delta_{c2}^{(1/2)}$  or (ii)  $\Delta_{c1}^{(1/2)} > \Delta_{c2}^{(1/2)}$ . If the case (i) is realized, the system undergoes only one phase transition at  $\Delta = \Delta_{c1}^{(1/2)} = \Delta_{c2}^{(1/2)}$  between the dimer phase and the gapless chiral phase with no dimer order. If the case (ii) is realized, on the other hand, the system undergoes two successive transitions on decreasing  $\Delta$ , first at  $\Delta = \Delta_{c1}^{(1/2)}$  from the dimer phase to the gapped chiral phase (or the ‘‘chiral dimer’’ phase) where both the dimer and chiral LRO’s coexist with gapfull excitations, and then at  $\Delta = \Delta_{c2}^{(1/2)}$  from the chiral dimer phase to the gapless chiral phase. Unfortunately, rather large error bars of  $\Delta_{c1}^{(1/2)}$  and  $\Delta_{c2}^{(1/2)}$  prevent us from determining which of the cases is realized although our result suggests that the chiral dimer phase, if it ever exists, appears only in a rather narrow region between the dimer and gapless chiral phases. The situation here is very much similar to the one encountered in the pure-XY case ( $\Delta=0$ ) with varying  $j$ .<sup>10</sup> Further work will be necessary to settle the question whether the chiral dimer phase exists in the  $S=1/2$  case.

Performing the calculations for several fixed values of  $j$  with varying  $\Delta$  and combining the result of Ref. 10, we determine the phase boundary between the dimer and the gapless chiral phases. The obtained transition points  $j_{c1}^{(1/2)}$  ( $\Delta_{c1}^{(1/2)}$ ) are plotted in Fig. 2 together with the SF-dimer transition points  $j_d^{(1/2)}$  determined by Nomura and Okamoto.<sup>20</sup> The transition line  $j_{c1}^{(1/2)}$  rises as  $j$  increases from the point in the XY case,  $j_{c1}^{(1/2)}(\Delta=0) \approx 1.26$ .<sup>10</sup> As can be seen from the phase diagram, the gapless chiral phase does exist in the large  $j$  region. At least within our present numerical precision, on the other hand, we did not find any evidence of the gapped chiral (chiral dimer) phase at all estimated points between the dimer and the gapless chiral phases.

Finally, we mention the reason why the ED analysis of Ref. 5 on the chain up to  $L=20$  sites failed to detect the chiral ordering in the  $S=1/2$  XY chain. We now consider that this failure can be ascribed to the finite-size effect discussed in Ref. 6. The wave number  $Q$  characterizing the incommensurability decreases rapidly from  $Q=\pi$  at  $j=j_L$  to  $Q=\pi/2$  at  $j \rightarrow \infty$  as  $j$  increases. In the  $S=1/2$  XY chain, the shift of  $Q$  from  $\pi/2$  turns out to be smaller than  $0.03\pi$  for

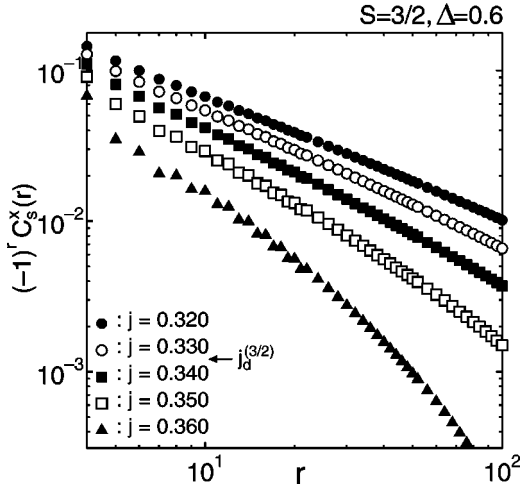


FIG. 3. The spin-correlation function  $(-1)^r C_s^x(r)$  of the  $S = 3/2$  chain for  $\Delta = 0.6$  and for several typical values of  $j$  around the SF-dimer transition. The number of kept states is  $m = 220$  for all  $j$ . The truncation errors are smaller than the symbols.

$j \gtrsim j_{c1}^{(1/2)} \approx 1.26$ . Meanwhile, in a finite open chain with  $L$  sites, the incommensurability smaller than  $2\pi/L$  cannot be taken into account because of the condition that the wave function should vanish on both ends of the chain. As a consequence, the system size must be larger than  $L \sim 70$  if one wishes to detect the shift of  $Q$  of order  $0.03\pi$ . Thus, the ED calculation on chains up to  $L = 20$  might fail to extract the true asymptotic properties of the chiral Binder parameter for  $j \gtrsim j_{c1}^{(1/2)}$ .

### B. Spin-3/2 case

In this subsection, we present the results for the  $S = 3/2$  case. The frustrated  $S = 3/2$  chain (1) was studied for the Heisenberg case ( $\Delta = 1$ ).<sup>16,22</sup> It was shown there that the system was in the SF phase for  $j < j_d^{(3/2)}$  while it was in the dimer phase for  $j > j_d^{(3/2)}$ . The phase transition of the KT type occurs at  $j = j_d^{(3/2)} \approx 0.33$ . The Lifshitz point was estimated to be at  $j = j_L^{(3/2)}(\Delta = 1) = 0.388$ .<sup>16</sup> Besides, the appearance of the gapped and gapless chiral phases was suggested recently for the  $XY$  case ( $\Delta = 0$ ) by the bosonization study.<sup>9</sup>

In Fig. 3, we show the DMRG data of the spin-correlation function  $C_s^x(r)$  for  $\Delta = 0.6$  and for several typical values of  $j$ . As can be seen from the figure, the spin correlation changes its behavior as  $j$  increases from a power-law decay ( $j < j_d^{(3/2)} \approx 0.335$ ) to an exponential decay ( $j > j_d^{(3/2)}$ ). We estimate the transition point between the gapless SF phase and the gapped dimer phase as  $j_d^{(3/2)}(\Delta = 0.6) = 0.335 \pm 0.015$ . By interpolating the transition points estimated in this way for various  $\Delta$ , we determine the SF-dimer transition line. The line runs from  $j_d^{(3/2)}(\Delta = 0) = 0.334 \pm 0.004$  in the  $XY$  case to  $j_d^{(3/2)}(\Delta = 1) = 0.335 \pm 0.015$  in the Heisenberg case, the latter being consistent with the estimate by Ziman and Schulz,  $j_d^{(3/2)}(\Delta = 1) \approx 0.33$ .<sup>22</sup>

Let us next consider the dimer-chiral transition. Figure 4(a) shows the chiral-correlation function  $C_\kappa(r)$  for  $\Delta = 0.6$

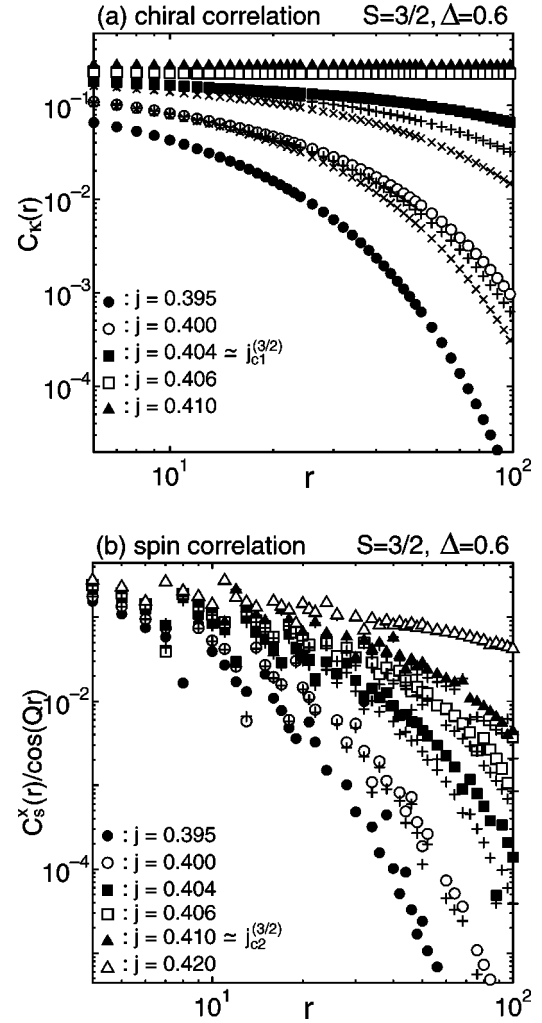


FIG. 4. Various correlation functions of the  $S = 3/2$  chain for  $\Delta = 0.6$  and for several typical values of  $j$  around the dimer-chiral transition: (a) chiral-correlation function  $C_\kappa(r)$ ; (b) spin-correlation function  $C_s^x(r)$  divided by the oscillating factor  $\cos(Qr)$ . The number of kept states is  $m = 260$ . We also indicate by crosses the data with  $m = 220$  and  $180$  for  $j = 0.400$  and  $0.404$  in (a), and the data with  $m = 220$  for  $j = 0.400$ ,  $0.404$ ,  $0.406$ , and  $0.410$  in (b). In other cases, the truncation errors are smaller than the symbols.

and for several typical values of  $j$ . As shown in the figure,  $C_\kappa(r)$  is bent upward for  $j > j_{c1}^{(3/2)} \approx 0.404$  suggesting a finite LRO, while it is bent downward for  $j < j_{c1}^{(3/2)}$  suggesting an exponential decay. Hence, the chiral-ordered phase is realized also in the  $S = 3/2$  case. The transition point at which the chiral LRO sets in is estimated to be  $j_{c1}^{(3/2)} = 0.404_{-0.006}^{+0.002}$ . The spin-correlation function  $C_s^x(r)$  for  $\Delta = 0.6$  is shown in Fig. 4 (b) where the data are divided by the oscillating factor  $\cos(Qr)$ . As in the  $S = 1/2$  case, the plots are largely scattered suggesting the existence of non-negligible correction terms. Nevertheless, it can be seen that the behavior of  $C_s^x(r)$  changes as  $j$  increases from an exponential decay to an algebraic decay at around  $j = j_{c2}^{(3/2)} = 0.410 \pm 0.010$ . We thus conclude that the system for  $j > j_{c2}^{(3/2)}$  is in the gapless chiral phase. Unfortunately, the error of our estimate of  $j_{c2}^{(3/2)}$  is quite large. This large error is ascribed to the poor  $m$  con-

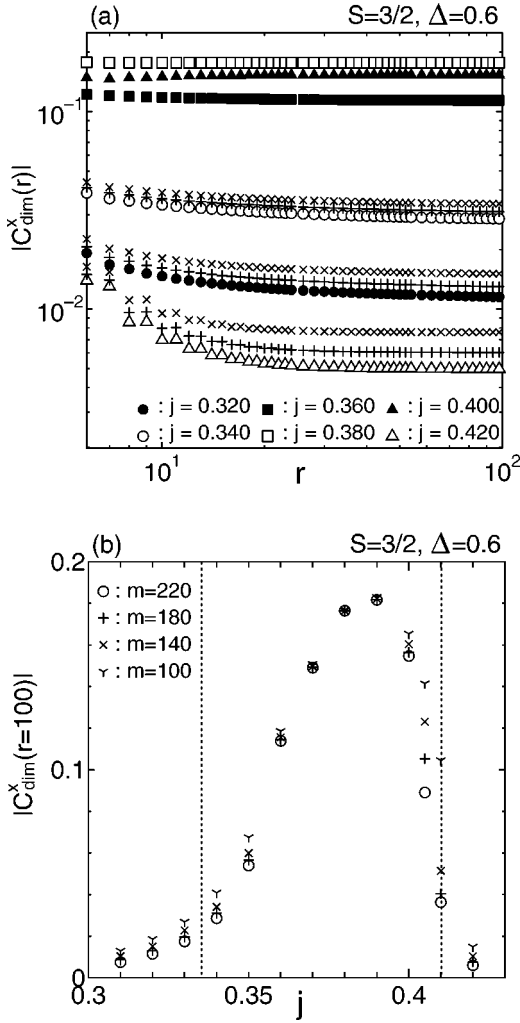


FIG. 5. (a) The  $r$  dependence of the dimer-correlation function  $C_{\text{dim}}^x(r)$  of the  $S=3/2$  chain for  $\Delta=0.6$  and for several typical values of  $j$ . The number of kept states is  $m=220$ . To illustrate the  $m$  dependence of the data, we also plot the data with  $m=180$  and  $140$  by crosses for  $j=0.320, 0.340$ , and  $0.420$ . The truncation errors for the other  $j$ 's are smaller than the symbols. (b) The  $j$  dependence of the value of  $C_{\text{dim}}^x(r=100)$  for various  $m$ . The dotted lines represent the phase boundaries,  $j=j_d^{(3/2)}(\Delta=0.6)\approx 0.335$  and  $j=j_{c1}^{(3/2)}(\Delta=0.6)\approx 0.410$ .

vergence of the data of  $C_s^x(r)$  shown in Fig. 4(b) and of the data of the dimer-correlation function  $C_{\text{dim}}^x(r)$  to be mentioned below. (Note that the situation here is different from the  $S=1/2$  case where the  $m$  convergence of the spin- and dimer-correlation functions is almost achieved at  $m=450$ : See Fig. 1.) Because of the errors in the estimates of  $j_{c1}^{(3/2)}$  and  $j_{c2}^{(3/2)}$ , we cannot determine whether  $j_{c2}^{(3/2)}$  is either larger than or equal to  $j_{c1}^{(3/2)}$ . Thus, in our present calculation, the gapped chiral phase has not been identified in the  $S=3/2$  case as well as in the  $S=1/2$  case. We have performed the same calculation for various  $\Delta$  with varying  $j$ , but have not been able to identify the gapped chiral phase at any  $j$  and  $\Delta$ .

In Fig. 5(a), we show the dimer-correlation function  $C_{\text{dim}}^x(r)$  for  $\Delta=0.6$  and for several typical values of  $j$ . At a glance, the data may look like indicating a finite dimer LRO

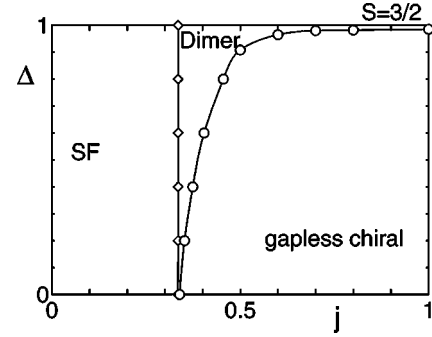


FIG. 6. The ground-state phase diagram of the  $S=3/2$  chain, where  $j$  and  $\Delta$  denote the ratio  $J_2/J_1$  and the exchange anisotropy, respectively, defined in Eq. (1). The diamonds and circles represent the transition points  $j_d^{(3/2)}$  and  $j_{c1}^{(3/2)}$ .

even in the SF phase ( $j < j_d^{(3/2)} \approx 0.335$ ) and in the gapless chiral phase ( $j > j_{c1}^{(3/2)} \approx 0.410$ ) where no dimer LRO is to be expected. The dimer correlations in these phases, however, rapidly decrease with increasing  $m$ , whereas the  $m$  convergence has almost been attained in the intermediate range of  $j$  corresponding to the gapped phase ( $j_d^{(3/2)} < j < j_{c1}^{(3/2)}$ ). To elucidate the  $m$  dependence of the long-distance value of the dimer correlation, we plot in Fig. 5(b) the value of  $C_{\text{dim}}^x(r=100)$ , which is expected to be a good approximation of  $C_{\text{dim}}^x(r \rightarrow \infty)$ .<sup>23</sup> The figure shows that  $C_{\text{dim}}^x(r=100)$  in the gapped phase converges to a nonzero value as  $m \rightarrow \infty$ , while it decreases toward zero in the SF and the gapless chiral phases. Thus, we infer that the apparent finite dimer LRO observed in  $C_{\text{dim}}^x(r)$  for  $j < j_d^{(3/2)}$  and  $j > j_{c1}^{(3/2)}$  is a spurious effect due to the truncation error.<sup>24</sup> The variation of the data with varying  $j$  near the expected phase boundaries is rather gentle, which prevents us from estimating the transition points accurately from Fig. 5(b). Nevertheless, we may conclude that the system in the gapped region  $j_d^{(3/2)} < j < j_{c1}^{(3/2)}$  possesses a true dimer LRO and is indeed in the dimer phase.

We show in Fig. 6 the obtained ground-state phase diagram of the  $S=3/2$  chain including the SF-dimer and the dimer-chiral transition lines,  $j_d^{(3/2)}$  and  $j_{c1}^{(3/2)}$ . We note that the dimer phase exists even in the XY case ( $\Delta=0$ ) for  $j_d^{(3/2)} \approx 0.334 < j < j_{c1}^{(3/2)} \approx 0.339$  although its width is quite narrow. The value of  $j_{c1}^{(3/2)}$  becomes larger as  $\Delta$  becomes larger, and the dimer-chiral phase boundary appears to tend to the Heisenberg line  $\Delta=1$  as  $j \rightarrow \infty$ .

### C. Spin-2 case

In this subsection, we present our results for the  $S=2$  case. It has been known that the  $S=2$  chain with only the nearest-neighbor coupling exhibits a phase transition between the SF and the Haldane phases.<sup>25,26</sup> The transition point was estimated to be at  $\Delta = \Delta_H^{(2)}(j=0) \approx 0.966$ .<sup>26</sup> Meanwhile, the Lifshitz point in the Heisenberg case was estimated to be at  $j = j_L^{(2)}(\Delta=1) = 0.325$ .<sup>16</sup> Very recently, the existence of the gapless and gapped chiral phases has been suggested by the large- $S$  approach<sup>8</sup> and the bosonization method.<sup>9</sup>

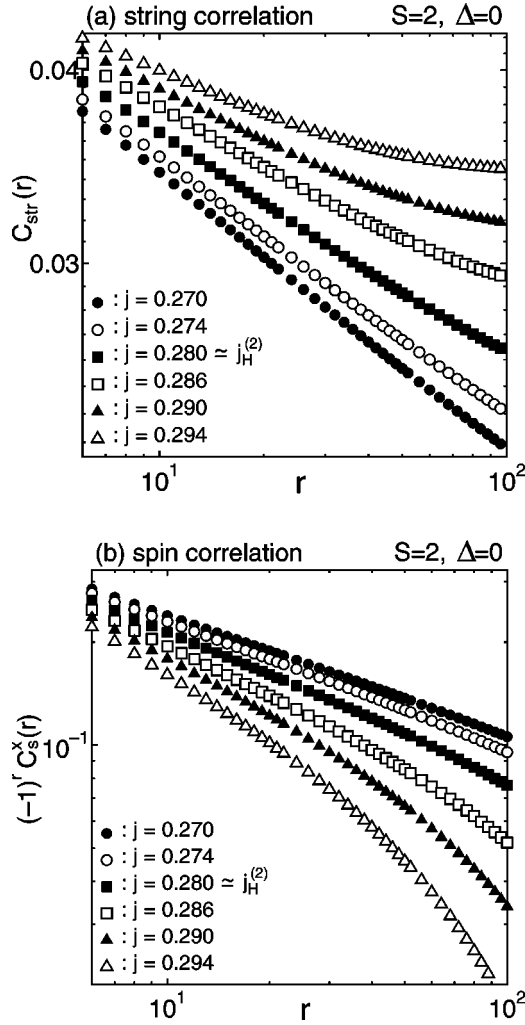


FIG. 7. Various correlation functions of the  $S=2$  chain for  $\Delta=0$  and for several typical values of  $j$  around the SF-Haldane transition: (a) generalized-string-correlation function  $C_{\text{str}}(r)$ ; (b) spin-correlation function  $(-1)^r C_s^x(r)$ . The number of kept states is  $m=220$ . The truncation errors are smaller than the symbols.

Let us first consider the SF-Haldane transition at  $j=j_H^{(2)}$ . In Fig. 7, we show the generalized-string- and spin-correlation functions  $C_{\text{str}}(r)$  and  $C_s^x(r)$  for  $\Delta=0$  and for several typical values of  $j$  on log-log plots. It can be seen in Fig. 7(a) that  $C_{\text{str}}(r)$  is bent upward for  $j>j_H^{(2)}\approx 0.280$  suggesting a finite LRO, while it shows a linear behavior for  $j<j_H^{(2)}$  suggesting an algebraic decay. Meanwhile, as shown in Fig. 7(b),  $C_s^x(r)$  decays exponentially for  $j>j_H^{(2)}$  indicating a finite gap, whereas it decays algebraically for  $j<j_H^{(2)}$ . We thus conclude that there occurs a phase transition at  $j=j_H^{(2)}$  between the SF and the Haldane phases. The critical value  $j_H^{(2)}$  is estimated to be  $j_H^{(2)}=0.280\pm 0.006$ . We estimate the critical points for various fixed  $\Delta$  ( $j$ ), and determine the phase boundary. The transition line smoothly connects the point  $j=j_H^{(2)}(\Delta=0)=0.280\pm 0.006$  in the XY case to the point of the case of no frustration,  $\Delta=\Delta_H^{(2)}(j=0)=0.96\pm 0.01$ . (See the phase diagram shown in Fig. 9.) The latter estimate is consistent with the previous estimate by Nomura and Kitazawa,  $\Delta_H^{(2)}(j=0)=0.966$ .<sup>26</sup>

Next, we consider the transition between the Haldane and the chiral phases. Figure 8(a) exhibits the chiral-correlation function  $C_\kappa(r)$  for  $\Delta=0$  and for several typical values of  $j$ . As can clearly be seen from the figure,  $C_\kappa(r)$  exhibits a finite LRO for  $j>j_{c1}^{(2)}\approx 0.318$  whereas it exhibits an exponential decay for  $j<j_{c1}^{(2)}$ . We estimate the transition point where the chiral LRO sets in to be  $j_{c1}^{(2)}=0.318\pm 0.001$ . As shown in Fig. 8(b), the generalized-string correlation  $C_{\text{str}}(r)$  exhibits a finite LRO for  $j<j_{c2}^{(2)}\approx 0.324$  whereas it decays algebraically for  $j>j_{c2}^{(2)}$ .<sup>27</sup> Meanwhile, as shown in Fig. 8(c), the spin-correlation function  $C_s^x(r)$  divided by the leading oscillating factor  $\cos(Qr)$  decays exponentially for  $j<j_{c2}^{(2)}$  whereas it decays algebraically for  $j>j_{c2}^{(2)}$ . From these observations, we estimate the transition point where the excitation spectrum becomes gapless and the generalized-string order vanishes to be  $j_{c2}^{(2)}=0.324_{-0.002}^{+0.006}$ . Here the estimate of  $j_{c2}^{(2)}$  is quite close to, but distinctly larger than that of  $j_{c1}^{(2)}=0.318\pm 0.001$ . Indeed, the data of  $j=0.320$  in Fig. 8 clearly show the existence of an intermediate phase, the gapped chiral phase, where the chiral and the generalized string LRO's coexist and the spin correlation decays exponentially. Hence, we conclude that, as in the case of the  $S=1$  chain, the gapped chiral (chiral Haldane) phase exists also in the  $S=2$  chain in a very narrow but finite region ( $j_{c1}^{(2)}<j<j_{c2}^{(2)}$ ) between the Haldane phase ( $j<j_{c1}^{(2)}$ ) and the gapless chiral phase ( $j>j_{c2}^{(2)}$ ). Performing the same calculations for various fixed  $\Delta$ , we estimate the transition points  $j_{c1}^{(2)}$  and  $j_{c2}^{(2)}$ . The chiral Haldane phase is also found in a certain range of  $j$  for  $\Delta=0.2, 0.4, 0.6$ , and  $0.8$ . By contrast, we cannot confirm its existence for  $\Delta>0.8$  corresponding to  $j\geq 0.5$  within our numerical accuracy. This is due to the large truncation error growing drastically with increasing  $j$ , which prevents us from precisely determining the transition points.

The obtained phase diagram of the  $S=2$  chain is shown in Fig. 9. The gapless chiral phase appears in a quite broad region of large  $j$ . The boundary of the region with the chiral LRO,  $j_{c1}^{(2)}$ , rises steeply as  $j$  increases from the point on the XY line,  $j_{c1}^{(2)}(\Delta=0)\approx 0.318$ , tending to the Heisenberg line  $\Delta=1$ . We note that, although our estimates of the points where the chiral LRO sets in are very close to  $\Delta=1$  for  $j\geq 0.6$ , i.e.,  $\Delta_{c1}^{(2)}=0.9975\pm 0.0025$  for all  $j=0.6, 0.7, 0.8$ , and  $1.0$ , the chiral LRO is not observed on the Heisenberg line  $\Delta=1$  where there no longer exists the twofold discrete chiral degeneracy.

We finally refer to our numerical results on the possible double-Haldane (DH) phase. The DH phase was first found in the large- $j$  region of the frustrated  $S=1$  Heisenberg chain.<sup>15</sup> In the DH phase, the next-nearest-neighbor coupling  $J_2$  is dominant and the system can be regarded as two Haldane subchains coupled by the weak inter-subchain coupling  $J_1$ . The DH phase is characterized by the absence of the string, spin, and chiral LRO's.<sup>28</sup> It has been shown that in the frustrated  $S=1$  XXZ chain with  $\Delta\geq 0.95$ , there occurs a first order phase transition between the Haldane and the DH phases.<sup>7,15</sup> The string order parameter vanishes discontinuously at the transition point. In our present study on the

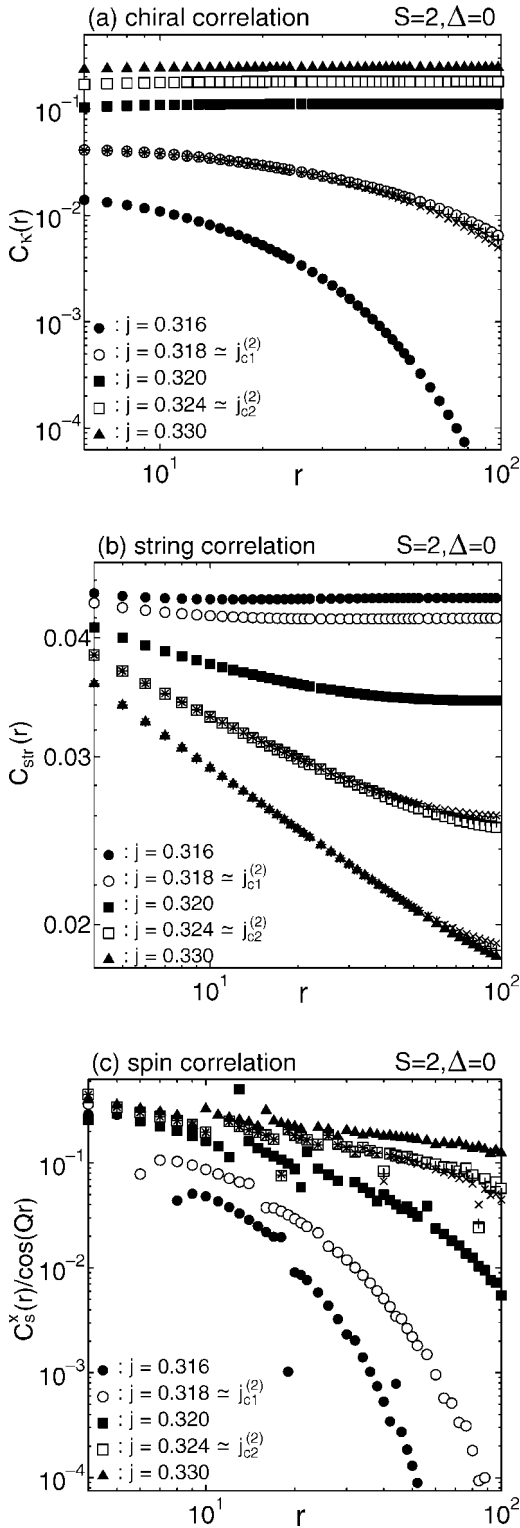


FIG. 8. Various correlation functions of the  $S=2$  chain for  $\Delta=0$  and for several typical values of  $j$  around the Haldane-chiral transition: (a) chiral-correlation function  $C_\kappa(r)$ ; (b) generalized-string-correlation function  $C_{\text{str}}(r)$ ; (c) spin-correlation function  $C_s^x(r)$  divided by the oscillating factor  $\cos(Qr)$ . The number of kept states is  $m=260$ . To illustrate the  $m$  dependence, we also indicate by crosses the data with  $m=220$  and  $180$  for  $j=0.318$  in (a),  $j=0.324$  and  $0.330$  in (b), and  $j=0.324$  in (c). In other cases, the truncation errors are smaller than the symbols.

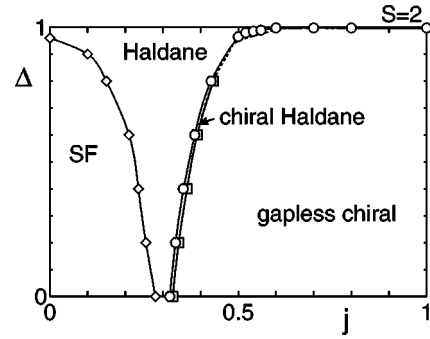


FIG. 9. The ground-state phase diagram of the  $S=2$  chain, where  $j$  and  $\Delta$  denote the ratio  $J_2/J_1$  and the exchange anisotropy, respectively, defined in Eq. (1). The diamonds, circles, and squares represent the transition points  $j_d^{(2)}$ ,  $j_{c1}^{(2)}$ , and  $j_{c2}^{(2)}$ , respectively.

frustrated  $S=2$  Heisenberg chain, such a vanishing of the string order has not been observed: The generalized-string-correlation function  $C_{\text{str}}(r)$  in the Heisenberg case ( $\Delta=1$ ) exhibits a finite LRO for an entire region studied here,  $0 \leq j \leq 1$ , while both the spin- and chiral-correlation functions  $C_s^x(r)$  and  $C_\kappa(r)$  show an exponential decay for  $0 \leq j \leq 1$  suggesting a gapful excitation. We note that, as  $j$  increases, the extrapolated value  $C_{\text{str}}(r \rightarrow \infty)$  decreases rapidly around  $j \approx 0.4$ . Although the rapid drop of the string LRO might be a sign of a phase transition from the Haldane phase to a new intermediate phase between the Haldane and the DH phases as suggested in Ref. 16, the situation here remains largely unclear. Further work is required to clarify the details of the transition at and near  $\Delta=1$  and the possible existence of the DH phase for  $j \geq 1$ .

#### IV. S DEPENDENCE

Based on our present results for  $S=1/2$ ,  $3/2$ , and  $2$  and our previous result for  $S=1$ ,<sup>7</sup> we now discuss how the ground-state phase diagrams change as  $S$  increases from  $S=1/2$  toward the classical limit  $S \rightarrow \infty$ . We are interested particularly in the way how the classical limit is achieved from the quantum phases analyzed above.

By comparing the obtained phase diagrams for  $S=1/2$ ,  $1$ ,  $3/2$ , and  $2$ , we deduce several features of the phase diagrams. The first is about the fate of the dimer and the Haldane phases. These phases are pure quantum ones in the sense that singlet spin pairs play an essential role in stabilizing them. Hence, it is natural to expect that the regions of these quantum phases become narrower as  $S$  gets larger. This feature can clearly be seen in the phase diagrams obtained for  $1/2 \leq S \leq 2$ : The dimer phase for  $S=3/2$  is narrower than that for  $S=1/2$ , while the Haldane phase for  $S=2$  is narrower than that for  $S=1$ . It thus seems reasonable to expect that the dimer and the Haldane phases continue to become narrower for  $S > 2$ , and eventually vanish in the classical limit  $S \rightarrow \infty$ .

The second feature concerns the chiral-ordered phases. Recently, the  $S$  dependence of the boundary of the chiral-ordered phases was examined via the field-theoretical large- $S$  approach.<sup>8</sup> It was shown there that, as  $S$  increased, the region of the gapless chiral phase converged smoothly to that of the



TABLE I. The estimates of  $j_d^{(S)}$ ,  $j_H^{(S)}$ ,  $j_{c1}^{(S)}$ , and  $j_{c2}^{(S)}$  in the XY case ( $\Delta=0$ ) for half-odd integer  $S$  ( $S=1/2$  and  $3/2$ ) and for integer  $S$  ( $S=1$  and  $2$ ). The data for  $S=1$  are from Ref. 7. The ratio  $(j_{c2}^{(S)} - j_{c1}^{(S)})/j_{c1}^{(S)}$  for integer  $S$  is also listed.

$S$	$j_d^{(S)}$	$j_H^{(S)}$	$j_{c1}^{(S)}$	$j_{c2}^{(S)}$	$(j_{c2}^{(S)} - j_{c1}^{(S)})/j_{c1}^{(S)}$
1/2	0.33 <sup>a</sup>		$1.26_{-0.03}^{+0.01}$	$1.26 \pm 0.01$	
3/2	$0.334 \pm 0.004$		$0.339 \pm 0.001$	$0.340_{-0.002}^{+0.004}$	
1		0	$0.473 \pm 0.001$	$0.490_{-0.005}^{+0.010}$	0.036
2		$0.280 \pm 0.006$	$0.318 \pm 0.001$	$0.324_{-0.002}^{+0.006}$	0.019

<sup>a</sup>Reference 20.

helical-ordered phase in the classical limit  $S \rightarrow \infty$ , whereas the gapped chiral phase vanished asymptotically. This feature of the chiral phases might be understood intuitively by considering the role of quantum fluctuations in the symmetry breaking. In the helical-ordered state with a finite magnetic LRO realized in the classical limit  $S \rightarrow \infty$ , both the discrete  $Z_2$  parity and the continuous  $U(1)$  spin symmetries are broken spontaneously. In the gapless chiral phase, quantum fluctuations marginally recover the continuous  $U(1)$  symmetry yielding the quasi-long-range spin order, with keeping the discrete  $Z_2$  parity symmetry broken. In this sense, the gapless chiral phases can be regarded as a quantum remnant of the classical helical phase. By contrast, the gapped chiral phase should be regarded as a pure-quantum phase since it exhibits a topological LRO, i.e., the string LRO, in the chiral-Haldane phase for integer  $S$ . (In the chiral-dimer phase for half-odd integer  $S$ , if any, the topological LRO is the dimer LRO, although we do not find evidence of such a phase in the present study.) We therefore expect that the gapped chiral phase should vanish in the classical limit  $S \rightarrow \infty$ . The observed behaviors of the chiral phases in the obtained phase diagrams are consistent with the above expectation. With increasing  $S$ , the chiral-transition line  $j_{c1}^{(S)}(\Delta)$  approaches that of the helical-ordered phase,  $j=1/4$ . Meanwhile, the region of the chiral-Haldane phase found for integer  $S$  shrinks as  $S$  increases. As an example, we list in Table I the estimated values of  $j_{c1}^{(S)}$  and  $j_{c2}^{(S)}$  in the XY case ( $\Delta=0$ ) and their ratio  $(j_{c2}^{(S)} - j_{c1}^{(S)})/j_{c1}^{(S)}$  for integer  $S$ , which is a measure of the relative stability of the chiral-Haldane phase.

The third feature concerns the SF phase. One may naturally expect that, as  $S$  increases, the region of the SF phase converges to that of the Néel phase in the classical limit  $S \rightarrow \infty$ . Somewhat unexpectedly, in the obtained phase diagrams, the SF phase grows as  $S$  becomes larger, *exceeding* the classical phase boundary of the Néel phase,  $j=1/4$ . (See the phase diagrams and Table I in which the estimates of  $j_d^{(S)}$  and  $j_H^{(S)}$  in the XY case are listed.) We consider that this ‘‘overshooting’’ is due to the rapid shrink of the dimer and the Haldane phases and that the boundary of the SF phase eventually ‘‘turns back’’ converging to the classical phase boundary  $j=1/4$  for large enough  $S$ . In order to confirm this conjecture, the analysis of larger  $S$  is needed, which is beyond the scope of the present work.

Finally, we wish to compare our numerical result on the decay exponent of the spin correlation with the prediction

from the bosonization analysis.<sup>4,9</sup> Applying the bosonization technique and the mean-field approximation, the authors of Refs. 4 and 9 predicted that for large enough  $j$  the spin-correlation function  $C_s^x(r)$  in the XY case should exhibit the asymptotic behavior,

$$C_s^x(r) = A \cos(Qr) r^{-\eta_x}, \quad (10)$$

where  $A$  is a numerical constant and the exponent  $\eta_x$  is given by  $\eta_x = 1/(8S)$ . We fit our numerical data for the  $S=1/2$ ,  $3/2$ , and  $2$  XY chains with Eq. (10), taking  $A$ ,  $Q$ , and  $\eta_x$  as fitting parameters. Resulting estimates of the decay exponent  $\eta_x$  are shown in Fig. 10 together with our previous estimate for the  $S=1$  XY chain.<sup>7</sup> The error bar is estimated by changing the region of the data used in the fitting and taking a difference of them. As can be seen from Fig. 10, the estimates of  $\eta_x$  decrease monotonically as  $j$  increases. For  $S \geq 1$ , the asymptotic  $j \rightarrow \infty$  value has almost been attained at around  $j \approx 1$ , which is in good agreement with the predicted value  $1/(8S)$ . For the  $S=1/2$  case, on the other hand, we can not reach the asymptotic  $j \rightarrow \infty$  regime: The estimated  $\eta_x$  still continues to decrease even around  $j \approx 1.5$ , the largest  $j$  value for which we can get reliable data. The estimated  $\eta_x$ , however, shows a tendency to further decrease toward the predicted value  $\eta_x = 1/4$  as  $j$  increases, which is consistent with the result of the bosonization study. Thus, our result can be considered as a numerical support of the bosonization analysis.

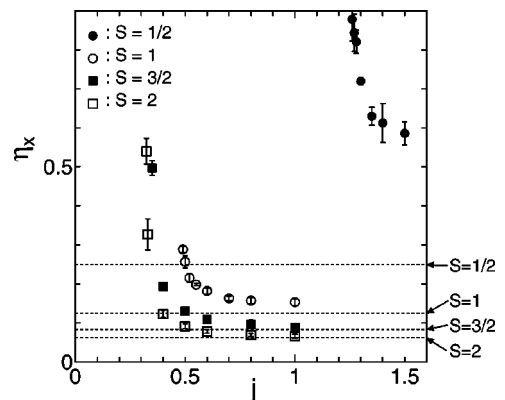


FIG. 10. The estimated decay exponent  $\eta_x$  as a function of  $j$  for the  $S=1/2$ ,  $1$ ,  $3/2$ , and  $2$  XY chains. The dotted lines represent the prediction of the bosonization analysis<sup>4,9</sup> at  $j \rightarrow \infty$ ,  $\eta_x = 1/(8S)$ .

## V. SUMMARY

In the present work, we have studied the ground-state properties of the frustrated spin- $S$  XXZ chains (1), especially paying attention to the chiral-ordered phases in which only the chirality exhibits a finite LRO without the standard magnetic LRO. We have used the infinite-system DMRG method to calculate the correlation functions associated with the spin-, chiral-, dimer-, and string-order parameters. By analyzing the long-distance behavior of the correlation functions, we have determined the ground-state phase diagrams of the  $S = 1/2$ ,  $3/2$ , and  $2$  chains for  $0 \leq \Delta \leq 1$  and  $j \geq 0$  (Figs. 2, 6, and 9).

By comparing the obtained results with our previous result for the  $S = 1$  chain, we reach the following picture of the ground-state phase diagram. In the integer  $S$  chains ( $S = 1$  and  $2$ ), the phase diagram consists of four different phases, i.e., the SF, Haldane, gapless chiral, and gapped chiral (chiral Haldane) phases. In the half-odd integer  $S$  chains ( $S = 1/2$  and  $3/2$ ), on the other hand, we have found three phases, i.e., the SF, dimer, and gapless chiral phases. It thus turns out that the gapless chiral phase appears for general  $S \geq 1/2$ . For integer  $S$ , the gapped chiral (chiral Haldane) phase exists in a narrow region between the Haldane and the gapless chiral phases. For half-odd integer  $S$ , by contrast, the gapped chiral (chiral dimer) phase has not been identified within our numerical precision: The rather large truncation error of the DMRG calculation prevents us from verifying whether the chiral dimer phase exists or not. Our results suggests, however, that the chiral dimer phase, if it ever exists, appears in a narrow region between the dimer and the gapless chiral phase. Further work will be required to solve the problem.

We have also discussed the  $S$  dependence of the phase

diagrams. The obtained phase diagrams indicate that, as  $S$  increases toward the classical limit  $S \rightarrow \infty$ , the region of the gapless chiral phase converge smoothly toward that of the classical helical phase, while the pure quantum phases, i.e., the dimer, Haldane, and gapped chiral phases, become narrower and eventually vanish in the  $S \rightarrow \infty$  limit. The prediction from the bosonization study that the decay exponent of the spin correlation in the XY case ( $\Delta = 0$ ) takes a value  $\eta_x = 1/(8S)$  in the  $j \rightarrow \infty$  limit has been verified.

Finally, we wish to touch upon the possible experimental realization of the gapless chiral phase in a quasi-one-dimensional compound  $\text{CaV}_2\text{O}_4$ . This material is expected to be described by the frustrated  $S = 1$  chain (1) where the AF next-nearest-neighbor coupling  $J_2$  is comparable to the AF nearest-neighbor coupling  $J_1$ . Recently, Kikuchi made measurements on magnetic susceptibility and on  $^{51}\text{V}$  NMR, and showed that the system had gapless excitations above the ground state.<sup>29</sup> For the frustrated  $S = 1$  chain (1), theoretical studies indicate that there is no gapless phase for  $j \geq 0$  and  $\Delta \geq 0$  except for the gapless chiral phase. Hence,  $\text{CaV}_2\text{O}_4$  might be a promising candidate for the realization of the chiral-ordered phase. For the future, it might be interesting to calculate thermodynamic properties at finite temperatures to compare them with the experimental data on this compound.

## ACKNOWLEDGMENTS

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- <sup>27</sup>In Fig. 8(b), the generalized string correlation for  $j=0.330$  is slightly bent upward for  $r \gtrsim 60$ . However we note that, in the range of  $r \gtrsim 60$ , the  $m$  convergence of the data has not been achieved yet and the observed bend up tends to be suppressed with increasing  $m$ . Thus, from the behavior of the string correlation for  $r \lesssim 50$  where the  $m$  convergence is achieved, we conclude that the string correlation for  $j=0.330$  exhibits an algebraic decay and the bend up observed for larger  $r$  is an artifact due to the truncation error eventually vanishing in the limit  $m \rightarrow \infty$ .
- <sup>28</sup>Since the system in the DH phase can be described approximately by the direct product of two Haldane subchains, one may expect the string correlations on each subchain to be the order parameter of the phase. Contrary to this naive expectation, however, the subchain string correlation in the DH phase does not exhibit a finite LRO but decays exponentially. (See Ref. 15.)
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