

Chiral order of Spin-1/2 frustrated quantum spin chains

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The ordering of the frustrated $S=1/2$ XY spin chain with the competing nearest- and next-nearest-neighbor antiferromagnetic couplings, J_1 and J_2 , is studied by using the density-matrix renormalization-group method. It is found that besides the well-known spin-fluid and dimer phases the chain exhibits gapless ‘chiral’ phase characterized by the spontaneous breaking of parity, in which the long-range order parameter is a chirality, $\kappa_l = S_l^x S_{l+1}^y - S_l^y S_{l+1}^x$, whereas the spin correlation decays algebraically. The dimer phase is realized for $0.33 \lesssim j = J_2/J_1 \lesssim 1.26$ while the chiral phase is realized for $j \gtrsim 1.26$.

Considerable attention has been paid to the ordering of frustrated quantum spin chains since these systems exhibit a wide variety of magnetic phases due to the interplay between quantum effect and frustration. We consider here an anisotropic frustrated quantum spin chain described by the XXZ Hamiltonian,

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

where S_{ℓ} is the spin- S spin operator at the ℓ th site, $J_{\rho} > 0$ is the antiferromagnetic interaction between the nearest-neighbor ($\rho = 1$) and the next-nearest-neighbor ($\rho = 2$) spin pairs, and Δ ($0 \leq \Delta \leq 1$) represents an exchange anisotropy. Note that $\Delta=0$ and $\Delta=1$ represent the XY and Heisenberg chains, respectively.

In the classical limit, $S \rightarrow \infty$, the system in the ground state exhibits a magnetic long-range order (LRO) characterized by a wavenumber q . The order parameter is defined by

$$\vec{m}(q) = \frac{1}{L} \sum_{\ell} \vec{S}_{\ell} e^{iq\ell}, \quad (2)$$

where L is the total number of spins. While the LRO is of the Néel-type ($q = \pi$) when the frustration is smaller than a critical value, i.e., $j \equiv J_2/J_1 \leq 1/4$, it becomes of helical-type for $j > 1/4$ with $q = \cos^{-1}(-1/4j)$. It should be noticed that both the time-reversal and the parity symmetries are broken in this helical ordered phase. In the XY -like case ($0 \leq \Delta < 1$), the helical ordered state possesses a two-fold 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 by¹

$$O_{\text{chiral}} = \frac{1}{L} \sum_{\ell} \kappa_{\ell}, \quad (3)$$

$$\kappa_{\ell} = S_{\ell}^x S_{\ell+1}^y - S_{\ell}^y S_{\ell+1}^x = \left[\vec{S}_{\ell} \times \vec{S}_{\ell+1} \right]_z.$$

The chiral order parameter changes its sign under the parity operation but is invariant under the time-reversal operation.

In contrast to the classical case $S = \infty$, in the quantum case $S < \infty$ the magnetic LRO (2) is completely destroyed by strong quantum fluctuations.² Nevertheless, for the case of the $S = 1$ XY -like chain, we have recently shown on the basis of the exact-diagonalization (ED) and the density-matrix renormalization-group (DMRG) methods that there exist novel chiral phases in which only the chirality (3) exhibits a LRO without the magnetic helical LRO (2).⁴ Two distinct chiral phases have been found, one gapless and the other gapped. With increasing j , the system exhibits two phase transitions first from the Haldane phase³ to the gapped chiral phase, and then from the gapped chiral phase to the gapless chiral phase. These chiral ordered phases break only the parity symmetry spontaneously, with preserving both the time-reversal and the translational symmetries. We also constructed the ground state phase diagram of the model (1) for the $S = 1$ case.^{5,6}

By contrast, the situation is less clear in the case of the $S = 1/2$ XY chain. There remains a discrepancy between the field-theoretical results⁷ and our numerical results:⁴ While the field-theoretical analysis based on the bosonization method predicted the occurrence of the chiral phase in the large j region, the Binder parameter of the chirality calculated via the ED method up to $L = 20$ exhibited no sign of the chiral phase. Although Aligia *et al.*⁸ recently pointed out that the system size $L = 20$ might be insufficient to deal with the chirality in the large j region, the question whether the chiral phase is realized in the $S = 1/2$ XY chain has not been clarified so far.

In the present paper, we try to resolve this discrepancy by determining the phase diagram of the $S = 1/2$ XY chain (1) based on the DMRG method. The method used is the same as that in the previous work.⁵ Using the DMRG method, we calculate appropriate correlation functions associated with each order parameter characterizing the phases, and analyze their long-distance be-

haviors. The results of our analysis strongly suggest the appearance of the chiral ordered phase for $j > j_c (\simeq 1.26)$.

Before going into details of our calculation, we briefly summarize the known properties of the ground-state phases of the $S = 1/2$ spin chain (1). The system undergoes a phase transition from the spin-fluid phase to the dimer phase at $j = j_d$ with increasing j .⁹⁻¹² The critical value j_d has been estimated to be $j_d \simeq 0.33$ for the XY case.¹² The spin-fluid phase realized at $j \leq j_d$ is characterized by gapless excitations above the ground state and an algebraic decay of spin correlations, while the dimer phase realized at $j > j_d$ 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 the translational symmetries are broken spontaneously. The order parameter characterizing the dimer phase is given as

$$O_{\text{dimer}}^\alpha = \frac{1}{L} \sum_\ell \tau_\ell^\alpha, \quad (\alpha = x, y, z) \quad (4)$$

$$\tau_\ell^\alpha = (-1)^\ell S_\ell^\alpha S_{\ell+1}^\alpha.$$

The dimer phase is further divided into two regions by the so-called Lifshitz line at $j = j_L$ according to the nature of the spin correlations: Whereas the structure factor $S(q)$ has a maximum at $q = \pi$ for $j \leq j_L$, the wavenumber q of the maximum of $S(q)$ shifts to an incommensurate value $q = Q < \pi$ for $j > j_L$. This incommensurate character is regarded as the vestige of the helical order in the classical case.¹³ Meanwhile, the question whether the chiral phase exists for larger j for the XY chain still remains controversial as mentioned above.

In order to probe the possible phases, we calculate the chiral, dimer and spin correlation functions defined by

$$C_\kappa(r) = \langle \kappa_{r_0-r/2} \kappa_{r_0+r/2} \rangle, \quad (5)$$

$$C_{\text{dim}}^x(r) = \langle S_{r_0-r/2}^x S_{r_0-r/2+1}^x \times (S_{r_0+r/2}^x S_{r_0+r/2+1}^x - S_{r_0+r/2+1}^x S_{r_0+r/2+2}^x) \rangle, \quad (6)$$

$$C_s^\alpha(r) = \langle S_{r_0-r/2}^\alpha S_{r_0+r/2}^\alpha \rangle \quad (\alpha = x, z) \quad (7)$$

which correspond to the order parameter (3), (4) and (2), respectively. Here r_0 represents the center position of open chain, i.e., $r_0 = L/2$ for even r and $r_0 = (L+1)/2$ for odd r . We employ the infinite-system DMRG algorithm introduced by White.¹⁴ The notation $\langle \dots \rangle$ represents the expectation value in the lowest energy state in the subspace of $S_{\text{total}}^z = 0$. Note that, since the chains treated in our calculation are sufficiently large,¹⁵ one can safely avoid the finite-size effect arising from the incommensurate character of the spin correlation as pointed out by Aligia *et al.*⁸

The calculated r -dependence of the chiral, dimer, and spin correlation functions are shown in Fig.1 (a)-(c) on log-log plots for several typical values of j . As can be seen from Fig.1 (a), the data of $C_\kappa(r)$ for $j > j_c \simeq 1.26$ are bent upward at larger r suggesting a finite chiral LRO, while for $j < j_c$ they are bent downward suggesting an

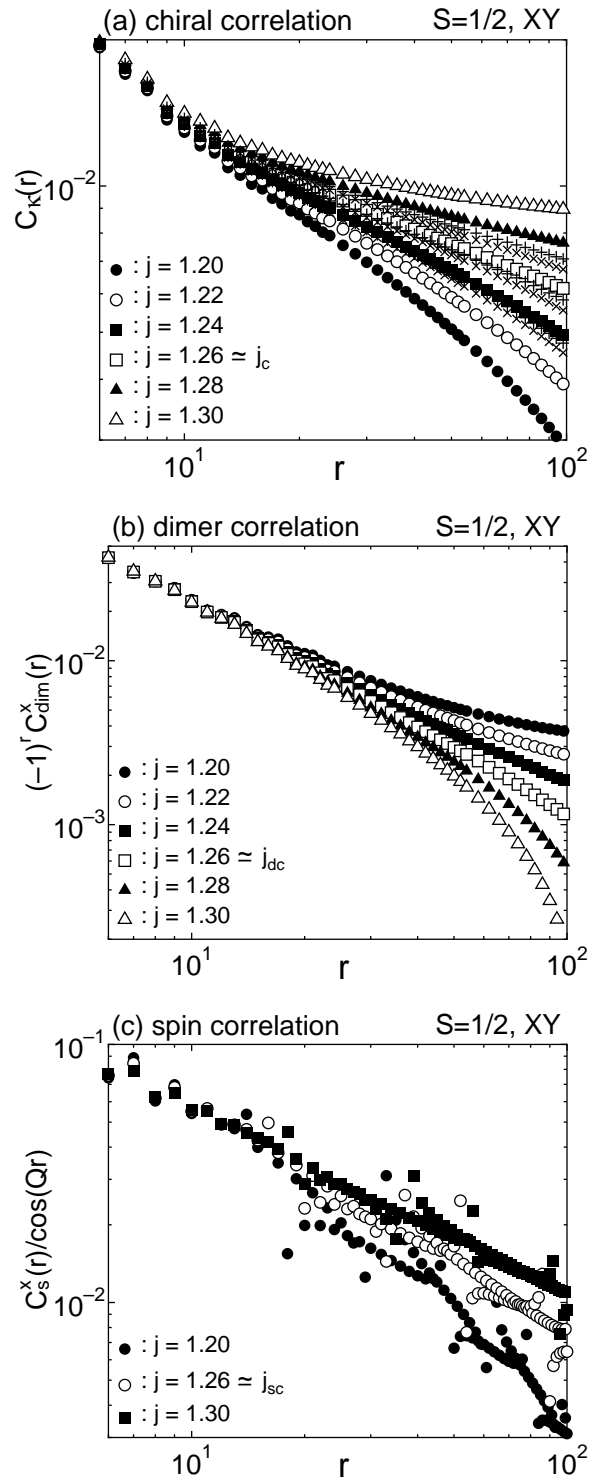


FIG. 1. Correlation functions versus r on log-log plots for various j : (a) chiral correlation $C_\kappa(r)$; (b) dimer correlation $(-1)^r C_{\text{dim}}^x(r)$; (c) spin correlation $C_s^x(r)$ divided by the oscillating factor $\cos(Qr)$. The number of block states kept in the DMRG calculation is $m = 450$. To illustrate the m -dependence, we also indicate by crosses the data for $m = 400$ and 350 for several cases where the m -dependence is relatively large. In other cases, the truncation errors are smaller than the symbols.

exponential decay of chiral correlations. Although the data around the transition point suffer from the truncation error inherent to the DMRG calculation, we estimate the transition point as $j_c = 1.26^{+0.01}_{-0.03}$ by taking account of the m -dependence of the data shown in the figure. The appearance of the chiral phase is consistent with the prediction of the field theory.^{7,16}

Meanwhile, as shown in Fig.1 (b), the data of $C_{\text{dim}}^x(r)$ for $j < j_{dc} \simeq 1.26$ are bent upward for larger r suggesting a finite dimer LRO, whereas they are bent downward for $j > j_{dc}$ suggesting an exponential decay of dimer correlations. The dimer transition point j_{dc} is then estimated to be $j_{cd} = 1.26 \pm 0.01$. Figure 1 (c) exhibits the spin correlation function $C_s^x(r)$ divided by the leading oscillating factor $\cos(Qr)$. The data of $C_s^x(r)$ are bent downward for $j < j_{sc} \simeq 1.26$ suggesting an exponential decay of spin correlations, while they exhibit a linear behavior for $j > j_{sc}$ suggesting a power-law decay of spin correlations.¹⁷ This behavior of spin correlations suggests that, as j increases, the system exhibits a transition from the gapped state ($j < j_{sc}$) to the gapless state ($j > j_{sc}$). We note that the absence of magnetic (spin) LRO has been proven rigorously for any j and for general $S < \infty$.²

The remaining problem is the relation among j_c , j_{dc} , and j_{sc} . Two possibilities seem to be allowed from our data, *i.e.*, (i) $j_c = j_{dc} = j_{sc}$ or (ii) $j_c < j_{dc} = j_{sc}$. If the case (i) is realized, the system undergoes only one phase transition at $j = j_c = j_{dc} = j_{sc}$ 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 increasing j , first at $j = j_c$ from the dimer phase to the ‘‘chiral dimer’’ phase where both the dimer and chiral LRO’s coexist with gapfull excitations, and then at $j = j_{dc} = j_{sc}$ from the chiral dimer phase to the gapless chiral phase. Although rather large error bars of j_c and j_{dc} prevent us from determining which of the cases is realized, our result suggests that the chiral dimer phase, if it ever exists, appears only in a rather narrow region, less than 3.2 % of $j_c \simeq 1.26$, between the dimer and gapless chiral phases. (We note that in the $S = 1$ XY chain the gapped chiral phase exists for $0.473 \lesssim j \lesssim 0.49$, whose width corresponds to about 3.6 % of $j_c \simeq 0.473$.^{4,5}) Further work will be necessary to solve the problem whether the chiral dimer phase exists.

In summary, from numerical studies of the ground-state properties of the frustrated $S = 1/2$ XY chain (1), we have found that

1. The chiral LRO is realized for a range of $j > j_c (\simeq 1.26)$. This is consistent with the prediction by Nersesyan *et al.*⁷
2. The dimer phase exists in the range $j_d (\simeq 0.33) < j < j_{dc} (\simeq 1.26)$.

Detailed results including the critical properties and the full phase diagram in the j - Δ plane will be reported elsewhere.

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 - ¹⁵ In the infinite-system DMRG algorithm, the system size increases by two at each DMRG step and the calculation is continued until the L -convergence of the data is attained. We have performed the calculation more than 750 DMRG steps (corresponding to the system with $L = 1500$ sites) and confirmed the L -convergence.
 - ¹⁶ We consider that the failure of the ED analysis of Ref. 4 can be ascribed to the finite-size effect discussed in Ref. 8. The wavenumber 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 0.03π for $j \gtrsim j_c \simeq 1.26$. Meanwhile, in a finite open chain with L sites, because of the condition that the wavefunction should vanish on both ends of the chain, the incommensurability smaller than $2\pi/L$ cannot be taken into account. As a consequence, the system size must be larger than $L \sim 70$ if one wishes to detect the shift of Q of order 0.03π . Thus, the calculation on chains up to $L = 20$ might fail to extract the true asymptotic properties for $j \gtrsim j_c$.
 - ¹⁷ The data of $C_s^x(r)$ shown in Fig.1 (c) are largely scattered, which might be attributed to the possible influence of cor-

rection terms characterized by wavenumbers $Q' \neq Q$. Nevertheless, we consider that we can judge the behavior of the leading term of $C_s^x(r)$ from the figure and make the conclusion in the text about $C_s^x(r)$.