Dynamics in a two-leg spin ladder with a four-spin cyclic interaction

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We study the two-leg Heisenberg ladder with four-spin cyclic interaction using the (dynamical) density-matrix renormalization-group method. We demonstrate the dependence of the low-lying excitations in the spin wave, staggered dimer order, and scalar-chirality order structure factors on the four-spin cyclic interaction. We find that the cyclic interaction enhances spin-spin correlations with wave vector around momentum $(q_x,q_y)=(\frac{\pi}{2},0)$. Also, the presence of long-range order in the staggered dimer and scalar-chirality phases is confirmed by a δ-function peak contribution of the structure factors at energy $\omega=0$.

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For many years, it had been generally believed that the magnetic properties of undoped high-T_c materials can be well described by the two-dimensional (2D) Heisenberg model with nearest-neighbor exchange interaction J. However, the four-spin cyclic interaction K has been increasingly recognized as a non-negligible correction to the Heisenberg model. The cyclic interaction comes from the fourth-order processes in the strong-coupling limit of the single-band Hubbard model at half filling.[1] The importance of this interaction was initially proposed in the 2D solid ^{3}He, which has the hard-core correlations between spin-$\frac{1}{2}$ fermions.[2]

In fact, a substantial value $K=0.24\ J$ was proposed for 2D copper oxide La_2CuO_4 by an accurate fit of the magnon dispersion.[3] A close value was also suggested by an analysis of the Raman-scattering data.[4] Such magnitude of the four-spin cyclic interaction must have a considerable influence at least quantitatively on the low-energy spin physics. Similar situations have been reported for several two-leg spin-ladder systems:[5] the exchange interactions were estimated as $J_\parallel=J_\perp=110$ meV and $K=16.5$ meV for $La_6Ca_8Cu_{24}O_{41}$ (Ref. 6); $J_\parallel=186$ meV, $J_\perp=124$ meV, and $K=31$ meV for $La_4Sr_{10}Cu_{24}O_{41}$ (Ref. 7); $J_\parallel=165$ meV, $J_\perp=150$ meV, and $K=15$ meV for $SrCu_2O_3$ (Ref. 8), where $J_\parallel$ and $J_\perp$ are exchange interactions in the leg and rung directions, respectively.

Motivated by those observations, the ground-state properties of the two-leg spin-$\frac{1}{2}$ Heisenberg ladder with the four-spin cyclic interaction have been intensively studied.[7,9–13] Also, the effect of magnetic field on the ground state has been investigated.[14–16] Furthermore, the spectral features of the spin structure factor have been examined by the exact diagonalization, perturbation-theory, and density-matrix renormalization-group (DMRG) methods.[17–20] The spin dynamics for small cyclic interactions is thus well understood, but the dynamical properties for other correlations and/or relatively large cyclic interactions are still open. In this Brief Report, we study the dynamical structure factors of staggered dimer order, scalar-chirality order, and spin waves for a wide range of the four-spin cyclic interaction to give a deeper insight into our knowledge of the low-lying excitations, using the dynamical DMRG (DDMRG) method.[21]

The Hamiltonian of the two-leg spin-$\frac{1}{2}$ Heisenberg ladder with the four-spin cyclic interaction is given by

$$H = J_\parallel \sum_{x,y} \vec{S}_{x,y}\cdot\vec{S}_{x+1,y} + J_\perp \sum_x \vec{S}_{x,1}\cdot\vec{S}_{x,2} + K\sum_x (P_x+P_x^{-1}), \tag{1}$$

with the cyclic permutation operator

$$\begin{aligned} P_x+P_x^{-1} = {} & \vec{S}_{x,1}\cdot\vec{S}_{x,2}+\vec{S}_{x+1,1}\cdot\vec{S}_{x+1,2}+\vec{S}_{x,1}\cdot\vec{S}_{x+1,1}+\vec{S}_{x,2}\cdot\vec{S}_{x+1,2} \\ & +\vec{S}_{x,1}\cdot\vec{S}_{x+1,2}+\vec{S}_{x,2}\cdot\vec{S}_{x+1,1}+4(\vec{S}_{x,1}\cdot\vec{S}_{x,2}) \\ & \times(\vec{S}_{x+1,1}\cdot\vec{S}_{x+1,2})+4(\vec{S}_{x,1}\cdot\vec{S}_{x+1,1})(\vec{S}_{x,2}\cdot\vec{S}_{x+1,2}) \\ & -4(\vec{S}_{x,1}\cdot\vec{S}_{x+1,2})(\vec{S}_{x,2}\cdot\vec{S}_{x+1,1}), \end{aligned} \tag{2}$$

where $\vec{S}_{x,y}$ is a spin-$\frac{1}{2}$ operator at a site (x,y) (see Fig. 1). For simplicity, we focus on the case of $J_\parallel=J_\perp=J$ and take $J=1$ as the unit of energy hereafter. The ground-state phase diagram was obtained in Ref. 10 as follows. The system has a rung-singlet phase for $-3.33\lesssim K\lesssim 0.23$, a staggered dimer long-range-order (LRO) phase for $0.23\lesssim K\lesssim 0.5$, a scalar-chirality LRO phase for $0.5\lesssim K\lesssim 2.8$, a dominant vector chirality phase for $2.8\lesssim K$, and a ferromagnetic phase for $K\lesssim -3.33$.

Let us define the dynamical structure factor as

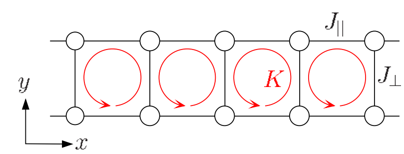

FIG. 1. (Color online) Lattice structure of the two-leg Heisenberg ladder. $J_\parallel(J_\perp)$ is the exchange interaction in the leg (rung) direction and K is the four-spin cyclic interaction. The x- (y-) axis is defined as the leg (rung) direction.

$$A(\vec{q},\omega) = \sum_{\nu} \langle \psi_0 | \hat{\mathcal{O}}_{-\vec{q}} | \psi_\nu \rangle \langle \psi_\nu | \hat{\mathcal{O}}_{\vec{q}} | \psi_0 \rangle \times \delta(\omega - E_\nu + E_0), \tag{3}$$

where $|\psi_\nu\rangle$ is the νth eigenstate with the eigenenergy E_ν and $\hat{\mathcal{O}}_{\vec{q}}$ is the Fourier transformation of the quantity-dependent operator $\hat{\mathcal{O}}_{\vec{r}}$. The δ function is replaced by a Lorentzian with width η in our numerical calculations. We now study the following three kinds of the dynamical structure factor corresponding to three phases at $-3.3 \lesssim K \lesssim 2.8$. The first is spin structure factor $S(\vec{q},\omega)$ with the operator

$$\hat{\mathcal{O}}_{\vec{r}} = S^z_{x,y}, \tag{4}$$

where $S^z_{x,y}$ is the z component of the total spin, the second is dimer-order structure factor $D(\vec{q},\omega)$ with

$$\hat{\mathcal{O}}_{\vec{r}} = \vec{S}_{x-1,y} \cdot \vec{S}_{x,y} - \vec{S}_{x,y} \cdot \vec{S}_{x+1,y}, \tag{5}$$

and the third is scalar-chirality structure factor $C(\vec{q},\omega)$ with

$$\hat{\mathcal{O}}_{\vec{r}} = \vec{S}_{x,1} \cdot (\vec{S}_{x+1,1} \times \vec{S}_{x+1,2}). \tag{6}$$

By integrating Eq. (3), we can easily obtain the static structure factor

$$A(\vec{q}) = \langle \psi_0 | \hat{\mathcal{O}}_{-\vec{q}} \hat{\mathcal{O}}_{\vec{q}} | \psi_0 \rangle. \tag{7}$$

We employ the DDMRG method[21] which is an extension of the standard DMRG method.[22] It has been developed for calculating dynamical correlation functions at zero temperature in quantum lattice models. This method has been successfully applied to the one-dimensional Heisenberg model.[23] We now calculate the dynamical structure factor (3) with applying the periodic boundary conditions in the leg (x) direction. We fix the system length $L=32$ and $\eta=0.1$ if not otherwise stated. In the DDMRG calculation, a required CPU time increases rapidly with the number of the density-matrix eigenstates (m) so that we would like to keep it as few as possible; meanwhile, the DDMRG approach is based on a variational principle so that we have to prepare a "good trial function" of the ground state with the density-matrix eigenstates as much as possible. Therefore, we keep $m=600$ to obtain true ground state in the first ten DDMRG sweeps and keep $m=300$ to calculate the spectral functions. In this way, the maximum truncation error, i.e., the discarded weight, is about 3×10^{-4}, while the maximum error in the ground-state and low-lying excited-states energies is about 10^{-2}.

To begin with, we consider the spin structure factor. In Fig. 2, we show the DMRG results of the static and dynamical spin structure factors for the rung singlet ($K=0.1$), staggered dimer LRO ($K=0.4$), and scalar-chirality LRO ($K=0.7$) phases. The dispersion relations $\omega(\vec{q})$ are also plotted in the insets. The spectra for $q_y=0$ and π exhibit the two-triplon and one-triplon contributions, respectively. In the absence of the cyclic interaction, i.e., $K=0$,[24,25] it is known that the spin dispersion has two minima at $q_x=0,\pi$ and a maximum at $q_x \sim 2\pi/3$ for $q_y=0$; whereas, two minima at $q_x=0,\pi$ and a maximum at $q_x \sim \pi/3$ for $q_y=\pi$. Those features have been confirmed to remain qualitatively unchanged at $K \lesssim 0.075$.[19] For $K=0.1$, however, the minima at $(q_x,q_y)=(\pi,0),(0,\pi)$ are no longer visible [see the insets of the top panels in Fig. 2(b)], i.e., the dispersions are nearly flat around $(q_x,q_y) \sim (\pi,0),(0,\pi)$. The one-triplon excitation ($q_y=\pi$) is in good agreement with the perturbative result.[17] This is also consistent with other numerical study.[18]

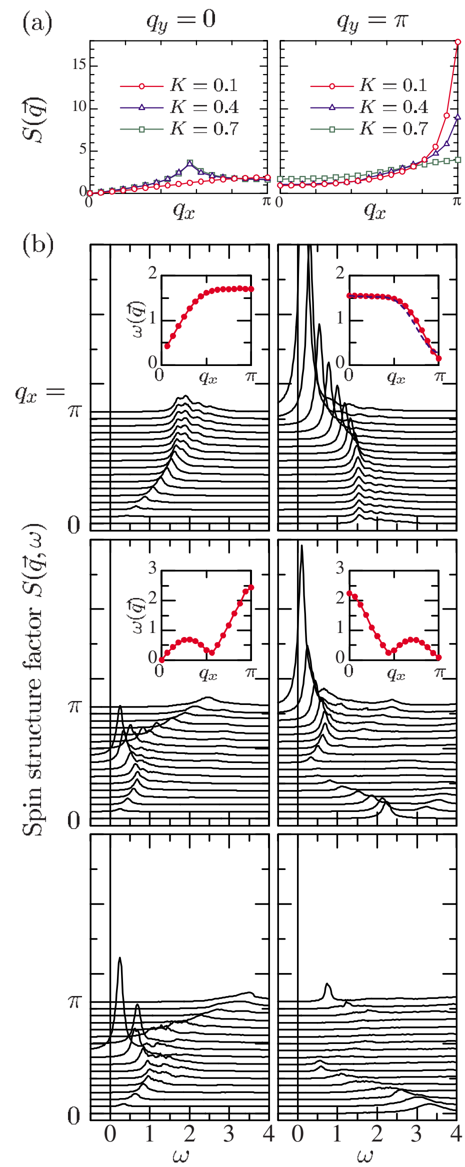

FIG. 2. (Color online) (a) Static spin structure factor. (b) Dynamical spin structure factor for $K=0.1$ (top), $K=0.4$ (middle), and $K=0.7$ (bottom). Left and right panels correspond to the results for $q_y=0$ and $q_y=\pi$, respectively. Insets: lower edge of the two-spinon continuum ($q_y=0$) and one-spinon dispersion ($q_y=\pi$). The dashed line denotes the perturbative result $\omega(q_x,q_y=\pi)=1.186+0.558\cos(q_x)-0.271\cos(2q_x)+0.071\cos(3q_x)$.

When the cyclic interaction is further increased to $K=0.4$, we can see a drastic change in the spectra for both $q_y=0$ and π: especially, an enhancement of peaks around $(q_x,q_y)=(\frac{\pi}{2},0)$ and a reduction in peaks around $(q_x,q_y)=(\pi,\pi)$ are derived. It is because the cyclic interaction leads to a repulsive interaction between neighboring rung triplets. In addition, a node emerges at $q_x=\frac{\pi}{2}$ for both q_y values and a relation $\omega(q_x,q_y=0)=\omega(\pi-q_x,q_y=\pi)$ appears to be satis-

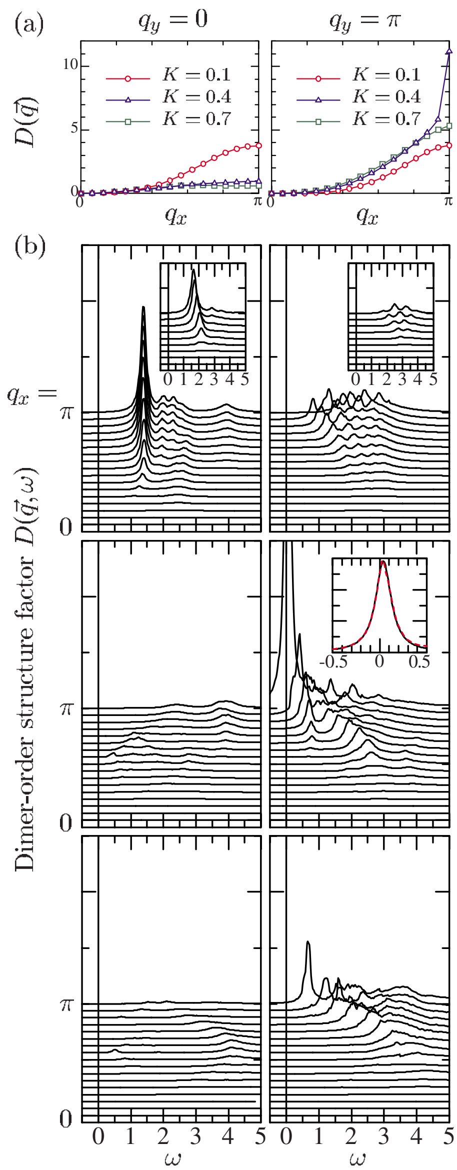

FIG. 3. (Color online) (a) Static dimer-order structure factor. (b) Dynamical dimer-order structure factors for K=0.1 (top), K=0.4 (middle), and K=0.7 (bottom). Left and right panels correspond to the results for q_y=0 and q_y=π, respectively. Insets of the top panels: $D(\vec{q},\omega)$ for K=0 with L=16 and η=0.2. Inset of the muddle panel: a Lorentzian fit of the peak at (q_x,q_y)=(π,π) and $\omega \sim 0$ with η=0.1.

fied. They would indicate a twofold-degenerate ground state with a broken translational symmetry, which is consistent with the staggered dimer-order state. For K=0.7, the peaks around (q_x,q_y)=$(\frac{\pi}{2},0)$ are still more enhanced, whereas, the low-energy spectral features for q_y=π seem to be much reduced. Actually, the one-triplon contribution is shunted off to the high-energy excitations since the static structure factor for q_y=π is not much suppressed. In short, from the standpoint of spin-spin correlation, the four-spin cyclic interaction may work for enhancing a spin-density wave with wave vector (q_x,q_y)=$(\frac{\pi}{2},0)$ and for reducing the antiferromagnetic correlation $S(\pi,\pi)$ [see Fig. 2(a)].

Next, we turn to the dimer-order structure factor. Figure 3

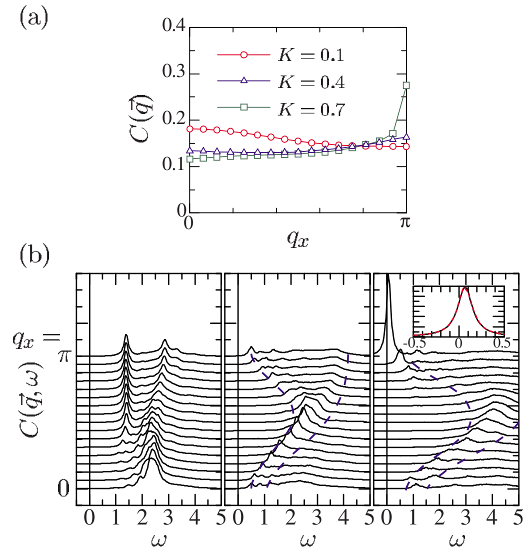

FIG. 4. (Color online) (a) Static scalar-chirality structure factor. (b) Dynamical scalar-chirality structure factors for K=0.1 (left), K=0.4 (center), and K=0.7 (right). Inset of the bottom panel: a Lorentzian fit of the peak at q_x=π and $\omega \sim 0$ with η=0.1. The dashed lines denote the lower and upper edges of the continuum.

shows the DMRG results of the static and dynamical dimer-order structure factors for K=0.1, 0.4, and 0.7. For comparison, the results of $D(\vec{q},\omega)$ for K=0 are shown in the insets of the top panels of Fig. 3(b). In the rung-singlet phase, the ground state is approximately expressed as the product of local rung singlets with gap $\Delta \sim \mathcal{O}(J_\perp)$. The lowest excitation comes from the formation of a leg singlet with coupling energy $\sim \frac{J_\parallel}{2}$ as well as the collapse of two rung singlets. For K=0, therefore, undispersive sharp peaks appear around $\omega = \mathcal{O}(2\Delta - \frac{J_\parallel}{2}) \sim 1.5$ for q_y=0; whereas, the spectra for q_y=π consist of broad continua at $\omega > \mathcal{O}(2\Delta - J_\parallel)$.

When small cyclic interaction (K=0.1) is introduced, we can see a strong influence on the continua around (q_x,q_y)=(π,π), i.e., they are significantly shifted toward lower energies. It implies that the gap Δ is reduced rapidly as K increases. For K=0.4, the continua are further drastically changed: a pronounced peak appears at (q_x,q_y)=(π,π) and $\omega \sim 0$; also, most of the spectral weight concentrates around the peak. On the other hand, the spectral weights for q_y=0 are totally suppressed. The pronounced peak is well fitted by a Lorentzian with η=0.1, as shown in the inset in the middle panel of Fig. 3(b). In other words, the spectrum for (q_x,q_y)=(π,π) may consist of a δ-function peak at ω=0 and a gapfull continuum. They would be a signature of long-range-staggered dimer order. For K=0.7, the spectral weights around (q_x,q_y)=(π,π) are much reduced and a gap opens. It means that the staggered dimer order is no longer dominant in the ground state. Nevertheless, the spectral weights around (q_x,q_y)=(π,π) are still significant, as seen in Fig. 3(a), so that the dimer-order correlation could just be changed from long-range order to short-range order. It is consistent with the fact that the staggered dimer-order parameter is finite even in the scalar-chirality LRO phase.[10]

Finally, we look at the scalar-chirality structure factor. The DMRG results of the static and dynamical scalar-chirality structure factors for $K=0.1$, $K=0.4$, $K=0.7$ are shown in Fig. 4. For $K=0.1$, the lowest excitations are described by (almost) undispersive peaks around $\omega \sim \mathcal{O}(2\Delta - \frac{J_\parallel}{2})$ in analogy with the dimer-order structure factor. For $K=0.4$, the spectra form a continuum bounded by the branches $\omega(q_x) \sim A \sin(q_x)$ and $\omega(q_x) \sim 2A \sin(q_x/2)$, except that a gap opens at $q_x=0$ and π. The existence of the gap implies that the scalar-chirality order still belongs to an excited state. If we assume a complete staggered dimer order, i.e., the ground state is the product of local dimer singlets, the scalar-chirality operator (6) may be effectively reduced as $\vec{S}_{x,1} \cdot (\vec{S}_{x+1,1} \times \vec{S}_{x+1,2})|\psi_0\rangle \approx (\vec{S}_{x,1}/2)|\psi_0\rangle$. Thus, the dispersions are similar to those of the spin structure factor in the one-dimensional spin-Peierls Heisenberg model.[26,27] For $K=0.7$, we can see the closing of the gap and, moreover, the appearance of a dominant peak at $q_x=\pi$ and $\omega \sim 0$. This peak is well fitted by a Lorentzian with $\eta=0.1$, as shown in the inset of the right panel in Fig. 4(b). Hence, the spectrum for $q_x=\pi$ is composed of a δ-function peak at $\omega=0$ and a gapfull continuum, as is $D(\vec{q},\omega)$ in the staggered dimer LRO phase. It must indicate the presence of the scalar-chirality LRO.

In summary, we study the two-leg Heisenberg ladder with the cyclic four-spin interaction. The static and dynamical structure factors for the spin waves, staggered dimer order, and the scalar-chirality order parameters are calculated with the DDMRG method. We find that the spin-spin correlation with wave vector $(q_x,q_y)=(\frac{\pi}{2},0)$ is enhanced by the cyclic interaction. We also confirm the presence of long-range order in the staggered dimer and scalar-chirality phases by a δ-function peak contribution of the structure factor at $\omega=0$.

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