PHYSICAL REVIEW B **78**, 104416 (2008)

Magnetization plateaus, Haldane-like gap, string order, and hidden symmetry in a spin-$\frac{1}{2}$ tetrameric Heisenberg antiferromagnetic chain

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(Received 7 May 2008; revised manuscript received 4 July 2008; published 18 September 2008)

The ground-state properties of a spin $S=1/2$ tetrameric Heisenberg antiferromagnetic chain with alternating couplings AF_1-AF_2-AF_1-F (AF and F denote antiferromagnetic and ferromagnetic couplings, respectively) are studied by means of the density-matrix renormalization-group method. Two plateaus of magnetization m are found at $m=0$ and 1/4. It is shown that in such a spin-1/2 AF system, there is a gap from the singlet ground state to the triplet excited states in the absence of a magnetic field. The spin-spin correlation function decays exponentially, and the gapped states have a nonvanishing string order, which measures a hidden symmetry in the system. By a dual transformation, the string order is transformed into a ferromagnetic order and the hidden symmetry is unveiled to be a $Z_2\times Z_2$ discrete symmetry, which is fully broken in the gapped states. This half-integer spin Heisenberg AF chain is in a Haldane-like phase suggesting that the present findings extend the substance of Haldane's scenario. A valence-bond-solid state picture is also proposed for the gapped states.

DOI: 10.1103/PhysRevB.78.104416 PACS number(s): 75.10.Jm, 75.40.Cx

I. INTRODUCTION

Even though many models have been extensively studied experimentally and theoretically, one-dimensional quantum spin systems are still an attractive field in low-dimensional quantum magnetism. One of their motivations is from Haldane's conjecture.[1] Haldane proposed that an isotropic Heisenberg antiferromagnetic chain (HAFC) with an integer spin has a finite gap from the singlet ground state to the triplet excited states, and the spin-spin correlation function decays exponentially; while the HAFC with half-integer spin has a gapless spectrum and a correlation function with power-law decay. Although Haldane's conjecture has been confirmed experimentally and numerically in many systems, there is not a rigorous proof until now. By means of the valence-bond states, a rigorous disordered ground state for the biquadratic Heisenberg Hamiltonian with spin $S=1$ was proposed by Affleck, Kennedy, Lieb, and Tasaki (AKLT).[2] This AKLT model was shown to have a spin gap from the singlet ground state to the triplet excited states, an exponentially decaying correlation function, and a nonlocal topological order, which is different from the long-range order of spin-spin correlation, thus confirming the Haldane's conjecture based on a specific model. This nonlocal string order, which is regarded as a hidden antiferromagnetic Néel order, was found by Den Nijs and Rommelse[3] in the spin-1 HAFC. Kennedy and Tasaki[4] introduced a nonlocal unitary transformation to reveal the hidden symmetry for this string order, which was found to be a discrete $Z_2\times Z_2$ symmetry. The Haldane phase of integer-spin HAFC is thus characterized by the complete breaking of the $Z_2\times Z_2$ symmetry.[4]

Besides the isotropic HAFC with integer spin, Haldane phase has also been found in other spin systems, like some $S=1/2$ spin ladders[5–7] and spin-1/2 ferromagnetic-antiferromagnetic (F-AF) alternating Heisenberg chain.[8] In these systems, the gap and the string order vary monotonically with the ratio between F and AF interactions (J_F/J_{AF}) and when $J_F\to-\infty$ recover the values obtained for the spin-1 HAFC. The weak F coupling phase belongs to the same phase as the strong F coupling case. When the F couplings dominate the AF ones, the dimers of two spins coupled by F interactions behave as spin-1, and the systems reduce to the spin-1 HAFC. The $Z_2\times Z_2$ symmetry is also fully broken in these systems, which indicates that the systems belong to the Haldane phase.

In this paper, we are concerned about the existence of a Haldane-like phase in an AF chain with half-integer spin, which, unlike the spin-1/2 F-AF alternating chain, could not be reduced to a HAFC with integer spin in any circumstance. The spin-1/2 trimerized F-F-AF Heisenberg chain might be a choice but its spectrum is gapless.[9] Here we consider a spin $S=1/2$ tetrameric HAFC with alternating couplings AF_1-AF_2-AF_1-F. As far as we know, there has been no report on any tetrameric antiferromagnet yet and only a tetrameric ferrimagnetic Heisenberg chain compound $Cu(3\text{-}Clpy)_2(N_3)_2$ (F-F-AF-AF) has been widely studied.[10–15] By means of the density-matrix renormalization-group (DMRG) method and dual transformation, we have found that this spin-1/2 tetrameric system is in a gapped phase; most properties of which are compared with the features of the Haldane phase. Most importantly, the phase we found has a string order and a hidden $Z_2\times Z_2$ symmetry, which is also fully broken in this system. This alternating tetrameric HAFC with spin-1/2 is in a Haldane-like gapped phase. In this sense, our findings extend the substance of Haldane's scenario, which implies that the spin gap can also appear in certain half-integer spin HAFCs.

The rest of this paper is organized as follows. In Sec. II, we shall introduce the model Hamiltonian and give a brief discussion on the isolated tetramer systems. In Sec. III, we shall present our DMRG results on the magnetic properties of the system in a longitudinal magnetic field, as well as the gap behaviors, spin-spin correlation function, and string order in the gapped ground states in the absence of the external field. A dual transformation is introduced to the model in Sec. IV to unveil the hidden symmetry. In Sec. V, we shall

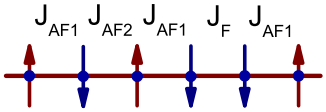

FIG. 1. (Color online) Schematic representation of the tetrameric Heisenberg spin chain with alternating couplings described by Hamiltonian (1).

propose a valence-bond-solid-state picture and a trial wave function for the gapped states. Finally, a summary and discussion will be given in Sec. VI.

II. SPIN-1/2 TETRAMERIC HEISENBERG ANTIFERROMAGNETIC CHAIN

The Hamiltonian of the isotropic tetrameric HAFC with alternating couplings AF_1-AF_2-AF_1-F in a longitudinal magnetic field is given by

$$H = \sum_j (J_{AF_1}\mathbf{S}_{4j-3}\cdot\mathbf{S}_{4j-2} + J_{AF_2}\mathbf{S}_{4j-2}\cdot\mathbf{S}_{4j-1} + J_{AF_1}\mathbf{S}_{4j-1}\cdot\mathbf{S}_{4j} - J_F\mathbf{S}_{4j}\cdot\mathbf{S}_{4j+1}) - h\sum_j S_j^z, \quad (1)$$

where $J_{AF_{1,2}}$ (>0) denote the different AF couplings, J_F (>0) denotes the F coupling, and h is the external magnetic field. We take $g\mu_B=1$ for convenience. The schematic spin configuration for the tetrameric HAFC is depicted in Fig. 1. Here we would like to remark that a spin-5/2 tetrameric HAFC compound, $C_{44}H_{36}N_{16}Mn_2$, with alternating couplings $AF_1AF_2AF_1$-F was synthesized experimentally.[16] Since the DMRG calculations on most physical properties of such a spin-5/2 tetrameric HAFC are impermissible for our present computing capacity, and considering that the spin-1/2 tetrameric HAFC is more fundamental and interesting and can be readily made as comparisons to other Haldane spin systems, we opt to pay attention to the tetrameric system with spin-1/2 in the following. Meanwhile, for reasons of comparison, some results on the spin-5/2 tetrameric HAFC will also be calculated.

Let us first discuss some cases of the present model. When $J_{AF_1}=0$, the system is decoupled into isolated dimers with J_{AF_2} or J_F couplings. The dimers coupled by J_{AF_2} form local singlets while those coupled by J_F form local triplets. Thus, the excitation of the system from $S^z_{tot}=0$ to $S^z_{tot}=\pm 1$ is gapless due to the triplets.

When $J_{AF_2}=0$, the system is decoupled into isolated tetramers, which becomes exactly soluble. In the absence of an external field, the ground state of the tetramer is antiferromagnetic with $S_{tot}=0$, and the first excited state is threefold degenerate with $S_{tot}=1$. The gap Δ is

$$\Delta = \frac{1}{2}(\sqrt{4J_{AF_1}^2 + 2J_{AF_1}J_F + J_F^2} - J_F), \quad (2)$$

which increases monotonically with J_{AF_1} but decreases with J_F. When $J_F \gg J_{AF_1}$, the gap has an asymptotic form $\Delta \sim J_{AF_1}(1+3J_{AF_1}/2J_F)/2$ and equals $J_{AF_1}/2$ when $J_F\to\infty$.

In the limit $J_F=0$, the ground state of the tetramer is also antiferromagnetic with $S_{tot}=0$, and the first excited state is threefold degenerate with $S_{tot}=1$. The gap Δ from the ground state to the first excited state is

$$\Delta = \frac{1}{2}(J_{AF_1} + \sqrt{4J_{AF_1}^2 - 2J_{AF_1}J_{AF_2} + J_{AF_2}^2} - \sqrt{J_{AF_1}^2 + J_{AF_2}^2}), \quad (3)$$

which enhances monotonically with J_{AF_1} but decreases with J_{AF_2}. When $J_{AF_2} \gg J_{AF_1}$, the gap behaves as $\Delta \sim J_{AF_1}^2/2J_{AF_2}$ and vanishes when $J_{AF_2}\to\infty$.

In the large J_F limit, the two spins coupled by J_F form a spin-1, and the model reduces to a Heisenberg chain with alternating spin-(1, 1/2, and 1/2),

$$H_{J_F\to\infty} = \sum_j \left(\frac{1}{2}J_{AF_1}\mathcal{S}_{3j-2}\cdot\mathbf{S}_{3j-1} + J_{AF_2}\mathbf{S}_{3j-1}\cdot\mathbf{S}_{3j} + \frac{1}{2}J_{AF_1}\mathbf{S}_{3j}\cdot\mathcal{S}_{3j+1}\right), \quad (4)$$

where $\mathcal{S}_j$ is the spin operator with $S=1$. This model appears to be rarely studied.

For arbitrary couplings, we will apply the DMRG (Refs. 17 and 18) method to explore the ground-state properties of the tetrameric chain defined in Eq. (1). In the following DMRG calculations, the chain length is taken as $N=160$, and the Hilbert space is truncated to 100 most relevant states. In the calculations for correlation function and string order, 160 optimal states are kept for accuracy. Open boundary conditions are adopted. The truncation error is less than 1×10^{-8} in all calculations.

III. MAGNETIZATION, HALDANE-LIKE GAP, CORRELATION FUNCTION, AND STRING ORDER

A. Magnetization

Due to the competition between interactions and the external magnetic field, a quantum magnet often shows exotic properties under magnetic fields. A field can close the zero-field gap and may induce magnetization plateaus under some conditions.[19–22] Therefore, we shall investigate the magnetic properties of the present alternating tetrameric system in a longitudinal field. Many cases with different couplings have been calculated. Here the results of the case with $J_{AF_1}:J_{AF_2}:J_F=1:1:1$ are presented for example. Figure 2(a) shows the magnetic-field dependence of the magnetization per site $m(h)$. The system exhibits two magnetization plateaus: a zero-field gap and a $m=1/4$ plateau, both of which satisfy the Oshikawa-Yamanaka-Affleck (OYA) (Ref. 21) condition $n(S-m)=$integer, with n as the period of the ground state, S as the magnitude of spin, and m as the magnetization per site. A similar magnetization curve has been found in the p-merized antiferromagnetic spin chain with $p=4$.[23] Both systems have shown all plateaus that the OYA condition permits. The $m=0$ plateau in the present system exhibits a spin gap in the spectrum, which is from the singlet ground state to the triplet excited states. Such a gap has also been found in the spin-1/2 F-AF alternating Heisenberg chain.[8] In such spin-1/2 chains with even lattice translation

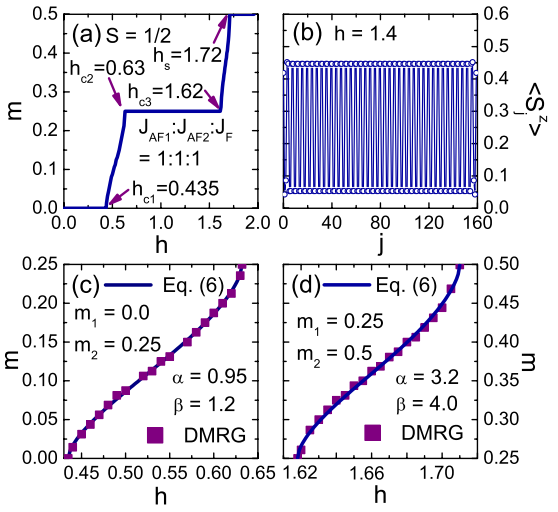

FIG. 2. (Color online) (a) The external field dependence of the magnetization per site $m(h)$ for the spin-1/2 tetrameric HAFC with couplings $J_{AF_1}:J_{AF_2}:J_F=1:1:1$. (b) The local magnetic moment $\langle S_j^z\rangle$ in the magnetization plateau states. The DMRG results of $m(h)$ in the gapless states can be fairly fitted by Eq. (6) for (c) $h_{c_1}<h<h_{c_2}$ and (d) $h_{c_3}<h<h_s$.

symmetry, the spectrum could have a gap even if the ground state has no spontaneous translation symmetry breaking.[21,24] In contrast, spin-1/2 chains with odd lattice sites per unit cell are gapless if the translation symmetry does not break spontaneously, like the spin-1/2 Heisenberg chain[25] and the spin-1/2 F-F-AF trimerized chain.[9] Further discussions on this gapped ground states will be presented below.

For the $m=1/4$ plateau, the local magnetic moment $\langle S_j^z\rangle$ and the spin-spin correlation function $\langle S_0^z S_j^z\rangle$ are calculated. These two quantities show a perfect sequence with a period of 4 and $\langle S_0^z S_j^z\rangle$ has a long-range order. It is shown that $\langle S_j^z\rangle$ behaves as $\{\ldots,(S_1,S_2,S_2,S_1),\ldots\}$ with $S_1=0.4468$ and $S_2=0.0532$ giving rise to the magnetization per site $m=1/4$ as shown in Fig. 2(b). The plateau state can be described by an approximate wave function,

$$\psi_i = a|\uparrow_{4i-3}\uparrow_{4i-2}\uparrow_{4i-1}\downarrow_{4i}\rangle + b|\uparrow_{4i-3}\uparrow_{4i-2}\downarrow_{4i-1}\uparrow_{4i}\rangle + c|\uparrow_{4i-3}\downarrow_{4i-2}\uparrow_{4i-1}\uparrow_{4i}\rangle + d|\downarrow_{4i-3}\uparrow_{4i-2}\uparrow_{4i-1}\uparrow_{4i}\rangle \quad (i=1,\ldots,N/4), \tag{5}$$

where $\uparrow_j$ ($\downarrow_j$) denotes spin up (down) on site j and N is the total site number. If the coefficients $a^2=d^2=S_2$ and $b^2=c^2=S_1$, the local magnetic moment and the spin-spin correlation function deduced from this wave function perfectly fit into the numerical results. The formation of the $m=1/4$ plateau in the limit $J_{AF_1}=0$ is quite simple, which is helpful in understanding the general case. When $J_{AF_1}=0$, the system is decoupled into the isolated dimers coupled by J_{AF_2} or J_F. After applying a magnetic field, the dimers coupled by J_F, which are in the triplet states, become polarized, and the system exhibits a magnetization plateau at $m=1/4$. The width of the plateau is determined by the upper critical field J_{AF_2} leading to full polarization.

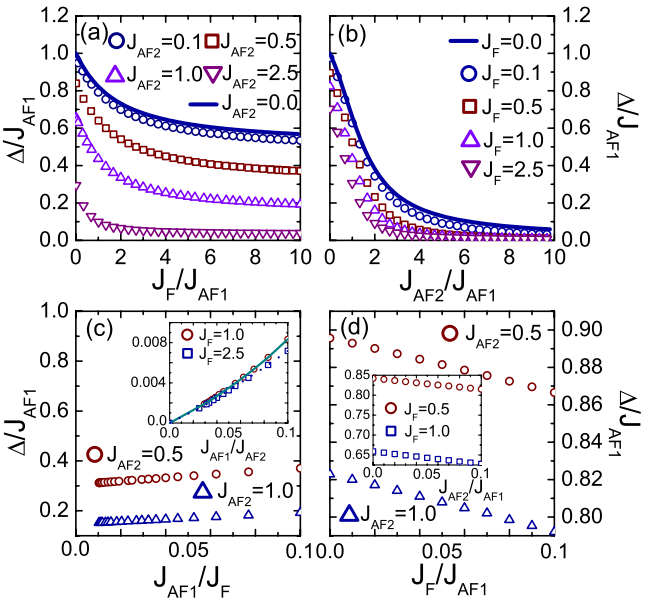

FIG. 3. (Color online) (a) The J_F dependence of the gap Δ for $J_{AF_2}=0.0$, 0.1, 0.5, 1.0, and 2.5. (b) The J_{AF_2} dependence of the gap Δ for $J_F=0.0$, 0.1, 0.5, 1.0, and 2.5. (c) The gap behaviors with J_{AF_1}/J_F for large J_F. The inset shows the gap behaviors with J_{AF_1}/J_{AF_2} for large J_{AF_2}. (d) The gap behaviors with J_F for large J_{AF_1}. The inset shows the gap behaviors with J_{AF_2} for large J_{AF_1}.

The magnetization process at $h_{c_1}<h<h_{c_2}$ and $h_{c_3}<h<h_s$ are shown in Figs. 2(c) and 2(d), respectively. It is found that the behaviors of the curves could be described as

$$m(h) = m_1 + (h-h_1)(m_2-m_1)/(h_2-h_1) + \alpha(h_2-h)\sqrt{h-h_1} - \beta(h-h_1)\sqrt{h_2-h}, \tag{6}$$

where h_1 (h_2) and m_1 (m_2) are the lower (upper) critical field and the corresponding magnetization per site, respectively, and α and β are two parameters. For $h_{c_1}<h<h_{c_2}$, $\alpha=0.95$ and $\beta=1.2$; while for $h_{c_3}<h<h_s$, $\alpha=3.2$ and $\beta=4.0$. The curves obtained from Eq. (6) are also shown in the figures, which fit into the DMRG results quite well.

B. Haldane-like gap

To understand the properties of the ground state of the spin-1/2 tetrameric alternating HAFC in the absence of a magnetic field, the spin gap, spin-spin correlation function, and string order are studied by means of the DMRG method in the whole parameter region, which will be compared with the features of Haldane phase.

We consider the spin gap Δ from the ground state to the triplet excited states, namely,

$$\Delta = E_1 - E_0, \tag{7}$$

where E_0 is the ground-state energy and E_1 is the lowest energy in the subspace with $S_{\text{tot}}^z=1$, and J_{AF_1} is chosen as the energy scale. J_F and J_{AF_2} dependences of the gap are presented in Figs. 3(a) and 3(b), respectively. Figure 3(a) shows the gap as a function of J_F for $J_{AF_2}=0.0$, 0.1, 0.5, 1.0, and

2.5. When $J_{AF_2}=0$, the gap is determined by Eq. (2). It is shown that with the increase of J_F, the gap Δ smoothly decreases and converges to a certain value Δ_c when $J_F \to \infty$. Δ_c is determined by J_{AF_2}. In the limit of $J_{AF_2}=0$, $\Delta_c=J_{AF_1}/2$. In the large J_F limit, the system is equivalent to the spin-(1, 1/2,1/2) model, which will be proved to have a gap by the nonlinear σ model below where Δ_c is related to the gap of this model. With the increase of J_F, the tetrameric system changes from a tetramer model to the spin-(1,1/2,1/2) model, and the gap decreases continuously. In Fig. 3(b), the gap is plotted as a function of J_{AF_2} for $J_F=0.0$, 0.1, 0.5, 1.0, and 2.5. When $J_F=0$, the gap is evaluated by Eq. (3). It is observed that the gap decreases rapidly with increasing J_{AF_2} and tends to zero when $J_{AF_2} \to \infty$. With the increase of J_{AF_2}, the tetrameric chain changes from a tetramer model to a system with relative small J_{AF_1} interactions, which is gapless when $J_{AF_1}=0$. From the above discussions, it can be seen that both J_F and J_{AF_2} give rise to the decrease of the gap but with different behaviors. The influence of J_{AF_1} on the gap is found to be distinct from those of J_{AF_2} and J_F. The gap would increase with J_{AF_1}. Because the gap only vanishes when $J_{AF_2}/J_{AF_1} \to \infty$, it is reasonable to conclude that a gap would be generated by an arbitrary small J_{AF_1}.

Next, let us consider the asymptotic behaviors of the gap. In Fig. 3(c), the gap as a function of J_{AF_1}/J_F is plotted in large J_F limit for $J_{AF_2}=0.5$ and 1.0. It is shown that the gaps linearly converge to Δ_c. J_{AF_2} alters the value of Δ_c but does not change this linear asymptotic behavior. Thus, the variations of the gap for large J_F could be evaluated by

$$\Delta = J_{AF_1}\left(\frac{\Delta_c}{J_{AF_1}} + \mu\frac{J_{AF_1}}{J_F}\right), \tag{8}$$

where Δ_c and the parameter μ are determined by J_{AF_2}. In the large J_{AF_2} limit, the isolated tetramer system with $J_F=0$ gives $\Delta \simeq J_{AF_1}^2/J_{AF_2}$. The inset of Fig. 3(c) shows the gap behaviors for $J_F=1.0$ and 2.5 for large J_{AF_2}, which exhibits an asymptotic behavior,

$$\Delta \sim \frac{J_{AF_1}^2}{J_{AF_2}} e^{\gamma J_{AF_1}/J_{AF_2}}, \tag{9}$$

where γ is a parameter, and $\gamma=3.2$ and 1.8 for $J_F=1.0$ and =2.5, respectively. The extrapolations show the linear behaviors near $J_{AF_1}=0$. When J_{AF_1} dominates, the gap behaviors are shown in Fig. 3(d). It can be seen that the gap decreases linearly with increasing both J_{AF_2} and J_F for large J_{AF_1}.

The DMRG results suggest that the system is in disordered spin liquid states with a spin gap. The gap varies monotonically with the couplings and does not show any singularity. We have calculated the ground-state energy against the couplings and found that the ground-state energy varies also monotonically with the interactions, and there is no any nonanalyticity. This nonanalyticity of the ground-state energy suggests an absence of the quantum phase transition in this system.[26]

It has been shown that the gap always exists if J_{AF_1} is finite. However, it is hard to identify the validity of this statement from numerical calculations when $J_{AF_2} \gg J_{AF_1}$. Thus, we consider the nonlinear σ model (NLSM) of this tetrameric system. Because the gap decreases with J_F, we consider the case in the limit of $J_F \to \infty$ when this tetrameric system is equivalent to the spin-(1,1/2,1/2) model, which is described by Eq. (4). The NLSM for such spin chains has been developed by Affleck,[27] Fukui and Kawakami,[28] and Takano.[29] The magnitude of $\mathbf{S}_j$ is denoted as s_j, which could be 1/2 or 1 here. The period of the system $2b$ is regarded as 6 for convenience. After a standard procedure,[29] we have the effective action for the spin-(1, 1/2, 1/2) Hamiltonian,

$$S_{\text{eff}} = \int_0^\beta d\tau \int_0^L dx \left\{ \frac{1}{2aJ^{(1)}}\left(\frac{J^{(1)}}{J^{(2)}} - \frac{J^{(0)}}{J^{(1)}}\right)(\partial_\tau \mathbf{m})^2 - i\frac{J^{(0)}}{J^{(1)}}\mathbf{m}\cdot(\partial_\tau \mathbf{m} \times \partial_x \mathbf{m}) + \frac{aJ^{(0)}}{2}(\partial_x \mathbf{m})^2 \right\}, \tag{10}$$

where $1/\beta$ denotes the temperature, α is the lattice spacing, L is the length of the chain, $\mathbf{m}$ presents the spin variables, and $\{J^n\}$ are defined by

$$\frac{1}{J^{(n)}} = \frac{1}{2b}\sum_{q=1}^{2b}\frac{(\tilde{s}_q)^n}{\tilde{J}_q} \quad (n=0,1,2), \tag{11}$$

with $\tilde{J}_q = J_q s_q s_{q+1}$ and $\tilde{s}_q = \Sigma_{k=1}^q (-1)^{k+1} s_k$. The topological angle θ is $4\pi J^{(0)}/J^{(1)}$, and the NLSM provides a gapless condition when $\theta/2\pi$ is a half-odd integer. After applying these equations to the spin-(1,1/2,1/2) model, we have the gapless condition

$$\frac{J_{AF_1}}{J_{AF_2}} = \frac{6l-11}{6-4l} \quad (l = \text{positive integer}). \tag{12}$$

As J_{AF_1} and J_{AF_2} are both positive, Eq. (12) could not be satisfied in any case, which indicates that even in the large J_F limit the present tetrameric chain is gapped for any $J_{AF_1} > 0$ and $J_{AF_2} > 0$. Considering the effect of J_F on the gap, we could conclude that this spin-1/2 tetrameric Heisenberg AF chain is always gapped if $J_{AF_1} \neq 0$.

For comparison, the gap of the spin-5/2 tetrameric HAFC is computed by utilizing the DMRG method. The chain length is taken as 140 and the Hilbert space is truncated to 400 optimal states. The truncation error is less than 10^{-13} in energy calculations. In Fig. 4, the DMRG results show that the extrapolations of the gap converge to nonzero values. Similar to the case with spin-1/2, the gap of this spin-5/2 tetrameric HAFC also decreases with both increasing J_{AF_2} and J_F. The gap diminishes more rapidly with increasing J_{AF_2}, which is also a feature of the spin-1/2 case. Although the gap of the spin-5/2 system is smaller than that in the spin-1/2 case, the qualitative behaviors of the gap for both systems appear to be similar.

C. Correlation function and static structure factor

To characterize the gapped ground states of the tetrameric spin chain, let us investigate the spin-spin correlation func-

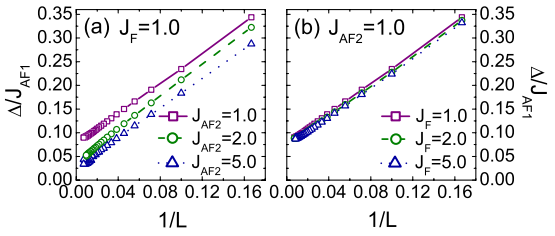

FIG. 4. (Color online) The gap Δ of the spin-5/2 tetrameric HAFC as a function of the inverse of chain length $(1/L)$ for (a) $J_F=1.0$, $J_{AF_2}=1.0$, 2.0, and 5.0, and (b) $J_{AF_2}=1.0$, $J_F=1.0$, 2.0, and 5.0.

tion $\langle S_i^z S_j^z \rangle$ and the static structure factor $S(q)$ that is defined as the Fourier transform of the correlation function,

$$S(q) = \frac{1}{N}\sum_{i,j} \langle S_i^z S_j^z \rangle e^{iq(i-j)}. \tag{13}$$

Our DMRG results show that the correlation function decays exponentially in the gapped states. For different couplings, the correlation length and the behavior of the correlation function have dramatic changes, which could be displayed more clearly in the static structure factor $S(q)$.

We have performed a large amount of calculations on the correlation function and static structure factor in a wide range of the parameter region. The changes of $S(q)$ are shown in Figs. 5(a) and 5(b) for some parameters as examples. In Fig. 5(a), for $J_F=0.1$, $J_{AF_2}=0.1$, 1.0, and 5.0, $S(q)$ shows an obvious maximum at $q=\pi$, and with the enhancement of J_{AF_2}, there are two small maxima appearing at $q=\pi/3$ and $5\pi/3$. When $J_{AF_2}=0.1$ and $J_F=5.0$, the maximum at $q=\pi$ becomes a valley and two small maxima appear near $q=3\pi/5$ and $7\pi/5$. With further increasing J_{AF_2}, $S(q)$ exhibits a totally different behavior showing four peaks at

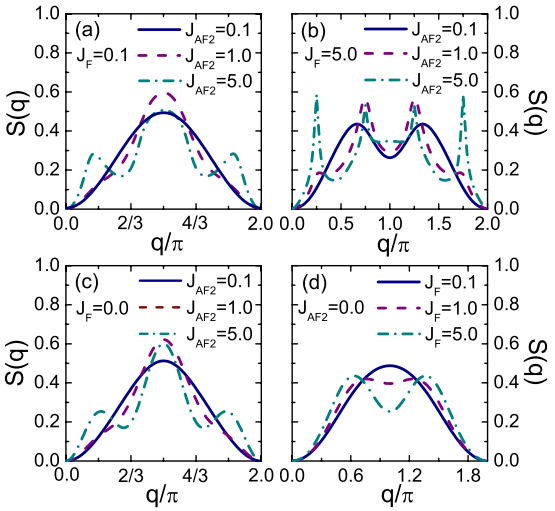

FIG. 5. (Color online) The DMRG results of the static structure factor $S(q)$ in the gapped ground states of the spin-1/2 tetrameric HAFC for (a) $J_F=0.1$, $J_{AF_2}=0.1$, 1.0, and 5.0; (b) $J_F=5.0$, $J_{AF_2}=0.1$, 1.0, and 5.0; (c) $J_F=0.0$, $J_{AF_2}=0.1$, 1.0, and 5.0; and (d) $J_{AF_2}=0.0$, $J_F=0.1$, 1.0, and 5.0.

$q=\pi/4$, $3\pi/4$, $5\pi/4$, and $7\pi/4$ as shown in Fig. 5(b). In these numerical results, $S(q)$ shows three different behaviors due to the competition of the couplings. It will be shown that some features of $S(q)$ mentioned above are determined by the short-range correlations, and some others are due to the increase of the correlation length and the translation symmetry of the ground states.

The correlation function of this model has no long-range order but exhibits a short-range order characterized by some $q_{\max}$ of $S(q)$. In the limit $J_{AF_2}=0$ and $J_F=0$, the tetrameric chain is decoupled into singlet dimers, and the static structure factor has a simple form $S(q)=(1-\cos q)/4$. The short-range correlations $\langle S_{2i-1}^z S_{2i}^z \rangle$ are reflected by the maximum of $S(q)$ at $q=\pi$. When J_{AF_2} is switched on, the tetrameric chain becomes a tetramer system. The short-range correlations of the tetramer produce another two maxima of $S(q)$ at $q=\pi/3$ and $5\pi/3$ as shown in Fig. 5(c). On the other hand, when J_F is turned on, the short-range correlations drive the maximum of $S(q)$ at $q=\pi$ to split into two small maxima, which move toward $q=3\pi/5$ and $7\pi/5$ with increasing J_F, as presented in Fig. 5(d). The distinct behaviors of $S(q)$ in the two situations are due to the different couplings of the tetramers. These results found in the tetramer systems also explain the behaviors of $S(q)$ for small J_{AF_2} or J_F shown in Figs. 5(a) and 5(b). When J_{AF_2} or J_F is smaller than J_{AF_1}, the correlation length of the system is quite short reflecting a highly disordered ground state, and the correlation function and static structure factor could be well characterized by the corresponding decoupled tetramer system.

When both J_{AF_2} and J_F are large enough, $S(q)$ exhibits a totally different behavior. There are four peaks at $q=\pi/4$, $3\pi/4$, $5\pi/4$, and $7\pi/4$ as shown in Fig. 5(b) when $J_{AF_2}=J_F=5.0$. In this case, the correlation function keeps exponentially decaying but shows a structure with a period of 4 and its correlation length becomes large. It is also observed that the correlation function has a characteristic such as $\langle S_i^z S_j^z \rangle \simeq \langle S_i^z S_{j+1}^z \rangle$ if the spins $\mathbf{S}_j$ and $\mathbf{S}_{j+1}$ are coupled by J_F, and $\langle S_i^z S_j^z \rangle \simeq -\langle S_i^z S_{j+1}^z \rangle$ if the spins $\mathbf{S}_j$ and $\mathbf{S}_{j+1}$ are coupled by J_{AF_2}. This feature reflects that the spins coupled by J_F behave like triplets, and the spins coupled by J_{AF_2} behave like singlets. As the correlation function that decays exponentially is modulated with a period of 4, the static structure factor $S(q)$ shows the peaks at $q=\pi/4$, $3\pi/4$, $5\pi/4$, and $7\pi/4$. Such a modulated structure of $S(q)$ has also been observed in the spin-1/2 alternating F-AF (Ref. 30) and spin-1/2 trimerized F-F-AF Heisenberg chains,[31] which show the peaks of $S(q)$ at $q=\pi/2$ and $3\pi/2$ and $q=\pi/3$, π, and $5\pi/3$, respectively. Generally speaking, for an exponentially decaying correlation function that is modulated with a period of n, the static structure factor $S(q)$ could show antiferromagnetic peaks at $q=\pi(1+2l)/n$ with $l=0,1,2,\ldots,n-1$.

Although the ground-state energy has no nonanalyticity in the parameter space, namely, no quantum phase transition happens, the static structure factor $S(q)$ shows rich features of the ground states for different couplings in this tetrameric system.

D. Topological string order

In order to investigate natures of the Haldane-like phase in the disordered phase of the tetrameric chain, we have cal-

culated the string order to detect the hidden symmetry in the gapped phase. The nonlocal string order was found in spin-1 antiferromagnetic Heisenberg chain by Den Nijs and Rommelse.[3] They found that although the spins with $S_i^z = 1, 0, -1$ are not ordered in position, their sequence has a hidden Néel order; that is, if all sites with $S_i^z = 0$ are removed, the left sites with $S_i^z = 1, -1$ have Néel orders. The string order was found to be a common feature of Haldane phase. Hida[8] suggested a string order for spin-1/2 F-AF chain, which was used to characterize the phase diagram of this spin chain.[32] The string order for spin ladders has also been considered in distinct gapped phases.[33]

Here we suggest a string order for this tetrameric system and use it to characterize the disordered spin liquid phase. Considering the basic feature of string order and the translation symmetry of the tetrameric Hamiltonian, we define four string operators for this tetrameric chain, which are denoted by $\Theta^{\alpha}_{4i-3,4j+2}$, $\Theta^{\alpha}_{4i-2,4j+3}$, $\Theta^{\alpha}_{4i-1,4j}$, and $\Theta^{\alpha}_{4i,4j+1}$. $\Theta^{\alpha}_{4i-3,4j+2}$ is defined as

$$\Theta^{\alpha}_{4i-3,4j+2} = -S^{\alpha}_{4i-3} \exp\left(i\pi \sum_{k=4i-2}^{4j+1} S^{\alpha}_{k}\right) S^{\alpha}_{4j+2}, \tag{14}$$

and the corresponding order parameter is

$$O^{\alpha}_{4i-3,4j+2} = \lim_{|j-i|\to\infty} \langle \Theta^{\alpha}_{4i-3,4j+2} \rangle, \tag{15}$$

where i and j denote the unit cell and $\alpha = x$, y, or z. The other three ones are defined in the similar way and they could be obtained by a translation of $\Theta^{\alpha}_{4i-3,4j+2}$. As the present model in the absence of a magnetic field has a $SU(2)$ symmetry, we need only to consider Θ^{z}. The spin configuration shows that $\Theta^{z}_{4i-3,4j+2}$ and $\Theta^{z}_{4i-1,4j}$ have the same topological structure, while $\Theta^{z}_{4i-2,4j+3}$ and $\Theta^{z}_{4i,4j+1}$ possess another same structure. The DMRG calculations have been performed on the four string orders. It was found that the string orders of the first structure have the same finite value, while the string orders of the second structure are both zero in the whole parameter space. For the spin-1/2 F-AF alternating chain, the two different definitions of string order also have two different values: one finite and one zero.[34] This difference would be explained in Sec. IV. Here we only consider the nonvanishing string order, which would be denoted as O^{z}_{string} below.

When both J_{AF_2} and J_{F} are equal to zero, the string order has its maximum 0.25 as shown in Fig. 6. After tuning up J_{F} or J_{AF_2}, the system becomes tetramer assemblies. In the limit $J_{\text{AF}_2} = 0$, the string order is evaluated from the wave function of the tetramer ground state as a function of $J_{\text{F}}/J_{\text{AF}_1}$,

$$O^{z}_{\text{string}} = \frac{4 + \frac{J_{\text{F}}}{J_{\text{AF}_1}} + \sqrt{4 + 2\frac{J_{\text{F}}}{J_{\text{AF}_1}} + \left(\frac{J_{\text{F}}}{J_{\text{AF}_1}}\right)^2}}{12\sqrt{4 + 2\frac{J_{\text{F}}}{J_{\text{AF}_1}} + \left(\frac{J_{\text{F}}}{J_{\text{AF}_1}}\right)^2}}, \tag{16}$$

while for $J_{\text{F}} = 0$, the string order as a function of $J_{\text{AF}_2}/J_{\text{AF}_1}$ is expressed as

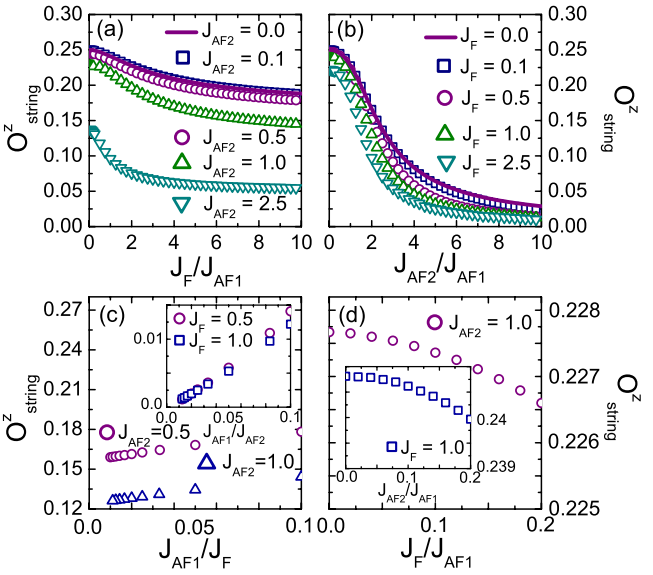

FIG. 6. (Color online) The string order as a function of $J_{\text{F}}/J_{\text{AF}_1}$ (a) and $J_{\text{AF}_2}/J_{\text{AF}_1}$ (b). The asymptotic behavior of the string order for (c) large J_{F} or J_{AF_2} and for (d) large J_{AF_1}.

$$O^{z}_{\text{string}} = \frac{4 - \frac{J_{\text{AF}_2}}{J_{\text{AF}_1}} + \sqrt{4 - 2\frac{J_{\text{AF}_2}}{J_{\text{AF}_1}} + \left(\frac{J_{\text{AF}_2}}{J_{\text{AF}_1}}\right)^2}}{12\sqrt{4 - 2\frac{J_{\text{AF}_2}}{J_{\text{AF}_1}} + \left(\frac{J_{\text{AF}_2}}{J_{\text{AF}_1}}\right)^2}}, \tag{17}$$

as shown with solid lines in Figs. 6(a) and 6(b), respectively. From these equations and numerical simulations, one may find that the string order in the case of $J_{\text{AF}_2} = 0$ has an asymptotic behavior,

$$O^{z}_{\text{string}} \sim \frac{1}{4} - \frac{1}{64}\left(\frac{J_{\text{F}}}{J_{\text{AF}_1}}\right)^2 e^{-J_{\text{F}}/2J_{\text{AF}_1}}, \tag{18}$$

when $J_{\text{F}} \ll J_{\text{AF}_1}$. In the case of $J_{\text{F}} = 0$, it behaves as

$$O^{z}_{\text{string}} \sim \frac{1}{4} - \frac{1}{64}\left(\frac{J_{\text{AF}_2}}{J_{\text{AF}_1}}\right)^2 e^{J_{\text{AF}_2}/2J_{\text{AF}_1}}, \tag{19}$$

when $J_{\text{AF}_2} \ll J_{\text{AF}_1}$. On the other hand, in the limit of $J_{\text{AF}_2} = 0$, the string order has an asymptotic form when $J_{\text{F}} \gg J_{\text{AF}_1}$,

$$O^{z}_{\text{string}} \sim \frac{1}{6} + \frac{1}{4}\frac{J_{\text{AF}_1}}{J_{\text{F}}} e^{-2J_{\text{AF}_1}/J_{\text{F}}}, \tag{20}$$

while it behaves as

$$O^{z}_{\text{string}} \sim \frac{1}{4}\frac{J_{\text{AF}_1}}{J_{\text{AF}_2}} e^{2J_{\text{AF}_1}/J_{\text{AF}_2}}, \tag{21}$$

when $J_{\text{AF}_2} \gg J_{\text{AF}_1}$ for the case $J_{\text{F}} = 0$.

Besides the limiting cases, the string order is evaluated as a function of the couplings by means of the DMRG method to detect the hidden symmetry in the gapped phase. Figure 6 presents the DMRG results of the string order as functions of $J_{\text{F}}/J_{\text{AF}_1}$ and $J_{\text{AF}_2}/J_{\text{AF}_1}$. In Fig. 6(a), the string order is shown

as a function of J_F/J_{AF_1} for $J_{AF_2}=0.1$, 0.5, 1.0, and 2.5. The string order decreases monotonically with J_F/J_{AF_1} and converges to a nonzero value when $J_F/J_{AF_1}\to\infty$. In Fig. 6(b), the string order as a function of J_{AF_2}/J_{AF_1} is evaluated for $J_F=0.1$, 0.5, 1.0, and 2.5. It is shown that it decreases rapidly with J_{AF_2}/J_{AF_1} and vanishes when $J_{AF_2}/J_{AF_1}\to\infty$. As is seen, the string order is always finite in the gapped phase indicating the existence of a hidden symmetry in this phase. The variations of the string order show the same tendencies as the gap behaviors. The string order has its maximum when $J_F=0$ and $J_{AF_2}=0$ where the system also shows the maximum of the gap. When the gap vanishes in the case of $J_{AF_1}=0$, the string order is also zero. This indicates that the opening of the gap and its behaviors could be characterized by this string order.

The asymptotic behaviors of the string order are shown in Figs. 6(c) and 6(d). Figure 6(c) shows the string orders when $J_F \gg J_{AF_1}$ for $J_{AF_2}=0.5$ and 1.0. The inset shows the string orders when $J_{AF_2} \gg J_{AF_1}$ for $J_F=0.5$ and 1.0. Figure 6(d) and the inset show the string orders when $J_{AF_1} \gg J_F$ and $J_{AF_1} \gg J_{AF_2}$, respectively. It is found that the asymptotic behaviors of the string orders preserve the features as those of the corresponding tetramer models, which are described by Eqs. (18)–(21).

It should be noticed that although the string order is nonlocal, it could measure some localized singlet correlation that depicts the singlet state. The string order has been found to characterize the behaviors of the gap perfectly as shown in Figs. 6(a) and 6(b). The gap monotonically increases with J_{AF_1} and is related to the singlet states of the spins coupled by J_{AF_1}, which could also be measured by the string order. When the system is the assembly of localized singlet spins coupled by J_{AF_1}, the string order has its maximum value of 0.25. With the disappearance of the singlet spins for $J_{AF_1}=0$, the string order also vanishes. In the spin-1/2 F-AF alternating chain, the gap is also related to the singlet dimers coupled by the AF interactions, and the string order could measure the singlet correlation.[8] Hida[8] pointed out that such a string order could distinguish the valence-bondlike disordered states from other disordered states. In this tetrameric chain, the valence bonds, namely, the singlet states in the spins coupled by J_{AF_1}, are characterized by the string order.

The finite string order reveals the hidden Néel order in the gapped states of the tetrameric chain, which is regarded as a feature of Haldane phase. For this tetrameric model, the valence-bond state could provide us a picture for the hidden Néel order. According to our definition of the string order, the exponent part of the string operator, which is between the spins at two boundaries, could be regarded as those constructed by the spin pairs coupled by J_{AF_2} or J_F. Consequently, the valence bonds form between spins coupled by J_{AF_1} leading to that the spin pairs coupled by J_{AF_2} or J_F could have $S_{tot}=1,0,-1$. After removing the spin pairs with $S_{tot}=0$, we can see a perfect Néel order of the spin pairs.

IV. DUALITY AND HIDDEN SYMMETRY

In the Haldane phase of the spin-1 Heisenberg chain[4] and spin-1/2 F-AF alternating chain,[35] the hidden symmetry measured by string order was found to be a Z_2 symmetry after a dual transformation, and the string order is transformed into a ferromagnetic order to measure such a Z_2 symmetry in the dual space. In general, the string orders in both x and z axes are considered to construct a $Z_2\times Z_2$ symmetry of the transformed Hamiltonian. The hidden symmetry could be revealed by means of the dual transformation,[35,36] and the Haldane phase was characterized by a fully breaking of the $Z_2\times Z_2$ symmetry.[4,32] It is interesting that this tetrameric chain also shows a hidden $Z_2\times Z_2$ symmetry, which is just measured by the string order defined above and fully breaking in this gapped phase. For simplicity, we start with the Hamiltonian rewritten in terms of Pauli matrices,

$$H=\sum_j (J_{AF_1}\sigma_{4j-3}\cdot\sigma_{4j-2}+J_{AF_2}\sigma_{4j-2}\cdot\sigma_{4j-1} + J_{AF_1}\sigma_{4j-1}\cdot\sigma_{4j}-J_F\sigma_{4j}\cdot\sigma_{4j+1}). \tag{22}$$

After applying the standard Kramers-Wannier[37] dual transformation D to the whole system, we get the transformed operators,

$$D\sigma_j^x\sigma_{j+1}^x D^{-1}=\sigma_{j-1+1/2}^z\sigma_{j+1+1/2}^z,$$

$$D\sigma_j^y\sigma_{j+1}^y D^{-1}=-\sigma_{j-1+1/2}^z\sigma_{j+1/2}^x\sigma_{j+1+1/2}^z,$$

$$D\sigma_j^z\sigma_{j+1}^z D^{-1}=\sigma_{j+1/2}^x, \tag{23}$$

where $\sigma_{j+1/2}^\alpha$ $(\alpha=x,y,z)$ are the Pauli operators in the dual space. In order to present the spins more clearly, we merely change the labeling of the lattice sites by the following rule:

$$R{:}r\to\frac{1}{2}\left(r+2-\frac{1}{2}\right). \tag{24}$$

After relabeling, we write the Pauli matrices on the half-odd-integer spins as τ and apply the inverse of the Kramers-Wannier dual transformation only on τ spins. As a result, the odd sites of both σ and τ spins are rotated by π about the x axis. Thus, the transformed Hamiltonian has the form of

$$\tilde{H}=-J_{AF_1}\sum_j(\sigma_j^z\sigma_{j+1}^z+\tau_j^z\tau_{j+1}^z+\sigma_j^z\sigma_{j+1}^z\tau_j^z\tau_{i+1}^z) + \sum_j(J_{AF_2}\sigma_{2j}^x+J_F\sigma_{2j+1}^x)+\sum_j(J_{AF_2}\tau_{2j}^x+J_F\tau_{2j+1}^x) + \sum_j(J_F\sigma_{2j+1}^x\tau_{2j+1}^x-J_{AF_2}\sigma_{2j}^x\tau_{2j}^x). \tag{25}$$

The tetrameric Heisenberg chain is transformed into a quantum Ashkin-Teller (AT) model in a transverse field, which is described by Eq. (25). This AT model consists of two Ising chains coupled by four-component interactions. The transverse field parts measured by J_{AF_2} and J_F in this model play the role of temperature in classical systems. They compete with J_{AF_1} to determine the behavior of the system, which has been demonstrated in our numerical results. Similar to the quantum Ising model,[26] a phase transition, which is referred to as a spontaneous breaking of the Z_2 symmetry and measured by the ferromagnetic order, may happen because of these competitions. The symmetry of this quantum AT model

can be easily read off. It is invariant under rotations of π about the x axis that are applied to σ spins alone or τ spins alone. Thus, it has a $Z_2 \times Z_2$ symmetry.

After the same dual transformation, the difference of the four string operators defined above is revealed. The vanishing string orders are transformed into

$$U\Theta^z_{4i-2,4j+3}U^{-1} = -\otimes_{k=2i}^{2j+2}\sigma^x_k,$$

$$U\Theta^z_{4i,4j+1}U^{-1} = -\otimes_{k=2i+1}^{2j+1}\sigma^x_k, \tag{26}$$

where U denotes the whole transformation. These two string operators are still expressed in terms of nonlocal operators and could not measure the spontaneous breaking of the discrete symmetry. In contrast, the nonvanishing string orders become ferromagnetic correlations in the dual space,

$$U\Theta^z_{4i-3,4j+2}U^{-1} = (-1)^{j-i}\tau^z_{2i-1}\tau^z_{2j+2},$$

$$U\Theta^z_{4i-1,4j}U^{-1} = (-1)^{j-i+1}\tau^z_{2i}\tau^z_{2j+1}, \tag{27}$$

where the factors $(-1)^{j-i}$ and $(-1)^{j-i+1}$ come from the rotation transformation on the odd spins. These order parameters measure possible spontaneous breaking of the Z_2 symmetry of τ spins. The ferromagnetic order of σ spins corresponds to the string order defined in the x component. When both $J_{\mathrm{AF}_2}=0$ and $J_{\mathrm{F}}=0$, the AT model becomes two ferromagnetic Ising chains coupled by the four-component interactions. The ferromagnetic correlation has the maximum 1, and the $Z_2 \times Z_2$ symmetry is totally broken because of the full polarization along the z axis. In contrast, when $J_{\mathrm{AF}_1}=0$, the AT model becomes isolated rungs in a transverse field. The ferromagnetic correlation is zero, and the $Z_2 \times Z_2$ symmetry is preserved. In our model, we are considering a $SU(2)$ symmetric model; thus the x component of the string order equals to that of the z component, namely, $O^x = O^z$. It turns out that O^z could also be used to measure the Z_2 symmetry of σ spins. The nonvanishing string order O^z indicates that the $Z_2 \times Z_2$ symmetry are fully breaking in the tetrameric system, which is an important evidence for the Haldane-like type of the gapped phase.

In this quantum AT model, the different effects of the couplings J_{AF_2} and J_{F} could be seen more clearly. As shown in the transformed AT Hamiltonian (25), the odd-site spins have an antiferromagnetic interaction $J_{\mathrm{F}}\sigma^x_{2j+1}\tau^x_{2j+1}$, which has an inverse effect on the transverse field part $J_{\mathrm{F}}(\sigma^x_{2j+1}+\tau^x_{2j+1})$, and thus counteracts the polarization of the odd-site spins on the x direction. In contrast, the even-site spins have a ferromagnetic interaction $-J_{\mathrm{AF}_2}\sigma^x_{2j}\tau^x_{2j}$, which promotes the polarization on the x direction. This difference could partly explain why the gap and string order would vanish when $J_{\mathrm{AF}_2} \to \infty$ but converge to finite values when $J_{\mathrm{F}} \to \infty$.

V. VALENCE-BOND GROUND STATE FOR THE HALDANE-LIKE PHASE

The nature of the spin-1 Heisenberg AF model can be demonstrated by the AKLT model where a Hamiltonian with the valence bond is constructed.[2] The Haldane-like gapped phase of this tetrameric system implies that it is reasonable to expect a valence-bond ground state that could explain the numerical results and support our analysis. As discussed above, the gap and string order are related to the singlet states of the spins coupled by J_{AF_1}. Therefore, a valence-bond-solid-(VBS) state picture for the ground state of the tetrameric chain can be proposed as shown in Fig. 7(a). The singlet valence bonds, which are represented as short lines, form between the spins coupled by J_{AF_1}. The gap, which is the energy needed to break the bonds, should increase with J_{AF_1}. This has been confirmed by our numerical results. After applying a magnetic field, the magnetization plateau at $m=1/4$ could appear when the bonds are broken, and the width of the plateau is thus mainly determined by J_{AF_2} as analyzed in Sec. III. In Figs. 7(b) and 7(c), the exponential parts of the two topologically different string orders are encircled by dashed lines. The numbers under the lines denote the spin $(S^z_i+S^z_{i+1})$. The nonvanishing string order has the hidden Néel order as shown in Fig. 7(b). But in Fig. 7(c), the vanishing string order does not exhibit the hidden Néel order in this picture.

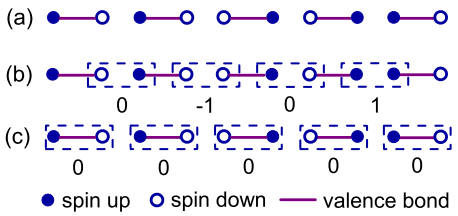

FIG. 7. (Color online) A schematic valence-bond picture for the gapped ground state of the tetrameric Heisenberg chain. (a) A typical configuration of the valence-bond state for the tetrameric chain in the absence of a magnetic field. The solid bullet denotes spin up, the hollow bullet denotes spin down, and the short line denotes the singlet bond. (b) The nonvanishing string order. (c) The vanishing string order.

In the absence of a magnetic field, we propose a trial wave function $|\Omega\rangle$, which is defined as a linear combination of two functions $|\Psi\rangle$ and $|\Phi\rangle$, i.e., $|\Omega\rangle = A|\Psi\rangle + B|\Phi\rangle$, for this VBS state picture. The wave function $|\Psi\rangle$ is defined as

$$|\Psi\rangle = \psi_{\alpha_1} \otimes \psi_{\alpha_2} \otimes \cdots \otimes \psi_{\alpha_{4L-1}} \otimes \psi_{\alpha_{4L}} \varepsilon^{\alpha_1\alpha_2} \cdots \varepsilon^{\alpha_{4L-1}\alpha_{4L}}, \tag{28}$$

where ψ_{α_i} $(\alpha_i = 1,2)$ denote the eigenstates of S^z with eigenvalues $1/2$ and $-1/2$ of the spin on the site i and $\varepsilon^{\alpha\beta}$ is the antisymmetric tensor with $\varepsilon^{12} = 1/\sqrt{2}$. These wave functions are written under periodic boundary conditions and thus L is even. This function is one of the ground states of the Majumdar-Ghosh model and qualitatively measures the ground states of this tetrameric system in large J_{AF_1} limit. In the state $|\Psi\rangle$, the system has the maxima for both the gap and the string order. The singlet correlation of the spins coupled by J_{AF_1} also has the maximum. In order to give a trial function that could depict the ground state, we introduce another wave function $|\Phi\rangle$, which is defined as

$$|\Phi\rangle = \psi_{\alpha_2} \otimes \psi_{\alpha_3} \varepsilon^{\alpha_2\alpha_3} \otimes \psi_{\alpha_4} \otimes \psi_{\alpha_5} \lambda^{\alpha_4\alpha_5} \otimes \cdots \otimes \psi_{\alpha_{4L-2}} \otimes \psi_{\alpha_{4L-1}} \varepsilon^{\alpha_{4L-2}\alpha_{4L-1}} \otimes \psi_{\alpha_{4L}} \otimes \psi_{\alpha_1} \lambda^{\alpha_{4L}\alpha_1}, \tag{29}$$

where $\lambda^{\alpha\beta}$ is the symmetric tensor with $\lambda^{11}=\lambda^{22}=0$ and $\lambda^{12}=1/\sqrt{2}$. $|\Phi\rangle$ measures the states in both large J_{AF_2} and J_{F} limit. In this state, the system is gapless and the string order is vanishing.

In the thermodynamic limit $L\to\infty$, $|\Psi\rangle$ and $|\Phi\rangle$ are orthogonal, namely, $\langle\Psi|\Phi\rangle=0$. The normalization of the trial function $|\Omega\rangle$ thus requires $A^2+B^2=1$. We have performed calculations of the physical properties on this trial function in the thermodynamic limit. It is found that the trial function $|\Omega\rangle$ has a vanishing local magnetic moment $\langle S_j^z\rangle$ and a short-range spin correlation function. The string order is found to be $O^z_{\mathrm{string}}=\frac{1}{4}A^2$, which is finite in the state $|\Omega\rangle$ and could well fit into the numerical results shown in Figs. 6(a) and 6(b) when the coefficient A is chosen as

$$A^2=\left(\frac{4-J_{\mathrm{AF}_2}/J_{\mathrm{AF}_1}}{3\sqrt{4-2J_{\mathrm{AF}_2}/J_{\mathrm{AF}_1}+(J_{\mathrm{AF}_2}/J_{\mathrm{AF}_1})^2}}+\frac{1}{3}\right)\times\left(\frac{4+J_{\mathrm{F}}/J_{\mathrm{AF}_1}}{3\sqrt{4+2J_{\mathrm{F}}/J_{\mathrm{AF}_1}+(J_{\mathrm{F}}/J_{\mathrm{AF}_1})^2}}+\frac{1}{3}\right). \tag{30}$$

The numerical results of the gap, as well as this valence-bond-state picture, indicate that the gap is induced by the valence bond, namely, the singlet state between the spins coupled by J_{AF_1}. The string order could well describe the gap and the singlet correlation that measures the singlet state of the spins coupled by J_{AF_1}. This above picture shows the crucial role of the valence bond in the formation of the Haldane-like gap and hidden symmetry.

VI. SUMMARY AND DISCUSSION

By means of the DMRG method, we have studied the magnetic properties, spin gap, spin-spin correlation function, and string order of the spin-1/2 tetrameric HAFC with alternating couplings AF_1-AF_2-AF_1-F. Two magnetization plateaus at $m=0$ and 1/4 are found, which satisfy the OYA condition for such a spin chain with a period of 4. For the $m=1/4$ plateau states, an approximate wave function is proposed, which fits into the numerical results of the local magnetic moment and spin-correlation function perfectly. The magnetization process of the two regions between the plateaus is fitted well by Eq. (6).

Besides the $m=1/4$ plateau, the gapped ground state in the absence of the magnetic field is also investigated. The system is found to have a gap from the singlet ground state to the triplet excited states. The gap changes monotonically with the couplings and does not show any level crossing. It decreases with J_{F} and J_{AF_2} but increases with J_{AF_1}. The ground-state energy has no nonanalyticity in the parameter space, which implies an absence of the quantum phase transition. The asymptotic behaviors of the gap have been calculated, which have the same features as those in the isolated tetramer systems. Combining the numerical results with the nonlinear σ model, it is shown that a gap would be generated by an arbitrary small J_{AF_1} and thus this system is always gapped if $J_{\mathrm{AF}_1}\neq 0$.

The spin-spin correlation function is uncovered to decay exponentially in the gapped states; but the correlation length and the behaviors of the correlation function show dramatic changes for different couplings, which are observed in the variations of the peaks of the static structure factor $S(q)$, reflecting a complex competition of the interactions. When J_{AF_2} or J_{F} is small compared with J_{AF_1}, $S(q)$ is dominated by short-range correlations. It would exhibit three maxima at $q=\pi/3,\pi$ and $5\pi/3$ when J_{F} is small. When J_{AF_2} is small, the maximum at $q=\pi$ becomes a valley and two small maxima appear near $q=3\pi/5$ and $7\pi/5$. In contrast, when both J_{F} and J_{AF_2} are large enough, $S(q)$ exhibits four peaks at $q=\pi/4$, $3\pi/4$, $5\pi/4$, and $7\pi/4$, which is due to the increase of the correlation length and the translation symmetry of the ground states.

In order to investigate the hidden symmetry of the gapped ground states, we proposed a string order and performed calculations to detect the hidden symmetry. The string order is found to be nonvanishing in the gapped phase indicating a hidden symmetry. More importantly, the behaviors of the string order have the same tendencies as that of the gap. The opening of the gap and its variations could be well described by this nonlocal order. The gap is related to the singlet state of the spins coupled by J_{AF_1} and increases with this interaction. Thus, it can be regarded that the gap is determined by the singlet correlation. The nonlocal string order could also measure this local singlet correlation. The singlet state of the spins coupled by J_{AF_1} provides a picture to understand the hidden Néel order reflected by the finite string order. Different from the conventional hidden Néel order, the order in the present system is not of the singlet spins but of the spin pairs coupled by J_{AF_2} or J_{F}.

The hidden symmetry measured by the string order is unveiled by a dual transformation. The present tetrameric Hamiltonian is transformed into a quantum AT model, which has a discrete $Z_2\times Z_2$ symmetry. The string order becomes a ferromagnetic order that is proper to measure this discrete symmetry. The nonvanishing string order indicates that this $Z_2\times Z_2$ symmetry is fully breaking in the gapped phase, which is the characteristic of Haldane phase. Thus, this tetrameric chain is in a Haldane-like gapped phase.

A valence-bond-solid-state picture and a trial function for the gapped states are proposed, most properties of which could be explained on the basis of this picture. The numerical results, as well as the VBS picture, indicate that the gap is induced by the valence bond of the spins coupled by J_{AF_1}. The valence bond is measured by the singlet correlation. The string order could well describe not only the gap but also the singlet correlation. The critical role of the valence bond on the formation of the Haldane-like gap and the hidden symmetry is unveiled.

Finally, we would like to state that unlike the spin-1/2 F-AF alternating HAFC, the present spin-1/2 tetrameric HAFC could not reduce to an integer-spin HAFC. Therefore, our findings extend the substance of Haldane's conjecture that was originally proposed for HAFCs with integer spin. We expect that our investigations would deepen further understanding on the physical properties of low-dimensional quantum magnetism.

ACKNOWLEDGMENTS

We are grateful to X. Chen, W. Li, X. L. Sheng, Z. C. Wang, Z. Xu, Q. B. Yan, L. Z. Zhang, Q. R. Zheng, and G. Q. Zhong for their useful discussions. This work was supported in part by the National Science Fund for Distinguished Young Scholars of China (Grant No. 10625419), the National Science Foundation of China (Grant Nos. 90403036 and 20490210), the MOST of China (Grant No. 2006CB601102), and the Chinese Academy of Sciences.

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