Exact ground state and elementary excitations of the spin tetrahedron chain

Shu Chen,[1,2] Yupeng Wang,[2] W. Q. Ning,[1,3] Congjun Wu,[4] and H. Q. Lin[1]
[1]*Department of Physics and Institute of Theoretical Physics, The Chinese University of Hongkong, Hongkong, People's Republic of China*
[2]*Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100080, People's Republic of China*
[3]*Department of Physics, Fudan University, Shanghai 200433, People's Republic of China*
[4]*Kavli Institute for Theoretical Physics, University of California, Santa Barbara, California 93106, USA*
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We study the antiferromagnetic spin exchange models with $S=1/2$ and $S=1$ on a one-dimensional tetrahedron chain by both analytical and numerical approaches. The system is shown to be effectively mapped to a decoupled spin chain in the regime of strong rung coupling, and a spin sawtooth lattice in the regime of weak rung coupling with spin $2S$ on the top row and spin S on the lower row. The ground state for the homogeneous tetrahedron chain is found to fall into the regime of strong rung coupling. As a result, the elementary excitation for the spin-1/2 system is gapless whereas the excitation for the spin-1 system has a finite spin gap. With the aid of the exact diagonalization method, we determine the phase diagram numerically and find the existence of an additional phase in the intermediate regime. This phase is doubly degenerate and is characterized by an alternating distribution of rung singlet and rung spin $2S$. We also show that the SU(3) exchange model on the same lattice has completely different kind of ground state from that of its SU(2) correspondence and calculate its ground state and elementary excitation analytically.

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I. INTRODUCTION

The study of quantum antiferromagnetic spin models with strong frustration has attracted great attention over the past decades. Early investigations of the frustrated quantum magnets were partly motivated by the work of Anderson to search the resonating-valence-bond (RVB) ground state in such systems.[1] In the frustrated quantum magnets, the magnetic ordering is generally suppressed by the frustration. Some well-studied frustrated magnetic systems include, for example, the kagome lattice and pyrochlore lattice, in which the interplay between frustration and quantum fluctuation leads to rich varieties of phenomena. Recently, the frustrated magnets are believed to be prominent candidates of realizing spin liquid states with exotic ground state and deconfined fractional excitations.[2–4] While the mechanism of deconfinment in two-dimensional (2D) magnetic systems is less clear, the deconfinement of spinons in quasi-one-dimensional magnetic system, which is closely related to the phenomenon of spin charge separation, is well investigated.[5–8] Since the 1980's, a large number of low-dimensional frustrated magnets have been synthesized experimentally.[9] Generally speaking, strongly geometrical frustration in these systems allows the simple dimerized state to be the ground state of the low-dimensional frustrated spin system and opens a spin gap. So far, a variety of quasi-one-dimensional frustrated models have been studied theoretically.[10–12] Additionally, important progress has been made in trapping cold atoms under a highly controllable way very recently, and thus it stimulates intensive investigation on how to simulate the magnetic systems using cold atoms. A number of schemes have been proposed to implement a variety of quantum spin models in optical lattices.[13]

In this paper, we investigate both the ground- and excited-state properties of the spin models on a one-dimensional (1D) tetrahedron chain as shown in Fig. 1, with site spins S_i residing in four corners of each tetrahedron. The basic unit, i.e., a tetrahedron is composed of four spins with equal antiferromagnetic exchanges between each pair of spins. The tetrahedron chain can be also viewed as a 1D pyrochlore strip in a 2D pyrochlore lattice, in which only two of four corners of each tetrahedron are shared by a neighboring tetrahedron. Generally, a three-dimensional (3D) pyrochlore lattice is a network of corner-sharing tetrahedra and a 2D pyrochlore model, named also as a checkerboard-lattice model, is obtained by a projection of the 3D lattice on a plane. Different from the 1D pyrochlore strip considered in this article, for both the 3D and 2D pyrochlore lattices, each corner of the tetrahedron is shared by a neighboring tetrahedron. As one of the most frustrated antiferromagnets, the model of spin pyrochlore lattice has been investigated by a variety of techniques including the semiclassical large-S

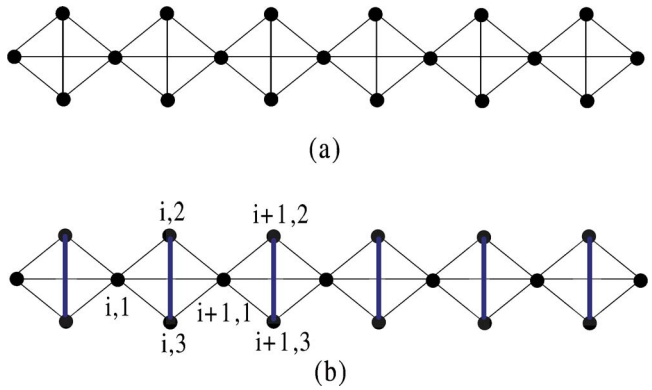

FIG. 1. (Color online) Schematic pictures of (a) the homogeneous spin tetrahedron chain, (b) the spin tetrahedron chain corresponding to model (2).

limit, large-N expansion of the SU(N) model, the contractor renormalization method based on the cluster expansion, and the bosonization method on the anisotropic limit.[14–17] In spite of the intensive research, even the ground state properties of the 3D pyrochlore lattice are not well understood. For the 2D pyrochlore lattice, the numerical results based on exact diagonizations have shown that the ground state has plaquette order.[18] However, for the 1D pyrochlore strip, we can determine its ground state and elementary excitation in an exact manner. With the aid of numerical diagonalization of the corresponding spin lattice systems with small sizes, we also investigate the quantum phase transitions of the ground state due to the change of exchange strengths along perpendicular rungs.

The spin model on a 1D pyrochlore strip as shown in Fig. 1 is described by the Hamiltonian:

$$H = J\sum_{\langle ij\rangle} \hat{S}_i \cdot \hat{S}_j, \tag{1}$$

where $\langle ij\rangle$ denotes sum over all the nearest neighbors along the tetrahedron chain and $\hat{S}_i$ represents the spin operator residing in site i. In this work, we study both the spin-1/2 and spin-1 models on the pyrochlore strip. Our results show that the excitation spectrum for the spin-1/2 system is gapless and the elementary excitation of the spin-1 system has a finite spin gap. This model can be extended to the cases where the strengths of bonds among the tetrahedra are not homogeneous. Here we only consider the inhomogeneous case as shown in Fig. 1(b), where we use $J_\perp$ to represent the exchange strength along the vertical rung of each tetrahedron. For convenience, we rewrite the Hamiltonian of the spin tetrahedron chain corresponding to Fig. 1(b) as follows:

$$H_A = J\sum_i [\hat{S}_{i,1}(\hat{S}_{i,2}+\hat{S}_{i,3}) + (\hat{S}_{i,1}+\hat{S}_{i,2}+\hat{S}_{i,3})\hat{S}_{i+1,1}] + J_\perp \sum_i \hat{S}_{i,2}\cdot\hat{S}_{i,3}. \tag{2}$$

It is obvious that model (2) reduces to model (1) when $J_\perp = J$, i.e., the homogeneous tetrahedron chain (1) is a special case of model (2). Since the model can be represented as a sum of local Hamiltonian on each tetrahedron, a classical ground state is obtained whenever the total spin in the tetrahedron is zero for a homogeneous model. It is straightforward that the classical ground states have a continuous local degeneracy.

II. SPIN-1/2 LATTICE

First, we consider the spin 1/2 case. As we have mentioned in the Introduction, there is a fundamental different property between the 1D pyrochlore strip and its high-dimensional analogies: not all spins on a tetrahedron are equivalent. The spins on the vertical rung of the tetrahedron are not coupled to the neighboring tetrahedron. We define the total spin on each vertical rung as $\hat{T}_i = \hat{S}_{i,2} + \hat{S}_{i,3}$. It is obvious that $\hat{T}_i^2$ is conserved. This property enables us to simplify the 1D model greatly.

For the tetrahedron chain model (2), it is convenient to reformulate the Hamiltonian as follows:

$$H_A = J\sum_i \hat{S}_{i,1}\hat{S}_{i+1,1} + J\sum_i (\hat{S}_{i,1}+\hat{S}_{i+1,1})\cdot\hat{T}_i + \frac{J_\perp}{2}\sum_i \hat{T}_i^2 - NJ_\perp S(S+1), \tag{3}$$

where $\hat{T}_i^2 = T_i(T_i+1)$ with $T_i = 0,\ldots,2S$. In the strong coupling limit $J_\perp \to \infty$, a pair of spins on each rung would form a singlet (spin dimer) with $T_i = 0$. This implies that the spins in the horizontal direction along the chain is effectively decoupled with the spins on the vertical rungs. Therefore, the ground state of H_A is a product of the ground state of spin chain and rung singlets. Explicitly, it is represented as follows:

$$|\mathrm{GS}\rangle = |BA\rangle \otimes \prod_i [S_{i,2}, S_{i,3}], \tag{4}$$

where $|BA\rangle$ denotes the Bethe-ansatz ground state wave functions of the 1D Heisenberg chain $H_{chain} = J\Sigma_i \hat{S}_{i,1}\hat{S}_{i+1,1}$ and $[S_{i,2}, S_{i,3}] = ([\uparrow]_{i,2}[\downarrow]_{i,3} - [\downarrow]_{i,2}[\uparrow]_{i,3})/\sqrt{2}$ is the dimer singlet across the ith vertical rung. The corresponding ground state energy is

$$E_g^A = E_g^{BA}(N) - \frac{3}{4}NJ_\perp, \tag{5}$$

where $E_g^{BA}(N)$ is the ground state energy of the N-site Heisenberg spin-1/2 chain. From the Bethe-ansatz solution of Heisenberg model, we know the exact ground state energy $E_g^{BA}(N)/N = -0.4431J$ at the infinite length limit.

In fact, utilizing the Raleigh-Ritz variational principle,[11,19–21] we can exactly prove the state given by Eq. (4) is the ground state of Hamiltonian (2) as long as $J_\perp \geqslant 2J$. To see it clearly, we can rewrite the Hamiltonian (2) with $J_\perp = 2J$ as the sum of a Heisenberg chain and $2N$ projection operators, which reads

$$H_A = J\sum_i \hat{S}_{i,1}\hat{S}_{i+1,1} + \sum_i \frac{3J}{2}\mathbf{P}^{3/2}(\hat{S}_{i,1},\hat{S}_{i,2},\hat{S}_{i,3}) + \sum_i \frac{3J}{2}[\mathbf{P}^{3/2}(\hat{S}_{i,2},\hat{S}_{i,3},\hat{S}_{i+1,1}) - 1], \tag{6}$$

where

$$\mathbf{P}^{3/2}(\hat{S}_{i,1},\hat{S}_{i,2},\hat{S}_{i,3}) = \frac{1}{3}\left[(\hat{S}_{i,1}+\hat{S}_{i,2}+\hat{S}_{i,3})^2 - \frac{3}{4}\right] \tag{7}$$

is a projection operator which projects a three-spin state composed of $S_{i,1}$, $S_{i,2}$, and $S_{i,3}$ into a subspace with total spin 3/2. Now it is clear that the state given by Eq. (4) is the ground state of the global Hamiltonian because it is simultaneously the ground state of each local sub-Hamiltonian.[11,20,21] With the same reasoning, the state (4) is of course the ground state of Hamiltonian Eq. (2) for $J_\perp > 2J$. It is not hard to check that the state (4) is an eigenstate of the global Hamiltonian H_A by utilizing the identities $(\hat{S}_{i,2}+\hat{S}_{i,3})[S_{i,2}, S_{i,3}] = 0$, however, such an eigenstate is not

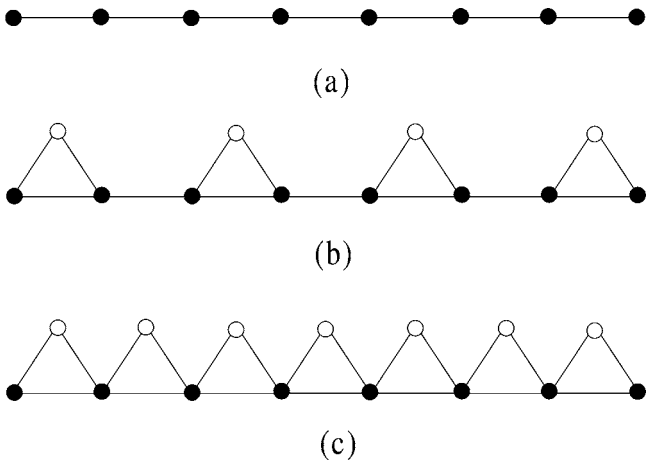

FIG. 2. Three types of ground state for the spin-1/2 and spin-1 pyrochlore strips. The open and close circles denote the spins with $S=1$ and $S=1/2$, respectively, for the spin-1/2 pyrochlore strip. For spin-1 pyrochlore strip, the open circles represent the spins with $S=2$ and the close circles represent the spins with $S=1$.

necessary the ground state for arbitrary $J_\perp$. We note that the condition $J_\perp \geqslant 2J$ for the existence of the ground state given by (4) is just a sufficient condition which is a very strong restriction. In fact, it can be released to a wider parameter regime. We expect that there is a critical value $J_\perp^c$ and the system evolves into another quantum ground state when $J_\perp$ is smaller than $J_\perp^c$.

For the homogeneous point $J_\perp=J$ which we are particularly interested in, although the above proof is no longer applicable, we can still argue that Eq. (4) remains the ground state, and prove this result by using the numeric exact diagonalization method. With the aid of numerical diagonalization, we may determine the phase boundary of the model (2) precisely. Since the total spin in every rung is conserved, the vertical rungs are either in singlets or triplets for a spin-1/2 pyrochlore strip. Therefore, the relevant eigenstate of the pyrochlore strip can be classified by the values of the total spins on the vertical rungs.[22,23] For convenience, we use $E(N,M)$ to represent the eigenenergy of the state with N-M spin singlets and M triplets on the vertical rungs. It follows that the eigenenergy is given by

$$E(N,M) = -\frac{3}{4}NJ_\perp + MJ_\perp + JE_{1/2,1}(N,M), \tag{8}$$

where $E_{1/2,1}(N,M)$ represents the energy of the lattice composed of N spins with $S=1/2$ on the sites of the lower row and M spins with $T=1$ on the top row. For each class of state with N-M spin singlets and M triplets on the vertical rungs, there are altogether C_N^M different configurations.

It is instructive to first consider the following two kinds of configuration which correspond to two opposite limits of the vertical exchange: (i) all the states on the vertical rungs are spin singlets and (ii) all the states on the vertical rungs are spin triplets. In the first case, the original model can be mapped to a spin chain model as displayed in Fig. 2(a) and the corresponding eigenenergy is given by

$$E(N,0) = -\frac{3}{4}NJ_\perp + JE_{1/2}(N), \tag{9}$$

where $E_{1/2}(N)=E_{1/2,1}(N,0)$ is the energy of the N-site Heisenberg spin-1/2 chain and the Bethe-ansatz ground state energy $E_{1/2}^g(N)/N=-0.4431$ as $N\to\infty$. In the second case, the tetrahedron chain can be effectively described by a Δ-chain model consisted of N spins with $S=1/2$ on the sites of the lower row and N spins with $T=1$ on the sites of top row as shown in Fig. 2(c) and the eigenenergy can be represented as follows:

$$E(N,N) = \frac{1}{4}NJ_\perp + JE_{1/2,1}(N,N), \tag{10}$$

where $E_{1/2,1}(N,N)$ denotes the eigenenergy of the corresponding Δ-chain model. The mixed spin Δ chain can be viewed as an alternating spin-1/2-spin-1 chain with an additional next-nearest neighbor interaction between the spins with $S_i=1/2$. It is well known that there is a ferrimagnetic long-range order in the ground state of quantum ferrimagnetic Heisenberg chain.[24–26] The additional interaction between the spins with $S=1/2$ is a kind of frustration which makes it harder to compensate the spin with $S=1$, therefore the long-range order still exists. Although no exact analytical results for the mixed spin Δ chain are known, its ground state energy may be determined by numerical exact diagonalization method. For a mixed spin Δ chain with size of $8+8$, we get its ground state energy given by $E_{1/2,1}^g(8,8)/16=-0.646\,773$. We note that the ground state of a spin Δ chain or a spin sawtooth model with $S_i=1/2$ is exactly known.[19,20,27]

It is clear that the state with all singlets or triplets on the rungs are the ground state of the tetrahedron chain in the limit of $J_\perp\to\infty$ and $J_\perp\to-\infty$, respectively. Flipping a rung singlet into triplet costs an energy of $J_\perp$, therefore the effect of the antiferromagnetic coupling $J_\perp$ is to prevent the spins on the rung forming triplet. On the other hand, a triplet in the rung acts effectively as a spin with $S=1$ which lowers the total energy by interacting with its neighboring spins with $S=1/2$ on the lower rung. The competition between the two processes gives rise to the complexity of the phase diagram for the tetrahedron chain. An interesting question arising here is whether some intermediate phases exist between the phases with fully paired singlets and triplets on the rungs. To determine the phase boundary of (2) numerically, in principle, we need consider all the different configurations of T_i on the rungs. Among a given class, we find that the configuration with the spins on the top row repelling each other has lower energy. For example, as shown in Fig. 2(b), the configuration with alternating spin 1 and spin 0 on the top row has the lowest energy among the $C_N^{N/2}$ configurations. After considering all the rung configurations, we get a phase diagram as shown in the Fig. 3. As expected, there is an intermediate phase which is effectively described by the ground state of its equivalent model as shown in Fig. 2(b). Corresponding to Fig. 2(b), there is another equivalent configuration which is obtained by totally shifting the spins on the top

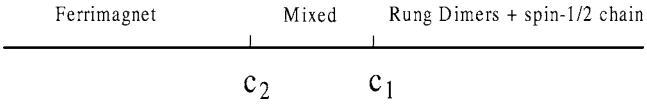

FIG. 3. The phase diagram for spin-1/2 tetrahedron chain with variable vertical exchange $J_\perp$ in the parameter space of $c=J_\perp/J$. For $c>c_1$, the system is in a decoupled phase whose ground state is a product of rung singlets and the critical spin liquid phase on the horizontal spin-1/2 chain; For $c_2<c<c_1$, the ground state is a double degenerate mixed state with the alternating spin singlet and spin triplet on the rungs; For $c<c_2$, the ground state is a ferrimagnetic state with spin triplet on the rungs.

row a lattice space. In this phase, the triplet and singlet on the rungs distribute in an alternating way and the ground state is doubly degenerate.

Next we will give a description on how to determine the phase diagram as shown in Fig. 3. Since the original pyrochlore strip can be classified by the values of the total spins on the vertical rungs or equivalently by M, labelling the numbers of the rung triplets, the ground-state energy of our tetrahedral spin chain, for a given value of J and $J_\perp$, will be given by the lowest value of Eq. (8) with $M=0,1,\ldots,N$. In Fig. 4, we show as a function of $c=J_\perp/J$ all the lowest eigenenergies for the lattice sizes with 4, 6, and 8 tetrahedra. The energies corresponding to the point of $c=0$ (intercept points with the vertical axis) are the lowest energies of $E_{1/2,1}(N,M)$, from above to below, with $M=0,1,\ldots,N$. The slope values of the straight lines depend upon the number M. Our numerical analysis shows that the ground state in the whole parameter space c is determined by three kinds of configurations with $M=0,N/2,N$, corresponding to the configurations of (a), (b), and (c) displayed in Fig. 2 and their crossing points determine the phase transition points. For simplicity, we omit all the excited energy levels for the case of $N=8$ in the Fig. 4. From our numerical results, we obtain the up critical value $c_1=0.9529$ and the down critical value $c_2=0.7214$ for the original pyrochlore strip with a size of 24 sites (8 tetrahedra or $N=8$). Similarly, we get $c_1=0.881\,86$ and $c_2=0.705\,46$ for $N=4$, $c_1=0.929\,52$ and $c_2=0.723\,51$ for $N=6$. Here c_1 corresponds to the crossing points of lines (a) and (b), whereas c_2 corresponds to the crossing points of lines (b) and (c). Since we need much smaller memory size to diagonalize systems of (a) and (b) than system of (c), therefore we can calculate even larger system to determine c_1. For example, we get $c_1=0.962\,28$ for $N=10$ and $c_1=0.967\,52$ for $N=12$. In Fig. 5, we analysis the finite size scaling of c_1 and c_2. The linear fit of c_1 and c_2 gives $c_1=0.9767\pm0.0020$ and $c_2=0.730\,21\pm0.005\,77$ for $N\to\infty$. We can also determine the phase boundaries c_1 and c_2 in an alternative way. By extrapolating the ground state energy of (a) and (b) to infinite size, we then determine c_1 and c_2 by the crossing of the energy levels of (a), (b) and (b), (c), respectively. In Fig. 6, we display the finite size scaling of the ground state energies of (a), (b), and (c). The ground state energies per site, obtained by linear fit to the infinite limit, corresponding to the configurations of (a), (b), and (c) are $0.442\,61\pm0.000\,19$, $0.620\,33\pm0.000\,91$ and $0.646\,75\pm0.000\,01$, respectively. By this way and using Eq. (8), we get $c_1=0.9757$ and $c_2=0.726\,01$ in the limit of infinite size. If we use the ground state energy obtained by Bethe ansatz for (a), we get $c_1=0.9748$.

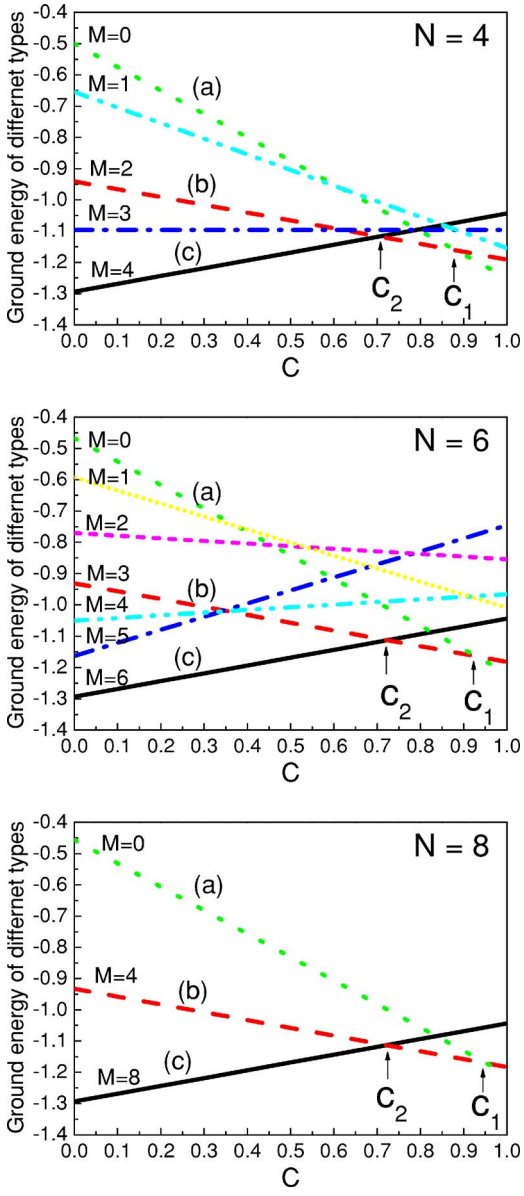

FIG. 4. (Color online) The lowest energies of $E(N,M)/\mathrm{J}$ as a function of $c=J_\perp/J$ for $N=4,6,8$. The solid, dashed, and dotted lines corresponding to the case with $M=N$, $M=N/2$, and $M=0$ or (c), (b), (a) as displayed in Fig. 2.

Before ending the discussion of the spin-1/2 pyrochlore strip, we would like to remark on a generalized spin pyrochlore strip where the horizontal exchange is variable. With the same reasoning as that of the model (2), we can easily get the sufficient condition for the existence of the fully dimerized state on all the vertical rungs, which reads $J_\perp \geqslant 2J$ and is irrelevant with the horizontal exchange. When the horizontal exchanges are zero, the model has totally different ground sates and it falls into the class of 1D diamond mode,[28,29] which has also fully dimerized state on the vertical rungs as the ground state but the ground state is highly degenerate with a degeneracy of 2^N because the unpaired N spins are completely free.

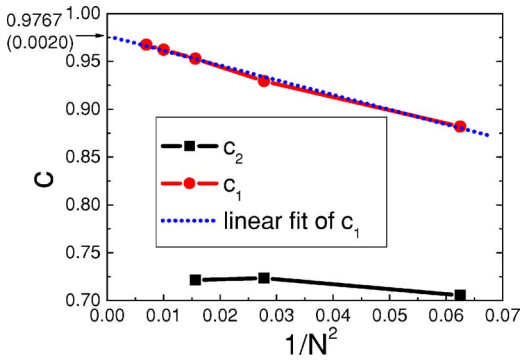

FIG. 5. (Color online) The phase boundaries c_1 and c_2 versus the sizes of the system.

III. SPIN-1 LATTICE WITH SU(2) SYMMETRY

The above method can be directly extended to deal with the spin-1 case. For the spin tetrahedron chain (2) with $S=1$, we can prove that the ground state of (2) is a product of fully dimerized singlets on the rungs and the ground state of horizontal spin-1 chain as long as $J_\perp \geqslant 4J$. Explicitly, the ground state can be represented as follows:

$$|\mathrm{GS}\rangle = |\mathrm{Haldane}\rangle \otimes \prod_i [S_{i,2}, S_{i,3}] \tag{11}$$

where $|\mathrm{Haldane}\rangle$ denotes the ground state of the 1D spin-1 chain and

$$[S_{i,2}, S_{i,3}] = \frac{1}{\sqrt{3}} \sum_{m=-1}^{1} (-1)^{m+1} |m\rangle_{i,2} |-m\rangle_{i,3}$$

is a spin singlet across the ith vertical rung. The proof is rather similar to its spin-1/2 correspondence and is straightforward when we rewrite the Hamiltonian (2) in the following form:

$$H_A = \sum_i [\mathbf{h}_\Delta(\hat{S}_{i,1}, \hat{S}_{i,2}, \hat{S}_{i,3}) + \mathbf{h}_\Delta(\hat{S}_{i,2}, \hat{S}_{i,3}, \hat{S}_{i+1,1})] + J \sum_i \hat{S}_{i,1} \hat{S}_{i+1,1} \tag{12}$$

with $\mathbf{h}_\Delta(\hat{S}_{i,1}, \hat{S}_{i,2}, \hat{S}_{i,3}) = J\hat{S}_{i,1}(\hat{S}_{i,2} + \hat{S}_{i,3}) + \frac{J_\perp}{2} \hat{S}_{i,2} \cdot \hat{S}_{i,3}$ and $\mathbf{h}_\Delta(\hat{S}_{i,2}, \hat{S}_{i,3}, \hat{S}_{i+1,1}) = J(\hat{S}_{i,2} + \hat{S}_{i,3})\hat{S}_{i+1,1} + \frac{J_\perp}{2} \hat{S}_{i,2} \cdot \hat{S}_{i,3}$. Now it is easy to find that the ground state of $\mathbf{h}_\Delta$ is a product of paired

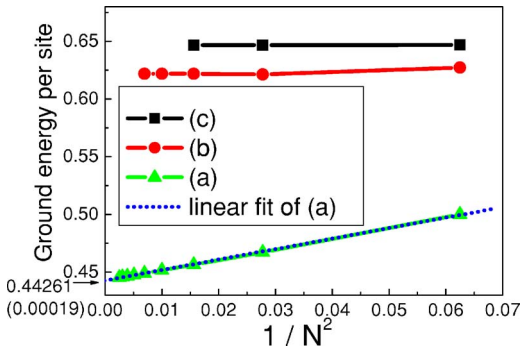

FIG. 6. (Color online) The ground state energies of systems (a), (b), and (c) versus the sizes of the system.

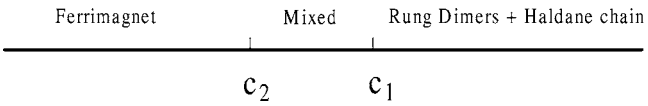

FIG. 7. The phase diagram for spin-1 tetrahedron chain. For $c > c_1$, the system is in a decoupled phase whose ground state is a product of rung singlets and Haldane phase on the horizontal chain; For $c_2 < c < c_1$, the ground state is a double degenerate mixed state with the alternating spin singlet and spin quintet on the rungs; For $c < c_2$, the ground state is a ferrimagnetic state with spin quintet on the rungs.

singlet on the rung and a free spin on the unpaired site as long as $J_\perp \geqslant 4J$. By the variational principle, we conclude that the state (11) is the ground state of the spin-1 model given by Eq. (2) for $J_\perp \geqslant 4J$. Certainly, the sufficient condition for the existence of a fully dimerized ground state on the rung can be released to a lower bound. In principle, we can determine it numerically following a similar scheme of the spin-1/2 case.

Since the total spin T_i on each vertical rung can be 0, 1 or 2, the spin-1 tetrahedron chain can be mapped to a mixed sawtoothlike model according to its configurations of the vertical rungs. Several relevant configurations are: (i) Spin singlets on all the vertical rungs with the eigenenergy given by

$$E_{T=0} = -2NJ_\perp + JE_1(N), \tag{13}$$

where $E_1(N)$ denotes the eigenenergy of a spin-1 chain of N sites. From the known numerical results,[30] we get ground state energy per site $E_1^g(N)/N = -1.4051$ in the large N limit. (ii) Spin triplets on all the vertical rungs with the eigenenergy given by

$$E_{T=1} = -NJ_\perp + JE_{1,1}(N,N). \tag{14}$$

Here $E_{1,1}(N,N)$ represents the eigenenergy of a spin-1 Δ chain of $2N$ sites.[31] (3) Spin quintet ($T=2$) on all the vertical rungs with the eigenenergy given by

$$E_{T=2} = NJ_\perp + JE_{1,2}(N,N). \tag{15}$$

Here $E_{1,2}(N,N)$ represents the eigenenergy of a mixed spin-1 and spin-2 Δ chain with spin 1 on the site of the lower row and spin 2 on the site of top row. Just similar to the spin-1/2 pyrochlore strip, we need to consider all the different configurations of the rungs. Numerically, we find the phase diagram is rather similar to that of the spin-1/2 case. As displayed in Fig. 7, there is also an intermediate phase between the fully paired singlet state with $T_i=0$ and state with all $T_i=2$. The intermediate state is twofold degenerate with the configuration of alternating singlet and quintet on rungs. Such a state can be schematized in terms of Fig. 2(b) with the open circle denoting the state with $T_i=2$. From our numerical results, we obtain $c_1=0.915\,96$ and $c_2=0.884\,04$ for the original tetrahedron chain with a size of 18 sites ($N=6$) as well as $c_1=0.9134$ and $c_2=0.8452$ for $N=4$. With similar reasoning as the spin-1/2 case, we can get $c_1=0.941\,89$ for an even larger system with $N=8$. Linear fitting of datum of c_1 versus $1/N^2$ and extrapolating it to the limit of the infinite

size, we get $c_1=0.959\,83\pm0.027\,48$ for $N\to\infty$.

As a natural generalization, it is straightforward to extend the spin pyrochlore model with SU(2) symmetry to the case with arbitrary spin S. For the spin-S model, a sufficient condition for the existence of rung-dimerized ground state is $J_\perp \geqslant 4-3/(s+1)$ for a half-integer spin and $J_\perp \geqslant 4$ for integer spin. In the dimerized phase, the horizontal chain is decoupled with the spins on the rungs and therefore the elementary excitation of the tetrahedron chain is gapless for half-integer-spin model or opens a gap for the integer-spin model.

IV. SPIN-1 LATTICE WITH SU(3) SYMMETRY

For the spin-1 system, the most general Hamiltonian has a biquadratic exchange term besides the bilinear term and it exhibits much richer quantum phase structures than the bilinear model.[32] When the biquadratic exchange has the same strength of the bilinear exchange, the Hamiltonian $H=J\Sigma_{\langle ij\rangle}h(i,j)$ with

$$h(\hat{S}_i,\hat{S}_j)=\hat{S}_i\cdot\hat{S}_j+(\hat{S}_i\cdot\hat{S}_j)^2 \tag{16}$$

owns the SU(3) symmetry. For spin-1 systems of transition metal compounds where two electrons are coupled ferromagnetically by Hund's rule, the biquadratic exchange term originates from a fourth order perturbation process. Its magnitude is thus small compared to the bilinear terms, and thus the SU(3) symmetry is not applicable. However, in the cold atomic physics, most atoms have high hyperfine multiplets, thus it is possible to achieve high symmetries. For example, the ^{6}Li atom is with nuclear spin 1 and electron spin 1/2. In a weak magnetic field, electron spin is polarized, while nuclear spin remains free. Recent studies indicated that the three nuclear spin components can be described by an approximate SU(3) symmetry.[33]

It is well known that the SU(3) exchange model on a chain has quite different properties from that of the SU(2) bilinear model. Therefore we may expect that the SU(3) tetrahedron chain

$$H=J_\perp\sum_i h(\hat{S}_{i,2},\hat{S}_{i,3})+J\sum_i\sum_{\alpha=1}^{3}h(\hat{S}_{i,\alpha},\hat{S}_{i+1,1})$$
$$+J\sum_i[h(\hat{S}_{i,1},\hat{S}_{i,2})+h(\hat{S}_{i,1},\hat{S}_{i,3})] \tag{17}$$

also displays different phase structure from that of its SU(2) correspondence (2). The model with $J_\perp=J$ was initially proposed by three of us with Zhang in Ref. 34 as an example of the SU(N) generalization of the Majumdar-Gosh model, however, no analytical results have been given there. Observing that the Hamiltonian can be written as a sum of the Casimir of the total spin in each tetrahedron and the representations with the smallest Casimir made out of four sites in the fundamental representations is three dimensional, we concluded that the state of trimer products is the GS of the SU(3) tetrahedron chain. The ground state is twofold degenerate. Explicitly, the ground state of the SU(3) spin tetrahedron chain can be represented as follows:

$$|\mathrm{GS}\rangle_1=\prod_i T(S_{i,1},S_{i,2},S_{i,3}) \tag{18}$$

or

$$|\mathrm{GS}\rangle_2=\prod_i T(S_{i,2},S_{i,3},S_{i+1,1}), \tag{19}$$

where

$$T(S_i,S_j,S_k)=\frac{1}{\sqrt{6}}\epsilon_{\alpha\beta\gamma}|\alpha_i,\beta_j,\gamma_k\rangle$$

represents a trimer state which is a singlet composed of three spins on site i,j, and k. Here α_i denotes the spin on site i with the value α taking 1, 0, or -1 and $\epsilon_{\alpha\beta\gamma}$ is an antisymmetric tensor.

In the following, we shall calculate the ground state energy and elementary excitation of Eq. (17) analytically. For convenience, we make a shift of constant to the Hamiltonian (17) by replacing $h(\hat{S}_i,\hat{S}_j)$ with $\hat{P}_{i,j}=h(\hat{S}_i,\hat{S}_j)-1$. We note that modification of $J_\perp$ does not lift the degeneracy of the left- and right-trimer states. For $J_\perp>J$, the state of trimer products is of course the ground state of the SU(3) tetrahedron chain and the corresponding ground state energy is

$$E_g=-2NJ-NJ_\perp.$$

Breaking a singlet of trimer will cost a finite energy, thus the elementary excitation of the SU(3) tetrahedron chain has an energy gap. For a three-site cluster, the trimer singlet is represented by a Young tableaux $[1^3]$ and the first excited state above the singlet are represented by the Young tableaux $[2^11]$. When a trimer singlet is broken, it decomposed into a monomer and a paired dimer. For a system with degenerate ground state, the monomer and dimer can propagate freely in the background of trimerized ground state and lower the energy further. In principle, two type of excitations are available in a pyrochlore chain, either a magnonlike excitation produced by flipping a trimer state into its excited state or a pair of deconfined objects composed of a dimer plus a monomer. For our system with doubly degenerate ground state, the spinonlike excitations have lower energy.

The deconfined excitations behave like domain-wall solitons which connects two spontaneously trimerized ground states. Explicitly, we represent an excited state with a dimer at site $2m-1$ and a monomer at site $2n$ is represented as

$$\Psi(m,n)=\cdots T(S_{m-1,1},S_{m-1,2},S_{m-1,3})m(S_{m,1}),$$
$$T(S_{m,2},S_{m,3},S_{m+1,1})\cdots T(S_{n-1,2},S_{n-1,3},S_{n,1}),$$
$$d(S_{n,2},S_{n,3})T(S_{n+1,1},S_{n+1,2},S_{n+1,3})\cdots,$$

where $d(S_i,S_j)=\frac{1}{\sqrt{2}}(|\alpha_i\beta_j\rangle-|\beta_i\alpha_j\rangle)$ with $\alpha\neq\beta$ represents a dimer. The corresponding momentum-space wave function is

$$\Psi(k_m,k_d)=\sum_{1\leqslant m\leqslant n\leqslant M}e^{imk_m+ink_d}\Psi(m,n).$$

The excitation spectrum can be calculated directly by using the above variational wave function. Because there exists no intrinsic mechanics responsible for binding the dimer and

monomer together to form a bound state in a spontaneously trimerized system, it is reasonable to assume that the dimer and monomer are well separated and they could be treated separately. Similar schemes have been used to evaluate the excitation spectrum in the spin-sawtooth system.[19,20] Under such an approximation, the excitation spectrum can be represented as a sum of monomer part and dimer part, i.e., $\omega(k_m,k_d)\approx\omega(k_m)+\omega(k_d)$. The state $\Psi(n)$ is not orthogonal with the inner product given by

$$\langle\Psi(n')||\Psi(n)\rangle=\left(\frac{1}{3}\right)^{|n'-n|},$$

thus $\Psi(k_d)$ has a nontrivial norm $\langle\Psi(k_d)||\Psi(k_d)\rangle=4/(5-3\cos k_d)$. With a similar scheme as solving the spectrum of excitations of the spin-1/2 model,[11,19,20] we get the spectrum for the dimer

$$\omega(k_d)=\frac{5}{4}\Delta_d-\frac{3\cos k_d}{4}\Delta_d \tag{20}$$

with $\Delta_d=2J$. In the large $J_\perp$ limit, a monomer can only hop around in the left and right phases along the horizontal direction without breaking additional trimer singlet, therefore its excitation spectrum forms a flat band, i.e., $\omega(k_m)=0$. When $J_\perp$ is close to J, the monomer actually can move around several corners, i.e., the monomer can be in the site of $(m,2)$ and $(m,3)$ either, therefore the wave function for a monomer has resonating structure at the mth triangle in the pyrochlore. The process of hopping from site $(m,1)$ to $(m,2)$ or $(m,3)$ accompanies with an energy cost of $J_\perp$-J, and thus the excitation spectrum is still a flat band for the homogeneous pyrochlore with $J_\perp=J$. For the inhomogeneous case, we take the monomer excitation as a three-site cluster consisting of three single monomers at sites $(m,1)$, $(m,2)$, and $(m,3)$, i.e.,

$$\Psi(m)=\frac{1}{\sqrt{3}}[\cdots m(S_{m,1})\cdots+\cdots m(S_{m,2})\cdots+\cdots m(S_{m,3})\cdots].$$

Similarly, after considerable algebra, we get the spectrum for the monomer

$$\omega(k_m)=\frac{2}{3}\Delta_m-\frac{6\cos k_m}{15}\Delta_m \tag{21}$$

with $\Delta_m=J_\perp$-J.

V. CONCLUSIONS

We have proposed and studied a class of frustrated lattice which can be viewed as a 1D strip of the pyrochlore lattice or a tetrahedron chain. For the general Heisenberg exchange model, we give an exact proof for the existence of the ground state consisting of the rung-dimerized state and the ground state of the decoupled chain. The phase diagrams of the spin-1/2 and spin-1 tetrahedron chain are given and the phase boundaries are precisely determined for the small-size systems. For both the spin-1/2 and spin-1 systems, there exist three phases, say, the fully dimerized singlets on the rungs plus a decoupled chain, a mixed phase with alternating spin singlet and state with total rung spin $2S$ on the rungs, and a ferrimagnetic phase with long-range order, as the strength of vertical exchanges varies from infinity to minus infinity. We also studied the SU(3) spin-exchange model on the 1D tetrahedron chain, for which the ground sate is a double degenerate trimerized state and the elementary excitations are fractionalized topological excitations. Our results indicate that the properties of the ground state for the pyrochlore systems with half-integer and integer spins or the systems with the same spins but different internal symmetries [SU(2) and SU(3) for spin-1 systems] are quite different.

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