Dimerizations in spin-S antiferromagnetic chains with three-spin interaction

Zheng-Yuan Wang,[1] Shunsuke C. Furuya,[2] Masaaki Nakamura,[3,4] and Ryo Komakura[1]
[1]*Department of Physics, Tokyo Institute of Technology, Oh-okayama, Meguro-ku, Tokyo, 152-8551, Japan*
[2]*DPMC-MaNEP, University of Geneva, 24 Quai Ernest-Ansermet CH-1211 Geneva, Switzerland*
[3]*Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany*
[4]*Institute of Industrial Science, the University of Tokyo, Meguro-ku, Tokyo, 153-8505, Japan*
(Received 31 October 2013; published 23 December 2013; corrected 3 February 2014)

We discuss spin-S antiferromagnetic Heisenberg chains with three-spin interactions, next-nearest-neighbor interactions, and bond alternation. First, we prove rigorously that there exist parameter regions of the exact dimerized ground state in this system. This is a generalization of the Majumdar-Ghosh model to arbitrary S. Next, we discuss the ground-state phase diagram of the models by introducing several effective field theories and the universality classes of the transitions are described by the level-2S SU(2) Wess-Zumino-Witten model and the Gaussian model. Finally, we determine the phase diagrams of $S = 1$ and $S = 3/2$ systems by using exact diagonalization and level spectroscopy.

DOI: 10.1103/PhysRevB.88.224419 PACS number(s): 78.30.−j, 75.40.Gb, 75.10.Jm

I. INTRODUCTION

Models with exact ground states have provided the foundations for investigating strongly correlated systems in a nonperturbative manner. The Affleck-Kennedy-Lieb-Tasaki (AKLT) model with an exact valence-bond-solid (VBS) ground state is a good example of such systems.[1] It is now widely accepted that the VBS state captures the qualitative nature of the Haldane phase in the integer-S antiferromagnetic Heisenberg (AFH) chain. For $S = 1/2$ systems, on the other hand, the Majumdar-Ghosh (MG) model is known to have a fully dimerized state as the exact ground state.[2] It has been shown that this state captures the dimer phases that appear in certain parameter regions of the frustrated AFH chain,[3] and experimentally observed states such as in $CuGeO_3$.[4] An extension of the exact dimerized ground state to higher dimensions has also been investigated, because it is relevant to experimental studies, such as those of the two-dimensional Shastry-Sutherland model[5] compound $SrCu_2(BO_3)_2$.[6]

In this paper, we consider an intriguing model which has a dimerized exact ground state in certain parameter regions: a general-S spin chain including three-spin, next-nearest-neighbor interactions, and bond alternation,

$$\mathcal{H} = J_1 \sum_i \{1 - \delta(-1)^i\} \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} + J_2 \sum_i \boldsymbol{S}_{i-1} \cdot \boldsymbol{S}_{i+1} + J_3 \sum_i [(\boldsymbol{S}_{i-1} \cdot \boldsymbol{S}_i)(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1}) + \text{H.c.}], \quad (1)$$

where H.c. denotes the Hermitian conjugate. The model (1) is schematically described in Fig. 1. As we will see below, our model (1) may be regarded as a natural, but not naive, extension of the $S = 1/2$ MG model to a general-S case. Note that, just as for several extensions of the MG model,[3,7,8] our model (1) has longer-range interaction than nearest neighbor.

Recently, Michaud *et al.* discussed a special case of this model with $J_2 = \delta = 0$.[9] They have shown that this "J_1-J_3" model is reduced to the MG model for $S = 1/2$, and that a doubly degenerate dimerized state appears as the exact ground state when the ratio of the couplings is $J_3/J_1 = 1/[4S(S + 1) - 2]$. In this sense, one may regard the J_1-J_3 model as a generalization of the MG model. Michaud *et al.* argued that the J_1-J_3 model has exact dimerized ground states for *any* S. While their conclusion is undoubtedly interesting, the mechanism that allows the J_1-J_3 model to possess an exact ground state is still unclear. In this paper, we prove rigorously that the fully dimerized state is the exact ground state of the J_1-J_3 model from a more comprehensive point of view. Namely, we present a proof of the fact that the general extension of the J_1-J_3 model, that is, the "J_1-J_2-J_3" model with bond alternation (1), has an exact dimerized ground state. Our proof, besides its rigorousness, gives a physical answer to the natural question of why an exact ground state is feasible in the general model (1).

One noteworthy feature of the model (1) is that it contains experimentally feasible interactions only.[9] This feature will be relevant to experimental studies directly or indirectly. Thus, it will be beneficial for experimental studies to investigate the spin chain (1) away from the exactly dimerized regions. For simplicity, we consider the phase diagram of Eq. (1) for $J_2 = 0$ in the δ-J_3/J_1 space. All the physical essence is encoded in this limited parameter region. Since the exact ground states are in the dimerized phase, there must be phase transition lines between the dimerized regions and the origin of the parameter space which corresponds to the pure Heisenberg model (i.e., $J_2 = J_3 = \delta = 0$). As discussed by Michaud *et al.*,[9,10] the phase transition occurs at a point $J_{3c}/J_1 > 0$ with $\delta = 0$ and it is expected that the level-2S SU(2) Wess-Zumino-Witten theory [$SU(2)_{2S}$ WZW theory] is realized there. This means that various relevant interactions are canceled at the critical point. On the other hand, for a fixed $J_3/J_1 < J_{3c}/J_1$, there

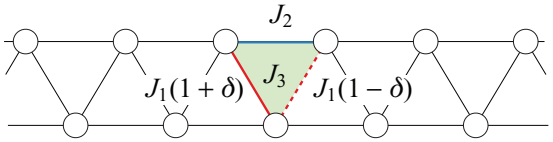

FIG. 1. (Color online) A schematic figure of the J_1-J_2-J_3 model with bond alternation δ (1). Alternating nearest-neighbor interactions $J_1(1 \pm \delta)$ are depicted by the red solid and dashed lines. The next-nearest-neighbor interaction J_2 is represented by the blue line. The three-spin interaction J_3 works on a triangle (green shaded area).

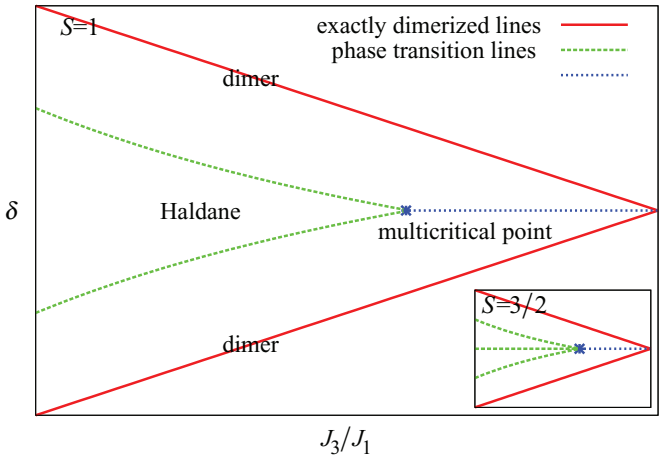

FIG. 2. (Color online) Schematic ground-state phase diagram for the model (1) with $J_2 = 0$ for $S = 1$ and 3/2. The solid lines correspond to the exact dimer ground-state regions. The dashed lines depict the critical lines between several dimerized phases including the Haldane phase. These critical lines are expected to be of the $c = 1$ Gaussian type. The stars denote multicritical points where the critical lines merge as described by $SU(2)_{2S}$ WZW theory with $c = 3S/(S+1)$.

should be $2S$ successive dimerization transitions between $2S+1$ phases with different VBS configurations when δ is varied from $\delta = -1$ to $\delta = 1$. These transitions are expected to be of Gaussian type. Therefore, the ground-state phase diagram of the general-S model (1) will consist of phase transitions of different universality classes. A field-theoretical point of view allows a comprehensive understanding of such complicated situations. The field-theoretical description also enables us to perform an accurate numerical analysis of the phase diagram by the level-spectroscopy method.[11] We will determine the phase diagram for the $S = 1, 3/2$ and $J_2 = 0$ systems of Eq. (1) numerically as shown in Fig. 2.

The rest of this paper is organized as follows: In Sec. II, we prove that there exist regions of the exact dimerized ground state of the spin-S AFH chain (1) in the (δ, J_1, J_2, J_3) parameter space. In Sec. III, we discuss the universality class of the phase transition of this model with $J_2 = 0$ based on a field-theoretical argument. Furthermore, we determine the phase diagrams of this model for $S = 1$ and $S = 3/2$ numerically, using exact diagonalization and the level-spectroscopy method. In the Appendix and Supplemental Material,[12] the detailed calculation for the proof of the exact ground state will be presented.

II. PROOF OF THE EXACT DIMERIZED GROUND STATES

In this section, we prove that Eq. (1) has parameter regions of exact dimer ground states for general S. First, let us reconsider the Majumdar-Ghosh model [Eq. (1) with $S = 1/2$, $\delta = J_3 = 0$, and $J_2 = J_1/2$],

$$\mathcal{H}_{\mathrm{MG}} = J_1 \sum_i \left(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} + \tfrac{1}{2} \boldsymbol{S}_{i-1} \cdot \boldsymbol{S}_{i+1} \right). \tag{2}$$

This model has two fully dimerized states as the exact ground state,

$$\begin{aligned} |\Psi_{\mathrm{odd}}\rangle &= \prod_{i \in \mathbb{Z}} |S(2i-1, 2i)\rangle \,, \\ |\Psi_{\mathrm{even}}\rangle &= \prod_{i \in \mathbb{Z}} |S(2i, 2i+1)\rangle \,, \end{aligned} \tag{3}$$

where $|S(i,i+1)\rangle$ denotes the singlet state formed by the spins at sites i and $i+1$. This can easily be proven if we rewrite Eq. (2) using the following projection operator:

$$Q_i = (\boldsymbol{S}_{i-1} + \boldsymbol{S}_i + \boldsymbol{S}_{i+1})^2 - S(S+1). \tag{4}$$

For the singlet states, the three spins form an $S = 1/2$ composite spin, so that $\langle Q \rangle_i = 0$ while $\langle Q \rangle_i \geqslant 0$ for other states. However, for $S \geqslant 1$, the singlet states (3) are no longer the ground states of this projection operator.

Next, we consider the J_1-J_3 model [Eq. (1) with $J_2 = \delta = 0$] which was discussed by Michaud *et al.*:[9]

$$\begin{aligned} \mathcal{H}_{J_1-J_3} &= J_1 \sum_j \boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1} \\ &\quad + J_3 \sum_i [(\boldsymbol{S}_{i-1} \cdot \boldsymbol{S}_i)(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1}) + \mathrm{H.c.}]. \end{aligned} \tag{5}$$

This Hamiltonian for $J_3/J_1 = 1/[4S(S+1) - 2]$ can be written as

$$\mathcal{H}_{J_1-J_3} = \frac{J_1}{16S(S+1) - 8} \sum_i P_i - \frac{J_1}{2} N S(S+1), \tag{6}$$

where N denotes the total number of the spins, and P_i is a local projection operator defined by

$$\begin{aligned} P_i &= (\boldsymbol{S}_{i-1} + \boldsymbol{S}_i) \cdot [(\boldsymbol{S}_i + \boldsymbol{S}_{i+1})^2 - 1] \cdot (\boldsymbol{S}_{i-1} + \boldsymbol{S}_i) \\ &= (\boldsymbol{S}_i + \boldsymbol{S}_{i+1}) \cdot [(\boldsymbol{S}_{i-1} + \boldsymbol{S}_i)^2 - 1] \cdot (\boldsymbol{S}_i + \boldsymbol{S}_{i+1}). \end{aligned} \tag{7}$$

It follows from $S_i^\alpha |S(i,j)\rangle = -S_j^\alpha |S(i,j)\rangle$ $(\alpha = x, y, z)$ that P_i projects out (i.e., annihilates) the singlet states,

$$P_i |S(i,i+1)\rangle = P_i |S(i-1,i)\rangle = 0. \tag{8}$$

Therefore, Eq. (3) is an exact *eigenstate* of the J_1-J_3 model.[9]

In order to show that Eq. (3) is the exact *ground state*, we have to prove that P_i is positive semidefinite. For this purpose, let us introduce the following two local projection operators:

$$R_i \equiv \tfrac{1}{2} P_i + (S+1) Q_i, \quad R_i' \equiv \tfrac{1}{2} P_i - S Q_i. \tag{9}$$

Since $[P_i, Q_i] = 0$ and also $[R_i, R_i'] = 0$, R_i and R_i' project out $|S(i-1,i)\rangle$ and $|S(i,i+1)\rangle$. Here one can show that R_i and R_i' are positive semidefinite, while Q_i is not. Let $|\psi\rangle$ be an eigenstate of R_i and R_i' simultaneously. We can confirm the non-negativity of its eigenvalues without making any *ad hoc* assumptions:

$$\langle \psi | R_i | \psi \rangle \geqslant 0, \quad \langle \psi | R_i' | \psi \rangle \geqslant 0, \tag{10}$$

where the equalities are satisfied for the singlet states. The relations (10) are proven by expanding the three-site wave functions explicitly into Ising-like bases (see the Appendix). Then P_i is also proven to be positive semidefinite due to the relation

$$P_i = \frac{S}{2S+1} R_i + \frac{S+1}{2S+1} R_i'. \tag{11}$$

Thus the J_1-J_3 model has an exact doubly degenerate dimerized ground state. In terms of R_i and R'_i, it is obvious that Q_i is not positive semidefinite:

$$Q_i = \frac{1}{2S+1}(R_i - R'_i). \tag{12}$$

Thus, the naive extension of the MG model $\mathcal{H}_{\rm MG} = (J_1/2)\sum_i Q_i + \text{const}$ to the general-S case fails to have an exact dimerized ground state.

The above argument enables us to generalize the J_1-J_3 model to Eq. (1) with $\delta = 0$, by constructing the Hamiltonian in the following form:

$$\tilde{\mathcal{H}}_{J_1-J_2-J_3} = \sum_i (AR_i + BR'_i), \quad A, B \geqslant 0, \tag{13}$$

where $\tilde{\mathcal{H}}_{J_1-J_2-J_3} \equiv \mathcal{H}_{J_1-J_2-J_3} - E_0$ with E_0 being the ground-state energy of $\mathcal{H}_{J_1-J_2-J_3}$. Furthermore, the model can be extended to $\delta \neq 0$ cases as

$$\mathcal{H}_{\delta-J_1-J_2-J_3} = \mathcal{H}_{J_1-J_2-J_3} + \sum_{i\in I_\delta} \delta'(\boldsymbol{S}_i + \boldsymbol{S}_{i+1})^2, \tag{14}$$

where I_δ stands for a set of odd (even) integers for $\delta > 0$ ($\delta < 0$). $\delta' > 0$ and the other parameters are related as

$$\delta' = \frac{1+\delta}{1-\delta}\left[A(2S^2+3S) + B(2S^2+S-1)\right], \tag{15}$$

$$\frac{J_3}{(1-|\delta|)J_1 - 2J_2} = \frac{1}{4S(S+1)-2}. \tag{16}$$

Since the operator $(\boldsymbol{S}_i + \boldsymbol{S}_{i+1})^2$ is obviously positive semidefinite and projects out the singlet state $|S(i,i+1)\rangle$, a nonzero δ lifts the doublet degeneracy of $|\psi_{\rm odd}\rangle$ and $|\psi_{\rm even}\rangle$. For $\delta > 0$ ($\delta < 0$), the fully dimerized state $|\psi_{\rm odd}\rangle$ ($|\psi_{\rm even}\rangle$) is the *unique* ground state of the model (14). The parameter regions of the exact ground state given by Eq. (16) are shown in Fig. 3.

The point of our proof lies in finding that the operator P_i in Eq. (6) can be written as two positive semidefinite operators R_i and R'_i, both of which project out the singlet states $|S(i-1,i)\rangle$ and $|S(i,i+1)\rangle$. Our proof clarifies that the operators R_i and R'_i that project out the singlet states are essential for realizing the exact dimerized ground state.

III. PHASE DIAGRAM OF $J_2 = 0$ CHAINS

In this section, we discuss the phase diagrams of the model (1) using a field-theoretical approach. For simplicity we consider only $J_2 = 0$ cases in the δ-J_3/J_1 space. The phase diagram of a related model including bond alternation and next-nearest-neighbor interaction J_2 is investigated in detail in Ref. 13.

A. Effective field theories

We introduce effective field theories of the AFH chain (1) for $J_2 = 0$, such as the O(4) and O(3) nonlinear σ models (NLSMs). All the field theories are derived from the $\mathrm{SU}(2)_k$ WZW theory. These field theories give the basic language needed to understand the statics and dynamics of this system.

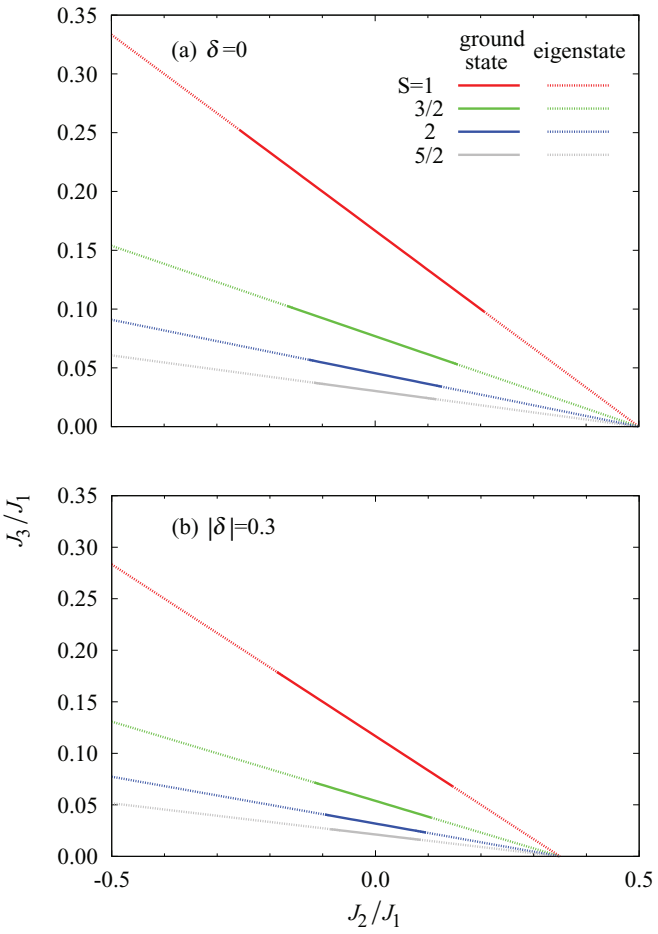

FIG. 3. (Color online) The parameter space of the model (1) for several $S \geqslant 1$ with (a) $\delta = 0$ and (b) $|\delta| = 0.3$. The solid (dotted) lines denote the regions where the dimerized state is the exact ground state (eigenstate).

1. The multicritical point

At a point $(\delta, J_3) = (0, J_{3c})$ with $J_{3c} > 0$, the Gaussian critical lines merge. This point is a multicritical point and the semi-infinite line $J_3 > J_{3c}$ on the horizontal axis is a first-order transition line. The low-energy physics at the multicritical point is described by the $\mathrm{SU}(2)_{2S}$ WZW theory and the central charge $c = 3S/(1+S)$.[9] The $\mathrm{SU}(2)_{2S}$ WZW theory has the following Euclidean action:

$$\mathcal{A}_{2S} = \frac{S}{8\pi}\int_{S^2} d^2x\, \mathrm{Tr}(\partial_\mu U \partial_\mu U^{-1}) + 2S\Gamma_{\rm WZ}. \tag{17}$$

$U \in \mathrm{SU}(2)$ is a primary field of the $\mathrm{SU}(2)_{2S}$ WZW theory. The second term is the Wess-Zumino term,

$$\Gamma_{\rm WZ} = -\frac{i}{24\pi}\int_{B^3} d^3x\, \epsilon^{\alpha\beta\gamma}\mathrm{Tr}(U^{-1}\partial_\alpha U U^{-1}\partial_\beta U U^{-1}\partial_\gamma U). \tag{18}$$

The two-dimensional space $\{(\tau,x)|\tau,x \in \mathbb{R}^2\}$ is identified as the two-dimensional sphere S^2 by a one-point compactification of infinity. B^3 is a three-dimensional ball whose boundary is $\partial B^3 = S^2$. The primary field $U \in \mathrm{SU}(2)$ can be represented

by a 2×2 matrix with four real parameters ϕ_α ($\alpha = 0,1,2,3$),

$$U = \phi_0 I + i\boldsymbol{\phi} \cdot \boldsymbol{\sigma}. \tag{19}$$

$I = \mathrm{diag}(1,1)$ is the 2×2 unit matrix. $\boldsymbol{\sigma} = (\sigma_1,\sigma_2,\sigma_3)$ denotes the Pauli matrices. The parameters ϕ_α are constrained to the three-dimensional sphere S^3,

$$\sum_{\alpha=0}^{3} {\phi_\alpha}^2 = {\phi_0}^2 + \boldsymbol{\phi}^2 = 1. \tag{20}$$

Therefore, the $\mathrm{SU}(2)_{2S}$ WZW theory is equivalent to the O(4) NLSM

$$\mathcal{A}_{2S} = \frac{S}{4\pi} \int d\tau dx \sum_{\alpha=0}^{3} (\partial_\mu \phi_\alpha)^2 + 2S\Gamma_{\mathrm{WZ}}. \tag{21}$$

The contraction $(\partial_\mu \phi_\alpha)^2 = (\partial_\tau \phi_\alpha)^2 + (\partial_x \phi_\alpha)^2$ is assumed. Whereas a $(2+1)$-dimensional version of the O(4) NLSM (21) is fully exploited to understand the deconfined quantum criticality of two-dimensional quantum antiferromagnets,[14,15] the $(1+1)$-dimensional version (21) is not used in one-dimensional quantum spin systems. In the following, we will see that the representation (21) also gives insight into the problem of one-dimensional quantum antiferromagnets. ϕ_0 and $\boldsymbol{\phi}$ represent order parameters of the dimerization and the Néel order, respectively:

$$\begin{pmatrix} S(S+1)\phi_0(x) \\ \sqrt{S(S+1)}\boldsymbol{\phi}(x) \end{pmatrix} \simeq \begin{pmatrix} (-1)^j \boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1} \\ (-1)^j \boldsymbol{S}_j \end{pmatrix}. \tag{22}$$

The SO(4) symmetry of the WZW theory is easily broken by relevant interactions. Indeed, the SO(4) group is homomorphic to $\mathrm{SU}(2)_L \times \mathrm{SU}(2)_R$. The subscripts L and R denote the holomorphic (right-moving) and the antiholomorphic (left-moving) degrees of freedom. The manifestation of the SO(4) symmetry means the decoupling of the holomorphic and antiholomorphic parts of the effective field theory, which is nothing but the fixed point theory (21). For instance, the most relevant interaction in the WZW theory is $\mathrm{Tr}U = 2\phi_0$. It apparently lowers the SO(4) symmetry to SO(3) if $\mathrm{Tr}U$ acquires a nonzero expectation value as in the dimerized phase.

The SO(4) symmetry is naturally manifested in the lattice model (1). Let us roughly determine a point where the SO(4) symmetry is realized in the phase diagram. First of all, it must be on the horizontal axis, $\delta = 0$, because the bond alternation $(-1)^j \boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1} \sim S(S+1)\phi_0$ cannot respect the SO(4) symmetry. The Hamiltonian (1) with $J_2 = 0$ and $\delta = 0$ is written in terms of the $(\phi_0,\boldsymbol{\phi})$ fields as follows:

$$\mathcal{H} \sim \int \frac{dx}{a} [-J_1 S(S+1)\boldsymbol{\phi}(x) \cdot \boldsymbol{\phi}(x+a) - J_3 [S(S+1)]^2 \phi_0(x)\phi_0(x+a) + \cdots]. \tag{23}$$

a is the lattice spacing of the spin chain. The SO(4) symmetry exists only when the right-hand side of Eq. (23) takes the form of $-JS(S+1)\sum_{\alpha=0}^{3} \phi_\alpha(x)\phi_\alpha(x+a) + \cdots$.

That is, the SO(4) symmetry is realized in the spin chain (1) at

$$\left(\delta, \frac{J_{3c}}{J_1}\right) = \left(0, \frac{C_S}{S(S+1)}\right). \tag{24}$$

C_S is a nonuniversal constant which may depend on the spin quantum number S. It is generally difficult to determine the precise value of C_S. But one can speculate that the constant C_S satisfies $0 < C_S \lesssim \frac{1}{4}$ because it lies between the origin (0,0) and the exactly dimerized point $(\frac{1}{4S(S+1)-2},0)$. In fact, $J_{3c}/J_1 = 0.111$ in the $S = 1$ AFH chain (1) leads to $C_{S=1} = 0.222$, which satisfies $0 < C_{S=1} < \frac{1}{4}$.

The effective field theory of the AFH chain (1) in the vicinity of the multicritical point has the following Euclidean action:

$$\mathcal{A} \simeq \mathcal{A}_{2S} - \int d\tau dx \, [c_\delta J_1 \delta \, \mathrm{Tr}\, U + c_3 (J_3 - J_{3c})(\mathrm{Tr}\, U)^2]. \tag{25}$$

c_δ and c_3 are positive dimensionless constants. Every effective field theory in distinctive regions of the phase diagram originates from the perturbed $\mathrm{SO}(2)_{2S}$ WZW theory (25).

The qualitative effects of the perturbations are easily seen as follows. When we move away from the multicritical point vertically ($J_3 = J_{3c}$), the ϕ_0 field is pinned to either of $\phi_0 = \pm 1$ in order to optimize the potential $\mathrm{Tr}\, U = 2\phi_0$. The pinning value depends on the sign of δ. But, irrespective of the sign, the spin chain (1) is drawn into the fully dimerized phase. On the other hand, when we move away horizontally ($\delta = 0$), the ϕ_0 field is pinned to ± 1 if $J_3 > J_{3c}$ and 0 if $J_3 < J_{3c}$. Only the former case corresponds to the fully dimerized phase where the one-site translational symmetry is spontaneously broken.

2. Between the multicritical point and the origin

The perturbed WZW theory (25) with $\delta = 0$ and $J_3 < J_{3c}$ is equivalent to the O(3) NLSM,[16]

$$\mathcal{A} = \int d\tau dx \, \frac{v}{2g} (\partial_\mu \boldsymbol{n})^2 + i\Theta Q \tag{26}$$

with a topological angle $\Theta = 2\pi S$. $\boldsymbol{n} = (n^x,n^y,n^z)$ is a three-dimensional unit vector. The $\boldsymbol{n}$ field is related to the original spin variable $\boldsymbol{S}_j$ via

$$\boldsymbol{S}_j \simeq (-1)^j S\boldsymbol{n}(x)\sqrt{1 - \left(\frac{\boldsymbol{L}(x)}{S}\right)^2} + \boldsymbol{L}(x). \tag{27}$$

Each component of $\boldsymbol{n}(x)$ represents a triplet one-magnon excitation near the wave number $q = \pi/a$, and $\boldsymbol{L}(x) = \frac{1}{gv}\boldsymbol{n} \times \partial_t \boldsymbol{n}$ describes two-magnon excitations near $q = 0$. The term $i\Theta Q$ in Eq. (26) is the so-called Θ term. $g = 2/S$ is a coupling constant. Q is an integer, which represents a winding number of the configuration of the $\boldsymbol{n}$ field on the two-dimensional sphere S^2. As Haldane first proposed,[17] the O(3) NLSM (26) describes a gapped spin chain when S is an integer.

3. On the critical line

Bond alternation modifies the coupling of the Θ term,[18]

$$\Theta = 2\pi S(1-\delta). \tag{28}$$

By increasing $|\delta|$ from zero, we can change the coupling Θ from $\Theta \equiv 0 \pmod{2\pi}$ to $\Theta \equiv \pi \pmod{2\pi}$ in the case of integer S, and from $\Theta \equiv \pi \pmod{2\pi}$ to $\Theta = 0 \pmod{2\pi}$ in the case of half-integer S. The O(3) NLSM (26) with $\Theta \equiv \pi$

(mod 2π) is equivalent to the massless free-boson theory,

$$\mathcal{A} = \frac{1}{2}\int d\tau dx\,(\partial_\mu \varphi)^2. \tag{29}$$

The boson field φ is compactified as $\varphi \sim \varphi + \sqrt{2\pi}$. For $S = 1$, the critical theory (29) describes the low-energy physics exactly on the $c = 1$ Gaussian critical line. This will also be the case for the $S = 3/2$ case.

B. Level spectroscopy

The phase diagrams of the $J_2 = 0$ chains for $S = 1$ and $S = 3/2$ are determined by level spectroscopy which identifies the phase transition as a level-crossing point of the lowest excitation levels obtained by exact diagonalization. The finite-size effect in this method is very small, since the logarithmic corrections are canceled at the level-crossing point, and only the power dependence of the size effect remains. The present Haldane-dimer and dimer-dimer transitions can be determined by level crossings of the lowest two excitations with different parities under antiperiodic boundary conditions.[11] These level crossings can also be interpreted as points of change of the (m,n)-type VBS configurations, which are defined as

$$\left|\Psi_{\rm VBS}^{(m,n)}\right\rangle \equiv \prod_{k=1}^{N/2}(B_{2k-1,2k}^{\dagger})^m (B_{2k,2k+1}^{\dagger})^n |{\rm vac}\rangle, \tag{30}$$

where $B_{i,j}^{\dagger} \equiv a_i^{\dagger} b_j^{\dagger} - b_i^{\dagger} a_j^{\dagger}$ and $|{\rm vac}\rangle$ is the vacuum with respect to bosons.[19] Here, the Schwinger boson operator $a_j^{\dagger}$ ($b_j^{\dagger}$) increases the number of up (down) $S = 1/2$ variables under symmetrization. The integers m and n satisfy $m + n = 2S$. The level-crossing points also correspond to zero points of the expectation values of the twist order parameters.[20] Moreover, for $S = 1$ the two excitation spectra for the level crossing can be related to the two different types of string order parameters.[21]

The phase diagrams obtained by this method are shown in Fig. 4. The extrapolation of the numerical data has been done assuming the function $\delta_c(N) = \delta_c(\infty) + A/N^2 + B/N^4$. The finite-size effect becomes larger for small-δ regions, but the extrapolated values [$(J_3/J_1)_c = 0.11$ for $S = 1$, $(J_3/J_1)_c = 0.062$ for $S = 3/2$] well agree with the ones obtained in Refs. 9 and 10. The global structure of the phase diagram Fig. 4(a) is similar to that for the $S = 1$ chain with a bilinear-biquadratic interaction. This is due to the fact that the three-spin interaction and the bilinear-biquadratic interaction will take almost the same form in the continuum limit.[22]

We calculate the conformal charge c along the critical line for the $S = 1$ system using the standard finite-size scaling of the ground state,

$$E_0(N) = \varepsilon_0 N - \frac{\pi v}{6N} c, \tag{31}$$

where the spin-wave velocity is calculated as

$$v = \lim_{N\to\infty} \frac{E(N, S = 1, k = 4\pi/N) - E_0(N)}{4\pi/N}. \tag{32}$$

As shown in Fig. 5, although the finite-size effect remains large, $c \to 1.5 = 3S/(S+1)$ around the multicritical point $\delta = 0$, whereas $c \to 1$ for $\delta \neq 0$ as was predicted by the field-theoretical arguments.

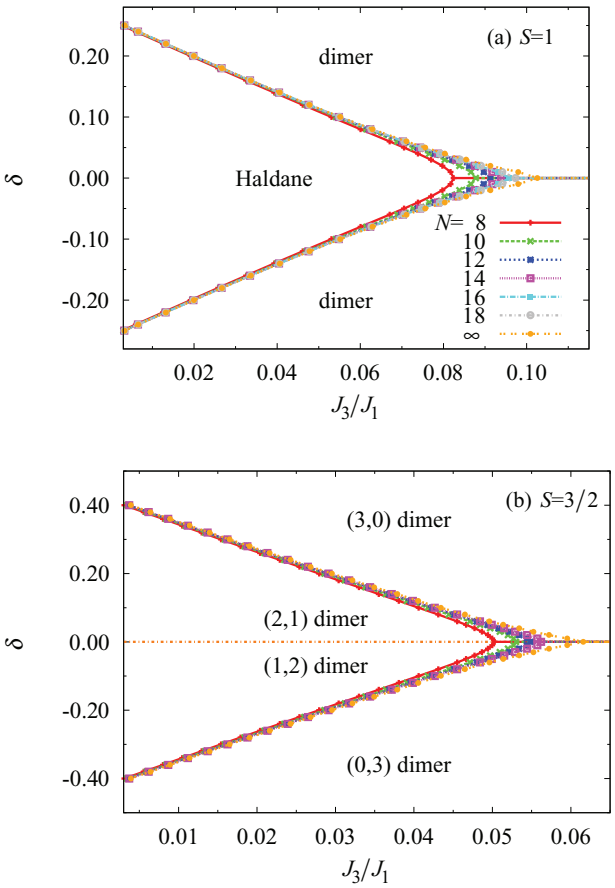

FIG. 4. (Color online) Ground-state phase diagram of the bond-alternating Heisenberg model with three-spin interactions [Eq. (1) with $J_2 = 0$] for (a) $S = 1$ and (b) $S = 3/2$. The multicritical points are located at $(J_3/J_1)_c = 0.11$ for $S = 1$ and at $(J_3/J_1)_c = 0.062$ for $S = 3/2$.

IV. SUMMARY

We have discussed the dimerizations of the spin-S AFH chains with three-spin interactions and bond alternations. We have rigorously proven that the AFH chains can possess exact dimerized ground states: Two local projection operators R_i and R_i' defined in Eqs. (A3) and (A4) are introduced and the Hamiltonians with exactly dimerized ground states are written as a linear combination of them. Then the exact ground states turn out to lie on the surface $\frac{J_3}{(1-\delta)J_1 - 2J_2} = \frac{1}{4S(S+1)-2}$. This argument is considered to be a generalization of the Majumdar-Ghosh model to arbitrary S. It is also possible to construct higher-dimensional versions of the present model, such as the Shastry-Sutherland model.

We have further discussed the ground-state phase diagram of the models whose Hamiltonian is defined by (1) by introducing several effective field theories. At the multicritical point the low-energy physics is described by the O(4) nonlinear σ model. However, on the phase transition lines except at the multicritical point, the low-energy physics is described by the O(3) nonlinear σ model. We have also obtained

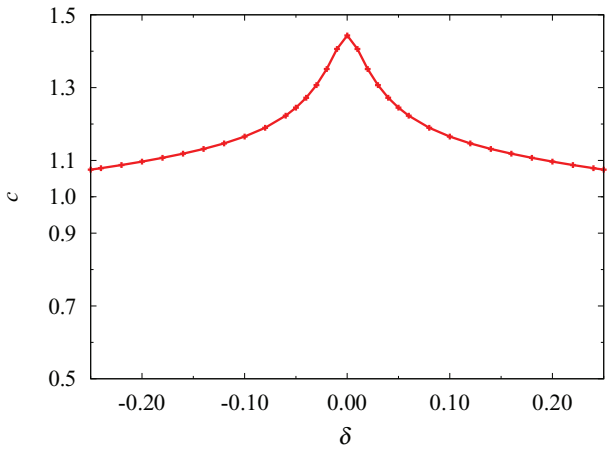

FIG. 5. (Color online) Conformal charge on the Haldane-dimer transition line in the $S = 1$ chain obtained from the size scaling of the ground state for $N = 8$–18. The value approaches $c = 1$ ($c = 3/2$) for $\delta \neq 0$ ($\delta = 0$).

the phase diagram for $S = 1$ and $S = 3/2$ chains by the level-spectroscopy method, and confirmed that the central charge on the critical lines changes rapidly from $3S/(S+1)$ to 1 when the bond alternation increases.

ACKNOWLEDGMENTS

The authors are grateful to Masaki Oshikawa for fruitful discussions. S.C.F. is supported by the Swiss National Foundation under MaNEP and Division II. M.N. acknowledges support from MEXT Grant-in-Aid No. 23540362.

APPENDIX: POSITIVITY OF R_i AND R_i'

We prove the positivity of the operators R_i and R_i' defined in Eqs. (A3) and (A4) for an arbitrary simultaneous eigenstate $|\psi\rangle$. Indeed, one can take such a state, because $[R_2, R_2'] = 0$. Thanks to the translational symmetry of the J_1-J_3 model, we may assume $i = 2$ without loss of generality. Since R_i and R_i' are involved with three neighboring spins $\boldsymbol{S}_{i-1}$, $\boldsymbol{S}_i$, and $\boldsymbol{S}_{i+1}$, one needs only a three-site subspace, in which an arbitrary state $|\psi\rangle$ can be written as

$$|\psi\rangle = \sum_{m_1,m_2,m_3} C_{m_1,m_2,m_3} |m_1,m_2,m_3\rangle , \tag{A1}$$

with

$$\sum_{m_1,m_2,m_3} \left|C_{m_1,m_2,m_3}\right|^2 = 1, \tag{A2}$$

where m_j ($j = 1,2,3$) is the S^z quantum number of each spin on site j and thus $|m_j| \leqslant S$.

After straightforward calculations,[12] one finds that the eigenvalues of the state $|\psi\rangle$ are non-negative,

$$\langle\psi| R_2 |\psi\rangle = \sum_{m_1,m_2,m_3} \left|\alpha C_{m_1,m_2,m_3} + \beta C_{m_1-1,m_2+1,m_3} + \gamma C_{m_1,m_2-1,m_3+1} + \theta C_{m_1-1,m_2,m_3+1}\right|^2, \tag{A3}$$

$$\langle\psi| R_2' |\psi\rangle = \sum_{m_1,m_2,m_3} \left|\alpha' C_{m_1,m_2,m_3} + \beta' C_{m_1-1,m_2+1,m_3} + \gamma' C_{m_1,m_2-1,m_3+1} + \theta' C_{m_1-1,m_2,m_3+1}\right|^2, \tag{A4}$$

where

$$\begin{aligned} \alpha &= \sqrt{(S+m_1)(S+m_2+1)(S-m_2+1)(S-m_3)}, \\ \beta &= \sqrt{(S-m_1+1)(S-m_2)(S-m_2+1)(S-m_3)}, \\ \gamma &= \sqrt{(S+m_1)(S+m_2)(S+m_2+1)(S+m_3+1)}, \\ \theta &= \sqrt{(S-m_1+1)(S-m_2+1)(S+m_2+1)(S+m_3+1)}, \end{aligned} \tag{A5}$$

and

$$\begin{aligned} \alpha' &= \sqrt{(S-m_1+1)(S-m_2)(S+m_2)(S+m_3+1)}, \\ \beta' &= \sqrt{(S+m_1)(S+m_2)(S+m_2+1)(S+m_3+1)}, \\ \gamma' &= \sqrt{(S-m_1+1)(S-m_2)(S-m_2+1)(S-m_3)}, \\ \theta' &= \sqrt{(S+m_1)(S-m_2)(S+m_2)(S-m_3)}. \end{aligned} \tag{A6}$$

When the pair 1,2 is a singlet state, one can find that

$$\begin{aligned} &\alpha C_{m_1,m_2,m_3} + \beta C_{m_1-1,m_2+1,m_3} \\ &\quad = \gamma C_{m_1,m_2-1,m_3+1} + \theta C_{m_1-1,m_2,m_3+1} \\ &\quad = \alpha' C_{m_1,m_2,m_3} + \beta' C_{m_1-1,m_2+1,m_3} \\ &\quad = \gamma' C_{m_1,m_2-1,m_3+1} + \theta' C_{m_1-1,m_2,m_3+1} = 0, \end{aligned} \tag{A7}$$

or when the pair 2,3 is a singlet state, we have

$$\begin{aligned} &\alpha C_{m_1,m_2,m_3} + \gamma C_{m_1,m_2-1,m_3+1} \\ &\quad = \beta C_{m_1-1,m_2+1,m_3} + \theta C_{m_1-1,m_2,m_3+1} \\ &\quad = \alpha' C_{m_1,m_2,m_3} + \gamma' C_{m_1,m_2-1,m_3+1} \\ &\quad = \beta' C_{m_1-1,m_2+1,m_3} + \theta' C_{m_1-1,m_2,m_3+1} = 0. \end{aligned} \tag{A8}$$

Therefore, R_i and R_i' are positive semidefinite and project out $|S(i-1,i)\rangle$ and $|S(i,i+1)\rangle$. It may also be possible to rewrite R_i and R_i' themselves into quadratic forms.

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