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Mass ratio of elementary excitations in frustrated antiferromagnetic chains with dimerization

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Excitation spectra of $S = 1/2$ and 1 frustrated Heisenberg antiferromagnetic chains with bond alternation (explicit dimerization) are studied using a combination of analytical and numerical methods. The system undergoes a dimerization transition at a critical bond alternation parameter $\delta = \delta_c$, where $\delta_c = 0$ for the $S = 1/2$ chain. The SU(2)-symmetric sine-Gordon theory is known to be an effective field theory of the system except at the transition point. The sine-Gordon theory has a SU(2)-triplet and a SU(2)-singlet of elementary excitation, and the mass ratio r of the singlet to the triplet is $\sqrt{3}$. However, our numerical calculation with the infinite time-evolving block decimation method shows that r depends on the frustration (next-nearest-neighbor coupling) and is generally different from $\sqrt{3}$. This can be understood as an effect of marginal perturbation to the sine-Gordon theory. In fact, at the critical frustration separating the second-order and first-order dimerization transitions, the marginal operator vanishes and $r = \sqrt{3}$ holds. We derive the mass ratio r analytically using form-factor perturbation theory combined with a renormalization-group analysis. Our formula agrees well with the numerical results, confirming the theoretical picture. The present theory also implies that, even in the presence of a marginally irrelevant operator, the mass ratio approaches $\sqrt{3}$ in the very vicinity of the second-order dimerization critical point $\delta \sim \delta_c$. However, such a region is extremely small and would be difficult to observe numerically.

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I. INTRODUCTION

Techniques of field theory have achieved growing success in interpreting physical properties in low dimensional magnets. The achievement stems from the close connection between one-dimensional quantum spin models and their effective theories. In particular, $S = 1/2$ Heisenberg antiferromagnetic (HAF) chains with various perturbations are important and also relevant for experimental studies of one-dimensional magnets. The bosonization scheme[1] is useful for analyzing these systems. A HAF chain with bond alternation, or under a staggered field, is described effectively by the sine-Gordon (SG) field theory. Elementary excitations in these systems are a soliton, an antisoliton, and breathers (bound states of the soliton and antisoliton). Materials such as Cu benzoate[2,3] and $\mathrm{KCuGaF_6}$ (Ref. 4) are described by HAF in a staggered field, and the soliton gap calculated from SG theory explains well the experimental results. For dimerized chains, the gap formula as a function of dimerization δ with logarithmic correction is obtained:[5] $\delta^{2/3}/|\log\delta|^{1/2}$, or it can also be represented as an effective power-law form with a renormalized exponent which deviates from 2/3.[6] Refined logarithmic correction is given in Ref. 7. Dimerized spin chains are an appropriate model for spin-Peierls materials such as $\mathrm{CuGeO_3}$ (Ref. 8) or Ni compounds.[9]

There are also a number of numerical studies on the frustrated HAF chain with next-nearest-neighbor coupling. We consider the Hamiltonian

$$\mathcal{H} = J\sum_j [\{1 + (-1)^j\delta\}\boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1} + \alpha\boldsymbol{S}_j \cdot \boldsymbol{S}_{j+2}], \tag{1}$$

where $J > 0$. The next-nearest-neighbor coupling $\alpha \geqslant 0$ introduces frustration.

This model exhibits a dimerization transition at $\delta = \delta_c$. For $S = 1/2$, the transition point is always $\delta_c = 0$, since the Lieb-Schultz-Mattis theorem implies either gapless excitations or twofold degeneracy of the ground states at $\delta = 0$. In fact, on the undimerized line $\delta = 0$, there exists a critical frustration parameter $\alpha_c \sim 0.2411$.[10,11] For $\alpha < \alpha_c$, the system is a gapless Tomonaga-Luttinger liquid (TLL); that is, the dimerization transition at $\delta = \delta_c = 0$ is of second order. In contrast, for $\alpha > \alpha_c$, the ground state is doubly degenerate, exhibiting a spontaneous dimerization. This implies a first-order dimerization transition at $\delta = \delta_c = 0$.

For $S = 1$, on the other hand, $\delta = 0$ (for a small α) belongs to the Haldane phase and does not represent a transition line. Instead, a dimerization transition between the Haldane phase and the dimerized phase occurs[12–15] at a finite δ_c, which depends on the frustration α. Although the shape of the phase diagram is thus different, the topology of the phase diagram is rather similar to that for $S = 1/2$. In fact, also for $S = 1$, there is a critical frustration α_c; the transition is second order with the critical point described by a TLL for $\alpha < \alpha_c$, and first order for $\alpha > \alpha_c$.

In the neighborhood of the gapless TLL line, the system acquires a small excitation gap, and would be described by the SG theory. Since our model (1) is SU(2)-invariant, the SG theory should also have SU(2)-symmetry. As a consequence, the mass ratio r of the second lowest breather to the soliton should be $\sqrt{3}$.

However, numerical results for $S = 1/2$ chains[16] show that r generally does not agree with the SG theory prediction $\sqrt{3}$. While r depends only weakly on δ, it does vary as a function of α. Only near the critical frustration $\alpha = \alpha_c$ does r agree with the SG prediction $\sqrt{3}$. In Ref. 16, it was pointed out that a marginal operator exists as a perturbation to the SG theory, and it would shift r from $\sqrt{3}$. However, how exactly the mass ratio r is affected by the marginal operator was not clarified.

The effect of the marginal perturbation to the SG theory on the mass ratio was discussed in terms of form-factor perturbation theory (FFPT) in Ref. 17. However, the theoretical prediction has not been tested. The mass ratio in the $S = 1$ case has also never been studied numerically.

In this paper, we study numerically the mass ratio of elementary excitations and the ground phase diagram of the frustrated HAF with bond alternation (1) for both $S=1/2$ and $S=1$. We employ the recently developed infinite time-evolving block decimation (iTEBD) method,[18] which allows high-precision calculation of infinitely long chains. The masses of elementary excitations are obtained from the asymptotic behavior of equal-time correlation functions instead of extrapolation of the finite-size energy spectrum. We confirm previous results when they are available, and we obtain the mass ratio for $S=1$ as a new result. Furthermore, we derive an explicit formula for the mass ratio r as a function of δ and α by combining FFPT and renormalization-group analysis. This agrees well with the numerical results for both $S=1/2$ and 1. Thus both cases are understood in terms of the unified framework of the SG theory with a marginal perturbation.

This paper is organized as follows. In Secs. II and III, respectively, we review direct bosonization of the $S=1/2$ chain and derivation of the SG theory for the general S case via the O(3) nonlinear sigma model (NLSM). In Secs. IV and V, we present numerical study on the mass ratio and phase diagram for $S=1/2$ and 1, respectively. We then discuss the mass ratio analytically based on FFPT and compare the theoretical formula with the numerical results in Sec. VI. Section VII is devoted to conclusions.

II. BOSONIZATION

We first review the bosonization of a spin-1/2 chain. Spin operators are represented as

$$S_j^z = \frac{a}{\pi}\partial_x\phi + a_1(-1)^j\cos(2\phi) + \cdots,$$
$$S_j^+ = e^{i\theta}[b_0(-1)^j + b_1\cos(2\phi) + \cdots],$$

where dual boson fields ϕ,θ satisfy the commutation relation $[\phi(x),\theta(x')] = -i\pi\vartheta(x-x')$ [$\vartheta(x-x')$ is the step function] with $x = ja$ (a is lattice spacing). ϕ and θ have periodicity $\phi\sim\phi+\pi$, $\theta\sim\theta+2\pi$. The effective Hamiltonian of the XXZ chain with dimerization is written with ϕ and θ as[1]

$$\mathcal{H}_{\text{eff}} = \frac{u}{2\pi}\int dx[K^{-1}(\partial_x\phi)^2 + K(\partial_x\theta)^2] + \frac{2g_1}{(2\pi a)^2}\int dx\cos(2\phi) + \frac{2g_2}{(2\pi a)^2}\int dx\cos(4\phi). \tag{2}$$

Irrelevant terms are omitted here. u and K denote spinon velocity and the Luttinger parameter, respectively. At the SU(2)-symmetric Heisenberg point, $u=\pi a/2$ and $K=1/2$. Since the operator $e^{iq\phi(x)}$ has scaling dimension $Kq^2/4$, the $\cos(2\phi)$ term is relevant while the $\cos(4\phi)$ term becomes marginal. The g_1 term arises from the bond alternation (i.e. dimerization). g_2 is known to decrease with increasing α and vanish at $\alpha=\alpha_{\text{c}}$ where the transition from TLL to the self-dimerized phase happens. Thus, coupling constants g_1 and g_2 are proportional to δ and $\alpha-\alpha_{\text{c}}$, respectively. When $g_1\neq 0$ and $g_2=0$, (2) is equivalent to the SG model. It is an exactly solved model, and the excitation spectrum is obtained.[19,20] There appear three types of elementary particles: a soliton, a corresponding antisoliton, and breathers. The number of breathers is $[2/K-1]$, where $[A]$ stands for the integer part of A. The mass of soliton M_{S} and the nth lightest breather M_{B_n} are related through the formula

$$M_{\text{B}_n} = 2M_{\text{S}}\sin\left(\frac{n\pi}{4/K-2}\right),\quad n=1,\ldots,[2/K-1]. \tag{3}$$

According to (3), in HAF chain with dimerization ($K=1/2$), the soliton, the antisoliton and the first breather form triplet while the second breather is a singlet which has $\sqrt{3}$ times as large mass as the triplet. Although the degeneracy of the triplet is protected thanks to SU(2)-symmetry, the mass ratio of singlet to triplet $r\equiv M_{\text{B}_2}/M_{\text{S}}$ is subject to correction caused by the marginal term g_2.

III. SG THEORY VIA THE NONLINEAR SIGMA MODEL

$S>1/2$ chains may be bosonized by introducing Hund coupling to $2S$ chains of spin-1/2. Each chain is bosonized separately, resulting in a theory of interacting $2S$ boson fields.[21] In the low-energy limit, however, one of the linear combinations of the boson fields becomes important. The SG theory (or TLL) would emerge as an effective theory of this linear combination.

However, it is rather cumbersome to pursue this explicitly. As an alternative, the SG theory can also be derived from the O(3) nonlinear sigma model (NLSM). The O(3) NLSM was derived in the semiclassical, large-S limit of the HAF chain. Nevertheless, it proved to be a useful effective theory even for $S=1$.

Let us define fields $\boldsymbol{n}(x)$ and $\boldsymbol{l}(x)$ by $\boldsymbol{S}_j/S\sim(-1)^j\boldsymbol{n}(x)+\boldsymbol{l}(x)$. Then the spin-$S$ HAF chain with bond alternation (1) can be generally mapped to the O(3) NLSM,

$$\mathcal{A}_\theta = \frac{1}{2g}\int d\tau\, dx\left\{v(\partial_x\boldsymbol{n})^2 + \frac{1}{v}(\partial_\tau\boldsymbol{n})^2\right\} + i\theta T,$$

where $g=2/S$ is some coupling constant and $v=2JS$ is the spin-wave velocity. $T=\frac{1}{4\pi}\int d\tau\, dx\,\boldsymbol{n}\cdot\partial_x\boldsymbol{n}\times\partial_\tau\boldsymbol{n}$ represents the integer-valued topological charge and $\theta=2\pi S(1+\delta)$. For the moment, let us assume that there is no frustration, $\alpha=0$.

O(3) NLSM is known to be integrable[22,23] at $\theta=0$ and π. At $\theta\equiv 0 \mod 2\pi$, the excitation consists of a triplet of massive particles. In contrast, the theory is massless at $\theta\equiv\pi \mod 2\pi$ and the infrared fixed point is a SU(2)$_1$ Wess-Zumino-Witten model, a conformal field theory (CFT) with central charge $c=1$. This is merely the TLL at the SU(2)-symmetric point $K=1/2$.

When bond alternation is absent ($\delta=0$), the system is massless ($\theta=\pi$) if S is a half-odd-integer, while it is massive ($\theta=0$) if S is an integer. This is the celebrated Haldane conjecture,[24] which is now established by intensive analytical, numerical, and experimental studies.

It is also interesting to consider the effect of bond alternation δ. By changing δ from -1 to 1, namely from the completely dimerized limit to the opposite completely dimerized limit, θ passes the critical point, $\pi \mod 2\pi$, $2S$ times. Thus, on $-1<\delta<1$, there are $2S$ successive phase transitions.[14] This could be understood as successive spontaneous breaking and restoration of hidden symmetry,[25] or more generally, symmetry-protected topological phase transitions.[26,27]

For $S = 1/2$, the transition occurs only at $\delta = 0$, consistent with the direct bosonization analysis. For $S = 1$, there are two transitions which separate the Haldane phase around $\delta = 0$ from the dimerized phases. The critical points are, according to the above argument, given by $\delta = \pm\delta_c = \pm 1/2$. However, in reality, the location of the critical points is renormalized. It was shown[15] numerically that $\delta_c \sim 0.25J$.

As discussed above, the critical point is described by the SU(2)-symmetric TLL with $K = 1/2$. By considering the possible perturbations to the TLL, the effective theory near the critical point $\delta = \delta_c$ is determined[17] to be the SG theory with marginal perturbation (2), which was derived previously for $S = 1/2$ by direct bosonization. Thus, the same theory (2) should describe the neighborhood of dimerization transitions for any S. In the following, we shall investigate the systems with $S = 1/2$ and 1 numerically and verify this universality.

IV. MASS RATIO AND PHASE DIAGRAM FOR $S = 1/2$

We study the excitation spectrum of the system numerically, and we focus in particular on the change of r due to the marginal term. We adopt a new strategy to extract the excitation spectrum from the equal-time correlation function obtained by iTEBD, shown as follows.

A single-particle excitation in the SG model can be parametrized by the rapidity θ, which defines its energy and wave number as $M_0 \cosh\theta$ and $(M_0/u)\sinh\theta$, respectively (M_0 is the mass of the particle). The one-particle form factor of operator O is specified by θ and the kind of particle a as $F_O(\theta,a) \equiv \langle 0|O|\theta,a\rangle$. O represents an operator which creates the single soliton, the antisoliton, or the breather. We can calculate the equal-time correlation function $\langle O(r)O(0)\rangle - \langle O(r)\rangle\langle O(0)\rangle$ by inserting the resolution of the identity $\hat{1} = \sum_{n=0}^{\infty} P_n$, where P_n is the projection operator defined as $P_0 = |0\rangle\langle 0|$ and $P_n = \frac{1}{n!}\sum_{a_1,\ldots,a_n}\int \frac{\prod_j d\theta_j}{(4\pi)^n}|\theta_1,a_1;\ldots;\theta_n,a_n\rangle\langle\theta_1,a_1;\ldots;\theta_n,a_n|$ $(n \geqslant 1)$. Then, the leading order of the correlation function[28] is

$$\langle O(r)O(0)\rangle - \langle O(r)\rangle\langle O(0)\rangle \approx \int \frac{d\theta}{4\pi} e^{iM_0 r \sinh\theta/u}|F_O(\theta,a)|^2.$$

In the limit of $l \to \infty$, it is calculated to be[29]

$$\langle O(l)O(0)\rangle - \langle O(l)\rangle\langle O(0)\rangle = [A(-1)^l + B]\frac{e^{-l/\xi}}{\sqrt{l}} \qquad (4)$$

consisting of a staggered and uniform part. We suppose that the effect of the marginal $\cos(4\phi)$ term is renormalized into mass M_0 and constants A,B.

In this way, the mass can be extracted from the correlation function, which we calculate with the iTEBD method. The truncation dimension, the number of conserved states in evolution, is fixed to be 200, large enough for the iTEBD calculation in gapped systems. $\langle S_0^x S_l^x\rangle$, $\langle S_0^y S_l^y\rangle$, $\langle S_0^z S_l^z\rangle$, and $\langle(\boldsymbol{S}_0\cdot\boldsymbol{S}_1)(\boldsymbol{S}_l\cdot\boldsymbol{S}_{l+1})\rangle$ are fitted with $Ce^{-l/\xi}/\sqrt{l}$ for sufficiently large and even l. $C(=A+B)$ and ξ are fitting parameters. Then we can obtain the mass of the soliton, the antisoliton, and the first and second breathers, respectively, through the relation $M = u/\xi$. Note that M is a renormalized mass. While the value u for $\alpha = 0$ is obtained exactly from the Bethe ansatz, it cannot be for $\alpha \neq 0$. Yet the value of u is not needed to calculate a mass ratio.

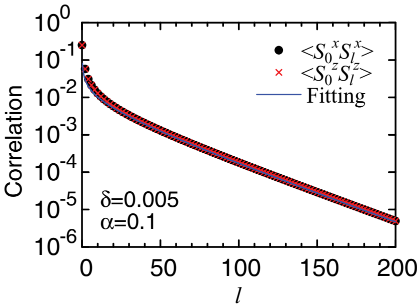

FIG. 1. (Color online) Correlation functions $\langle S_0^x S_l^x\rangle$ and $\langle S_0^z S_l^z\rangle$ calculated with the iTEBD method. The solid line represents the fitting with the function $Ce^{-l/\xi}/\sqrt{l}$.

Since $S_{\text{tot}}^z \equiv \sum_j S_j^z$ commutes with the Hamiltonian, S_{tot}^z is a good quantum number. The ground state is in $S_{\text{tot}}^z = 0$ Hilbert space, and the soliton (antisoliton) is an excitation to the lowest energy level in $S_{\text{tot}}^z = 1(-1)$ Hilbert space. Hence, their mass corresponds to the inverse correlation length of the operator changing S_{tot}^z by ± 1,[30] i.e., $\langle S_0^x S_l^x\rangle = \langle S_0^y S_l^y\rangle$. On the other hand, the first breather is the lowest excitation in $S_{\text{tot}}^z = 0$ Hilbert space; it corresponds to $\langle S_0^z S_l^z\rangle$. In the case of the antiferromagnetic XXZ model, the mass of the soliton/antisoliton and the first breather is different. For a Heisenberg chain, however, SU(2)-symmetry requires $\langle S_0^x S_l^x\rangle = \langle S_0^y S_l^y\rangle = \langle S_0^z S_l^z\rangle$, which indicates that the mass of the soliton, the antisoliton, and the first breather is all the same, and these three particles constitute a triplet. The second breather has to be a singlet, and the operator corresponding to it does not change S_{tot}^z. The most relevant operator with such properties is $\boldsymbol{S}_j\cdot\boldsymbol{S}_{j+1}$, and we expect that the second breather corresponds to $\langle(\boldsymbol{S}_0\cdot\boldsymbol{S}_1)(\boldsymbol{S}_l\cdot\boldsymbol{S}_{l+1})\rangle$.

An example of fitting for correlation functions is shown in Fig. 1. $\langle S_0^x S_l^x\rangle$ and $\langle S_0^z S_l^z\rangle$ calculated with the iTEBD method are equal up to eight digits, which is consistent with the SU(2)-symmetry. The solid line represents the fitting with the function $Ce^{-l/\xi}/\sqrt{l}$. The correlation functions are well fitted with the function.

We show numerically the calculated mass ratio r as a function of α and δ in Fig. 2(a). r is larger than 2 for $\alpha = 0$ (nonfrustrated HAF chain with bond alternation) and decreases with increasing α. r becomes $\sqrt{3}$ at $\alpha \sim 0.25$. It is very close to $\alpha = 0.2411$, where the transition from TLL to the self-dimerized phase happens without bond alternation, and the marginal $\cos(4\phi)$ term vanishes.[11] This result indicates that the deviation of r from $\sqrt{3}$ is attributed to the effect of the marginal term. While r is subject to correction as α moves away from this point, its δ dependence is quite small.

A similar result was obtained through a gap evaluation by exact diagonalization.[16] However, the mechanism of the variation of r has not been made clear. We will theoretically analyze the dependence of r on the frustration α later in Sec. VI. The α-δ phase diagram is shown in Fig. 2(b). Note that the universality class of the transition from positive to negative δ is of $c = 1$ CFT for $\alpha < 0.25$ and of first order for $\alpha > 0.25$.[31]

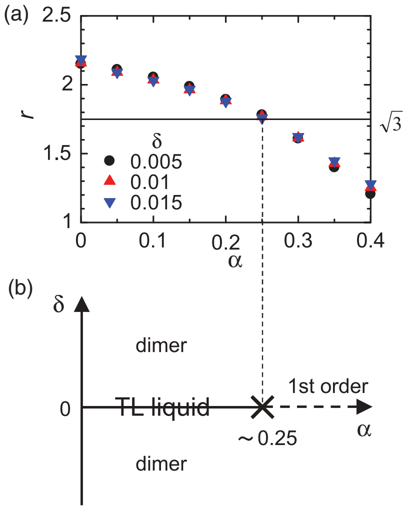

FIG. 2. (Color online) (a) Triplet-singlet mass ratio r as a function of α and δ in the $S = 1/2$ bond-alternating chain with frustration. (b) Phase diagram of the $S = 1/2$ bond-alternating chain with frustration. Solid and dashed lines represent second order (TLL, $c = 1$ CFT) and first order transition, respectively. Universality class of transition changes at $\alpha \sim 0.25$, where r becomes $\sqrt{3}$.

V. MASS RATIO AND PHASE DIAGRAM FOR $S = 1$

Next, we numerically investigate the excitation spectrum and the phase diagram of the $S = 1$ HAF chain with dimerization and frustration. The method for evaluating particle mass is the same as for the $S = 1/2$ chain. As can be seen in Fig. 3, when α is small enough, r is always larger than 2, at least in $|\delta - \delta_c| \geqslant 0.005$ [δ_c can be determined from the divergence of ξ or the jump of $|\langle(-1)^j \boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1}\rangle|$ as explained in the following part; see Fig. 4], and does not depend much on δ. Since particles heavier than $2M_{\mathrm{S}}$ become resonance, the second breather cannot be a stable particle even in the vicinity of δ_c. The above result again seems inconsistent with the prediction in Ref. 17.

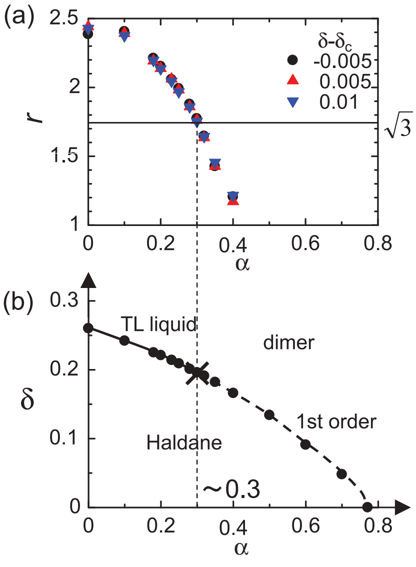

FIG. 3. (Color online) (a) Triplet-singlet mass ratio r as a function of α and δ in the $S = 1$ bond-alternating chain with frustration. The transition point δ_c corresponds to circles in (b). (b) Phase diagram of the $S = 1$ bond-alternating chain with frustration. The solid and dashed lines, which represent the second-order (TLL, $c = 1$ CFT) and first-order transition, respectively, are guides for the eye. The circles show transition points determined from Fig. 4. The universality class of the transition changes approximately at $\alpha = 0.3$, where r becomes $\sqrt{3}$.

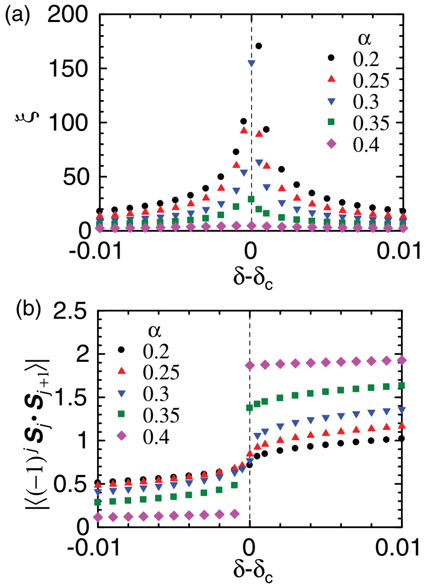

FIG. 4. (Color online) (a) Correlation length ξ as a function of $\delta - \delta_c$ and α. ξ diverges when the transition is second order. (b) Dimerization order parameter $|\langle(-1)^j \boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1}\rangle|$ as a function of $\delta - \delta_c$ and α. $|\langle(-1)^j \boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1}\rangle|$ jumps when the transition is first order. Therefore, δ_c can be determined from the divergence of ξ or the jump of $|\langle(-1)^j \boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1}\rangle|$.

The deviation of r from $\sqrt{3}$ would be attributed to the existence of the marginal term as in the spin-1/2 chain. We introduce the next-nearest-neighbor coupling α in order to confirm it. As shown in Fig. 3(a), r decreases with increasing α and becomes $\sqrt{3}$ around $\alpha = 0.3$. The transition point δ_c from the Haldane phase to the dimerized phase also decreases, which is natural because next-nearest-neighbor coupling favors the dimerized phase. Figure 4 shows the behavior of correlation length ξ and dimerization order parameter $|\langle(-1)^j \boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1}\rangle|$ near δ_c. ξ diverges at δ_c for $\alpha \lesssim 0.3$, which is not the case for $\alpha > 0.3$. In addition, $|\langle(-1)^j \boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1}\rangle|$ jumps at δ_c for $\alpha > 0.3$ while the variation is continuous for $\alpha \lesssim 0.3$. These results indicate that the universality class of transition at δ_c changes from $c = 1$ CFT to first order when α goes beyond 0.3. From the viewpoint of field theory, the $\cos(4\phi)$ term changes from a marginally irrelevant to a marginally relevant operator at this point. The situation is very analogous to the spin-1/2 case. The α-δ phase diagram is summarized in Fig. 4(b). It is consistent with Ref. 13. The transitions along the lines $\delta = 0$ and $\alpha = 0$ are studied in Refs. 12 and 15, respectively.

VI. MASS RATIO FROM THE FORM-FACTOR PERTURBATION THEORY

Now let us discuss the variation of the mass ratio r theoretically. In Ref. 17, the δ dependence of r was discussed as follows. The excitation structure at the very vicinity of $\delta = \delta_c$ would be described by the pure SG theory without the marginal perturbation; r is then equal to $\sqrt{3}$. On the other hand, O(3) NLSM with $\theta = 0$ also has triplet lowest excitation, which is smoothly connected to the triplet in the SG model thanks to SU(2)-symmetry, but does not have the second breather. Therefore, r increases as δ decreases from δ_c to 0, and it exceeds 2 at some point. This argument was further augmented by a FFPT calculation in terms of the marginal perturbation.

However, their predictions[17] do not seem to be consistent with numerical results. In the absence of frustration α, r is substantially larger than $\sqrt{3}$ even when δ is closest to δ_c within the precision of the numerical calculations. This already contradicts the picture presented in Ref. 17. Moreover, the effect of the frustration α was not discussed.

Here, we will improve the FFPT by supplementing it with a RG analysis. Let us define a dimensionless coupling constant $y_2 \equiv g_2/(\pi u)$. With the FFPT of the marginal operator in the SG theory, mass corrections arising from the marginal term y_2 to the triplet and the singlet, which we denote, respectively, as ΔM_t and ΔM_s, were found[17] to be

$$\begin{aligned} \Delta M_t &= 4\sqrt{3} y_2, \\ \Delta M_s &= 12\sqrt{3} y_2. \end{aligned} \tag{5}$$

Here, we argue that the renormalized coupling constant should be used for y_2. In the following, we derive the renormalized form of y_2. Since the system has SU(2)-symmetry, y_2 is renormalized according to the Kosterlitz-Thouless renormalization equation,[5,32]

$$\frac{dy_2}{ds} = y_2^2. \tag{6}$$

The solution of (6) is $y_2 = -1/(s + \text{const})$. y_2 becomes a function of energy scale by the parametrization $s = \ln(E/\Lambda)$ (Λ is the infrared cutoff) as follows:

$$y_2(E) = \frac{1}{\ln(\Lambda'/E)}.$$

Constant Λ' can be fixed from the condition that bare y_2 corresponds to the original spin chain, where the energy scale is of order of J, i.e., $y_2(E \sim J) = C_1(\alpha_c - \alpha)$, where C_1 is a nonuniversal positive constant. Therefore, the renormalized form of y_2 is

$$y_2(E) = \frac{1}{\ln(J/E) + \frac{1}{C_1(\alpha_c - \alpha)}}.$$

When the system is renormalized until the energy scale is equal to the soliton mass, y_2 becomes $y_2(M_S)$. From Eq. (5), the mass ratio r is

$$r = \frac{\sqrt{3} + \frac{12\sqrt{3}}{\ln(J/M_S) + 1/(C_1[\alpha_c - \alpha])}}{1 + \frac{4\sqrt{3}}{\ln(J/M_S) + 1/[C_1(\alpha_c - \alpha)]}}. \tag{7}$$

A fitting of the numerical results with the function (7) is shown in Fig. 5. The only fitting parameter is the nonuniversal constant C_1. For the $S = 1/2$ chain, we use an excitation gap with $\alpha = 0$ as the value of M_S since the value of M_S can be estimated through $M = u/\xi$, where $u = \pi J a/2$. The solid, dashed, and dashed-dotted lines in Fig. 5(a) are Eq. (7) with $C_1 = 0.3$ for $\delta = 0.005$, 0.01, and 0.015, respectively. The variation of Eq. (7) by changing δ is quite small since the only δ-dependent variable is M_S and it is present only inside a logarithm. It is difficult to estimate M_S with good precision for $S = 1$ because the value of u is not known. However, as we have discussed, the M_S dependence is rather weak in Eq. (7). Thus, in a practical range to compare with the numerical results, we can set $M_S/J = 0.1$. Equation (7) with $C_1 = 0.6$ is shown as a solid line in Fig. 5(b). The fitting curves agree well with numerical data for both $S = 1/2$ and 1 in the vicinity of $\alpha = \alpha_c$, where the marginal perturbation is small. The deviation away from the theory (7) can be attributed to higher-order correction in both FFPT and the renormalization equation.

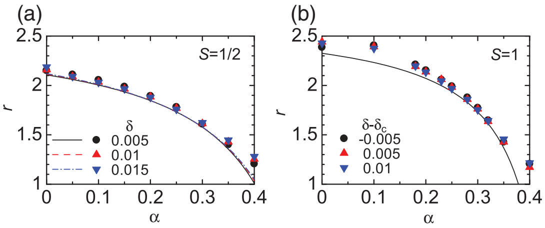

FIG. 5. (Color online) Triplet-singlet mass ratio r as a function of δ and α. (a) The case of $S = 1/2$. The circle, triangle, and down-pointing triangle represent numerically obtained r for $\delta = 0.005$, 0.01, and 0.015, respectively. The solid, dashed, and dashed-dotted lines are Eq. (7) with $C_1 = 0.3$. M_S is a function of δ and α, and M_S for $\alpha = 0$ is used here. (b) The case of $S = 1$. The circle, triangle, and down-pointing triangle represent numerically obtained r for $\delta - \delta_c = -0.005$, 0.005, and 0.01, respectively. δ_c is determined from Fig. 4. The solid line is Eq. (7) with $M_S = 0.1J$ and $C_1 = 0.6$.

Let us come back to the argument in Ref. 17. As we have seen, their idea that r evolves from $\sqrt{3}$ as θ is changed from π mod 2π does not seem to agree with the numerical results. On the other hand, however, where the dimerization transition is second order ($\alpha < \alpha_c$), the marginal operator is marginally irrelevant. Thus, in the limit $\theta \to \pi \mod 2\pi$ ($\delta \to \delta_c$ in our spin-chain model), the SG theory without the marginal operator becomes exact, and $r = \sqrt{3}$ should follow. In this sense, their idea is still qualitatively correct. However, the marginally irrelevant operator is renormalized to zero very slowly (logarithmically), and thus the mass scale must be exponentially small in order to probe this regime. This can indeed be seen in the logarithmic dependence of r on the soliton mass M_S in Eq. (7). Thus, for $\alpha < \alpha_c$, the mass ratio deviates very quickly from $r = \sqrt{3}$ as δ is shifted from the critical point δ_c. As a consequence, it would be impractical to observe this behavior numerically.

VII. CONCLUSION

We have investigated the excitation spectrum of $S = 1/2$ and 1 frustrated HAF chains with dimerization δ. To evaluate particle mass $M = u/\xi$, we calculate the corresponding correlation function numerically and extract the correlation length by using a fitting function $Ce^{-l\xi}/\sqrt{l}$ for a range of large enough and even l. The ratio r of the singlet (the second breather) to the triplet (soliton, antisoliton, and the first breather) is expected to be $\sqrt{3}$ from bosonized SG effective field theory, but r is subject to correction from a marginal term. $r = \sqrt{3}$ is recovered at the critical next-nearest-neighbor coupling $\alpha = \alpha_c$, for which the marginal term vanishes. At $\alpha = \alpha_c$, the dimerization transition with varying δ changes from second order, with the critical behavior described by $c = 1$ CFT, to first order. We give δ and α dependences of r in Eq. (7) through FFPT and RG analysis. r obtained by the iTEBD method is well fitted by Eq. (7). Our analysis indicates that, for $\alpha < \alpha_c$, the mass ratio r asymptotically approaches $\sqrt{3}$ when $\delta \to \delta_c$, consistent with the argument in Ref. 17. However, this asymptotic behavior occurs only for exponentially small $|\delta - \delta_c|$, and could not be observed in numerical studies in the literature and in the present work.

Finally, we comment on the general-S case. When the dimerization δ is changed from 1 to -1, the phase transition happens once for the $S = 1/2$ case (from one dimerized to the other dimerized phase), and twice for the $S = 1$ case (from one dimerized to the Haldane phase and from the Haldane to the other dimerized phase). In the general-S case, there are $2S$ transitions from one fully dimerized to the other fully dimerized phase, and they are the transitions between the partially dimerized phases. Around those transition points, the system is represented by the same effective field theory as explained in this paper.

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