Mass ratio of elementary excitations in frustrated antiferromagnetic chains with dimerization

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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 magnets. The achievement stems from the close connection between one-dimensional quantum spin models and magnets. The bosonization scheme is useful for analyzing such systems. A HAF chain with bond alternation, or under a staggered field, is described effectively by the sine-Gordon field theory. Elementary excitations in these systems are a soliton, an antisoliton, and breathers (bound states of a soliton and antisoliton). Materials such as Cu benzoate and KCuGaF₄ are described by HAF in a staggered field, and the soliton gap calculated from SG theory explains well the experimental 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

Excitation spectra of \( S = 1/2 \) and \( S = 1 \) 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.

\[ \mathcal{H} = J \sum_j \left[ (1 + (-1)^j \delta) S_j \cdot S_{j+1} + \alpha S_j \cdot S_{j+2} \right], \]

where \( J > 0 \). The next-nearest-neighbor coupling \( \alpha \geq 0 \) 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 two-fold degeneracy of the ground states at \( \delta = 0 \). 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 \( \alpha \)) 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 at \( \delta_c \) at a finite \( \delta_c \), which depends on the frustration \( \alpha \). 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 \( \alpha_c \); 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 \( \mathcal{H} \) 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 \( \mathcal{H} \) show that \( r \) generally does not agree with the SG theory prediction \( \sqrt{3} \). While \( r \) depends only weakly on \( \delta \), it does...
vary as a function of $\alpha$. Only near the critical frustration $\alpha = \alpha_c$ does $r$ agree with the SG prediction $\sqrt{3}$. In Ref. 14, 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 for both $S = 1/2$ and $S = 1$. We employ the recently developed infinite time-evolving block decimation (iTEBD) method 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 as a function of $\delta$ and $\alpha$, by combining FFPT and renormalization-group analysis. This agrees well with the numerical results for both $S = 1/2$ and $S = 1$. 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, we review direct bosonization of the $S = 1/2$ chain and derivation of the SG theory for 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, respectively for $S = 1/2$ and $S = 1$. We then discuss the mass ratio analytically based on FFPT and compare the theoretical formula with the numerical results in Sec. VI. Sec. VII is devoted to conclusions.

II. BOSONIZATION

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

$$S_j^z = \frac{a}{\pi} \partial_x \phi + a_1 (-1)^j \cos(2\phi) + \cdots$$

$$S_j^x = e^{i\theta} \left[ b_0 (-1)^j + b_1 \cos(2\phi) + \cdots \right],$$

where dual boson fields $\phi, \theta$ satisfy the commutation relation $[\phi(x), \theta(x')] = -i\pi \delta(x-x')$ ($\delta(x-x')$ is the step function) with $x = j a$ ($a$ is lattice spacing). $\phi$ and $\theta$ have periodicity $\phi \sim \phi + \pi, \theta \sim \theta + 2\pi$. Effective Hamiltonian of XXZ chain with dimerization is written with $\phi$ and $\theta$

as

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

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 $e^{i\phi(x)}$ 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 $\alpha$ and vanish at $\alpha = \alpha_c$ where the transition from TLL to the self-dimerized phase happens. Thus, coupling constants $g_1$ and $g_2$ are proportional to $\delta$ and $\alpha - \alpha_c$, respectively. When $g_1 \neq 0$ and $g_2 = 0$, (4) is equivalent to the SG model. It is an exactly solved model, and the excitation spectrum is obtained. 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 $n$-th lightest breather $M_{B_n}$ are related through the formula

$$M_{B_n} = 2M_S \sin \left( \frac{n\pi}{4/K - 2} \right), \quad n = 1, \cdots, [2/K - 1].$$

According to (4), 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 $r = M_{B_2}/M_S$ is subject to correction caused by the marginal term $g_2$.

III. SG THEORY VIA 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 $\phi$. 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 $O(3)$ non-linear sigma model (NLSM). The $O(3)$ NLSM was derived in the semi-classical, large-$S$ limit of the HAF chain. Nevertheless, it proved to be a useful effective theory even for $S = 1$.

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

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

where \( g = 2/S \) is some coupling constant and \( v = 2JS \) is the spin-wave velocity. \( T = \frac{1}{2\pi} \int d\tau dx \cdot \partial_x n \times \partial_n n \) 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 at \( \theta = 0 \) and \( \pi \). 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)-symmetric TLL, the effective theory \( (\text{CFT}) \) 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 which is now established by intensive analytical, numerical, and experimental studies.

It is also interesting to consider the effect of bond alternation \( \delta \). By changing \( \delta \) from 1 to 0, namely from the completely dimerized limit to the opposite completely dimerized limit, \( \theta \) passes the critical point, \( \pi \mod 2\pi \), \( 2S \) times. Thus, on \( -1 < \delta < 1 \), there are \( 2S \) successive phase transitions. This could be understood as successive spontaneous breaking and restoration of hidden symmetry or more generally, symmetry-protected topological phase transitions.

For \( S = 1/2 \), the transition occurs only at \( \delta = 0 \), consistently 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 numerically that \( \delta_c \approx 0.25J \).

As discussed above, the critical point is described by the SU(2)-symmetric TLL with \( K = 1/2 \). By considering some perturbations to the TLL, the effective theory near the critical point \( \delta = \delta_c \) is determined to be the SG theory with marginal perturbation \( (3) \), which was derived previously for \( S = 1/2 \) by direct bosonization. Thus, the same theory \( (3) \) should describe the neighborhood of dimerization transitions for any \( S \). In the following, we shall investigate the systems with \( S = 1/2 \) and \( S = 1 \) 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 parameterized by the rapidity \( \theta \), which defines its energy and wave number as \( M_0 \cosh \theta \) and \( (M_0/\alpha) \sinh \theta \), respectively. \( M_0 \) is the mass of the particle. The one-particle form factor of operator \( O \) is specified by \( \theta \) and the kind of particle \( a = F_0(\theta, a) = \langle 0|O(\theta, a) \rangle \). \( O \) 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 \( I = \sum_{n=0}^{\infty} P_n \) where \( P_n \) is the projection operator defined as \( P_0 = |0\rangle\langle 0| \) and \( P_n = \frac{1}{\pi} \int \frac{d\theta}{(2\pi)^n} \langle \theta_1, a_1; \cdots; \theta_n, a_n | \theta_1, a_1; \cdots; \theta_n, a_n \rangle \) \( (n \geq 1) \). Then, the leading order of the correlation function \( (4) \) is

\[
\langle O(r)O(0) \rangle - \langle O(r) \rangle \langle O(0) \rangle \approx \frac{1}{4\pi} \int \frac{d\theta}{e^{imqr \sinh \theta / u} |F_0(\theta, a)|^2}.
\]

In the limit of \( l \to \infty \), it is calculated to be

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

consisting of a staggered and uniform part. We suppose that the effect of the marginal \( \cos(4\theta) \) 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. \( \langle S_0^\alpha S_0^\beta \rangle, \langle S_0^\alpha S_0^\beta \rangle, \langle S_0^\alpha S_0^\beta \rangle \) and \( \langle (S_0\cdot S_1)(S_1\cdot S_{i+1}) \rangle \) are fitted with \( Ce^{-l/\xi} / \sqrt{l} \) for sufficiently large and even \( l \). \( C(= A + B) \) and \( \xi \) 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.

Since $S_{\text{tot}}^z = \sum_j S_j^z$ commutes with the Hamiltonian, $S_{\text{tot}}^z$ 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 $S_{\text{tot}}^z$ by $\pm 1$, i.e. $\langle S_0^z S_l^z \rangle = \langle S_0^z S_l^z \rangle$. 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 $\langle S_0^z S_l^z \rangle = \langle S_0^z S_l^z \rangle = \langle S_0^z S_l^z \rangle$, 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 $S_{\text{tot}}^z$. The most relevant operator with such properties is $S_j^z S_{j+1}^z$, and we expect that the second breather corresponds to $\langle (S_0^z S_1^z)(S_l^z S_{l+1}^z) \rangle$.

An example of fitting for correlation functions is shown in Fig. 3(a) and 3(b). The solid lines represent the fitting with the function $C e^{-1/\xi}/\sqrt{\xi}$. The correlation functions are well fitted with the function.

We show numerically the calculated mass ratio $r$ as a function of $\alpha$ and $\delta$ in Fig. 3(a). $r$ is larger than 2 for $\alpha = 0$ (nonfrustrated HAF chain with bond alternation) and decreases with increasing $\alpha$. $r$ 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. 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 $\alpha$ moves away from this point, its $\delta$ dependence is quite small.

A similar result was obtained through a gap evaluation by exact diagonalization. However, the mechanism of the variation of $r$ has not been made clear. We will theoretically analyze the dependence of $r$ on the frustration $\alpha$ later in Sec. VI. The $\alpha-\delta$ phase diagram is shown in Fig. 3(b). Note that the universality class of the transition from positive to negative $\delta$ is of $c = 1$ CFT for $\alpha < 0.25$ and of first order for $\alpha > 0.25$. In the case of $\delta = 0$ and $\alpha > 0.25$, the transition becomes discontinuous.

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(b), when $\alpha$ is small enough, $r$ is always larger than 2 at least in $|\delta - \delta_c| \geq 0.005$ ($\delta_c$ can...
Fig. 4 shows the behavior of correlation length \( \xi \) as a function of \( \delta - \delta_c \) and \( \alpha \). \( \xi \) diverges when the transition is second order. (b) Dimerization order parameter \( |\langle (-1)^j S_j \cdot S_{j+1} \rangle| \) as a function of \( \delta - \delta_c \) and \( \alpha \). \( |\langle (-1)^j S_j \cdot S_{j+1} \rangle| \) jumps when the transition is first order. Therefore, \( \delta_c \) can be determined from the divergence of \( \xi \) or the jump of \( |\langle (-1)^j S_j \cdot S_{j+1} \rangle| \).

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 \( \delta \) 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 \( \delta \) decreases from \( \delta_c \) 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 do not seem to be consistent with numerical results. In the absence of frustration \( \alpha, r \) is substantially larger than \( \sqrt{3} \) even when \( \delta \) is closest to \( \delta_c \) within the precision of the numerical calculations. This already contradicts the picture presented in Ref. [17]. Moreover, the effect of the frustration \( \alpha \) 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 \( \Delta M_t \) and \( \Delta M_s \), were found to be

\[
\Delta M_t = 4\sqrt{3} y_2, \\
\Delta M_s = 12\sqrt{3} y_2.
\]

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 [23]

\[
\frac{dy_2}{ds} = y_2^2.
\]

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

\[
y_2(E) = \frac{1}{\ln(N/E)}.
\]

Constant \( N \) 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 non-universal 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

be determined from the divergence of \( \xi \) or the jump of \( |\langle (-1)^j S_j \cdot S_{j+1} \rangle| \) as explained in the following part. See Fig. 4, and does not depend much on \( \delta \). Since particles heavier than \( 2M_S \) become resonance, the second breather cannot be a stable particle even in the vicinity of \( \delta_c \). The above result again seems inconsistent with the prediction in Ref. [17].

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 \( \alpha \) in order to confirm it. As shown in Fig. 3(a), \( r \) decreases with increasing \( \alpha \) and becomes \( \sqrt{3} \) around \( \alpha = 0.3 \). The transition point \( \delta_c \) from the Haldane phase to the dimerized phase also decreases, which is natural because next-nearest-neighbor coupling favors the dimerized phase.

Fig. 3 shows the behavior of correlation length \( \xi \) and dimerization order parameter \( |\langle (-1)^j S_j \cdot S_{j+1} \rangle| \) near \( \delta_c \). \( \xi \) diverges at \( \delta_c \) for \( \alpha \lesssim 0.3 \), which is not the case for \( \alpha > 0.3 \). In addition, \( |\langle (-1)^j S_j \cdot S_{j+1} \rangle| \) jumps at \( \delta_c \) for \( \alpha > 0.3 \) while the variation is continuous for \( \alpha \lesssim 0.3 \). These results indicate that the universality class of transition at \( \delta_c \), changes from c = 1 CFT to first order when \( \alpha \) 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 \( \alpha-\delta \) 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 [13], respectively.
and it is present only inside a logarithm. It is difficult to \( \delta \)
respectively. The variation of Eq. (7) by changing \( \alpha \) we can set
shown as a solid line in Fig. 5 (b). The fitting curves agree
the renormalization equation.

A fitting of the numerical results with the function (7)
is quite small since the only \( \delta \) is present inside a logarithm. It is difficult to
value of \( M \) for \( \delta \) is not known. However, as we have discussed,
the marginal term vanishes. At \( \alpha = \alpha_c \), the dimerization transition with varying \( \delta \)
changes from second order, with the critical behavior described by \( e = 1 \) CFT, to first order. We give \( \delta \) and \( \alpha \) 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 \( \delta \to \delta_c \), consistently 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 \( \delta \) 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 2\( S \) 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.

VII. CONCLUSION

We have investigated the excitation spectrum of \( S = 1/2 \) and 1 frustrated HAF chains with dimerization \( \delta \). To evaluate particle mass \( M = u/\xi \), we calculate the corresponding correlation function numerically and extract the correlation length by using a fitting function \( C e^{-l/\sqrt{1}} \) 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.

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