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Elementary excitations in dimerized and frustrated Heisenberg chains

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We present a detailed numerical analysis of the low-energy excitation spectrum of a frustrated and dimerized spin $S=1/2$ Heisenberg chain. In particular, we show that in the commensurate spin-Peierls phase the ratio of the singlet and triplet excitation gap is a universal function which depends on the frustration parameter only. We identify the conditions for which a second elementary triplet branch in the excitation spectrum splits from the continuum. We compare our results with predictions from the continuum limit field theory. We discuss the relevance of our data in connection with recent experiments on $CuGeO_3$, NaV_2O_5, and $(VO)_2P_2O_7$.
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I. INTRODUCTION

Low-dimensional quantum spin systems have attracted considerable attention from theorists over the decades. Most of the interesting and fascinating features observed in these systems are pure quantum effects uniquely due to their low dimensionality. Peculiar properties of one-dimensional quantum antiferromagnets such as e.g., exotic ground states or unconventional excitation spectra are not accessible to traditional methods such as spin-wave or perturbation theory, but require the use of numerical or field-theoretical approaches. These methods are complementary to each other and together with exact Bethe ansatz solutions of particular models they allow for a complete description of low-dimensional quantum spin systems. In particular, the field-theoretical methods have been used successfully to predict the scaling behavior of the one-dimensional spin $S=1/2$ Heisenberg model,[1] the existence of gapless and gapped phases in the $S=1/2$ frustrated Heisenberg chain,[2] and the existence of an excitation gap in the spin $S=1$ Heisenberg chain.[3] On the other hand, only numerical methods allow us to determine the critical value of frustration beyond which the gapped phase appears[4,5] and to determine details of the ground state properties[6] or the behavior of the excitation gap itself.[7,8]

Recently the interest in one-dimensional spin systems has been particularly boosted by the discovery of various nonorganic quasi-one-dimensional compounds, in particular, the spin-Peierls materials $CuGeO_3$ (Ref. 9) and NaV_2O_5 (Refs. 10–13) and spin ladder compounds such as $SrCu_2O_3$, $Sr_2Cu_3O_5$, or possibly $(VO)_2P_2O_7$.[14–17] A common feature of these compounds is an excitation spectrum which is dramatically different from the spin $S=1/2$ Heisenberg chain. A remarkable fact about the Heisenberg chain is that its excitation spectrum consists of spin-1/2 particles (spinons).[18] Physically such excitations can be created only in pairs because upon flipping one spin the total spin projection is changed by $\Delta S_z=1$. Thus, in the Heisenberg chain the conventional magnons carrying spin 1 are deconfined into spin-1/2 spinons. In dimerized spin-Peierls compounds the excitation spectrum is always gapped and the low lying excitations are triplets. In addition, a massive singlet branch may exist above the triplet excitation branch in frustrated systems. As it will be shown in the following, even a second triplet branch can appear below the continuum. Hence in these systems spinons are confined back into triplet magnons. The interaction between magnons can lead to massive singlet and triplet excitations below the continuum[19,20] and even a sequence of further massive excitations.[21] Furthermore the dimerized frustrated Heisenberg model can also describe the two-leg ladder with frustration.[22]

In recent years the field-theoretical continuum-limit approaches were successfully used to study spin-Peierls compounds and spin-ladder systems.[2,23,24] These studies show mechanisms for spinon confinement from the alternation of exchange couplings in spin-Peierls compounds and from the interchain coupling in spin-ladder systems. Although universal features of the physical system are usually properly captured in field theoretical studies, important details governed by the physics at short length scales remain out of range for the applicability of these methods. Moreover, due to the perturbative nature of the continuum-limit approach, its predictions are less accurate in the physically more realistic strong coupling limit where details of the short-distance physics are very important. Therefore, there is still a number of open questions motivating further theoretical studies of spin-Peierls and spin-ladder systems — especially in the strong coupling limit — by using exact methods.

In this paper we present specifically a detailed numerical analysis of the low-energy excitation spectrum of the $S=1/2$ antiferromagnetic Heisenberg chain with frustration and dimerization, as proposed in particular to describe the magnetic properties of $CuGeO_3$.[5] The Hamiltonian reads

$$H=J\sum_i \{[1+\delta(-1)^i]\mathbf{S}_i\cdot\mathbf{S}_{i+1}+\alpha\mathbf{S}_i\cdot\mathbf{S}_{i+2}\}, \qquad (1)$$

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where i denotes the sites of a chain with length L and $\mathbf{S}_i$ are $S=1/2$ spin operators. $J>0$ is the nearest-neighbor exchange coupling, α the frustration parameter from next-nearest-neighbor coupling and δ is the dimerization parameter.

Besides its relevance to real spin-Peierls compounds the model is interesting purely from a theoretical point of view as it contains two independent mechanisms for spin-gap formation. At $\delta=0$ the model is characterized by a critical value of frustration α_c (Ref. 2) which was accurately determined by numerical studies: $\alpha_c=0.2412$.[4,5] For $\alpha<\alpha_c$ the frustration is irrelevant, the system renormalizes to the Heisenberg fixed point: the ground state corresponds to a spin liquid and the elementary excitations are massless spinons. At $\alpha=\alpha_c$ there is a transition into a spontaneously dimerized ground state. The spectrum acquires a gap and the elementary excitation is a massive spinon.[2] On the other hand, at any $\delta\neq 0$ the singlet ground state of the model is also dimerized with a gap in the spin excitation spectrum, but the elementary excitation is a magnon.[2,24]

For the special case $2\alpha+\delta=1$ the ground state of the spin Hamiltonian Eq. (1) is known exactly to be a product wave function of nearest-neighbor singlet pairs.[25,19] This line in the (α,δ) parameter plane separates two distinct regimes: for $2\alpha+\delta-1\leqslant 0$ the dominant peak in the static magnetic structure factor is at $q^*=\pi$, while in the other case $\pi/2<q^*<\pi$. In this latter incommensurate phase, q^* continuously decreases from π with increasing α and δ, and asymptotically approaches $\pi/2$.[7,8]

In a recent work,[26] the existence of a massive singlet excitation has been confirmed numerically for the Hamiltonian Eq. (1) with $\alpha=0.35$ and $\delta=0.012$. In addition to the elementary triplet and singlet excitations and depending on the set of parameters (α,δ) another triplet excitation was found to split from the continuum.[26,27]

In this paper we will analyze in detail the intriguing structure of the excitation spectrum for different frustration and dimerization parameters, and we compare our numerical data with the available results from field theoretical methods. The paper is organized as follows. In Sec. II we summarize the procedure and the results of the continuum limit field theory and outline the open questions inaccessible by these analytical methods. In Sec. III we focus our attention on the singlet to triplet energy gap ratio $R(\alpha,\delta)=\Delta_s/\Delta_t$ and show that $R(\alpha,\delta)$ only depends on α when $2\alpha+\delta<1$; the field theory prediction $R=\sqrt{3}$ is precisely realized for all δ *only* when $\alpha=\alpha_c$. In Sec. IV we discuss the conditions for which a second triplet excitation branch may exist below the continuum. Finally, in Sec. V we connect our results to recent experimental data on different spin chain compounds.

II. THE CONTINUUM-LIMIT FIELD-THEORY APPROACH

The first insight into the structure of the excitation spectrum of the model Eq. (1) is obtained from bosonization and the continuum limit renormalization group approach.[28] In terms of the continuum field $\phi(x)$ the bosonized version of the initial spin model is the double sine-Gordon (SG) model

$$H_{\rm bos}=\int dx\left\{\frac{u}{2}\left[K\,\Pi^2+K^{-1}\left(\frac{d\phi}{dx}\right)^2\right]+M_\delta\cos\,(\beta_\delta\phi)+M_\alpha\cos\,(\beta_\alpha\phi)\right\}, \tag{2}$$

where u is the spin wave velocity, $\beta_\alpha=\sqrt{8\pi}$, $\beta_\delta=\sqrt{2\pi}$, $K=\sqrt{[1-(\alpha-\alpha_c)]/[1+(\alpha-\alpha_c)]}$, $M_\alpha=J(\alpha-\alpha_c)$, and $M_\delta=\delta$.

The value of the critical frustration α_c is determined by the behavior of the system at short distances, i.e., it depends on nonuniversal parameters of the continuum limit theory. Therefore, differently constructed continuum limit theories give rather different values of this parameter.[2,29,30] The exact value of α_c was determined only within numerical studies,[4,5] but the nonuniversal parameters of the continuum limit Hamiltonian could be always chosen in such a way to ensure the proper value of the critical frustration α_c.

Contrary to the standard SG model [Hamiltonian (2) with only 1 ''cosine term'' $M\cos(\beta\phi)$], which is exactly solvable and well understood,[31] the theory of the quantum double SG model is much less developed. However, in two limiting cases the model Eq. (2) reduces to the SG theory and provides exact knowledge about the characteristic properties of the system.

Let us first consider the case $\delta=0$ $(M_\delta=0)$ corresponding to the frustrated Heisenberg chain. The behavior of this model is determined by the marginal interaction which is controlled by the frustration: $\beta=\beta_\alpha=\sqrt{8\pi}$. For $\alpha<\alpha_c$ the interaction is irrelevant and the system scales to the Gaussian fixed point: elementary excitations are massless spinons. For $\alpha>\alpha_c$ the interaction is marginally relevant and the effective interaction renormalizes to large values. An exponentially small gap $M^*\propto\exp[-c/(\alpha-\alpha_c)]$ is dynamically generated in the excitation spectrum, the field ϕ is ordered leading to a spontaneously dimerized ground state with the finite order parameter

$$\langle\hat{O}_d\rangle=\frac{1}{L}\left\langle\sum_i\,(-1)^i(\mathbf{S}_{i-1}\cdot\mathbf{S}_i-\mathbf{S}_i\cdot\mathbf{S}_{i+1})\right\rangle. \tag{3}$$

Thus, the elementary excitations in the massive phase of the frustrated Heisenberg chain are described by solitons (''kinks'') of the quantum SG model with $\beta=\sqrt{8\pi}$.[2] There are no soliton-antisoliton bound states in this case and the system is characterized by the only one scale spin gap $\Delta=2M^*$. Excitations above the given vacuum are created by breaking singlet bonds. Each broken bond gives rise to a pair of decoupled spins 1/2 on neighboring sites. Once created, these isolated spins can propagate coherently along different sublattices and constitute elementary excitations of the massive spinon type.

We now consider the case $\delta\neq 0$ and $\alpha=\alpha_c$ $(M_\alpha=0$ and $M_\delta\neq 0)$. The excitation spectrum of the SG model at $\beta=\beta_\delta=\sqrt{2\pi}$ is exactly known[31] and at this point consists of soliton and antisoliton excitations with masses $M_s=M_{\bar{s}}=M$ and two bound states (breathers) with masses $M_1=M$ and $M_2=\sqrt{3}M$. The soliton excitation carries spin $S^z=1$, the antisoliton excitation $S^z=-1$, and the two breathers with opposite parity $S^z=0$. The lower-energy breather mode is degenerate with the kink and antikink and these three exci-

tations correspond to a triplet excitation branch in the original spin model language. The second bound state, in fact, has its counterpart in a spin singlet excitation.[2] These two modes are the only elementary excitations in this case and the ratio of their excitation gaps is exactly $\sqrt{3}$.

The standard renormalization group (RG) approach[24,30,32] to the double SG model Eq. (2) is based on the fact that the critical dimensions of the two cosine terms arising from the smooth and staggered part of the exchanges, respectively, are different:

$$\dim \cos(\sqrt{2\pi}\phi)=1, \quad \dim \cos(\sqrt{8\pi}\phi)=2. \tag{4}$$

Thus, the $\delta \cos(\sqrt{2\pi}\phi)$ term is strongly relevant, while the $J(\alpha-\alpha_c)\cos(\sqrt{8\pi}\phi)$ term is marginal. Therefore, the essential physics as determined by the relevant term is — at least for $\delta \ll 1$ — similar to that of the above discussed SG model with $\beta=\sqrt{2\pi}$, and the marginal interaction leads to logarithmic corrections only. Therefore one assumes that the excitation spectrum of the spin-Peierls state consists of two excitation branches with gaps Δ_t (triplet excitation) and $\Delta_s = R\Delta_t$ (singlet excitation) with R slightly different from $\sqrt{3}$ due to the logarithmic corrections.[24,32] However, since frustration and dimerization provide two principally different mechanisms for spin gap formation, interference between these interactions is nontrivial especially in the limit of strong initial interactions. A very sensitive tool to study these particular effects is to explore the detailed structure of the excitation spectrum. Moreover, the exact excitation spectrum of the dimerized and frustrated Heisenberg chain Eq. (1) provides another way for the determination of the critical parameter α_c. Only for $\alpha=\alpha_c$ is the structure of the excitation spectrum exactly the same as that of the SG model with $\beta=\sqrt{2\pi}$. Therefore, α_c is determined from the condition $R(\delta,\alpha_c)=\sqrt{3}$.

Due to the different critical dimensions of the cosine terms in the double SG model one may attempt, in a first approximation, to neglect the $\cos(\sqrt{8\pi}\phi)$ term and to consider the usual SG model with the $\cos(\sqrt{2\pi}\phi)$ term only. However, as we demonstrate in the subsequent sections, we have to conclude from our numerical results that this commonly accepted procedure is not valid and the structure of the excitations is quite different. For example, we find $R=2$ in the absence of frustration $\alpha=0$ which means that there is no long wavelength singlet excitation branch and the singlet excitation energy coincides with the edge of the continuum. Furthermore we obtain that for $\alpha<\alpha_c$ and small δ the ratio $R=\Delta_s/\Delta_t$ is a ''universal'' function of α alone. So although the continuum limit Hamiltonian is a proper description of the spin lattice model Eq. (1) the commonly adopted field theoretical tools for the double SG model are not sufficient for a complete understanding of the excitation spectrum as we will show from our exact diagonalization data.

III. GAP RATIO

Our numerical study is performed using exact diagonalization techniques with periodic boundary conditions for chains with up to $L=26$ sites. As previously reported in Ref. 26 the triplet and singlet gaps Δ_t and Δ_s have different finite size scaling behavior. While Δ_t is a monotonically decreasing function of $1/L$, Δ_s is nonmonotonic in $1/L$ and develops a minimum for a particular chain length which varies with the model parameters. Thus, in order to extrapolate the values for Δ_t and Δ_s to the infinite chain limit, we need two different finite size scaling fit functions. For the triplet gap we have used the three-parameter ansatz[26]

$$\Delta_t(L)=\Delta_t+\frac{A}{L}\exp\left(-\frac{L}{L_t}\right). \tag{5}$$

On the other hand, in order to account for the nonmonotonic behavior of Δ_s we have chosen the four-parameter ansatz

$$\Delta_s(L)=\Delta_s+\exp\left(-\frac{L}{L_s}\right)\left(\frac{A}{L}+B\right), \tag{6}$$

with $A>0$ and $B<0$. Note that both fit functions proved to give an excellent agreement with density matrix renormalization group (DMRG) data with L of order 100, in particular in the region where the spin-spin correlation length is shorter than the chain length.[26,33]

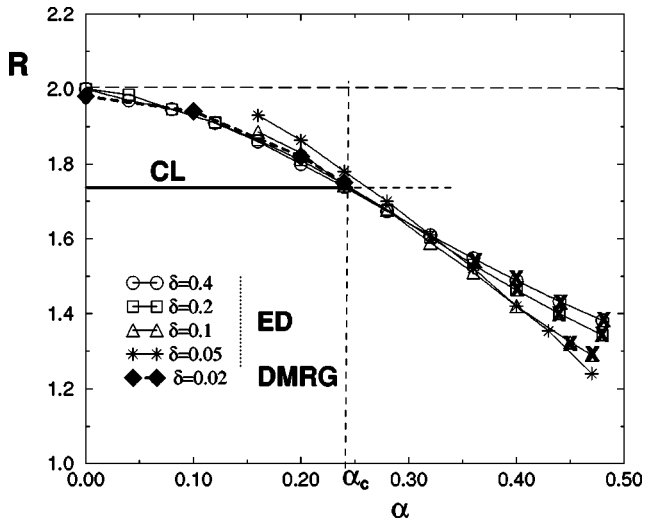


FIG. 1. Extrapolated singlet-triplet gap ratio $R(\alpha,\delta)=\Delta_s/\Delta_t$ vs frustration α for different dimerization parameters δ. The symbols marked with a cross have been calculated in the incommensurate phase. ED indicates exact diagonalization results extrapolated to the infinite chain limit. In addition we have added data points from density matrix renormalization group (DMRG) calculations (Ref. 33).

In Fig. 1 we show the ratio $R(\alpha,\delta)$ as a function of α for different values of the dimerization parameter ($0.02<\delta<0.4$) using the extrapolated values of Δ_t and Δ_s. Since we find that the width of the singlet dispersion is smaller than the width of the triplet dispersion, the necessary condition for the singlet excitation branch to split from the continuum over the whole Brillouin zone is $R(\alpha,\delta)<2$. Figure 1 clearly shows that the ratio depends on the frustration parameter in an *essential* way. For $\alpha<\alpha_c$ we obtain $R(\alpha,\delta)>\sqrt{3}$ implying that the $\cos(\sqrt{8\pi}\phi)$ term in the double SG model is indeed relevant for all $\alpha\neq\alpha_c$ and cannot be omitted. We recall the field theoretical expectation that the deviations from $\sqrt{3}$ should be logarithmically small. Furthermore, the exact diagonalization data show that the ratio R is for α

$<\alpha_c$ insensitive to the dimerization parameter δ (to be more precise, for $\delta>0.05$ within the accuracy of our finite size studies) which in the continuum limit field theory controls the relevant interaction in the double SG model. $R=\sqrt{3}$ is indeed obtained at criticality $\alpha=\alpha_c$ for any finite δ, weak or strong. In the absence of frustration, $\alpha=0$, and for any dimerization we find $R(\alpha=0,\delta)=2$. Therefore, there is no well defined singlet excitation at $q=0$ (or equivalently $q=\pi$) since $\Delta_s=2\Delta_t$ coincides with the lower edge of the continuum.

In addition we find that (i) $R(\alpha,\delta)$ is a *universal* function of α for $2\alpha+\delta\leqslant 1$ and (ii) $R(\alpha,\delta)$ depends on both parameters in the incommensurate phase for $2\alpha+\delta>1$. We note that the deviations observed for weak values of δ (i.e., $\delta=0.05$) in Fig. 1 result from a lack of precision in the determination of the extrapolated Δ_s. High precision is lost when the spin-spin correlation length becomes comparable to or longer than the chain length for small δ. On the other hand the comparison with DMRG calculations for $L\leqslant 100$ shows that the ansatz for the scaling of the singlet gap Δ_s, Eq. (5), remains very accurate even in the region of long correlation lengths (small gap). To demonstrate the consistency with the diagonalization data we have added in Fig. 1 DMRG data points calculated for $\delta=0.02$.[33] The DMRG data support the observation that the ratio $R(\alpha,\delta)$ depends on α *only* in the commensurate phase, i.e., as long as $2\alpha+\delta\leqslant 1$. We have indicated in Fig. 1 (with a cross) the data points for which the parameter pairs (α,δ) belong to the incommensurate phase. We emphasize that for these sets of parameters the finite size effects are extremely small and the values of $R(\alpha,\delta)$ are thus very accurate.

A similar behavior has recently been found by Yokoyama *et al.* for the leading δ power law dependence of the triplet excitation gap $\Delta_t\propto\delta^{\gamma}$, where the exponent γ is a monotonic continuous function of α.[27] In this work it was shown that the Cross-Fisher value $\gamma=\frac{2}{3}$ (Ref. 34) is realized only for $\alpha=\alpha_c$, but $\gamma\neq\frac{2}{3}$ for $\alpha<\alpha_c$.

IV. A SECOND TRIPLET BRANCH

Another peculiar observation is made when the parameters (α,δ) are increased towards stronger dimerization in that a second triplet excitation branch splits from the continuum. In analogy to the singlet excitation this second triplet may be interpreted as a bound state between a triplet and a singlet excitation. In order to investigate this feature we fix the dimerization parameter $\delta=0.2$ and discuss the low-energy spectrum as a function of frustration in the subsector of total momentum $q=0$. For this purpose we have show in Fig. 2(a) the energies of the three lowest excited states, extrapolated to $L\to\infty$, as a function of α. In this figure the lower edge of the continuum at $2\Delta_t$ is indicated by a continuous bold line. We observe that for $\alpha<0.28$, there are only two well defined excitations below the continuum, one triplet and one singlet as discussed above. The energy of the next excited state is found to scale to the lower edge of the continuum with $L\to\infty$. In contrast to the triplet, the singlet excitation gap remains almost constant with changing α. However, we observe that for $\alpha>0.28$ another triplet excitation T_2 splits from the continuum (i.e., $E_{T_2}<2\Delta_t$). This is

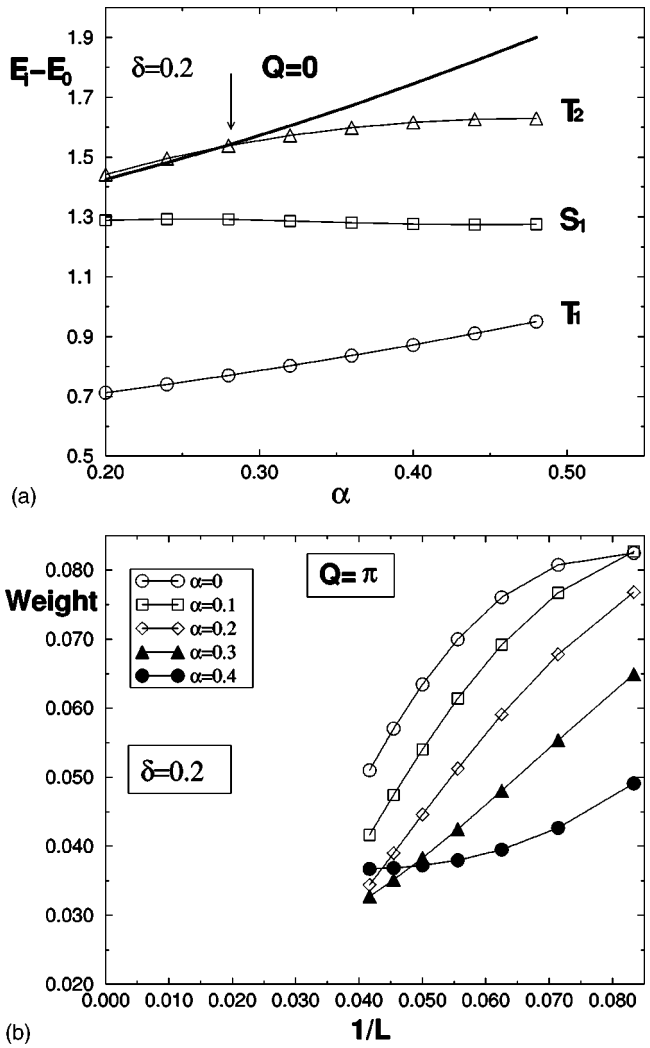
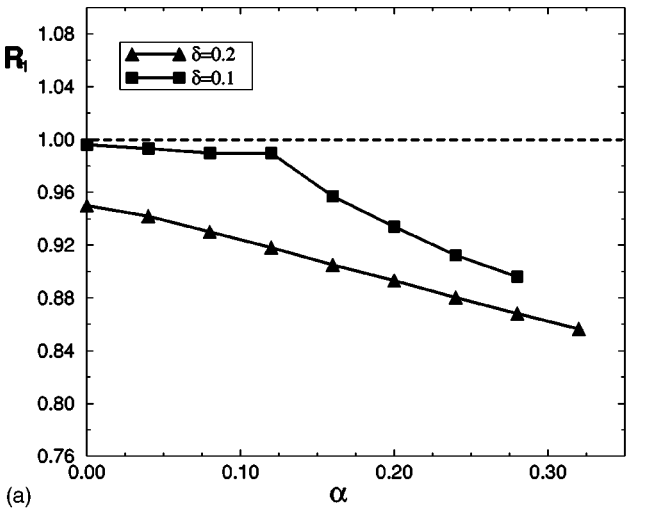


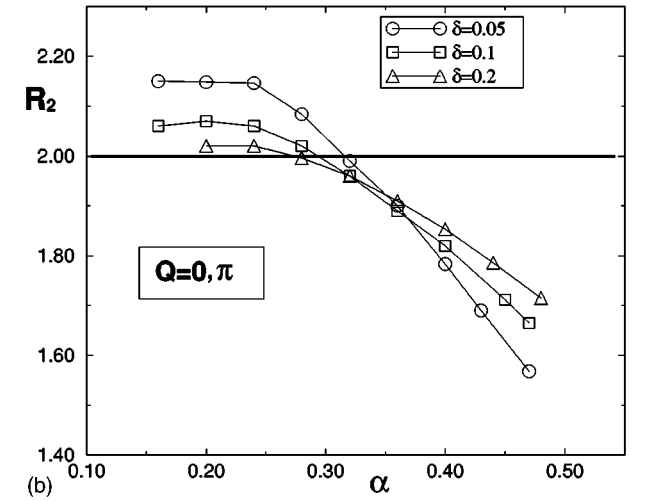
FIG. 2. (a) Energy of the three lowest excitations vs frustration calculated at fixed dimerization $\delta=0.2$ and momentum $q=0$ (resp. π). The continuous line indicates the edge of the continuum at $2\Delta_t$. $T_{1,2}$ are triplet excitations and S_1 is the lowest singlet excitation. (b) Spectral weight W of the triplet T_2 as a function of $1/L$ (L is the size of the system) for $\delta=0.2$ and different values of α. The full symbols correspond to cases for which W scales to finite values in the infinite chain limit.

in agreement with the results reported previously in Ref. 26.

In order to verify that the triplet T_2 is indeed a well defined elementary excitation at $q=\pi$ only when $\alpha>0.28$ (for $\delta=0.2$), we have also evaluated its spectral weight $W=|\langle T_2|\hat{O}|0\rangle|^2$ versus $1/L$ in the dynamical structure factor $S(\pi,\omega)$ for different frustration parameters α [see Fig. 2(b)] where $|0\rangle$ is the ground state wave function and $\hat{O}=S^z(\pi)=(1/\sqrt{L})\Sigma_l \exp(i\pi l)S^z_l$. We observe that for $\alpha<0.28$, W has a strong size dependence, and the data indicate that $W\to 0$ with $L\to\infty$. However, for $\alpha>0.28$ the curvature of $W(1/L)$ changes indicating that the weight $W(1/L)$ scales to a finite value consistent with the identification of T_2 as an elementary excitation below the continuum.

By evaluating the excitation spectrum in different momentum sectors we find that the triplet T_2 splits from the continuum first at $q=\pi/2$. In Fig. 3(a), we have plotted the ratio





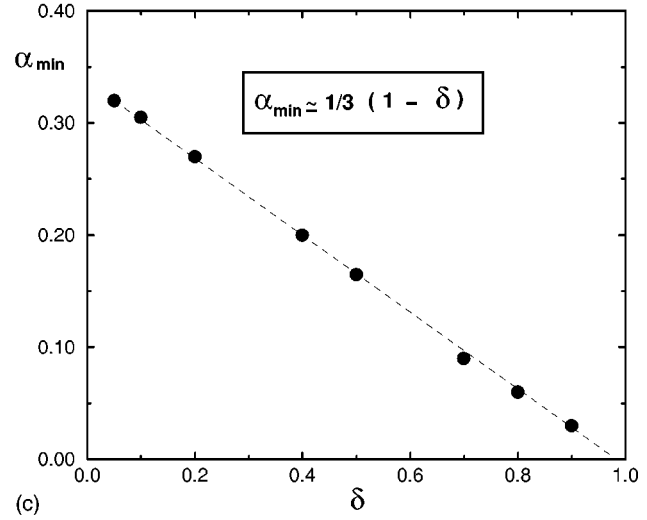


FIG. 3. (a) R_1 and (b) R_2 as a function of α calculated for different values of the parameter δ. For the definitions of the ratios R_1 and R_2 see Eqs. (7) and (8), respectively. In (c), we have plotted $\alpha_{\min}$ as a function of δ, the dashed line is a linear fit of the data.

$$R_1=\frac{E(S=1,\pi/2,2)-E(S=1,\pi/2,1)}{\Delta_t}, \tag{7}$$

versus α where $E(S,q,n)$ is the nth energy level in the subsector with total momentum q and spin S extrapolated to L

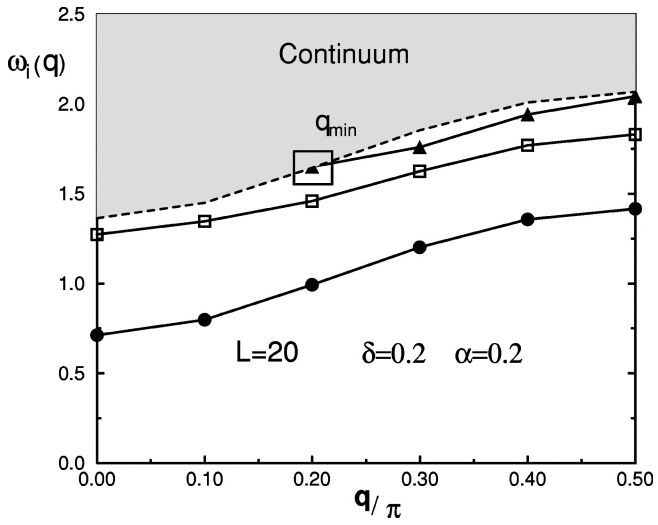


FIG. 4. Dispersion $\omega_i(q)=E_i(q)-E_0$ of the three lowest excitations for $\alpha=0.2$ and $\delta=0.2$. The full symbols correspond to the triplets T_1 and T_2 and the open symbols to the singlet S_1. The continuum is indicated by the shaded area.

$\rightarrow\infty$. $R_1<1$ implies that the excitation is split from the continuum at $q=\pi 2$. Figure 3(a) shows that for large enough dimerization (e.g., $\delta=0.2$) the triplet T_2 is well defined at $q=\pi/2$ for any α. However, as we reduce the dimerization parameter (e.g., to $\delta=0.1$), we observe that stronger frustration is needed in order to separate T_2 from the continuum. In fact, for $\delta=0.1$ and $\alpha<0.12$, $R_1\approx 1$, i.e., the energy of the second triplet excitation scales to the lower edge of the continuum. Thus our data suggest that in the absence of frustration, there is a minimal value $\delta_{\min}>0.1$ above which the triplet T_2 appears. The fact that $R_1\approx 0.98$ instead of 1, for $\delta=0.1$ and $\alpha<0.12$ shows that this excitation is not well defined, the finite size analysis is not valid for excitations in the continuum. The kink in R_1 clearly indicates the minimum value of the frustration for which the excitation separates from the lower edge of the continuum. Similarly, the value $\alpha=0.28$ [see Fig. 2(a)] is the minimal frustration $\alpha_{\min}(\delta=0.2)$ for the second triplet to be a well defined excitation branch over the entire Brillouin zone. In other words, for a given δ, the momentum range for which the triplet T_2 is split from the continuum is centered around $q=\pi/2$ increasing continuously with increasing α. As an example, we show in Fig. 4 the dispersion of the three lowest excitations for $\alpha=0.2$ and $\delta=0.2$, for which the triplet T_2 is split from the continuum in the momentum range $4\pi/5>q>q_{\min}\approx\pi/5$.

In order to determine the δ dependence of $\alpha_{\min}$, we have plotted in Fig. 3(b) the ratio

$$R_2=\frac{E(S=1,\pi,2)-E_0}{\Delta_t}, \tag{8}$$

versus α for different values of δ. The excitation T_2 is split from the continuum when $R_2<2$. Figure 3(b) shows that $\alpha_{\min}$ increases when δ is reduced, for instance, $\alpha_{\min}(0.2)\approx 0.28$ and $\alpha_{\min}(0.05)\approx 0.32$. We have plotted in Fig. 3(c) $\alpha_{\min}$ as a function of δ for $\delta<1$. Our results suggest that $\alpha_{\min}$ is within a good approximation a simple linear function of the parameter δ, $\alpha_{\min}\approx(1-\delta)/3$. Thus, in the special limiting case $\delta\rightarrow 1$, and restricting ourselves to the commensu-

rate region we observe that $\alpha_{\min} \to 0$. Note that the result cannot be extended at the special point $\delta = 1$, since the spectrum at this point consists of a discrete set of eigenvalues $E_n = n\Delta_t$, thus there is no continuum in the vicinity of $2\Delta_t$. However, for $0.5 < \delta < 1$, the spectrum consists of minibands with finite band gaps, thus the notion of continuum has a meaning in the vicinity of $2\Delta_t$. Furthermore our result suggests that the spectrum is completely dense (no band gap), when $\delta < 0.5$. The other interesting point corresponds to the limit $\delta \to 0$. Indeed, if the linear approximation is still valid in this limit, our data shows that $\alpha_{\min} \to 1/3$.

V. DISCUSSION OF EXPERIMENTAL DATA

We now try to connect these results to some recent experimental data on $CuGeO_3$, NaV_2O_5, and $(VO)_2P_2O_7$. $CuGeO_3$ (Ref. 9) and NaV_2O_5 (Refs. 10,35,11) are spin-Peierls systems with transition temperatures $T_{SP} \approx 14$ and 35 K, respectively. Previously it has been shown that the magnetic susceptibility of $CuGeO_3$ in the uniform phase can be accurately reproduced by a frustrated Heisenberg chain model with Ref. 37; from this fit the frustration was estimated to be $\alpha \approx 0.35$, close to the previous estimate of Riera and Dobry.[38] With an exchange coupling $J \approx 160$ K and $\alpha = 0.36$ the experimental value for the gap $\Delta_t = 2.1$ meV as determined by inelastic neutron scattering[36] is obtained within the frustrated and dimerized Heisenberg chain model with a dimerization $\delta = 0.012$.[26] With this parameter set a singlet-triplet gap ratio $R(0.35,0.012) \approx 1.50$ follows (see Fig. 1). However, the experimental ratio is $R_{\exp} = 1.72 \approx \sqrt{3}$; according to Fig. 1, this would corresponds to $\alpha \approx \alpha_c$, a value for α which was previously proposed by Castilla *et al.*[5]

There are different possibilities how to resolve this quantitative problem. First, the effects of interchain coupling along the crystal b direction in $CuGeO_3$ are experimentally well established but little is known from theoretical studies.[39] Second, the dynamics resulting from the spin-lattice coupling is expected to play an important role. Indeed, including dynamical phonons will renormalize the spin excitation spectrum and as a direct consequence the ratio R.[40]

Recently, it has been proposed that the low-temperature phase of the compound NaV_2O_5 is well described by an unfrustrated ($\alpha = 0$) dimerized chain model.[10] Following the same procedure as used for $CuGeO_3$, the dimerization was estimated to be of order $\delta \approx 0.048$.[41] If we assume that this is indeed the case then — according to our results — we expect a singlet-triplet gap ratio $R(0,0.048) = 2$, i.e., there is no well defined long wavelength singlet excitation below the continuum. As a consequence, we expect no magnetic Raman response at frequencies below the lower edge of the continuum at $2\Delta_t$. However, in a recent Raman scattering experiment on NaV_2O_5 (Ref. 42) it has been observed that the energy of the lowest excitation in the dimerized phase is at 64 cm^{-1}; for this compound the measured triplet excitation gap from inelastic neutron scattering is $\Delta_t \approx 59$ cm^{-1}.[11] Thus the energy of the lowest excitation in the Raman spectra is very close to the singlet-triplet gap Δ_t. Furthermore, it was observed that this feature remains unchanged for different photon polarization geometries suggesting that this excitation is probably not of magnetic origin. An alternative origin is a charge excitation due to a local charge transfer from a V^{4+} to a V^{5+} chain. All these observations indicate some important qualitative differences between the spin chain compounds $CuGeO_3$ and NaV_2O_5.

Finally we discuss the case of $(VO)_2P_2O_7$ — a spin chain compound whose magnetic properties have given rise to controversial interpretations. This compound has been initially considered as an ideal realization of a two-leg antiferromagnetic Heisenberg spin ladder.[43] Subsequently, however, it has been shown that the susceptibility data on polycristalline material could be well fitted by either a ladder or an alternating chain model.[44] Early neutron scattering data indicated a spin gap of about 50 K and supported the two-leg ladder picture.[45] Recently, inelastic neutron scattering experiments have been performed on a collection of many oriented single crystals.[15] Observed features such as, e.g., the strong dispersion in the rung direction lead to the conclusion that the data are not consistent with a spin ladder description and that $(VO)_2P_2O_7$ is better described as an alternating spin chain directed in the rung direction. Remarkably, in addition to the lowest triplet another well defined higher energy triplet excitation below the continuum was observed near $q = \pi$. If we assume that this compound is well described by an unfrustrated ($\alpha = 0$) dimerized chain with a dimerization of order $\delta \approx 0.1$ (i.e., an alternating exchange coupling in the rung direction), then we find a contradiction with our present results. In fact, for $\delta \approx 0.1$ and $\alpha = 0$, there is no well defined second triplet at $q = \pi$. The microscopic structure of $(VO)_2P_2O_7$, however, does not allow us to identify any obvious superexchange path which can lead to frustration. At this point we can only point out that both pictures — a two-leg ladder or an unfrustrated alternating chain — do not properly describe the low-energy excitation spectrum in this compound. The correct modeling of the magnetic properties of $(VO)_2P_2O_7$ remains an unresolved problem.

VI. SUMMARY AND CONCLUSION

In this paper we have studied the elementary excitations of frustrated and dimerized Heisenberg chains. We have shown that in the commensurate dimerized phase the singlet-triplet gap ratio $R(\alpha,\delta)$ only depends on the frustration parameter for arbitrary values of the dimerization ($\delta \geqslant 0.02$). The magnitude of this ratio gives a direct measure for the strength of the frustrating exchange coupling. Without frustration $R(\alpha = 0,\delta) = 2$ implying the absence of a long wavelength singlet excitation below the continuum. We have shown that away from criticality $\alpha \neq \alpha_c$ the frustration term plays an important role for the low-energy excitation spectrum. Therefore, the commonly adopted procedure of disregarding the frustration term in the bosonized continuum limit Hamiltonian for $\alpha < \alpha_c$ is at least questionable since it is not marginally irrelevant. However, for $\alpha = \alpha_c$, our exact diagonalization results give precisely $R(\alpha_c) = \sqrt{3}$ in perfect agreement with the field theoretical treatment of the SG model. Furthermore, we have demonstrated the conditions for the existence of another triplet excitation branch which we interpret as a bound state of elementary triplet and singlet excitations. Depending on the dimerization strength the second

triplet excitation branch is observable at $q=0$ (or $q=\pi$) only if the frustration parameter is large enough. As we have discussed we consider our results relevant for the magnetic excitations in the spin chain compounds $CuGeO_3$, NaV_2O_5, and $(VO)_2P_2O_7$. For the latter material we conclude from our results that neither a two-leg ladder nor an alternating, unfrustrated Heisenberg chain model captures the experimental facts on the excitation spectrum in $(VO)_2P_2O_7$.

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