From spinons to magnons in explicit and spontaneously dimerized antiferromagnetic chains

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We reconsider the excitation spectra of a dimerized and frustrated antiferromagnetic Heisenberg chain. This model is taken as the simpler example of competing spontaneous and explicit dimerization relevant for spin-Peierls compounds. The bosonized theory is a two-frequency sine-Gordon field theory. We analyze the excitation spectrum by semiclassical methods. The elementary triplet excitation corresponds to an extended magnon whose radius diverges for vanishing dimerization. The internal oscillations of the magnon give rise to a series of excited states until another magnon is emitted and a two-magnon continuum is reached. We discuss, for weak dimerization, the manner in which the magnon forms as a result of a spinon-spinon interaction potential. [S0163-1829(99)05213-3]

One-dimensional (1D) antiferromagnetic systems have attracted a great deal of interest over the last decades. They are typical examples where the low dimensionality enhances quantum fluctuations, producing effects completely different than the ones expected by classical theories of magnetism. Interest in one-dimensional magnetic system has recently been strongly renewed in view of the discovery of a new class, in general inorganic compounds, with definite one-dimensional character. Detailed spectral characterizations are now available and the theory is pushed to make precise predictions on how different microscopic interactions influence the spectral response of this system. We discuss in this work the case of a gapped antiferromagnetic chain and analyze how an explicit dimerization and a frustrated interaction compete between them and how the magnetic spectra evolve with the microscopic parameters. A similar subject has recently been analyzed by different numerical techniques.[1,2] An analytical approach for the case of the weak dimerization limit has been also proposed.[3] We will discuss the similarities and differences with our results. We take the recently discovered inorganic material $CuGeO_3$ (Ref. 4) as a reference even though our result could be more general. Our starting model Hamiltonian reads

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

where J is the nearest-neighbor (NN) exchange coupling, α is the frustration parameter, and δ measures the amount of explicit dimerization. There are two different motivations to associate this model Hamiltonian with the magnetic spectra of a spin-Peierls compound. First, the temperature dependence of the magnetic susceptibility of $CuGeO_3$ could only be accounted for if an important next-nearest neighbor (NNN) is included in the 1D Heisenberg model used to describe this material.[5,6] It is therefore natural to include an explicit dimerization on the exchange interaction to describe the magnetic excitations in the low-temperature Peierls phase and this has been in fact the approach used in various theoretical studies.[7,8] Second, if the adiabatic hypothesis is left out, the system turns into a coupled spin-phonon one. Even though the magnetic interactions have mainly one-dimensional character, they interact with the three-dimensional phonons. The excitations of the low-temperature phase are strongly affected by the interchain elastic coupling. In fact, topological solitons (kink) which are genuine excitations of the isolated chain can no longer exist as free excitations because they create a zone with an opposite dimerization phase relative to the surrounding chains. A kink and an antikink are strongly interacting excitations. Their interactions were accounted for in previous work by a linear confined potential[3,9] or as producing a kind of domain configuration where the kink and antikink oscillate around an equilibrium distance.[10] As has been recently remarked the model Hamiltonian (1) is the simplest example where these processes could be studied. In this context the first term of Eq. (1) accounts for the explicit dimerization imposed by neighboring chains and the second term for the tendency to spontaneous dimerization as we will discuss in the following.

For $\alpha=0$ and strong dimerization (δ) the ground state is a product of the singlet over the strong bonds. The first excitations correspond to replacing a singlet for a triplet and then delocalize it to build states of definite momentum. They form a band of spin-1 magnon excitations. In the opposite limit ($\delta=0$) translational symmetry is not explicitly broken. However, for α greater than a critical value ($\alpha_c\sim 0.23$) the system spontaneously dimerizes and a gap in the spectra is opened. At $\alpha=1/2$ (Majumdar-Ghosh point) the exact ground state is the double-degenerate product of singlets over the NN bonds. The excitations have been variationally evaluated by Shastry and Sutherland[11] (SS). They are massive $S=1/2$ spinons which correspond to an uncoupled spin separating two regions of singlet dimers. The two previously discussed cases represent the extreme situation of a correlation length equal to the lattice constant. As we discuss below

the structure of the lower-energy triplet excitations remains similar for other values of the correlation length in the limits previoulsy discussed.

The main question we address in this work is how the spectra evolve from one limit to another, i.e., how the massive spinons bind in a magnon. To address this question we analyze this system in the limit of small δ and α slightly larger than the critical value. In this region the low-energy spectrum could be studied by bosonization. The bosonized Hamiltonian is[14]

$$H_{bos}=\int dx\left\{\frac{u\beta^2}{2}\Pi^2+\frac{u}{2\beta^2}(\partial_x\phi)^2+g_1\sin\phi+g_2\cos(2\phi)\right\}, \tag{2}$$

where $g_1\sim\delta$ and $g_2\sim\alpha-\alpha_c$. The proportionality constants are of the order of unity depending on the short-range cutoff in the bosonization procedure. $\beta=\sqrt{2\pi}$ for the isotropic model, and u is the spin-wave velocity. The spectrum of this double-frequency sine-Gordon (DFSG) field theory is not known in general. We start by analyzing both limits of $g_1=0$ and $g_2=0$ where the theory reduces to a single sine-Gordon model and a lot of information is available. In particular the semiclassical method of Dashen, Hasslasher, and Neveu[12] (DHN) gives the exact mass spectrum of the particles for this model.

For $g_2=0$ (we are indeed analyzing the whole zone $g_2<0$ because this marginal interaction renormalizes to zero in this case) the excitation spectra consist of a kink, an antikink, and two breathers. In the original spin language, the kink excitation carries $S_z=1$, the antikink $S_z=-1$, and the breathers $S_z=0$. The lower-energy breather is degenerate with the kink and antikink and these three excitations give rise to a triplet branch, the correlate of the previously discussed magnon band. For $g_1=0$ the only one-particle excitations of the resulting SG theory are a kink and an antikink; no breather is found. This kink carries spin one-half and is the analog of the massive spinons of the SS variational wave function. However, note that in this parameter regime where the continuum approximation is reliable the characteristic width of these excitations is large compared with the lattice space.

We are now in position to discuss the excitations in the intermediate zone. We start by implementing a semiclassical calculation of the spectra of the theory (2). Even though the method is not expected to give exact results for this nonintegrable model, it gives valuable nonperturbative information which will allow us to interpolate between the desired limits. The time-independent equation of motion corresponding to Eq. (2) is

$$\frac{u}{2\beta^2}(\partial_x^2\phi_0)+g_1\cos\phi_0-2g_2\sin 2\phi_0=0. \tag{3}$$

The lowest-energy (homogeneous) configuration is $\phi_0=-\pi/2 \pmod{2\pi}$ (it is not degenerate with $\phi_0=\pi/2$ as it would if $g_1=0$). Solitons are x-dependent solutions of the equation of motion with finite energy with respect to this homogeneous solution. Owing to the fact that the system is Lorentz invariant, moving solitons are obtained from static ones by a Lorentz transformation. To look for these static configurations we write a first integral of Eq. (3):

$$\frac{(1+B)\xi^2}{2}(\partial_x\phi_0)^2-B\sin\phi_0-\frac{1}{4}\cos 2\phi_0=cte, \tag{4}$$

where we have introduced the quantity $B=g_1/(4g_2)$ as a characteristic parameter to analyze the evolution of the spectrum from one limit to another. $\xi=u/\Delta$ and $\Delta=\beta\sqrt{u(g_1+4g_2)}$ is the mass gap to create a particle (let it call a meson) above the homogeneous vacuum. ξ is the correlation length of the theory and measure the width of the kinks. The boundary conditions for finite energy are $\lim_{x\to\pm\infty}\phi_0=-\pi/2 \pmod{2\pi}$ and $\lim_{x\to\pm\infty}\partial_x\phi_0=0$. They fix the $cte=B+\frac{1}{4}$. Equation (4) can now be integrated. The solution center at the origin is

$$t(x)\equiv\sin(\phi_0)=1-2\cosh^2[x_0/\xi]\operatorname{sech}[(x-x_0)/\xi]\times\operatorname{sech}[(x+x_0)/\xi], \tag{5}$$

with

$$x_0=\frac{1}{2}\ln\left[\frac{2+B+\sqrt{1+B}}{B}\right]. \tag{6}$$

The quantity x_0 defines a length scale which can be identified as the ''radius'' of this excitation. In the limit of $B\ll 1$ we have $x_0\gg 1$ and $t(x)$ can be approximated by $\tanh(x-x_0)\tanh(x+x_0)$, i.e., a kink-antikink pair of the system without explicit dimerization. In the opposite limit $x_0=0$ and Eq. (5) becomes a kink solution of the static sine-Gordon equation corresponding to the dimerized chain, so that $t(x)$ interpoles between these limiting cases.

$\phi_0(x)=\arcsin[t(x)]$ winds a complete round clockwise or counterclockwise. Therefore this excitation carries $S_z=\pm 1$. The $S_z=0$ component of this triplet excitation could be taken into account in our semiclassical approach by including the periodic time-dependent solution of the field equation which cannot be obtained by a boosting of the static solution $t(x)$. After quantization, this solution will give additional singlet states which are not taken into account in the quantum states generated by the quantization of $t(x)$. For the single sine-Gordon equation these are the breatherlike solutions. Furthermore, DHN have shown that the first breather is nothing but a renormalized meson. In this context the n-excited breather state is considered as a bound state of n mesons. For our DFSG equation there are no analytic expressions for these breather solutions. We will consider in the following that a renormalized meson corresponds to the $S_z=0$ component of our triplet excitation. That is to say, for the SU(2)-invariant model we should expect that after an appropriated resummation of the perturbative series the meson mass Δ will be equal to the soliton mass to be introduced below.

To discuss the physical content of solution (5) we show in Fig. (1) the unstaggered part of the local magnetization $\langle S_i^z\rangle[(1/2\pi)\partial_x\phi$ in the bosonic representation] for different values of the ratio of the parameters B corresponding to g_1 smaller than, equal to, or greater than g_2. The correlation length (ξ) has been fixed to be 10 times the lattice constant

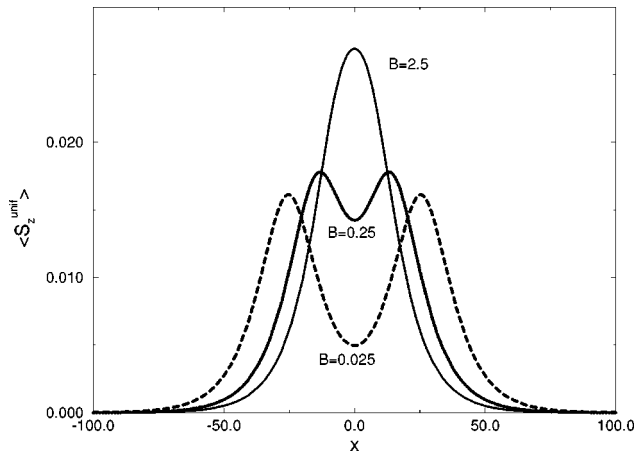

FIG. 1. Uniform part of the local magnetization carried by the configuration defined by $t(x)$ for three values of the parameter B.

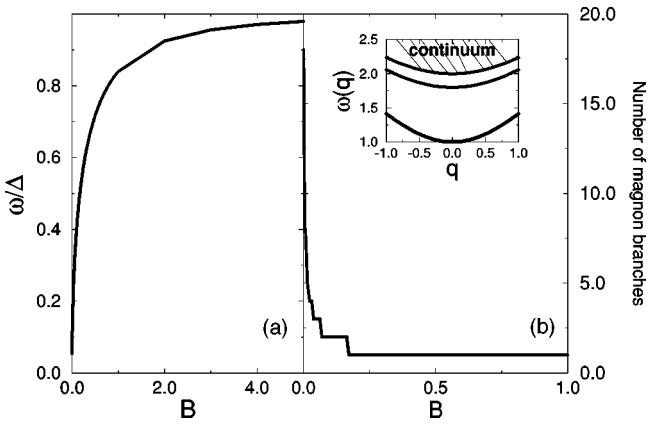

FIG. 2. (a) The evolution of the nonzero eigenfrequency of the fluctuation operator as obtained by numerical integration of Eq. (7). (b) The number of magnon branches predicted by the semiclassical calculation. The inset shows a typical low-energy spectrum.

in this figure. The figure has been obtained by freezing $t(x)$. This corresponds to the physical situation where two nonmagnetic impurities cut the chain and fix the dimerization phase at the border. This situation has been recently studied by different numerical techniques.[1] Note the similarities of the behavior shown in Fig. 1 and the one of Fig. 3(a) of Ref. 1. For the clean translational-invariant system the local magnetization is x independent as the result of the combination of this pattern center at the different sites of the chain.

Only for very low B are there two well-separated peaks corresponding to two spin-1/2 excitations at a distance of the order x_0/ξ. For increasing B these two peaks are washed up and a single spin-1 excitation emerges at the chain center. All the intermediate spins in this configuration are excited from their value in the ground state. The excitation we are dealing with is therefore an extended spin-1 magnon which dissociates into two independent spinons for very weak dimerization and collapses in the magnon of the dimerized chain in the opposite strong dimerization limit. Note that at this leading order of our semiclassical expansion this is a rigid configuration which translates as a whole.

We now include Gaussian fluctuations around this classical solution. The eigenvalue problem of the fluctuation operator corresponds to a Schrödinger-like equation which reads as

$$[-\partial_x^2+V(x)]\psi=E\psi,$$

$$V(x)=-\frac{1}{1+B}\{Bt+[1-2t(x)^2]\}, \tag{7}$$

where we have made the substitution $x\to x/\xi$. The eigenfrequencies are given by $\omega=\Delta\sqrt{E}$. Equation (7) has a zero-energy solution (with eigenfunction $\psi=\partial_x\phi_0$); this is connected with the translational mode arising in the broken of translational invariance of $t(x)$. We recall that this is the only bound state of the fluctuation operator for the case of single sine-Gordon solitons. For the present case we find in addition another bound state which split from this zero mode for finite B. For increasing B the energy of this mode increases going to the continuum spectra of $V(x)$ for $B\to\infty$. In Fig. 2 we show the evolution of this eigenvalue with B. This figure has been obtained by numerical integration of Eq. (7).

The excitation spectra of the theory in the sector of $Sz=\pm 1$ is spanned by the following states.

(i) The state of the quantum particle (of mass M) built around $t(x)$. We identify this as belonging to a one-magnon branch with dispersion $E(p)=u\sqrt{p^2+M^2}$.

(ii) The excited states of the magnon of mass $M^*=M+n\omega$. There are as much as additional triplet branches as $n\omega$ reaches the value Δ where the continuum of the Schrödinger equation starts. This continuum corresponds to (iii), next.

(iii) Labeling by q the continuum of level of Eq. (7), they are $\omega(q)=u\sqrt{q^2+1/\xi^2}$. This is just the kinetic energy of a meson with momentum q. Therefore this state corresponds to the scattering of a meson in the presence of a soliton. Moreover, when one of the continuum modes is excited once, we get a two-particle meson-soliton state. As we have associated a meson with the elementary $S_z=0$ excitation of the theory these excitations correspond to the $S_z=1$ component of the two-magnon continuum of our original spin chain.

The semiclassical calculation predicts the appearance of additional equispaced magnon branches. The number of these additional branches diverges as B goes to zero; this is nothing but the two-spinon continuum of the undimerized chain. For decreasing dimerization or increasing frustration the number of excited magnon states decreases until a critical value of B. Beyond this critical value only two magnon branches are found. In Fig. 2(b) we show the behavior previously discussed. The insert gives our prediction for the low-energy spectra for B greater than the critical value. Previous exact diagonalization studies of the spectra of Hamiltonian (1) have shown the appearance of an additional triplet branch[7,2] confirming this picture. The increase of the number of the triplet branches with δ has also recently seen in numerical studies of this system.[1]

Now, we address the question of the contact of this semiclassical approach and previous work assuming a linear confinement potential between the spinons.

For $B\ll 1$ (weak dimerization limit) it is customary to think the problem as one of two interacting kinks as has been recently proposed.[3,1] If they are well separated, their interaction is given by an attractive linear potential, the one arising in the term proportional to g_1 in Eq. (2). At low energy the

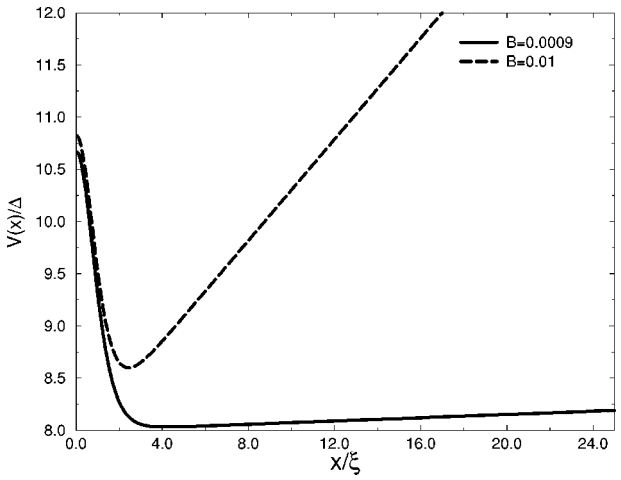

FIG. 3. Kink-antikink interaction potential as defined in the text.

spectra of the system correspond to one of two particle interacting via this linear potential. A ladder of bound states is obtained by solution of an effective Schrödinger equation. At high enough energy these bound states are truncated because it becomes favorable to create a new kink-antikink pair than to excite one of them. This is essentially the scenario discussed in Ref. 3.

Let us define an effective kink-antikink potential by the following procedure: take Eq. (5) as a suitable kink-antikink form with x_0 a variable distance; replace this form in Eq. (2) so that the x_0 dependence of the total energy gives our kink-antikink interaction energy. The result is shown in Fig. 3 for two small values of B where the kinks are expected to be well-defined excitations.

Two competing interactions could be clearly identified. An attractive linear interaction and a repulsive one acting at a small distance. The repulsive interaction originates on the finite width of the kinks. The value of x_0 given in Eq. (6) represents the minimum of the total potential. For very small B the slope of the linear potential is small and this minimum is not well defined. The kinks and antikinks will be always far apart and they never ''see'' the barrier. Therefore the linear approximation for the kink-antikink potential will give essentially the same result as a potential like the one shown in the figure. The semiclassical approach gives only poor quantitative results in this zone because it describes the problem as the one of harmonic oscillators with a very small frequency. However, the general qualitative behavior of the spectra is well reproduced, i.e., the divergence of the number of excited states in the limit of no dimerization.

For increasing B, a well-defined minimum appears in the potential energy. Now, at low energy the kink-antikink pair oscillates around this minimum as bounded by a spring. Our system behaves as a vibrating molecule made by a kink and an antikink. The semiclassical approximation previously discussed precisely describes the quantum state of this harmonic oscillator.

By further increasing B the kinks lose their identity; $t(x)$ becomes almost a kink solution of the SG theory with $g_2 = 0$. The semiclassical result represents an internal oscillation mode in which the kink wave form undergoes a harmonically varying shape change localized about the kink center.

Note that even for very small B the kinks are not well separated in the order of their width; therefore, we should associate the excitation in a broad range of the parameters as a unique magnon dispersed over a great number of spins.

Finally we analyze the experimental situation in $CuGeO_3$. Neutron scattering measurements of the magnetic spectra [13] show only one dispersive excitation before the continuum. The excited states previously discussed have not been found in these experiments. Two possible reasons could be given. As has recently been shown by numerical diagonalization[1] the spectral weight of these states is very small. Moreover, in the original spin-phonon model the inclusion of the interchain elastic coupling[10] implies that spins interact with transversal acoustic phonons. Therefore this excited state could decay in acoustic phonons, thus broadening the magnon peak. More experimental and theoretical work will be needed to elucidate this point.

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