Soliton approach to spin-Peierls antiferromagnets: Large-scale numerical results

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A simple intuitive picture of spin-Peierls antiferromagnets arises from regarding the elementary excitations as $S=1/2$ solitons. We investigate these excitations numerically in a phononless model where spontaneous dimerization arises from frustration and the interchain coupling is treated in mean field theory. It is shown that in a strictly one-dimensional system without any explicit dimerization, soliton-antisoliton bound-states do not form and the solitons are repelled by impurities. Couplings to the three-dimensional lattice produce an effective confining potential and we show that in this case solitons bind to antisolitons and to impurities, with the number of such bound-states increasing as the interchain coupling goes to 0. [S0163-1829(98)52746-4]

The discovery of a spontaneous lattice dimerization induced by quasi-one-dimensional antiferromagnetic interactions, the spin-Peierls effect, in CuGeO$_3$ has sparked renewed experimental$^{1-10}$ and theoretical interest in this field. Subjects of current interest include the nature of the excitations in the dimerized phase,$^{11-15}$ the effect of impurities,$^{16-18}$ and the effect of a magnetic field.$^{19-21}$ Sharp resonances have been observed in inelastic neutron$^8$ and light$^9$ scattering experiments. A simple intuitive picture of these phenomena is provided by the soliton model, introduced in the context of frustrated spin chains by Shastry and Sutherland$^{22}$ and discussed for example by Khomskii and collaborators$^{23}$ as well as others.$^{13,24-27}$ This model is based on the assumption that all interchain interactions, both magnetic and elastic, are weak. While this assumption may not be very good for CuGeO$_3$, it is possible that other spin-Peierls systems may be found which are more one-dimensional.

In the absence of any explicit dimerization a completely decoupled single $S=1/2$ chain can still have a *spontaneously* dimerized ground state due to spin-phonon interactions or due to frustrating next-nearest-neighbor interactions. The ground state is two-fold degenerate, corresponding to the two possible dimerizations $A$ and $B$, and the fundamental excitations are expected to be massive $S=1/2$ solitons $s$, and antisolitons $\bar{s}$, with a gap $\Delta_{sol}$, living on different sublattices, separating the two different dimerizations. It is sometimes assumed that no soliton-antisoliton bound states form in this model and that solitons are repelled by nonmagnetic impurities, i.e., by the ends of an open chain, as we demonstrate below. Neither of these assumptions is obvious and indeed some approaches make assumptions in contradiction to these.$^{16}$

It follows from general principles that spontaneous dimerization disappears at any non-zero $T$, due to a finite density of solitons, for a strictly one-dimensional (1D) system. Inter-chain interactions, either magnetic or elastic, can fundamentally change the situation. Spontaneous dimerization is now robust against the appearance of solitons. A soliton-antisoliton pair on a particular chain separated by some distance $r$ leaves a region of the chain in the wrong ground state relative to the neighboring chains. The consequence is an energy cost $\lambda r$ where $\lambda$ is determined by the interchain interactions. Such a linear potential is confining; the soliton and antisoliton cannot escape from each other and behave analogously to quark-antiquark pairs. Associated with this stabilization of the spontaneously dimerized phase is a drastic change in the excitation spectrum. As proposed by one of us,$^{25}$ low-lying excitations corresponding to soliton-antisoliton bound states now have to occur. These excitations will have spin $S=1$ or 0 and energy $E=2\Delta_{sol}+E_b$, where $E_b$ is the binding energy. There is no soliton continuum due to the confining nature of the interaction (i.e., the fact that it grows without limit at large separation), however a $s\bar{s}-s\bar{s}$ continuum can occur beginning at the lowest lying $S=2$ states. At this energy $E_b$ exceeds $2\Delta_{sol}$ and it becomes energetically favorable to create a new $s\bar{s}$ pair. Furthermore, a soliton is bound by a linear potential to each nonmagnetic defect. It is convenient to model the linear potential using a mean field treatment of interchain couplings. In this approach the interchain couplings simply provide a term in the single-chain Hamiltonian which favors one or the other of the two dimerized states. It is important to realize that the soliton picture is only expected to be useful if the interchain couplings are relatively small so that the solitons, although confined, still behave in a quasigneindependent fashion at short distances. If the interchain couplings are large then the soliton and antisoliton never get far apart compared to their intrinsic size (Compton wavelength) and behave effectively as a single well-defined magnon. Consequently, the soliton picture ceases to have much utility.
In this paper we make an extensive numerical investigation of this soliton picture using the simplest possible model:

\[ H = J \sum_i \{ [(1 + \delta(-1)^i)]S_i \cdot S_{i+1} + J_2 S_i \cdot S_{i+2} \} \]

where \( \delta \) is a spin only Hamiltonian with spontaneous dimerization arising from a second nearest-neighbor interaction \( J_2 \), and explicit dimerization (representing the effect of the neighboring chains) due to an alternating nearest-neighbor interaction \( \delta \). For \( \delta = 0 \) this model exhibits a second-order phase-transition to a dimerized phase at \( J_{2c} = 0.2411 \). As a representative of the dimerized phase we shall take the vicinity of the Majumdar-Ghosh (MG) model, \( J_{2c} = \frac{1}{2} \), since at this point the correlation length is vanishing and we therefore expect only minimal finite-size corrections. We have performed exact diagonalizations of up to 32 sites as well as density matrix renormalization group (DMRG) calculations with \( m = 128 \) states. Our main results are as follows: When \( \delta = 0 \) we find that there are no low-energy bound states near zero crystal momentum for \( J_2 \ll \frac{1}{2} \). For \( J_2 > J_{2c} \) the solitons behave as free massive particles; we explicitly calculate the gap and dispersion of the solitons and show numerically that the soliton is repelled by the ends of an open chain, behaving like a massive particle in a box. When \( \delta \neq 0 \) we demonstrate that a ladder of \( S = 1.0 \) soliton-antisoliton bound states is formed, increasing in number with decreasing \( \delta \) and giving rise to a range of well-defined peaks in the dynamical structure factor close to \( q = \pi \). In this case, an isolated soliton will bind to one of the chain ends. We begin by discussing our results for \( \delta = 0 \).

Odd-length systems. The behavior of an isolated soliton can be studied by considering odd-length systems for which the ground state has \( S_{\text{tot}} = 1/2 \). In Fig. 1(a) we show results for the lowest-lying \( S_{\text{tot}} = 1/2, 3/2 \) states (open and full circles) of a 23-site chain at the MG point. The ground-state energy per spin of an even-length system, for \( J_2 = 1/2 \) and open boundary conditions, is \(-3J/8\) and we use this value to define zero energy for the odd-site system. A well-defined \( S = 1/2 \) mode corresponding to the dispersion of the soliton is clearly visible around \( k = \pi/2 \). Approximating the soliton as a single unpaired spin between the two dimer ground states gives a rigorous upper bound on the soliton dispersion relation of \( E = (J/2)(5/4 + \cos 2k) \). This is shown as the solid line in Fig. 1 and agrees very well with the numerical data. Including three- and five-spin structures in the variational soliton wave function reduces the rigorous upper bound on the soliton gap \( \Delta_s / J \) (at \( k = \pi/2 \)) from 0.125 to 0.11701 in remarkably good agreement with our best DMRG estimate of 0.1170(2). In Fig. 1(b) \( \langle S_z^2 \rangle \) is shown for a \( L = 101 \)-site system in the \( S_{\text{tot}} = 1/2 \) ground state. Clearly the soliton is repelled by the open ends and enters approximately a particle in a box state \( \langle S_z^2 \rangle \approx \{ \text{const} + \langle -1 \rangle \sin^2[\pi L / (L+1)] \} \) indicated by the solid circles. We have calculated the soliton gap defined as the \( \Delta_{s/o} = \lim_{L \to \infty} E_{L+1} - \{ E_L + E(L+2) \}/2 \) (L even) as a function of \( J_2 \). Our DMRG results are shown in Fig. 2. As \( J_2 \) is increased from \( J_{2c} \) the soliton gap should increase exponentially:

\[ \Delta_{s/o} = \exp \left[-b(J_2 - J_{2c})\right] \]

The numerical data seem largely consistent with such a behavior as can be seen in the inset of Fig. 2 although \( \Delta_{s/o} \) quickly becomes too small for a reliable determination.

Even-length systems. DMRG calculations can be performed using spin inversion as a symmetry in which case even and odd multiplets can be distinguished. Performing such calculations for \( J_2 = 1/2 \) we find that the gap to the lowest-lying triplet and singlet excitations are degenerate in the thermodynamic limit of \( \Delta_{00} / J = \Delta_{01} / J = 0.2340(2) \), precisely twice \( \Delta_{s/o} \). This degeneracy persists for \( J_2 < 1/2 \) and we conclude that there are no low-energy bound states near zero crystal momentum, although such states could possibly occur for \( J_2 > 1/2 \). On the other hand, at the MG point, Caspers and Magnus (CM) (Ref. 33) have shown that there are exact singlet and triplet bound states at \( q = \pi/2 \), degenerate with energy \( E/J = 1 \). The triplet state saturates the total weight of the dynamical structure factor which is a single delta peak at \( q = \pi/2, E = J \). The lowest-lying \( S = 2 \) state at \( q = \pi/2 \) marking the onset of the continuum has \( E \approx 1.2J \) and is clearly separated from the bound state. Exact diagonaliza-

![Figure 1](image1.png)

**FIG. 1.** (a) The single soliton dispersion relation at the MG point for a 23-site chain. The solid line indicates the Shastry-Sutherland variational estimate \( \omega_{\text{var}}(k) = (J/2)(5/4 + \cos 2k) \). (b) \( \langle S_z^2 \rangle \) as a function of \( \delta \). DMRG results are shown for \( L = 101 \), with \( S_{\text{tot}} = 1/2, m = 128 \).

![Figure 2](image2.png)

**FIG. 2.** The soliton gap as a function of \( J_2 \).
tion results are consistent with the occurrence of bound states for a small range of momenta close to $q = \pi/2$. It is interesting to compare this with the predictions of the sine-Gordon field theory, expected to be valid near $J_2$. This relativistic field theory for coupling constant $\beta^2 = 8\pi$ has no bound states. By Lorentz invariance, if there are no bound states at zero momentum there cannot be any at finite momentum either. However, a resonance with a finite lifetime would become longer lived at finite momentum due to relativistic time dilation. Clearly the non-Lorentz invariance at the MG point is important in allowing for bound states only at finite momentum.

Explicitly dimerized systems. We next investigate the model with an alternating interaction $\delta \neq 0$, added. From a numerical perspective two effects complicate such an investigation; the exponentially diverging correlation length $\xi$ as $J_2$ is approached and the size $l_{x,3}$ of a $s\bar{s}$ bound state, diverging as $\delta \to 0$. Note that $l_{x,3}$ increases with the energy of the bound state. We need to have $L \gg \xi, l_{x,3}$. In Fig. 3(a) we show DMRG results for the on-site magnetization $\langle S_i^z \rangle$ in the lowest-lying two-soliton state $J_2=1/2, S_{z,0}=1, P=-1, L=100$ for various different values of $\delta$. For $\delta = 0$ two well-defined peaks can be seen in the uniform part of $\langle S_i^z \rangle$, separated by $L/2$. As $\delta$ is increased the formation of a soliton bound state is clearly visible and the excitation becomes more and more magnonlike. In all cases the chain starts and ends with a strong link. Chains starting and ending with a weak link will have edgelike excitations. In Fig. 3(f) we show DMRG results for $\langle S_i^z \rangle$ at the MG point for different values of $\delta$ as calculated in the $S_{z,0}=1/2$ ground state. In this case $L=51$ is odd and the first link of the chain is weak. Clearly the soliton binds to the end of the chain, in agreement with other recent results. However, as $\delta$ is decreased the maximum in $\langle S_i^z \rangle$ moves further and further inside the chain; only for the largest value of $\delta$ is the maximum at the first chain site, as has also been found in the impurity susceptibility. From these results we can roughly estimate the size of a bound state $l_{x,3}$ as a function of $\delta$. We see that we can only hope to determine the excited states if $J_2 \approx 1/2$, if $\delta > 0.05$ due to finite-size effects.

We now examine the excitation spectrum for $\delta \neq 0$. In Fig. 4(a) we show the lowest-lying triplet, singlet, and quintuplet excitations vs $k=2q$ for a system with $L=28, J_2=1/2, \delta=0.05$. Three well-defined triplet branches are clearly visible below the continuum (the quintuplet $S=2$ states) as well as two singlet branches. The third and highest-lying singlet appears to remain marginally below the continuum at $k=0$ as can be seen for the $L=32$ results shown to the left of the panel. The inset in Fig. 4(a) shows the same spectrum but for $L=20, J_2=0.45, \delta=0.1$. In this case finite-size corrections are significantly smaller and we see that only two triplet and two singlet branches are below the continuum. We take these results as clear evidence that the number of bound states increases as $\delta \to 0$. At still larger $\delta = 0.2, J_2=0.35$ only two triplets and one singlet are found. The point $J_2=0.45, \delta=0.1$ is along the disorder line $\delta=1-2J_s$ where the excited states of Caspers and Magnus remain exact, as noted by Brehmer et al., but they are no longer degenerate. These two states are indicated by an arrow in the inset (CM). As was the case at the MG point the triplet state saturates the structure factor at $k=\pi$ along the disorder line, i.e., $S(k, \omega)$ is a single delta peak at the energy of the triplet. In Fig. 4(b) we show results for the dynamical structure factor $S^{21}(q, \omega)$ for the $L=28$ results in panel 4(a). Note the change between $k$ and $q$ from panel (a) to (b), $k = n \pi / 7, q = n \pi / 14$. Here, $S^{21}(q, \omega) = \sum_n \langle \Phi_n | S_z(q) | \Phi_0 \rangle^2 \delta(\omega - E_n + E_0)$, where $E_0 (E_n)$ is (are) the energy(ies) of the ground state $\Phi_0$ (triplet states $\Phi_n$), $S_z(q) = \sum \exp(iqL) S_i^z / \sqrt{L}$ is the Fourier transform of $S_i^z$. 

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**FIG. 3.** (a) The on-site magnetization for an open even-length chain, $L = 100$, at the MG point, in the two-soliton state $S_{z,0}=1$ and parity $P=-1$. DMRG results with $m=128$ for different values of the explicit dimerization $\delta$ is shown. $m=128$ was used in the calculation. The solid line, for $\delta = 0$, indicates the uniform part of the magnetization. (f) The on-site magnetization for an open odd-length chain, $L = 51$, at the MG point, with $S_{z,0}=1/2$. DMRG results with $m=128$ for different values of the explicit dimerization $\delta$ is shown. The chain begins with a weak link.

**FIG. 4.** (a) The lowest-lying triplet (solid circles), singlets (open circles), and quintuplets (crosses) for $J_2=0.5, \delta=0.05, L=28$, as a function of $k=2q$. Results for $L=32, k=0$ are shown to the left. The inset shows the same spectrum for $J_2=0.45, \delta=0.10, L=20$. (b) The dynamical structure factor $S^{21}(q, \omega)$ for $J_2=0.5, \delta=0.05, L=28$ and a broadening of $\epsilon=0.04J$. The solid, dashed, and dotted lines indicate the three-triplet branches.
and $\delta_c$ is a Lorentzian of width $\varepsilon$. The three triplet branches are most clearly visible around $q = \pi$. Neutron-scattering experiments on CuGeO$_3$ have so far only seen evidence for a single triplet branch at $q = \pi$ (Ref. 8) which can be interpreted as a $s\bar{s}$ bound state. CuGeO$_3$ can be approximately described by Eq. (1) with $J_2 = 0.36, \delta = 0.014$. Hence, it is possible, but not necessary, that more bound states exist. However, the weight of a peak due to an eventual second triplet branch should be much smaller and could have been missed. In addition, Raman-scattering experiments$^9$ have shown clear evidence for the accompanying singlet bound state below the continuum.$^{9,35}$ Hence, at least one pair of triplet-singlet excitations have been experimentally observed. More importantly, it is possible that other compounds with $J_2 > J_{2c}$ and a small explicit dimerization $\delta \neq 0$, may yield more clear evidence for a ladder of soliton bound states which would consolidate the soliton picture. In conclusion we have demonstrated that well-defined soliton excitations occur in frustrated spin chains for $J_2 > J_{2c}$. In the absence of interchain coupling ($\delta = 0$) the solitons do not bind and are repelled by the chain ends. In the presence of interchain coupling ($\delta \neq 0$) a number of stable bound states occur and isolated solitons are attracted to the chain ends.

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35We have numerically checked that singlet bound states yield significant weight in the Raman spectrum.