Soliton Approach to Spin-Peierls Antiferromagnets: Large-Scale Numerical Results

Erik Sørensen[a], Ian Affleck[b], David Augier[a] and Didier Poilblanc[a]
[a]*Laboratoire de Physique Quantique & UMR CNRS 5626, Université Paul Sabatier, 31062 Toulouse, France*
[b]*Department of Physics and Astronomy, and Canadian Institute for Advanced Research, University of British Columbia, Vancouver, BC, V6T 1Z1, Canada*
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A simple intuitive picture of spin-Peierls antiferromagnets arises from regarding the elementary excitations as S=1/2 solitons. In a strictly one-dimensional system these excitations are assumed not to form bound-states and to be repelled by impurities. Couplings to the three-dimensional lattice are assumed to produce an effective confining potential which binds solitons to antisolitons and to impurities, with the number of bound-states increasing as the interchain coupling goes to 0. We investigate these various assumptions numerically in a phononless model where spontaneous dimerization arises from frustration and the interchain coupling is treated in mean field theory.

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]. A simple intuitive picture of these phenomena is provided by the soliton model, first 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 Δ_{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 non-magnetic 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 ones [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. Interchain 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 λr where λ 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 anti-quark 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 non-magnetic 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 quasi-independent 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:

$$H = J\sum_i [(1 + \delta(-1)^i)\mathbf{S}_i \cdot \mathbf{S}_{i+1} + J_2 \mathbf{S}_i \cdot \mathbf{S}_{i+1}], \qquad (1)$$

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, δ. For $\delta = 0$ this model exhibits a second order phase-transition to a dimerized phase at $J_{2c} \simeq 0.2411$ [28]. As a representative of the dimerized phase we shall take the vicinity of the Majumdar-Ghosh (MG) model [29], $J_2 = \frac{1}{2}$, 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 $J_2 \leq \frac{1}{2}$. For $J_2 > J_{2c}$ the solitons behave as free massive particles [30]; 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 anti-soliton bound-states is formed, increasing in number with decreasing δ 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

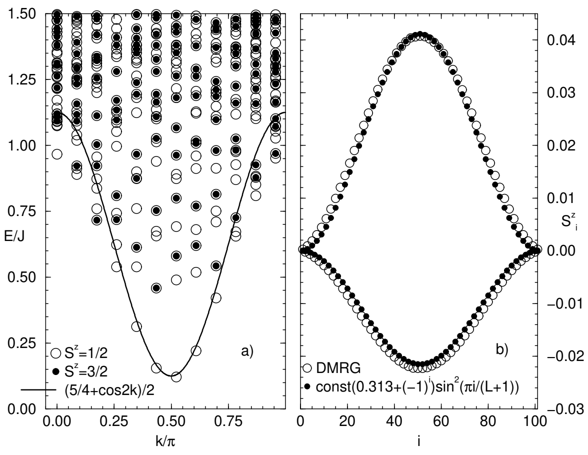

figure 1: a) The single soliton dispersion relation at the MG point for a 23 site chain. The solid line indicates the Shastry-Sutherland variational estimate $\omega_{sol}(k) = (J/2)(5/4+\cos 2k)$. b) $< S^z_i >$ as a function of i. DMRG results are shown for L=101, with $S^z_{tot} = 1/2$, $m = 128$.

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 $S_{tot} = 1/2$. In Fig. 1a we show results for the lowest-lying $S^z_{\rm tot} = 1/2, 3/2$ states (open and full circles) of a 23 site chain at the MG point. The ground-state energy per spin of an even length sys-

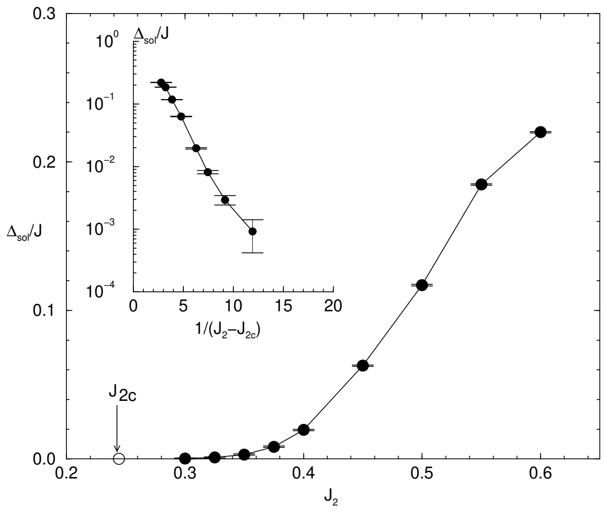

figure 2: The soliton gap as a function of J_2.

tem, 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 [22,31] 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 3 and 5 spin structures in the variational soliton wave-function reduces [32] the rigorous upper bound on the soliton gap, Δ_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) [30]. In Fig. 1b $< S^z_i >$ is shown for a $L = 101$ site system in the $S^z_{tot} = 1/2$ ground-state. Clearly the soliton is repelled by the open ends and enters approximately a particle in a box state $< S^z_i > \simeq \text{const} + (-1)^i \sin^2(\pi i/(L+1)$ indicated by the solid circles. We have calculated the soliton gap defined as the $\Delta_{sol} = \lim_{L\to\infty} E(L+1) - (E(L) + E(L+2))/2$ (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 [25]: $\Delta_{sol} = \exp(-b/(J_2 - J_{2c}))$. The numerical data seems largely consistent with such a behavior as can be seen in the inset of Fig. 2 although Δ_{sol} 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 $\Delta_{00}/J = \Delta_{01}/J = 0.2340(2)$, precisely twice Δ_{sol}. 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) [33] have shown that there are exact singlet and triplet bound-state 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 on-set of the continuum has $E \simeq 1.2J$ and is clearly separated from the bound-state. Exact diagonalization 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_{2c}. This relativistic field theory, for coupling constant, $\beta^2 \approx 8\pi$ 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 life-time 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.

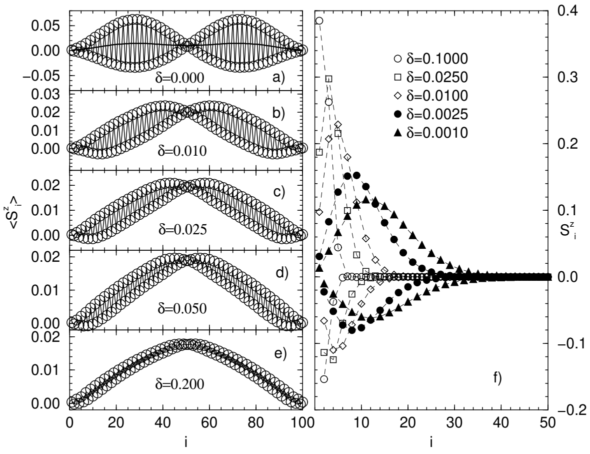

figure 3: a) The on-site magnetization for an *even* length chain, $L = 100$, at the MG point, in the two soliton state $S^z_{tot} = 1$ and parity $P = -1$. DMRG results with $m = 128$ for different values of the explicit dimerization δ is shown. $m = 128$ was used in the calculation. The solid line,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

Explicitly dimerized systems. We next investigate the model with an alternating interaction, $\delta \neq 0$, added. From a numerical perspective two effects complicate such

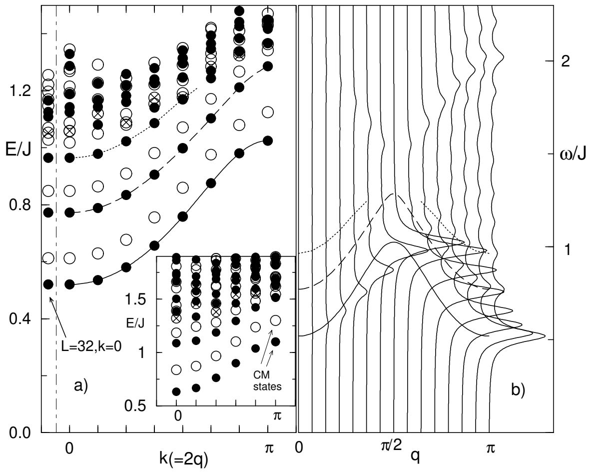

figure 4: a) The lowest lying triplet (solid circles), singlets (open circles) and quintuplets (crosses) for $J_2 = 0.5$, $\delta = 0.05$, $L = 28$, as a function of $k = 2q$. Results for $L = 32$, $k = 0$ are shown to the left. The inset shows the same spectrum from $J_2 = 0.45$, $\delta = 0.10$, $L = 20$. b) The dynamical structure factor $S^{zz}(q,\omega)$ for $J_2 = 0.5$, $\delta = 0.05$, $L = 28$ and a broadening of $\varepsilon = 0.04J$. The solid, dashed and dotted lines indicate the 3 triplet branches.

an investigation; The exponentially diverging correlation length ξ as J_{2c} is approached and the size, $l_{s\bar{s}}$, of a $s\bar{s}$ bound-state, diverging as $\delta \to 0$. Note that $l_{s\bar{s}}$ increases with the energy of the bound-state. We need to have $L \gg \xi, l_{s\bar{s}}$. In Fig. 3a we show DMRG results for the on-site magnetization $< S^z_i >$ in the lowest-lying two soliton state $J_2 = 1/2, S^z_{tot} = 1, P = -1, L = 100$ for various different values of δ. For $\delta = 0$ two well-defined peaks can be seen in the uniform part of $< S^z_i >$, separated by $L/2$. As δ is increased the formation of a soliton bound-state is clearly visible and the excitation becomes more and more magnon like. In all cases the chain starts and ends with a strong link. Chains starting and ending with a weak link will have edge like excitations [17]. In Fig. 3f we show DMRG results for $< S^z_i >$ at the MG point for different values of δ as calculated in the $S^z_{tot} = 1/2$ 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 [17]. However, as δ is decreased the maximum in $< S^z_i >$ moves further and further inside the chain, only for the largest value of δ is the maximum at the first chain site, as has also been found in the impurity susceptibility [17]. From these results we can roughly estimate the size of a bound-state, $l_{s\bar{s}}$, as a function of δ. 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. 4a 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. 4a 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 a one singlet is found [15]. The point $J_2 = 0.45, \delta = 0.1$ is along the disorder line $\delta = 1 - 2J_2$ where the excited states of Caspers and Magnus [33] remain exact, as noted by Brehmer et al [13], however, 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. 4b we show results for the dynamical structure factor $S^{zz}(q, \omega)$ for the $L = 28$ results in panel a. Note the change between k and q from panel a to b, $k = n\pi/7$, $q = n\pi/14$. Here, $S^{zz}(q, \omega) = \sum_n |\langle \Phi_n | S_z(q) | \Phi_0 \rangle|^2 \delta_\varepsilon(\omega - E_n + E_0)$, where E_0 (E_n) is (are) the energy(ies) of the ground-state Φ_0 (triplet states Φ_n), $S_z(q) = \sum_j e^{iqr_j} S_j/\sqrt{L}$ is the Fourier transform of S_z^j and δ_ε is a Lorentzian of width ε. 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 $q = \pi$. However, the weight of a peak due to an eventual second triplet branch should be much smaller and could have been missed. Secondly, it is possible that other compounds 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. 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 occurs and isolated solitons are attracted to the chain ends. We thank IDRIS (Orsay) for allocation of CPU time on the C94 and C98 CRAY supercomputers. The research of IA is supported in part by NSERC of Canada.

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