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Elementary excitations in the gapped phase of a frustrated $S = 1/2$ spin ladder: from spinons to the Haldane triplet

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Abstract. We use the variational matrix-product *ansatz* to study elementary excitations in the $S = \frac{1}{2}$ ladder with additional diagonal coupling, equivalent to a single $S = \frac{1}{2}$ chain with alternating exchange and next-nearest-neighbour interaction. In the absence of alternation, the elementary excitation consists of two free $S = \frac{1}{2}$ particles ('spinons') which are solitons in the dimer order. When the nearest-neighbour exchange alternates, the 'spinons' are confined into one $S = 1$ excitation which is a soliton in the generalized string order. The variational results are found to be in qualitative agreement with the exact-diagonalization data for 24 spins. We argue that such an approach gives a reasonably good description over a wide range of the model parameters.

1. Introduction

Spin ladders continue to attract much attention as structures intermediate between one- and two-dimensional forms and possibly important for the understanding of high-T_c superconductivity [1]. On the other hand, there exists a close relationship between 'generalized' spin ladders (with an additional diagonal coupling), antiferromagnetic chains with frustrating next-nearest-neighbour interaction, and the Haldane systems.

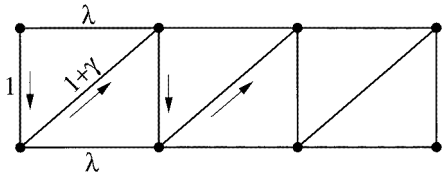

Figure 1. The generalized spin ladder with additional diagonal (frustrating) coupling. The arrows show the way in which the sites are numbered to map this system onto a single chain with nearest- and next-nearest-neighbour interactions.

In the present paper we study elementary excitations of the generalized $S = \frac{1}{2}$ spin ladder model (equivalent to a single-zigzag spin chain with alternation and frustration). The model is described by the Hamiltonian (see figure 1)

$$\widehat{H} = \sum_n \boldsymbol{S}_{1,n} \cdot \boldsymbol{S}_{2,n} + (1+\gamma) \sum_n \boldsymbol{S}_{1,n} \cdot \boldsymbol{S}_{2,n+1} + \lambda \sum_n (\boldsymbol{S}_{1,n} \cdot \boldsymbol{S}_{1,n+1} + \boldsymbol{S}_{2,n} \cdot \boldsymbol{S}_{2,n+1}) \quad (1)$$

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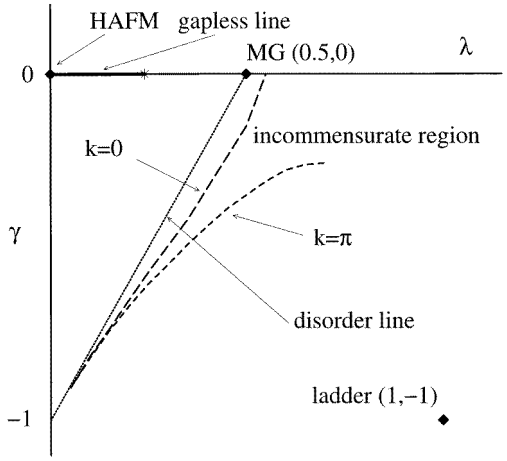

Figure 2. The phase diagram of the generalized ladder. The interval of the line $\gamma = 0$ for $0 < \lambda < \lambda_c \approx 0.2411$ is gapless, and the other part of the diagram is gapped. The $k = 0$ and $k = \pi$ boundaries of the incommensurate region are variational estimates for the corresponding Lifshitz lines determined from the variation of the wave vector k of the lowest excitation mode. The disorder line, where spin–spin correlations in the real space become incommensurate, for the $k = 0$ boundary is known [34, 2] to be $\gamma = 2\lambda - 1$; for the $k = \pi$ boundary the exact position of the disorder line is unknown.

where $\lambda > 0$ determines the strength of the next-nearest-neighbour interaction, and γ corresponds to alternation of the nearest-neighbour exchange, whose strength is set to be unity. This model has rich behaviour depending on the values of parameters λ and γ, and its phase diagram (see figure 2) is rather well understood [2, 3] (at least for the half-plane $\lambda > 0$; for negative λ the situation is less clear [4]). Without loss of generality, we will assume that $\gamma < 0$, since there is an obvious symmetry transformation [3] relating the half-plane $\gamma > 0$ with the strip $-1 < \gamma < 0$. The 'symmetry line' $\gamma = 0$ is peculiar because it is the line of transition between dimerized phases with different signs of the dimer order. Within the interval $0 < \lambda < \lambda_c \approx 0.24$ this transition is of second order, the ground state is unique and nondimerized, and the corresponding spectra are gapless; on the other part of this line the transition is of first order, so for $\lambda > \lambda_c$, $\gamma = 0$ there are two degenerate dimerized ground states, and the system is gapped. The transition at $\lambda = \lambda_c$ has been well studied; see reference [5] for a review. Everywhere except at the symmetry line, the model (1) has a unique ground state with a finite gap above it. In the limit $\gamma \to -\infty$ the diagonal spins form effective $S = 1$ units, and the system becomes equivalent to the $S = 1$ Haldane chain, with the effective coupling constant $(1 + 2\lambda)/4$.

Elementary excitations of the generalized ladder, however, have been studied to a much lesser extent than its ground-state properties. The Heisenberg model ($\lambda = 0$, $\gamma = 0$) is exactly solvable by means of the Bethe *ansatz* technique, and the elementary excitations are pairs of noninteracting $S = \frac{1}{2}$ entities ('spinons') [6]. The ground state contains the Fermi sea of spinons, and the excitations are of the particle–hole type.

It is also known that at the so-called Majumdar–Ghosh (MG) point ($\gamma = 0$, $\lambda = \frac{1}{2}$), where the exact (twofold-degenerate) ground state is a simple product of singlet dimers [7], the elementary excitation can be approximately constructed as a pair of unbound spins above the completely dimerized state [8]. The elementary excitation is composed of two $S = \frac{1}{2}$ entities which are kinks in the dimer order and resemble spinons in that they

are 'almost free' (i.e. form scattering states for most values of momenta) in the case of unbroken translational invariance. When nonzero alternation is present, one may expect those 'spinons' to be confined into a single $S = 1$ particle [9–11].

In the Haldane limit (infinite alternation), the system has long-range hidden (string) order [12], and the elementary excitation is known [13–15] to be a soliton in the string order. The concept of string order was generalized to spin ladders [16–18] and it was shown that several ladder models exhibit long-range generalized string correlations [18]. It was argued [18] that the gapped phase of the spin ladder is the same as the Haldane phase of the effective $S = 1$ chain.

We construct the variational *ansatz* for the wave function of the elementary excitation in the form of a matrix product, using the recently proposed [3] matrix-product-states approach to the description of the ground-state properties of spin ladders. The ground state in this approach has a built-in generalized string order, and we construct the excitation as the $S = 1$ composite particle, which is a kink in the string order and consists of two bound $S = \frac{1}{2}$ entities. The wave function of the kink pair contains only one variational parameter, ξ, having the meaning of the average pair size (the localization length). We show that at the MG point ξ is infinite, and our *ansatz* reduces to that of Shastry and Sutherland [8]; on moving away from the MG point, ξ drops down very quickly to a value of about a few lattice constants. At the 'regular' ladder point ($\gamma = -1$, $\lambda = 1$) the dispersion relation as obtained from our *ansatz* agrees well with the results obtained by other authors using different techniques (see reference [1] and references therein). In the Haldane limit, ξ goes to zero, and our wave function transforms into the 'crackion' *ansatz* introduced by Fáth and Sólyom [14] (see also reference [19]) for the description of the Haldane triplet in the Affleck–Kennedy–Lieb–Tasaki (AKLT) model. We compare our variational results with the numerical data obtained through the exact diagonalization of a finite (24-spin) ladder system, and find a reasonable agreement between the two approaches. We conclude that our simple variational *ansatz* allows us to study analytically at a qualitative level the crossover from free to strongly bound spinons, giving a reasonably good description over a wide range of physical models.

The paper is organized as follows: in section 2 we introduce our *ansatz* for the elementary excitation. In section 3 we present results from the variational calculation and compare them with numerical data. The elementary excitations in different regions of the phase diagram are discussed. Finally, section 4 contains concluding remarks.

2. The two-spinon 'composite particle' *ansatz*

Recently, a variational wave function for the description of the ground-state properties of generalized spin ladders was proposed [3] in the form of a matrix-product (MP) state. The MP representation was first discussed by Fannes *et al* [20] in an abstract manner, and later by Klümper *et al* [21] for the $S = 1$ deformed VBS chain, and has found since then numerous applications in exact and variational calculations [22–25]. It should also be mentioned that the MP structure naturally appears in the thermodynamic and large-m limits of the density matrix renormalization group calculations [26, 27]. For periodic boundary conditions, the trial wave function for the ground state of the ladder consisting of $2N$ spins can be written as

$$|\Psi_0\rangle = \mathrm{Tr}(g_1 g_2 \cdots g_N) \tag{2a}$$

where

$$g_i(u, v) = u\left(\hat{1}|s\rangle_i\right) + v \sum_{\mu=0,\pm1} \widehat{\sigma}_\mu |t_\mu\rangle_i. \tag{2b}$$

Here the elementary matrix g_i is constructed from the singlet state $|s\rangle_i$ and three triplet states $|t_\mu\rangle_i$ of the ladder diagonals; $\widehat{\sigma}_\mu$ are the Pauli matrices in a spherical basis; $\sigma_0 = \sigma_z$ and $\sigma_{\pm1} = \mp(1/\sqrt{2})(\sigma_x \pm \mathrm{i}\sigma_y)$. The parameters u and v in the case of the absence of an external magnetic field can be chosen real, and they satisfy the normalization condition $u^2 + 3v^2 = 1$.

The wave function (2*a*) has the following remarkable properties [3]:

(i) for arbitrary u and v it is a global singlet (see also reference [25] for details);

(ii) it has a built-in generalized string order defined as 'diluted antiferromagnetic order': $|t_{+1}\rangle$ and $|t_{-1}\rangle$ should occur in perfect antiferromagnetic sequence, arbitrarily diluted by $|s\rangle$s and $|t_0\rangle$s;

(iii) both degenerate dimer ground states at the Majumdar–Ghosh point can be written in the above form, as can the 'valence-bond' AKLT state [28] which approximates the ground state in the effective $S = 1$ Haldane limit. The two dimer ground states at the MG point correspond to $u = 1$, $v = 0$ and $u = v = \frac{1}{2}$ respectively, and the AKLT state corresponds to zero singlet weight ($u = 0$, $v = 1/\sqrt{3}$).

The state (2*a*) has very short-ranged correlations and therefore cannot be considered as a good approximation in the gapless region of the phase diagram; we will thus restrict ourselves to the study of the gapped phase only.

The variational energy $E_0 = \langle\Psi_0|\widehat{H}|\Psi_0\rangle$ calculated with the trial function (2*a*) has at most two minima as a function of u, v: one is always located at $u = 1$, $v = 0$ and corresponds to singlets on the diagonal links, and the position of the other minimum (u_0, v_0) depends on λ and γ; this latter minimum is absent in certain regions of the phase diagram. The two minima have equal energies only at the MG point, and for any other choice of the model parameters they are inequivalent [3].

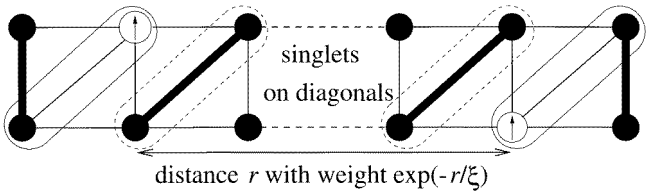

Figure 3. The structure of the variational two-spinon *ansatz* (3), (4). Ovals show the locations of matrices; solid ovals denote $g^{(0)}$ and dashed ones denote $\widetilde{g}$. Thick solid links represent singlet bonds (bonds inside dashed ovals are *always* pure dimer bonds, and bonds between the solid ovals become purely singlet only on the disorder line $\gamma = 2\lambda - 1$).

We construct the trial wave function for the elementary excitation, requiring the following:

(i) it should be a triplet;

(ii) it should be a soliton in the generalized string order as defined above;

(iii) it should be able to reproduce the *ansatz* of Shastry and Sutherland for the MG point [8], i.e. a pair of unbound spins connecting two degenerate dimer ground states, and the 'crackion' *ansatz* of Fáth and Sólyom [14].

One can check that the following construction satisfies the above requirements:

$$|n, n'; \mu\rangle = \mathrm{Tr}\left\{ \Big(\prod_{i=1}^{n} g_i^{(0)} \Big) \widehat{\sigma}_\mu^\dagger \prod_{i=n+1}^{n'} \widetilde{g}_i \prod_{i=n'+1}^{N} g_i^{(0)} \right\}. \tag{3}$$

Here $g_i^{(0)} = g_i(u_0, v_0)$ denotes the matrix corresponding to the variational ground state, and $\widetilde{g}_i = g_i(u = 1, v = 0)$ is the matrix describing singlet dimers on the diagonals (it is easy to see from (2*a*) that $\widetilde{g}_i$ is proportional to the unit matrix). In fact, the state (3) describes two domain walls which correspond to transitions between the two inequivalent variational ground states mentioned above; it is worth remarking that the states $|n, n'; \mu\rangle$ are not mutually orthogonal. The presence of $\widehat{\sigma}_\mu^\dagger$ ensures that this state breaks the generalized string order and has the total spin $S = 1$ and the z-projection $S_z = \mu$ (the general technique for constructing MP states with the given quantum numbers S, S_z can be found in reference [25]). The structure of the *ansatz* (3) is schematically shown in figure 3.

At the MG point, $u_0 = v_0 = \frac{1}{2}$, and one can straightforwardly check that in this case equation (3) describes a pair of unbound spins $\frac{1}{2}$ separating two completely dimerized regions, i.e. it reduces to the *ansatz* of Shastry and Sutherland. On the other hand, if $n = n'$ and $u_0 = 0$, then the state (3) is exactly the same as the 'crackion' of Fáth and Sólyom.

We use the following (unnormalized) trial wave function of the composite two-spinon excitation with a given total momentum k:

$$|k, q; \mu\rangle = \sum_{n' \geqslant n} \mathrm{e}^{\mathrm{i}k(n+n')/2} \mathrm{e}^{\mathrm{i}q(n-n')/2} \mathrm{e}^{-(n'-n)/\xi} |n, n'; \mu\rangle. \tag{4}$$

It contains two variational parameters, q and ξ, which can be considered as the real and imaginary parts of the relative momentum of the two spin-$\frac{1}{2}$ entities forming our composite particle. The parameter ξ has the meaning of a localization length, or the average size of the composite object, and nonzero q corresponds to the excitation of some internal degree of freedom. If the localization length diverges, $\xi \to \infty$, the wave function describes a triplet scattering state of two spinons, and finite ξ corresponds to a bound state.

On the disorder line $\gamma = 2\lambda - 1$, according to reference [3], the parameters u_0 and v_0 both equal $\frac{1}{2}$, and the structure of our variational *ansatz* becomes rather obvious: it describes a bound state of two Shastry–Sutherland kinks ('free spins' in a completely dimerized chain) with the localization length ξ.

The energy for such an excitation can be calculated in the usual way:

$$E(q, \xi, k) = \frac{\langle k, q; \mu | \widehat{H} - E_0 | k, q; \mu \rangle}{\langle k; \mu | k; \mu \rangle} \tag{5}$$

and has to be minimized over ξ and q, separately for any given k (as we will see below, it turns out that optimal ξ strongly depends on k). In this way one looks for a lowest variational state in a subspace with the total spin $S = 1$ and certain momentum k. Calculating the averages in (5) involving MP states can be done with the help of the standard technique [21, 24]. The final expression for $E(q, \xi, k)$ is quite cumbersome because of the complicated structure of our trial wave function (3), so we present here only the resulting dispersion plots for a number of representative points of the phase diagram. The minimization has been performed numerically.

Another, simpler *ansatz* can be obtained if one forces (4) to be strongly localized, i.e. $\xi \to 0$. Then only the configurations with $n = n'$ survive, and we obtain

$$|k; \mu\rangle = \sum_n \mathrm{e}^{\mathrm{i}kn} |n; \mu\rangle \tag{6a}$$

where

$$|n;\mu\rangle = \mathrm{Tr}\{(g_1^{(0)} g_2^{(0)} \cdots g_n^{(0)})\widehat{\sigma}_\mu^\dagger (g_{n+1}^{(0)} g_{n+2}^{(0)} \cdots g_N^{(0)}\}. \tag{6b}$$

Such an *ansatz* may be called 'regular', or localized crackion (in contrast to our two-spinon *ansatz* (4), describing an 'extended crackion'), because it exactly reproduces the structure of the wave function proposed by Fáth and Sólyom, and the only difference is in the generalized concept of the string order (or, in other words, in the fact that matrices $g_i^{(0)}$ are allowed to contain singlet states). This 'regular' crackion *ansatz* is essentially equivalent to the construction introduced recently by Nakamura *et al* [29] within a slightly different approach using the Kennedy–Tasaki unitary transformation.

3. Variational results for the excitations, and comparison with numerical data

In this section we present variational and numerical results for dispersion relations, lowest modes, and their corresponding wave vectors for various points of the phase diagram. In the first subsection we study the spinon-type excitations on the symmetry line $\gamma = 0$ in the vicinity of the MG point. Variational energies for scattering states and bound states are computed at the MG point, $\lambda = \frac{1}{2}$, and the difference in behaviour of the spectrum for $\lambda > \frac{1}{2}$ and $\lambda < \frac{1}{2}$ is discussed. In the second subsection we investigate the consequences of alternation. When one moves off the symmetry line, the crossover from spinon-type excitations to ladder-type ('crackion') excitations occurs, which is characterized by the change of the localization length $\xi(k_0)$ from infinity to zero; here k_0 denotes the wave vector of the lowest-energy mode. We show that this crossover takes place at the $k_0 = \pi$ boundary of the incommensurate region where k_0 changes gradually from 0 to π. These results are compared with numerical data from exact diagonalization for 24 spins. Because the correlation lengths for the points taken into account are rather small, the numerical data are very close to the thermodynamic limit, and therefore we do not perform any finite-size extrapolation.

3.1. Elementary excitations on the symmetry line $\gamma = 0$

The *ansatz* (3), (4) obviously becomes inadequate close to the symmetry line $\gamma = 0$ (except for the MG point), because two variational minima of the ground-state energy are inequivalent while the true ground state is twofold degenerate on this line. However, the interval of the symmetry line in the vicinity of the MG point (i.e. $\gamma = 0$ and λ close to $\frac{1}{2}$) can be studied with the help of the Shastry–Sutherland-type *ansatz*: it is sufficient to put $u_0 = v_0 = 1/2$ in (3), (4). In the limit $\xi \to \infty$ one gets exactly the *ansatz* of reference [8] and can thus calculate variational energies for the scattering states. On the other hand, if we do not force $\xi = \infty$, the energy of the lowest bound state can be calculated for each value of the total momentum k. For the scattering states it is possible to obtain a compact analytical expression for the energy of such a two-particle excitation:

$$\begin{aligned} E(k,q) &= \varepsilon\left(\frac{k+q}{2}\right) + \varepsilon\left(\frac{k-q}{2}\right) \\ \varepsilon(k) &= \frac{\lambda}{4}(5+4\cos k) + (1-2\lambda)\left\{\frac{3}{8} + \frac{5\cos k + 4}{5+4\cos k}\right\}. \end{aligned} \tag{7}$$

Here $\varepsilon(k)$ has the meaning of the spinon dispersion. At $\lambda = \frac{1}{2}$ it coincides with the result of reference [8]. (It should be mentioned that since in this paper we consider the general case of an alternated chain, momenta in equations (4), (7) are defined in the halved Brillouin

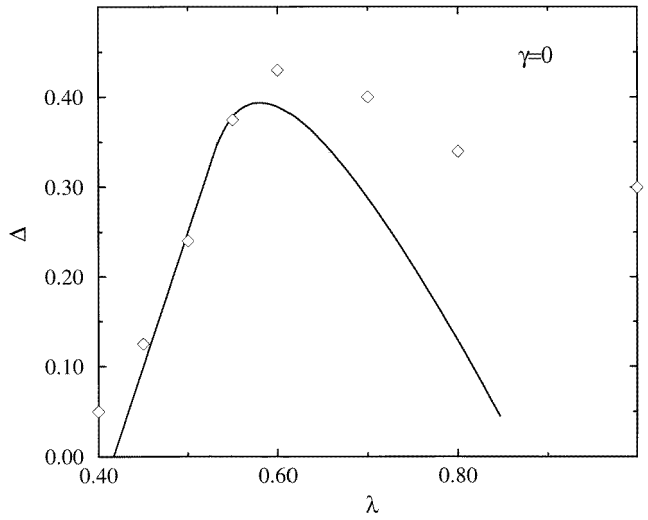

Figure 4. The dependence of the gap on λ on the symmetry line $\gamma = 0$ in the vicinity of the MG point; the full line represents the variational result according to (7), and the diamonds are numerical (DMRG) results given by White and Affleck [30].

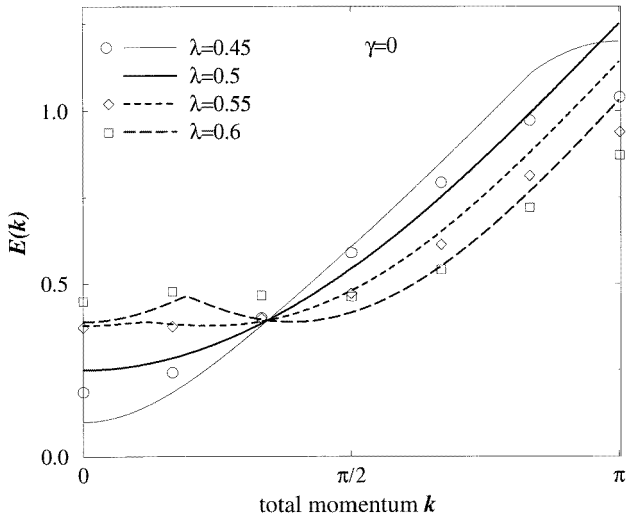

Figure 5. Typical plots of the lower boundary of the two-spinon continuum on the symmetry line $\gamma = 0$ in the vicinity of the MG point: the lines correspond to the formula (7) and the points (□, ◇, ○) are exact-diagonalization data for a 24-spin system .

zone, in contrast to the case in reference [8]). The dispersion relation is determined by the lower boundary of the two-particle continuum. The resulting λ-dependence of the gap Δ is shown in figure 4, together with the numerical results by White and Affleck [30]. One can see that quantitatively this approach yields reasonable results only in the close vicinity of the MG point; nevertheless, at the qualitative level it correctly predicts closing of the gap on decreasing λ and the existence of a maximum in $E_g(\lambda)$ at λ slightly greater than $\frac{1}{2}$.

Characteristic plots of the dispersion of scattering states in the vicinity of the MG point are shown in figure 5. From (7) one can see that for λ less than $\lambda_\pi = \frac{9}{17}$ the single-spinon dispersion has a minimum at $k = k_0 = \pi$, and for larger λ this minimum shifts towards k_0 lower than π. Thus, the lower boundary of the two-spinon continuum always has the minimum at $k = 0$ (corresponding to $q = 2k_0$), and for $\lambda > \lambda_\pi$ there appears another minimum at $k = k_0 = 2(\pi - k_0)$ (which corresponds to $q = 0$). When λ increases, this second minimum gets more pronounced.

The appearance of the lowest mode with an incommensurate wave vector is closely related to the existence of the so-called disorder points [31–33] where spin–spin correlations in real space become incommensurate. Strictly speaking, the point at which the wave vector of the lowest mode becomes incommensurate corresponds not to the disorder point itself, but to the so-called Lifshitz point where the correlation function peak in momentum space (i.e., the peak in the structure factor $S(q)$) starts moving from commensurate to incommensurate q. Generally, the Lifshitz point does not coincide with the disorder point and is situated at some small distance from the boundary of the incommensurate region. In our variational calculation the wave vector starts to change at $\lambda_\pi = \frac{9}{17}$, while the disorder line (the line of disorder points) is numerically established [34, 2] to be $\gamma = 2\lambda - 1$, which means that at $\gamma = 0$ the disorder point is $\lambda = \frac{1}{2} < \lambda_\pi$, in agreement with the above.

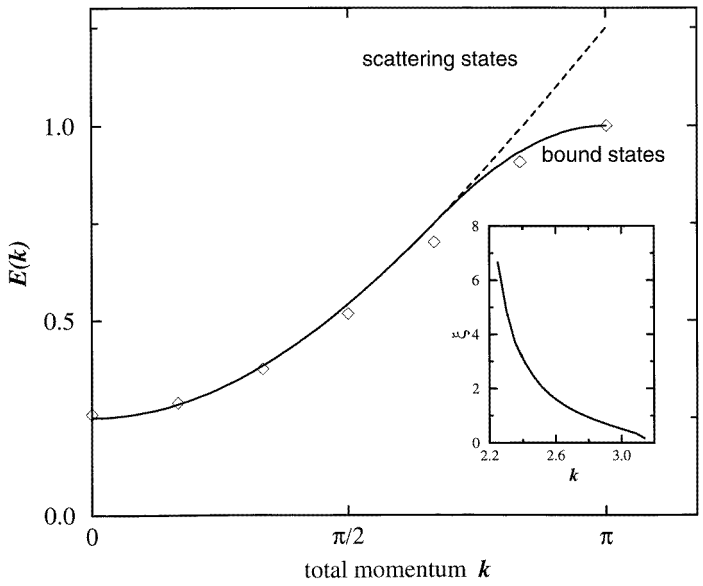

Figure 6. The variational result for the dispersion at the MG point $\gamma = 0$, $\lambda = \frac{1}{2}$ (solid line) in comparison with the numerical data for 24 spins (diamonds); the inset shows the momentum dependence of the localization length $\xi(k)$ for the bound states.

We would like to end this subsection by pointing out the role of bound states. At the MG point it is known [8] that bound states are lower in energy than scattering states for wave vectors k close to the zone boundary. This was shown in reference [8] by using the variational estimate for the upper bound of the dispersion (see below). We can capture the dispersion of the lowest bound state in our approach if we minimize with respect to ξ for each k. For values of the total momentum $0.68\pi < k \leqslant \pi$ we obtain $1/\xi_{\min} > 0$ as shown in figure 6. The same feature, namely the appearance of bound states as the lowest-

energy excitations, can be expected for $\lambda > \lambda_\pi$ and k around the midpoint in between the two dispersion minima, but we did not perform this calculation. Generally, more than one bound state may exist [35]; unfortunately, within the present approach one can access only the *lowest* bound state.

3.2. Dispersion relations and the crossover from loosely bound to tightly bound spinons

First of all, we would like to focus on the disorder line $\gamma = 2\lambda - 1$. As soon as one moves away from the MG point ($\lambda = \frac{1}{2}$, $\gamma = 0$) towards the dimer point ($\lambda = 0$, $\gamma = -1$), the energy of the MG ground state with singlets on diagonals picks up an energy proportional to the size of the system, while the other MG ground state with singlets on the rungs remains the true ground state. As a consequence, only bound states of spinons can survive: this is a typical confinement situation. The wave vector of the lowest mode is still $k = 0$.

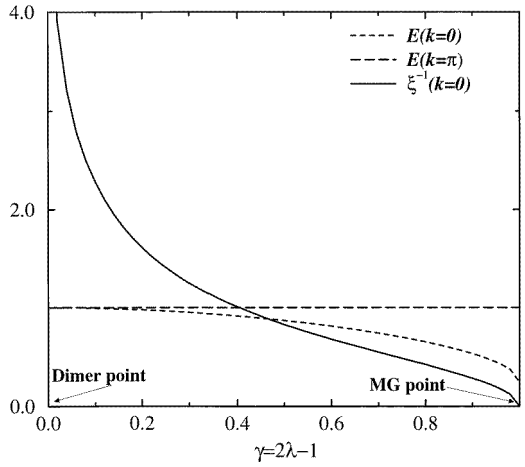

Figure 7. The bandwidth $E(0) - E(\pi)$ and the localization length ξ of the lowest-energy mode on the disorder line $\gamma = 2\lambda - 1$.

The main feature of this excitation is the k-dependent delocalization: the ground state is formed as a product of rung singlets. If we now replace one singlet by a triplet and superpose with wave vector π, we obtain an exact eigenstate on the disorder line, whose energy gives the upper bound of the dispersion [36]. To obtain the lowest mode we delocalize the up spins, which make up the triplet, with the amplitude $e^{-\xi/r}$ as shown in figure 3, and superpose with the wave vector $k = 0$. The bandwidth for this excitation is illustrated in figure 7; one can see that the bandwidth increases along with the increase of the localization length ξ from 0 to ∞ on the way from the dimer point to the MG point (here ξ is not to be confused with the spin-correlation length!) At the MG point we reproduce the result of Shastry and Sutherland for the gap $\Delta = 1/4$. One may say that here we observe the crossover from loosely bound spinons (the 'extended crackion', $1 \ll \xi < \infty$) to spinons tightly bound into the Haldane triplet (the 'crackion', $\xi \ll 1$), even though the crackion at the dimer point is a trivial (dispersionless) excitation.

The same physical picture of crossover should be valid for any path beginning somewhere on the symmetry line and ending somewhere at sufficiently negative γ; on the symmetry line, $\xi(k_0)$ should be infinite (k_0 denotes the lowest-mode wave vector), and it decreases to zero when $-\gamma$ is large enough. In the present approach we can observe this $\xi \to \infty$ behaviour only for the MG point, because for any other point on the symmetry line our two variational ground states become inequivalent and we lose the feature of twofold

degeneracy. However, we believe that our approach remains reasonable for points which are far enough from the symmetry line, where the translational symmetry is explicitly broken and this effect overrides the built-in dimerization of our variational *ansatz*.

It is worthwhile to make a few remarks concerning the behaviour of the real part of relative momentum q. Because of the confinement, the energy of states with internal motion, i.e. with $q \neq 0, 2\pi$, has to be much higher compared to that of the states with zero relative momentum. In our variational calculations we were able to detect only one minimum which always occurred at $q = 0$ or 2π (strictly speaking, $q = 0$ for $\pi < k < 2\pi$ and $q = 2\pi$ for $0 < k < \pi$, so sets with $q = 0$ and $q = 2\pi$ correspond to physically equivalent states).

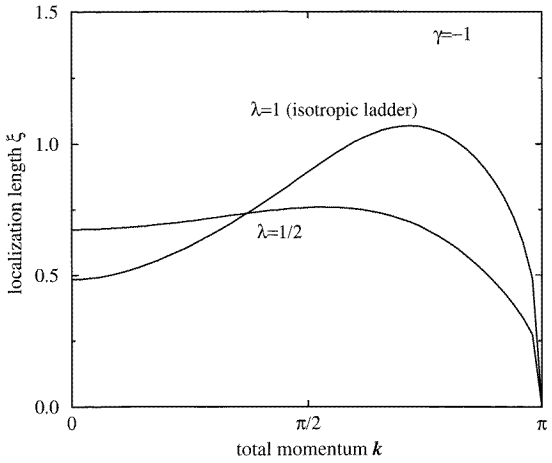

Figure 8. The momentum dependence of the localization length ξ for two points on the line $\gamma = -1$. Note that $\xi(\pi) = 0$.

The crossover from the 'extended crackion' to the crackion is related to the change of wave vector k_0 of the lowest mode, due to the following remarkable feature which we observed from our calculations and which is illustrated by figure 8: *everywhere in the gapped region of the phase diagram, the property* $\lim_{k\to\pi} \xi(k) = 0$ *holds.* Thus, once k_0 has changed from 0 to π, we know that the lowest mode is a 'usual' crackion because $\xi(\pi) = 0$, so the crossover takes place at the $k_0 = \pi$ boundary of the incommensurate region. In order to determine the boundaries of the incommensurate region, we used our variational approach and compared the results with exact-diagonalization data. In figure 9(a) dispersion relations for a few points on the vertical line $\lambda = \frac{1}{2}$ are presented. The numerical data and variational results are in good agreement even though the lowest wave vectors are at slightly different positions (one should keep in mind that numerical dispersions for finite chains consist of a finite number of points). Figure 9(b) illustrates the change of k_0 when crossing the disorder line. Similarly to the situation on the symmetry line as described in the previous subsection, one can see that k_0 starts to change from 0 not exactly at the disorder line but slightly above it (i.e., the Lifshitz line is not identical to the disorder line). The comparison with the numerical data, as is shown in figure 9(b), confirms this property, within the numerical accuracy (exact diagonalization of 24 spins leads to 12 values for the wave vector which is not sufficient to mark the incommensurate region precisely but allows qualitative comparison). The boundaries of the incommensurate region obtained by the variational calculation are presented in figure 2. It should be pointed out that our result for the $k_0 = \pi$ boundary does not agree with that of Pati *et al* [37]. For example, we obtain that the $k_0 = \pi$ boundary goes through the dimer point $\gamma = -1$, $\lambda = 0$, while the corresponding curve C of figure 2 from reference [37] crosses the $\gamma = -1$ line at $\lambda \approx 0.6$.

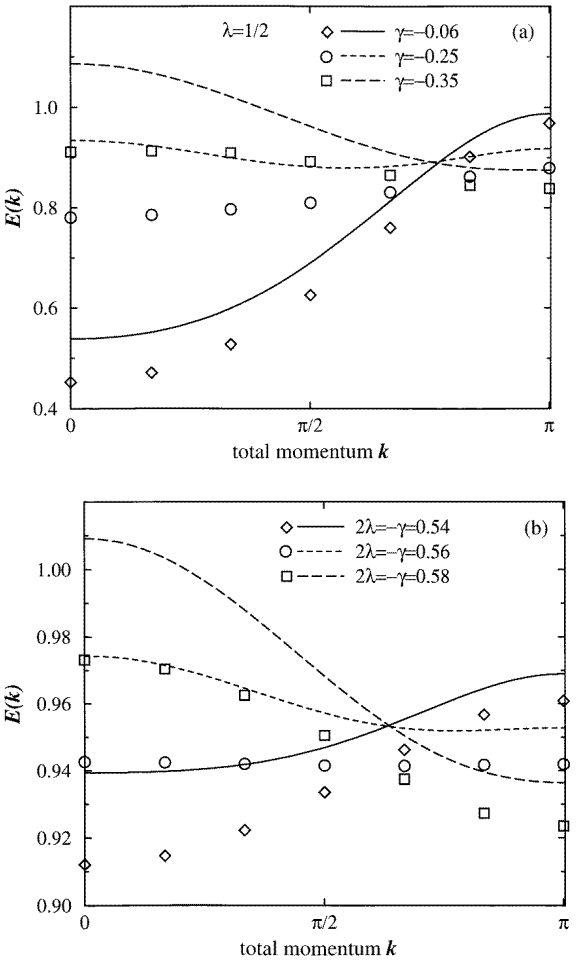

Figure 9. The dispersion curves from the variational *ansatz* in comparison with the numerical data from exact diagonalization for 24 spins: (a) three points on the line $\lambda = \frac{1}{2}$; (b) three points on the line $\gamma = -2\lambda$ in the vicinity of its crossing with the disorder line $\gamma = 2\lambda - 1$ (the numerical data are taken from reference [3]).

At present we cannot comment on the origin of this strong discrepancy.

Finally, we would like to discuss the vicinity of the line $\gamma = -1$ which includes the experimentally relevant ladder point ($\lambda = 1$, $\gamma = -1$). Figure 10 shows the dispersion curves for the 'regular' crackion and the 'extended' crackion, and the numerical data for two points on this line (we should mention that our data agree rather well with those of reference [38]). The dispersion curve of the extended crackion is located slightly below the curve of the crackion and coincides with it for $k = \pi$, in agreement with the general property $\lim_{k\to\pi} \xi(k) = 0$ (see also figure 8). One can also observe that the $k = 0$ gap is slightly larger than $2E(k = \pi)$, which indicates the repulsive character of the effective interaction between the elementary excitations in the ladder. Figure 11 displays the lowest crackion mode ($k = \pi$) in comparison with exact-diagonalization data along the horizontal line $\gamma = -1$, $0 < \lambda < 1$. We conclude that the ladder excitations can be described by the usual crackion *ansatz*, and that isotropic spin ladder has the same type of elementary excitation as

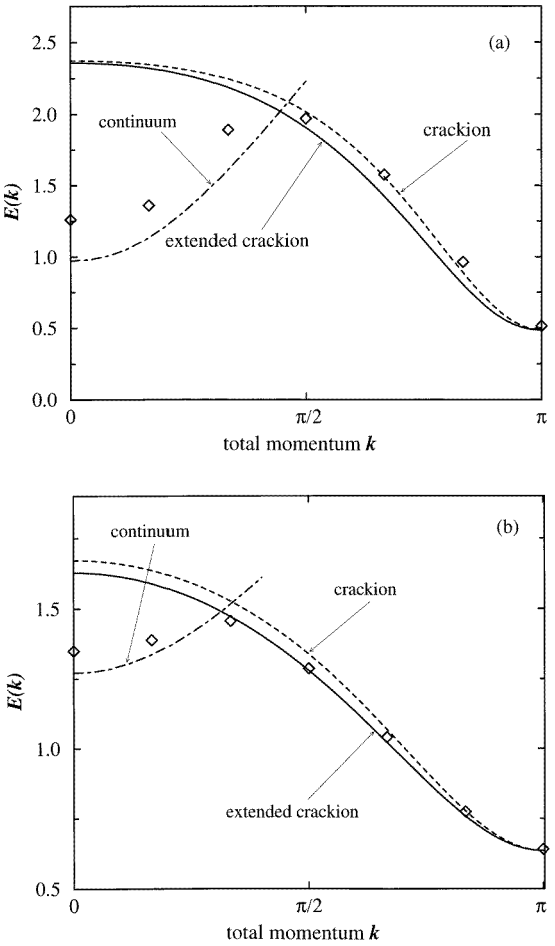

Figure 10. The dispersion of the elementary excitations on the line $\gamma = -1$: (a) the ladder point $\lambda = 1$; (b) $\lambda = \frac{1}{2}$. The variational results from the 'extended-crackion' ($\xi = \xi_{\min}(k)$) and 'crackion' ($\xi = 0$) approaches are shown along with the numerical data ($\diamondsuit$) from exact diagonalization. The chain curve shows the lower boundary of the two-particle continuum for the 'extended-crackion' *ansatz*.

the effective $S = 1$ chain which appears as the limit $\gamma \to -\infty$ of the generalized frustrated ladder. In that limit the localization length ξ collapses for all values of k because creation of singlets on the diagonals would cost infinite energy.

4. Conclusion

We have presented a variational matrix-product *ansatz* for elementary excitations in the gapped phase of the $S = \frac{1}{2}$ ladder with an additional frustrating diagonal coupling $1 + \gamma$, $\gamma < 0$; the strength of interaction along the legs is λ, and the interaction along the rungs is chosen to be unity. This system is equivalent to the antiferromagnetic spin-$\frac{1}{2}$ zigzag chain with alternating exchange (the magnitude of the alternation is proportional to γ) and next-nearest-neighbour interaction λ. Our *ansatz* describes a triplet state of two $S = \frac{1}{2}$ entities

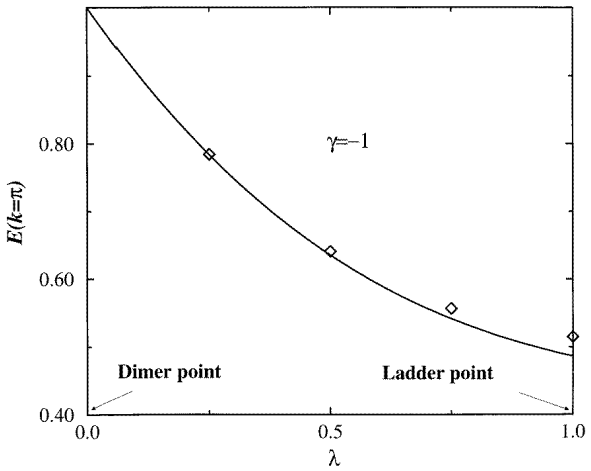

Figure 11. The energy of the lowest mode $E(k = \pi)$ along the line $\gamma = -1$; the solid line represents the variational result, and diamonds ($\Diamond$) are numerical points from exact diagonalization for 24 spins.

('spinons') and allows one to interpolate between free and bound spinons by varying the parameter ξ which has the meaning of a localization length (the average distance between spinons in the pair). This state is constructed to be a soliton in generalized string order [3], and in the limit $\gamma \to -\infty$ of the effective $S = 1$ Haldane chain it coincides with the 'crackion' *ansatz* proposed by Fáth and Sólyom [14] if the localization length $\xi \to 0$; for that reason we call our *ansatz* an 'extended crackion'. The limit $\xi \to \infty$ leads to the two-particle excitation of Shastry and Sutherland [8], which corresponds to free spinons existing in the absence of the alternation (i.e., on the symmetry line $\gamma = 0$).

Using our variational *ansatz*, we calculated dispersion relations for various points in the phase diagram. These results were compared to exact-numerical-diagonalization data for 24 spins, and showed a reasonable agreement of the two approaches. The variational parameter ξ was determined separately for each value of the total momentum k; it turns out that $\xi(k)$ has nontrivial behaviour; in particular, the property $\lim_{k\to\pi} \xi = 0$ was observed numerically over the entire range of model parameters studied.

We determined the boundaries of the incommensurate region (strictly speaking, the corresponding Lifshitz lines) by locating the wave vector k_0 of the lowest mode: for $\gamma > 2\lambda - 1$ the wave vector is pinned at $k_0 = 0$, slightly after crossing this line it starts to change from 0 to π, and, finally, at some other line it again gets pinned at $k_0 = \pi$ (in terms of the full Brillouin zone of the chain this corresponds to the change from π to $\pi/2$).

We show that in the interval between the symmetry line $\gamma = 0$ and the $k_0 = \pi$ boundary of the incommensurate region the dispersion of elementary excitations is well described by our bound-spinon *ansatz*. The crossover of the lowest mode from the 'extended crackion' to the 'localized' crackion (i.e., from finite $\xi(k_0)$ to $\xi(k_0) = 0$) occurs at the $k_0 = \pi$ boundary of the incommensurate region, due to the above-mentioned property of the function $\xi(k)$. For the isotropic ladder point ($\gamma = -1$, $\lambda = 1$) a localized-crackion *ansatz* with $\xi = 0$ is sufficient to describe the excitations.

To conclude, we propose a simple *ansatz* providing a reasonably good description of the elementary excitations in the gapped phase of the frustrated $S = \frac{1}{2}$ chain with alternation for over wide range of the model parameters.

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