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

S. Brehmer, A. K. Kolezhuk, H.-J. Mikeska, and U. Neugebauer
Institut für Theoretische Physik, Universität Hannover, Appelstr. 2, D-30167 Hannover, Germany
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We use the variational matrix-product ansatz to study elementary excitations in the $S = 1/2$ ladder with additional diagonal coupling, equivalent to a single $S = 1/2$ chain with alternating exchange and next-nearest neighbor interaction. In absence of alternation the elementary excitation consists of two free $S = 1/2$ particles (“spinons”) which are solitons in the dimer order. When the nearest-neighbor exchange alternates, the “spinons” are confined into one $S = 1$ excitation being a soliton in the generalized string order. Variational results are found to be in a qualitative agreement with the exact diagonalization data for 24 spins. We argue that such an approach gives a reasonably good description in a wide range of the model parameters.

I. INTRODUCTION

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

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

$$\hat{H} = \sum_n \mathbf{S}_{1,n} \mathbf{S}_{2,n} + (1 + \gamma) \sum_n \mathbf{S}_{1,n} \mathbf{S}_{2,n+1} + \lambda \sum_n (\mathbf{S}_{1,n} \mathbf{S}_{1,n+1} + \mathbf{S}_{2,n} \mathbf{S}_{2,n+1}),$$

(1)

where $\lambda > 0$ determines the strength of the next-nearest neighbor interaction, and $\gamma$ corresponds to alternation of the nearest-neighbor exchange, whose strength is set to be unity. This model has rich behavior depending on the values of parameters $\lambda$ and $\gamma$, and its phase diagram (see Fig. 2) is rather well understood (at least for the half-plane $\lambda > 0$; for negative $\lambda$ the situation is less clear). Without loss of generality, we will assume that $\gamma < 0$, since there is an obvious symmetry transformation 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 the 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 the first order, so that for $\lambda > \lambda_c$, $\gamma = 0$ there are two degenerate dimerized ground states, and the system is gapped. The transition at $\lambda = \lambda_c$ is well studied, see Ref. [3] for a review. Everywhere except at the symmetry line the model [4] has 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 much less extent than its ground state properties. The Heisenberg point ($\lambda = 0$, $\gamma = 0$) is exactly solvable by means of the Bethe ansatz technique, and the elementary excitations are pairs of noninteracting $S = 1/2$ entities (“spinons”). 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 ($\gamma = 0$, $\lambda = 1/2$), where the exact (twofold degenerate) ground state is a simple product of singlet dimers, the elementary excitation can be approximately constructed as a pair of unbound spins above the completely dimerized state. The elementary excitation is composed of two $S = 1/2$ 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 case of unbroken translational invariance. When nonzero alternation is present, one may expect that those “spinons” are confined into a single $S = 1$ particle.

In the Haldane limit (infinite alternation) the system has long-range hidden (string) order [8], and the elementary excitation is known [3] to be a soliton in the string order. The concept of string order was generalized to spin ladders [9] and it was shown that several ladder models exhibit long-range generalized string correlations [10]. It was argued [11] 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 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 being a kink in the string order and consisting of two bound \( S = \frac{1}{2} \) entities. The wave function of the kink pair contains only one variational parameter \( \xi \) having the meaning of the average pair size (the localization length). We show that at the MG point \( \xi \) is infinite and our ansatz reduces to that of Shastry and Sutherland when moving away from the MG point, \( \xi \) drops down very quickly to the 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 of other authors using different technics (see Ref. and references therein). In the Haldane limit \( \xi \) goes to zero, and our wave function transforms into the “crack-ion” ansatz introduced by Fáth and Sólyom (see also Ref. 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 spins) 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 in a wide range of physical models.

The paper is organized as follows: in Sect. we introduce our ansatz for the elementary excitation. In Section we present results from the variational calculation in comparison with numerical data. The elementary excitations in different regions of the phase diagram are discussed. Finally, Sect. contains concluding remarks.

II. TWO-SPINON “COMPOSITE PARTICLE” ANSATZ

Recently, a variational wave function for the description of the ground state properties of generalized spin ladders was proposed in the form of a matrix-product (MP) state. The MP representation was first discussed by Fannes et al. in an abstract manner and later by Klümper et al. for the \( S = 1 \) deformed VBS chain, and has found since then numerous applications in exact and variational calculations. For periodic boundary conditions, the trial wave function for the ground state of the ladder consisting of \( 2N \) spins can be written as

\[
|\Psi_0\rangle = \text{Tr} \left( g_1 g_2 \cdots g_N \right), \quad \text{where}
\]

\[
g_i(u, v) = u \left( \mathbb{1} \cdot |s\rangle_i \right) + v \sum_{\mu=0,\pm 1} \bar{\sigma}_\mu \cdot |t_\mu\rangle_i \quad (2)
\]

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; \( \sigma_\mu \) are the Pauli matrices in a spherical basis, \( \sigma_0 = \sigma_x, \sigma_\pm = \mp 1/\sqrt{2}(\sigma_x \pm i\sigma_y) \). The parameters \( u \) and \( v \) in case of absence of external magnetic field can be chosen real and satisfy the normalization condition \( u^2 + 3v^2 = 1 \).

The wave function \( \langle \Psi_0|H|\Psi_0\rangle \) has the following remarkable properties: (i) for arbitrary \( u \) and \( v \) it is a global singlet (see also Ref. 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 \(|t_0\)'s; (iii) both degenerate dimer ground states at the Majumdar-Ghosh point can be written in the above form, as well as the “valence-bond” AKLT state 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 \( u = v = \frac{1}{\sqrt{3}} \) respectively, and the AKLT state corresponds to zero singlet weight \( (u = 0, v = 1/\sqrt{3}) \). The state \( \langle \Psi_0|H|\Psi_0\rangle \) 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 \( E_0 = \langle \Psi_0|H|\Psi_0\rangle \) calculated with the trial function \( \langle \Psi_0|H|\Psi_0\rangle \) 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 \( \lambda \) and \( \gamma \); this latter minimum is absent in certain region 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.

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 i.e. a pair of unbound spins connecting two degenerate dimer ground states, and the “crack-ion” ansatz of Fáth and Sólyom. One can check that the following construction satisfies the above requirements:

\[
|n, n'; \mu\rangle = \text{Tr} \left( \prod_{i=1}^{n} g_i^{(0)} \bar{\sigma}_\mu \prod_{i=n+1}^{n'} \bar{g}_i \prod_{i=n'+1}^{N} g_i^{(0)} \right). \quad (3)
\]

Here \( g_i^{(0)} = g_i(u_0, v_0) \) denotes the matrix corresponding to the variational ground state, and \( \bar{g}_i = g_i(u = 1, v = 0) \) is the matrix describing singlet dimers on the diagonals (it is easy to see from (2) that \( \bar{g}_i \) 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 worthwhile to remark that the states \(|n, n'; \mu\rangle\) are not mutually orthogonal. The presence of \( \bar{\sigma}_\mu \) ensures that this state breaks the generalized string order and has the total spin \( S = 1 \) and its \( z \)-projection \( S_z = \mu \) (the general technique of constructing MP states with given quantum
numbers $S$, $S_z$ can be found in Ref. [22]. The structure of the ansatz (4) is schematically shown in Fig. 3.

At the MG point $v_0 = v_0 = 1/2$, and one can straightforwardly check that in this case Eq. (3) describes a pair of unbound spins $1/2$ 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 (5) 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 $k$:

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

(4)

It contains two variational parameters $q$ and $\xi$ which can be considered as real and imaginary part of the relative momentum of the two spin-$1/2$ entities forming our composite particle. The parameter $\xi$ has the meaning of a localization length, or the average size of the composite particle. The parameter $q$ correspond 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 $\xi$ corresponds to a bound state.

On the disorder line $\gamma = 2 \lambda - 1$, according to Ref. 3, the parameters $u_0$ and $v_0$ both equal $1/2$, 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 $\xi$.

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

$$
E(q, \xi, k) = \langle k, q; \mu|\hat{H} - E_0|k, q; \mu\rangle \langle k; \mu|k; \mu\rangle^{-1},
$$

(5)

and has to be minimized over $\xi$ and $q$, separately for any given $k$ (as we will see below, it turns out that optimal $\xi$ 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. The final expression for $E(q, \xi, k)$ is quite cumbersome because of the complicated structure of our trial wave function (4), so that 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

$$
|k; \mu\rangle = \sum_n e^{ikn} |n; \mu\rangle,
$$

where

$$
|n; \mu\rangle = \text{Tr}\left\{ (g_1^{(0)} g_2^{(0)} \cdots g_n^{(0)}) \sigma_\mu g_{n+1}^{(0)} g_{n+2}^{(0)} \cdots g_N^{(0)} \right\}.
$$

(6)

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. within a slightly different approach using the Kennedy-Tasaki unitary transformation.

### III. 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 $\lambda = 1/2$, and the difference in behavior of the spectrum at $\lambda > 1/2$ and $\lambda < 1/2$ 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, being 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 $\pi$. 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.

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

The ansatz (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 $\lambda$ close to $1/2$) can be studied with the help of the Shastry-Sutherland-type ansatz: it is sufficient to put $u_0 = v_0 = 1/2$ in (4). In the limit $\xi \to \infty$ one gets exactly the ansatz of Ref. 3 and can 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:

$$E(k, q) = \varepsilon \left( \frac{k + q}{2} \right) + \varepsilon \left( \frac{k - q}{2} \right),$$

$$\varepsilon(k) = \frac{\lambda}{4} (5 + 4 \cos k) + (1 - 2\lambda) \left\{ \frac{3}{8} + \frac{5 \cos k + 4}{5 + 4 \cos k} \right\},$$

where $\varepsilon(k)$ has the meaning of the spinon dispersion. At $\lambda = \frac{1}{2}$ it coincides with the result of Ref. 3. (It should be mentioned that since in this paper we consider the general case of an alternated chain, momenta in Eqs. (2-3) are defined in the halved Brillouin zone, in contrast to Ref. 8.) The dispersion relation is determined by the lower boundary of the two-particle continuum. The resulting $\lambda$-dependence of the gap $\Delta$ is shown in Fig. 4, together with the numerical results by White and Affleck. 2

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 when decreasing $\lambda$ and the existence of a maximum in $E_{\gamma}(\lambda)$ at $\lambda$ slightly greater than $\frac{1}{2}$.

Characteristic plots of the dispersion of scattering states in the vicinity of the MG point are shown in Fig. 3. From (2) one can see that for $\lambda$ less than $\lambda_x = \frac{2}{9}$ the single-spinon dispersion has a minimum at $k = k_0 = \pi$, and for larger $\lambda$ this minimum shifts towards $k_0$ lower than $\pi$. Thus, the lower boundary of the two-spinon continuum always has the minimum at $k = 0$ (corresponding to $q = 2k_0$), and for $\lambda > \lambda_x$ there appears another minimum at $k = k_0 = 2(\pi - k_0)$ (which corresponds to $q = 0$). When $\lambda$ increases, this second minimum gets more pronounced.

Appearance of the lowest mode with incommensurate wave vector is closely related to the existence of the so-called disorder points, where spin-spin correlations in real space become incommensurate. Strictly speaking, the point where 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., 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 $\lambda_x = \frac{2}{9}$, while the disorder line (line of disorder points) is numerically established to be $\gamma = 2\lambda - 1$, which means that at $\gamma = 0$ the disorder point is $\lambda = \frac{1}{2} < \lambda_x$, in agreement with the above.

We would like to end this subsection by pointing out the role of bound states. At the MG point it is known that bound states are lower in energy than scattering states for wave vectors $k$ close to the zone boundary. This was obtained in Ref. 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 $\xi$ for each $k$. For values of the total momentum $0.68 \pi < k \leq \pi$ we obtain $1/\xi_{\min} > 0$ as shown in Fig. 4. The same feature, namely the appearance of bound states as the lowest energy excitations, can be expected for $\lambda > \lambda_x$ 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, unfortunately, within the present approach one can access only the lowest bound state.

**B. Dispersion relations and 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 off 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 $k = 0$.

The main feature of this excitation is the $k$-dependent delocalization: The ground state is formed by a product of rung singlets. If we now replace one singlet by a triplet and superpose with wave vector $\pi$, we obtain an exact eigenstate on the disorder line, whose energy gives the upper bound of the dispersion. 23 To obtain the lowest mode we delocalize the up spins, which make up the triplet, with the amplitude $e^{-\xi/\tau}$ as shown in Fig. 3 and superpose with the wave vector $k = 0$. The bandwidth for this excitation is illustrated in Fig. 3. One can see that the bandwidth increases along with the increase of the localization length $\xi$ from 0 to $\infty$ on the way from the dimer point to the MG point (here $\xi$ 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 (“extended crackion,” $1 < \xi < \infty$) to spinons tightly bound into the Haldane triplet (“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 at the symmetry line and ending somewhere at sufficiently negative $\gamma$; 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 $\xi \to \infty$ behavior 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 behavior 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 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 \(2\pi\) (strictly speaking, \(q = 0\) for \(\pi < k < 2\pi\) and \(q = 2\pi\) for \(0 < k < \pi\), so that sets with \(q = 0\) and \(q = 2\pi\) correspond to physically equivalent states).

The crossover from ‘extended crackion’ to 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 Fig. 3(a), 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 \(\pi\), we know that the lowest mode is a ‘usual’ crackion because \(\xi(\pi) = 0\), so that 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 Fig. 3(a) dispersion relations for a few points on the vertical line \(\lambda = \frac{1}{2}\) are presented. Numerical data and variational results are in a 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). Fig. 3(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 Fig. 3(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 Fig. 3. It should be pointed out that our result for the \(k_0 = \pi\) boundary does not agree with that of Pati et al.\(^{12}\). 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 Fig. 2 from Ref. \(^{12}\) crosses the \(\gamma = -1\) line at \(\lambda \approx 0.6\). 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 4 shows the dispersion curves for the “regular” crackion, the “extended” crackion and the numerical data for two points on this line (one should mention that our data agree rather well with those of Ref. \(^{33}\)). 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 Fig. 3). 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. Fig. 4 displays the lowest crackion mode \((k = \pi)\) in comparison with exact diagonalization data along the horizontal line \(\gamma = -1, \lambda = 0 \ldots 1\). We conclude that the ladder excitations can be described by the usual crackion ansatz, and the isotropic spin ladder has the same type of elementary excitation as the effective \(S = 1\) chain which appears as the limit \(\gamma \to -\infty\) of the generalized frustrated ladder. In that limit the localization length \(\xi\) collapses for all values of \(k\) because creation of singlets on the diagonals would cost infinite energy.

**IV. 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 \(\lambda\), 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 alternation is proportional to \(\gamma\) and next-nearest neighbor interaction \(\lambda\)). Our ansatz describes a triplet state of two \(S = \frac{1}{2}\) entities (“spinons”) and allows one to interpolate between free and bound spinons by varying the parameter \(\xi\) which has the meaning of a localization length (average distance between spinons in the pair). This state is constructed to be a soliton in generalized string order and in the limit \(\gamma \to -\infty\) of effective \(S = 1\) Haldane chain it coincides with the “crackion” ansatz proposed by Fáth and Sólyom\(^{12}\) 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\(^{13}\) which corresponds to free spinons existing in 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 \(\xi\) was determined separately for each value of the total momentum \(k\); it turns out that \(\xi(k)\) has nontrivial behavior, particularly the property \(\lim_{k \to \pi} \xi = 0\) was numerically observed in the entire range of studied model parameters.

We determined the boundaries of the incommensurate region (strictly speaking, the corresponding Lifshitz
reasonably good description of the elementary excitations
excitations. $\gamma$ the isotropic ladder point ($\xi$ crackion ansatz with
$k \xi$ the above-mentioned property of the function crackion (i.e., from finite
the lowest mode from “extended crackion” to “localized”
described by our bound spinons ansatz. The crossover of
the rate region the dispersion of elementary excitations is well
line
$\gamma > 2 \lambda - 1$ the wave vector is pinned at $k_0 = 0$,
slightly after crossing this line it starts to change from 0 to $\pi$, and, finally, at some other line it gets again pinned
at $k_0 = \pi$ (in terms of the full Brillouin zone of the chain
this corresponds to the change from $\pi$ 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 spinons ansatz. The crossover of
the lowest mode from “extended crackion" to “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 a wide range of the model parameters.

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* Permanent address: Institute of Magnetism, 36(b) Vernad-
skii avenue, 252142 Kiev, Ukraine.

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FIG. 1. Generalized spin ladder with additional diagonal (frustrating) coupling. Arrows show the way of numbering the sites to map this system onto a single chain with nearest and next-nearest neighbor interactions.

FIG. 2. 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. $k = 0$ 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 $k = 0$ boundary is known to be $\gamma = 2\lambda - 1$; for $k = \pi$ boundary the exact position of the disorder line is unknown.
FIG. 3. The structure of the variational two-spinon ansatz (4). Ovals show the location of matrices; solid ovals denote $g^{(0)}$ and dashed ones denote $\tilde{g}$. 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 $\gamma = 2\lambda - 1$).

FIG. 4. Dependence of the gap on $\lambda$ on the symmetry line $\gamma = 0$ in the vicinity of the MG point; full line represents the variational result according to (5), and squares are numerical (DMRG) results by White and Affleck.
FIG. 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: lines correspond to the formula and points ($\square, \diamond$, $\circ$) are exact diagonalization data for a 24-spin system.

FIG. 6. 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 insert shows the momentum dependence of the localization length $\xi(k)$ for the bound states.
FIG. 7. The bandwidth $E(0) - E(\pi)$ and the localization length $\xi$ of the lowest energy mode on the disorder line $\gamma = 2\lambda - 1$.

FIG. 8. Momentum dependence of the localization length $\xi$ for two points on the line $\gamma = -1$. Note that $\xi(\pi) = 0$. 
FIG. 9. Dispersion curves from 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 $\gamma = 2\lambda - 1$ (numerical data are taken from Ref. 3).
FIG. 10. The dispersion of elementary excitations on the line $\gamma = -1$: (a) the ladder point $\lambda = 1$; (b) $\lambda = \frac{1}{2}$. Variational results from “extended crackion” ($\xi = \xi_{\text{min}}(k)$) and “crackion” ($\xi=0$) approaches are shown along with the numerical data (◇) from exact diagonalization. The dash-dotted curve shows the lower boundary of the two-particle continuum for ‘extended crackion’ ansatz.
FIG. 11. The energy of the lowest mode $E(k = \pi)$ along the line $\gamma = -1$; solid line represents the variational result and diamonds (◇) are numerical points from exact diagonalization for 24 spins.