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Dressed solitonic excitations for the AKLT Hamiltonian

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Abstract. In contrast to the ground state of the Affleck–Kennedy–Lieb–Tasaki (AKLT) isotropic spin-1 Hamiltonian its elementary excitations are not known exactly in general. Based on a simple variational *ansatz* we construct approximate excitations in the form of dressed hidden domain walls. This allows us to give an improved upper bound for the gap of the AKLT Hamiltonian which is only 1% larger than the best currently available numerical result. We compare the one- and two-soliton dispersion curves with low-lying excitations for a chain of 16 sites as given by Fath and Solyom and find excellent agreement. Spin and string correlations are calculated and found to agree in leading order with the corresponding correlations for the bare kinks. Finally the weight of the string-ordered part of the lowest excited state is calculated and compared with the exact numerical result.

Haldane's conjecture [1] about the isotropic antiferromagnetic Heisenberg chain for integer spin prompted numerous investigations of spin chains with a disordered singlet ground state and a gap in the excitation spectrum (see [2, 3] for reviews). A model well understood and believed to be in the same universality class as the isotropic Heisenberg chain is a spin-1 chain with an isotropic biquadratic nearest-neighbour Hamiltonian [4]. It has the form of a sum of spin-2 projectors on neighbouring sites:

$$H = \sum_n \left(\frac{1}{2} S_n \cdot S_{n+1} + \frac{1}{6} (S_n \cdot S_{n+1})^2 + \frac{1}{3} \right). \quad (1)$$

The ground state Ω for this Hamiltonian can be constructed explicitly. It is a valence bond state which is annihilated by each of the projectors. For open boundary conditions there are four ground states which only differ in their behaviour at the boundaries and can be classified into eigenstates of S^2 and S^z of the boundary spins S_N and S_1 . These states have exponentially decaying spin correlations and are separated from the excited states by an energy gap. They have *hidden* order, though, as was pointed out in [5] and further explored in [6, 7].

The energetically lowest-lying excited states come as a triplet of spin-1 excitations at $k = \pi$. They are not known exactly but have been investigated with the help of the Bijl–Feynman single-mode approximation [8]. (For exactly known bound two- and three-particle states higher up in the spectrum see [9].) These approximate states also come in triplets: $S_k^\alpha \Omega$ with $\alpha = z, \pm$ where $S_k^\alpha = N^{-1/2} \sum_n e^{ikn} S_n^\alpha$. They have the following dispersion relation:

$$E(k) = \frac{5}{27} (5 + 3 \cos k). \quad (2)$$

This allows for a first upper bound for the gap: $\Delta < E(\pi) = \frac{10}{27}$.

As an alternative approach, convincing evidence was presented that the underlying elementary excitations do not have the form of spin waves but are hidden domain walls or kinks [10, 11]. They can be written in the form of linear combinations of the differences of two states (Ω_n^α and Ω_{n-1}^α) which can be generated from the ground state Ω by breaking one bond [11, 12]. The resulting edge spins of this 'dangling bond' add up to $S_{\text{tot}} = 1$.

For the infinite chain the states Ω_n^α have the form of domain walls between different ground states for the left and right half-infinite chain distinguished by their boundary spins. In the case of periodic boundary conditions the special nature of the hidden order allows for introducing a single kink by breaking a single bond. Details can be found in [11, 12]. The transitions between the domains being quite abrupt, a spatial smoothing of the domain wall should result in an improved approximation for the gap. In the following we quickly summarize the steps necessary to achieve this and give some explicit results.

The strongly correlated valence bond ground state Ω for periodic boundary conditions ($S_{\text{tot}} = 0, S_{\text{tot}}^z = 0$) can be put in a factorizing form with the help of a non-local unitary transformation [7]:

$$\Phi = U\Omega = \frac{1}{2}(\Phi^{(1)} + \Phi^{(2)} - \Phi^{(3)} - \Phi^{(4)}) \quad (3)$$

with $\Phi^{(i)} = \phi^{(i)} \otimes \phi^{(i)} \otimes \dots \otimes \phi^{(i)}$ and $i = 1, \dots, 4$, and

$$\begin{aligned} \phi^{(1/2)} &= \begin{pmatrix} \pm a \\ b \\ 0 \end{pmatrix} \\ \phi^{(3/4)} &= \begin{pmatrix} 0 \\ -b \\ \mp a \end{pmatrix} \end{aligned} \quad (4)$$

with $a = \sqrt{2/3}$ and $b = 1/\sqrt{3}$. This state is normalized for $N \rightarrow \infty$.

The approximate excited states Ω_n^α transform in a way which we illustrate for Ω_n^z :

$$\Phi_n^z = U\Omega_n^z = \Phi^{(1)} \otimes \Phi^{(2)} + \Phi^{(2)} \otimes \Phi^{(1)} + \Phi^{(3)} \otimes \Phi^{(4)} + \Phi^{(4)} \otimes \Phi^{(3)}. \quad (5)$$

Here we use the same notation $\Phi^{(i)}$ to denote the state of the full chain as well as the state of a part of the chain since there appears no danger of confusion. The broken bond between sites n and $n+1$ divides the states 1 and 2, and 3 and 4, respectively. Explicitly this means for example:

$$\Phi^{(1)} \otimes \Phi^{(2)} = \begin{pmatrix} a \\ b \\ 0 \end{pmatrix} \otimes \dots \otimes \begin{pmatrix} a \\ b \\ 0 \end{pmatrix}_n \otimes \begin{pmatrix} -a \\ b \\ 0 \end{pmatrix}_{n+1} \otimes \dots \otimes \begin{pmatrix} -a \\ b \\ 0 \end{pmatrix}_N. \quad (6)$$

This state is normalized and orthogonal to the ground state for $N \rightarrow \infty$. We introduce a dressing of this state in the following non-normalized form:

$$\Phi_n^{(1,2)} = \frac{1}{2} \Phi^{(1)} \otimes \left\{ \begin{pmatrix} a \\ b \\ c \end{pmatrix}_n \otimes \begin{pmatrix} -a \\ b \\ c \end{pmatrix}_{n+1} + \begin{pmatrix} a \\ b \\ -c \end{pmatrix}_n \otimes \begin{pmatrix} -a \\ b \\ -c \end{pmatrix}_{n+1} \right\} \otimes \Phi^{(2)}. \quad (7)$$

c will be considered as variational parameter. From a physical point of view this state smears the domain wall over three lattice sites and also mixes in components which locally have additional domain walls. In that respect it is similar to a recent variational *ansatz* of Kennedy [14] which leads to an improved ground state energy of the antiferromagnetic

Heisenberg chain by adding to the states considered in [7] states with additional domain walls. The state of equation (7) can also be written in operator form:

$$\Phi_n^{(1,2)} = \left(1 - \frac{c^2}{4a^2} \left(e^{ix S_n^x} - e^{ix S_n^y} \right) \left(e^{ix S_{n+1}^x} - e^{ix S_{n+1}^y} \right) \right) \Phi^{(1)} \otimes \Phi^{(2)}. \quad (8)$$

Substituting $\Phi^{(1)} \otimes \Phi^{(2)}$ by $\Phi^{(i)} \otimes \Phi^{(j)}$ with $i \neq j$ one can construct 16 different states $\Phi^{(i,j)}$. Four of these are the four ground states of the valence bond model; the remaining 12 states are the excited states investigated in the following.

Upon Fourier transformation one finds the same dispersion relation for all these states:

$$\begin{aligned} E(k) &= \frac{11\sqrt{R} - 579 + 306 \cos k}{6(\sqrt{R} - 49 + 30 \cos k)} \\ R &= 3121 - 2508 \cos(k) + 900 \cos^2(k) \\ c^2 &= \frac{\sqrt{R} - 49 + 30 \cos k}{6(5 + 3 \cos k)}. \end{aligned} \quad (9)$$

An improved upper bound for the gap Δ is therefore given by $E(k = \pi)$:

$$E(k = \pi) = \frac{11\sqrt{6529} - 885}{6(\sqrt{6529} - 79)} = 0.353\,683\,1\dots \quad (10)$$

This should be compared with the result of the Bijl–Feynman approximation: $\Delta = \frac{10}{27} = 0.370\,370\dots$, and with the finite-size scaling result from exact diagonalization of chains with N up to 16 [11, 13], which gives $\Delta \approx 0.350\dots$. For $k = \pi$ we have $c^2 \approx 0.150\dots$

Noting that $E(k = 0) = 1.297\,245\dots$ and $E(k = \pi/2) = 0.862\,35\dots$ one can see that $2E(\pi) < E(0)$, but $E(0) + E(\pi) < 2E(\pi/2)$. The two-kink dispersion curve therefore has vanishing slope for $k = 0$ as well as for $k = \pi$ (in contrast to the Bijl–Feynman curve) and its two parts join smoothly around $k = k_c \approx 0.95\pi$. For smaller wavevectors the two-kink dispersion relation is given by $E_2(k) = 2E(\pi + k/2)$. Only for k sufficiently close to π is it given by $E((k + \pi)/2) + E((k - \pi)/2)$.

In figure 1 we compare the dispersion relations for single-kink, two-kink, and three-kink excitations with numerical results by Fath and Solyom [11] for the chain with $N = 16$ sites and periodic boundary conditions and find excellent agreement with their finite-size scaling results for the gaps at $k = 0$ and $k = \pi$ denoted by asterisks. The single-kink branch enters the continuum for $k/\pi = 0.442\,078\dots$. Around this value the numerical results for the finite chain deviate visibly from our approximation and from the thermodynamic limit as well for which our one- and two-kink approximation should give reliable results.

We remark that we can obtain an even better upper bound for the gap by treating also the parameter b in the *ansatz* of equation (6) as a variational parameter: this leads to $E(k = \pi) = 0.350\,63\dots$, within 10^{-3} of the numerical value.

The variational states that have been constructed are neither eigenstates of S_{tot}^z nor of S_{tot}^2 . To compare spin and string correlations for these variational solutions with the exact results it is necessary to linearly superpose the former solutions to become eigenstates of S_{tot}^z and S_{tot}^2 . So far this goal could only be achieved partially.

As H and S_{tot}^2 commute we can obtain an even better bound by projecting a given variational solution on the subspace with given S_{tot} . Unfortunately the states found in this way in general have no simple local form any longer. On the other hand it turns out that it is quite simple to construct a variational state for $S_{\text{tot}}^z = 0$ following the lines given in [11] but using the variational states. The resulting state, however, is not an eigenstate of

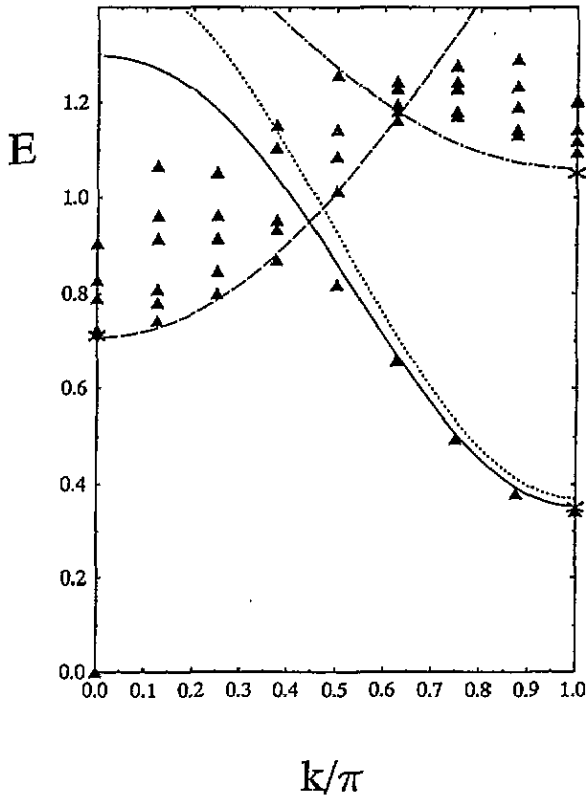


Figure 1. Low-lying eigenvalues of the AKLT Hamiltonian with periodic boundary conditions for $N = 16$ sites taken from [11] compared with the variational single-kink dispersion curve as given in equation (9) (full curve) and the two-kink (dashed curve) and three-kink (dashed-dotted curve) dispersion curves derived from it. The two- and three-soliton continua lie above these curves. The finite-size scaling results of [11] are indicated by asterisks. For comparison we also show the single-kink dispersion curve as given in equation (2) based on the Feynman-Bijl single-mode expansion (dotted line).

S_{tot}^z and therefore mixes contributions from several S_{tot}^z subspaces. Here we only give the result after back-transforming it with U :

$$\Psi_k^z = \frac{1}{\sqrt{N}} \sum_{n=1}^N e^{ikn} S_n^z \left(1 + \frac{c^2}{2a^2} e^{i\pi S_n^z} \left(e^{i\pi S_{n-1}^z} S_{n-1}^z{}^2 + e^{i\pi S_{n+1}^z} S_{n+1}^z{}^2 \right) \right) \Omega \quad (11)$$

with parameters and dispersion relation as in equation (9). Direct calculation for $k = \pi$ shows that $\sum_m S_m^z \Psi_{k=\pi}^z = 0$.

The ground state Ω has complete string order. Numerical results show that the string order of the exact low-lying excited states with $S_{\text{tot}}^z = 0$ at $k = \pi$ is only negligibly perturbed and a description in terms of effective fermions becomes feasible [15, 16]. A measure for the completeness of the string order of a state Ψ_k is given by the weight $w_k^{(\text{string})}$ of the string-ordered part of Ψ_k . Upon using the non-normalized states $\Psi_k^z(c)$ this quantity can be seen to be

$$w_k^{(\text{string})} = \frac{\langle \Psi_k^z(0) | \Psi_k^z(0) \rangle}{\langle \Psi_k^z(c) | \Psi_k^z(c) \rangle}. \quad (12)$$

Upon normalization this gives the weight of the part $\Psi_k^z(0)$ of the state $\Psi_k^z(c)$ which has perfect string order. $\Psi_k^z(0)$ is a linear combination of states with antiferromagnetic order being diluted by sites with $s_z = 0$ (spin-zero defects).

For $k = \pi$ this gives $w_{k=\pi}^{(\text{string})} = 0.9888\dots$, which should be compared with the numerical result for the exact excited state $0.9866\dots$ found for $N = 14$ and periodic boundary conditions.

Finally we want to communicate our results for the string and the spin correlations for the state $\Psi_{k=\pi}^z$. The string order operator σ_{mn}^α for $\alpha = x, z$ and $i < j$ is defined as follows [7]:

$$\sigma_{ij}^\alpha = -S_i^\alpha e^{i\pi \sum_{l=i+1}^j S_l^\alpha} S_j^\alpha. \quad (13)$$

The unitary operator U transforms spin and string operators into each other:

$$U^\dagger \sigma_{ij}^\alpha U = S_i^\alpha S_j^\alpha. \quad (14)$$

Neglecting terms of the order $O(1/N)$ one calculates:

$$\begin{aligned} \frac{\langle \Psi_k^z | \sigma_{mn}^x | \Psi_k^z \rangle}{\langle \Psi_k^z | \Psi_k^z \rangle} &= \left(\frac{2}{3} \delta_{mn} + \frac{4}{9} (1 - \delta_{mn}) \right) \left(1 - \frac{2|n-m|}{N} \right) + O(1/N) \\ \frac{\langle \Psi_k^z | \sigma_{mn}^z | \Psi_k^z \rangle}{\langle \Psi_k^z | \Psi_k^z \rangle} &= \left(\frac{2}{3} \delta_{mn} + \frac{4}{9} (1 - \delta_{mn}) \right) + O(1/N). \end{aligned} \quad (15)$$

This result is independent from c and coincides with the result for the bare kinks ($c = 0$) to the given order in $1/N$. Comparison with numerical results for chains with $N \leq 14$ show qualitative agreement. Extrapolation for $N \rightarrow \infty$ was, unfortunately, not possible.

Similar calculations for the spin correlations give to leading order

$$\frac{\langle \Psi_k^z | S_m^\alpha S_n^\alpha | \Psi_k^z \rangle}{\langle \Psi_k^z | \Psi_k^z \rangle} = \left(\frac{2}{3} \delta_{mn} + \frac{4}{3} (-1/3)^{|n-m|} (1 - \delta_{mn}) \right) \left(1 + O\left(\frac{2|n-m|}{N}\right) \right) + O(1/N) \quad (16)$$

for both $\alpha = x$ and $\alpha = z$. Again, in leading order these results agree with the result for bare kinks. Comparison with numerical results again shows qualitative agreement.

Our results confirm the picture given in [11] and independently in [12] that the elementary excitations of the AKLT Hamiltonian are hidden string order domain walls with a spatial extension of a few lattice sites. Numerical results for the string order correlation of two-kink states in finite chains [17] show that they repel each other. This feature already goes beyond our simple independent two-soliton *ansatz* used to determine $E_2(k)$.

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References

- [1] Haldane F D M 1983 *Phys. Rev. Lett.* **50** 1153; 1983 *Phys. Lett.* **93A** 464
- [2] Affleck I 1989 *J. Phys.: Condens. Matter* **1** 3047
- [3] Mikeška H J 1995 *Chaos, Solitons, and Fractals* at press
- [4] Affleck I, Kennedy T, Lieb E and Tasaki H 1987 *Phys. Rev. Lett.* **59** 799
- [5] den Nijs M and Rommelse K 1989 *Phys. Rev. B* **40** 4709

- [6] Girvin S M and Arovas D P 1989 *Phys. Scr.* T **27** 156
- [7] Kennedy T and Tasaki H 1992 *Phys. Rev.* B **45** 304
- [8] Arovas D P, Auerbach A and Haldane F D M 1988 *Phys. Rev. Lett.* **60** 531
- [9] Arovas D P 1989 *Phys. Lett.* **137A** 431
- [10] Knabe S 1988 *J. Stat. Phys.* **52** 627
- [11] Fáth G and Sólyom J 1993 *J. Phys.: Condens. Matter* **5** 8983
- [12] Neugebauer U 1993 *Thesis*
- [13] Scharf R 1993 unpublished
- [14] Kennedy T 1994 *J. Phys.: Condens. Matter* **6** 8015
- [15] Gomez-Santos G 1989 *Phys. Rev. Lett.* **63** 790
- [16] Mikeska H J 1992 *Europhys. Lett.* **19** 39
- [17] Elstner N and Mikeska H J 1988 *Phys. Rev.* **50** 3907