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Solitonic excitations in the Haldane phase of an $S = 1$ chain

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Abstract. We study low-lying excitations in the 1D $S = 1$ antiferromagnetic valence-bond-solid (VBS) model. In a numerical calculation on finite systems the lowest excitations are found to form a discrete triplet branch, separated from the higher-lying continuum. The dispersion of these triplet excitations can be satisfactorily reproduced by assuming approximate wavefunctions. These wavefunctions are shown to correspond to moving hidden domain walls, i.e. to one-soliton excitations.

1. Introduction

It was almost a decade ago that Haldane [1] conjectured the existence of a new type of ground state for isotropic Heisenberg antiferromagnets (HAF) of integer spin S . The Haldane phase was proposed to be characterized by a unique disordered ground state with exponential decay of the correlation functions and a finite energy gap to the excited states. Since then one-dimensional quantum spin chains with $S = 1$ have been studied intensively and it is claimed that the gapful behaviour is a generic feature of integer-spin models [2].

The first rigorous example of an $S = 1$ antiferromagnetic model with Haldane phase was given by Affleck and co-workers [3]. They showed that the $S = 1$ isotropic bilinear-biquadratic model defined by the Hamiltonian

$$H = \sum_{j=1}^N h_j(\beta) = \sum_{j=1}^N \left[\frac{1}{2} S_j \cdot S_{j+1} + \frac{1}{2} \beta (S_j \cdot S_{j+1})^2 + \frac{1}{3} \right] \quad (1)$$

has a short-range valence-bond-solid ground state for $\beta = 1/3$ (the VBS or AKLT model). At that point $h_j(1/3)$ is a special projection operator, which projects out the quintuplet state of the two neighbouring spins, and which is positive semi-definite. Therefore, a state Ω for which $h_j \Omega = 0$ for any j is necessarily a ground state with ground-state energy $E_{GS} = 0$. Such an Ω state could be constructed using nearest-neighbour valence bonds. They were also able to prove rigorously [3] that in the infinite-chain limit this state (i) is the only ground state, (ii) is separated by a finite gap from the excited states and (iii) the two-point correlation functions decay exponentially.

According to Haldane's conjecture such a phase should not appear for half-integer values of the spin. This was proven rigorously by Affleck and Lieb [4] and independently by Kolb [5]. It was shown for a wide class of models that in the case when the ground state is a spin singlet, the energy spectrum as a function of momentum k is symmetric under reflections with respect to $k = m\pi/2$ (m integer), and therefore the ground state should be at least doubly degenerate.

A similar proof fails in the integer- S case, allowing for the existence of a unique singlet ground state [4, 5]. The excitation spectrum is in general symmetric with respect to $k = m\pi$ only. Of course, higher symmetry can also appear in integer- S chains as, for example, in the spontaneously dimerized phase of the general bilinear–biquadratic $S = 1$ model [6].

The $S = 1$ bilinear–biquadratic model is integrable [7] at the critical point $\beta = 1$ which separates the dimerized phase from the Haldane phase. Although the spin is an integer, at this point the excitations can be described in exactly the same way as for the spin-1/2 HAF. More generally, it has been known since the work of Faddeev and Takhtajan [7] that there are integrable-spin models for arbitrary S in which the elementary excitations are in fact spin-1/2 solitons with a dispersion independent of the spin length S . The observable excitations are composite particles, since for topological reasons the solitons can only appear in singlet or triplet pairs. As the energy of such a soliton pair can be described by two parameters, the excitations form a continuum in momentum space.

Away from the integrable point, where the symmetry properties of the excitation spectra are different for integer and half-integer S , the above-mentioned picture of composite excitations may not hold. In this paper we will study this problem.

We will restrict ourselves to the $S = 1$ case, where the non-integrability appears in the most dramatic way in the Haldane phase. We will show that the lowest excitations are real spin-1 one-particle excitations which cannot be decomposed into pairs of spin-1/2 solitons. These triplet excitations are, however, not usual antiferromagnons but rather some sort of *hidden spin-1 solitons*.

The solitonic nature of the excitations of the integer-spin models was predicted by Haldane. This assumption became less astonishing after the discovery of the hidden order in the Haldane phase. Recently, in a very inspiring work, den Nijs and Rommelse [8] have introduced a non-local string operator σ_{ij}^α defined by

$$\sigma_{ij}^\alpha := -S_i^\alpha \exp\left(i\pi \sum_{l=i+1}^{j-1} S_l^\alpha\right) S_j^\alpha. \quad (2)$$

They argued that, although in the Haldane phase the ground state is disordered in the conventional sense, it has a hidden long-range order that could be characterized by the string order parameter

$$O_{\text{string}}^\alpha(H) = \lim_{|i-j| \rightarrow \infty} {}_H \langle \sigma_{ij}^\alpha \rangle_H \quad \alpha = x, y, z \quad (3)$$

where ${}_H \langle \cdot \rangle_H$ denotes the expectation value in the ground state of the Hamiltonian H .

This prediction was later verified numerically by several authors [9]. The appearance of the hidden long-range order was further discussed by Kennedy and Tasaki [10]. They showed, using a non-local unitary transformation, that $O_{\text{string}}^\alpha > 0$ corresponds to the spontaneous breaking of a hidden $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry of the model. Similarly, the fact that the four lowest states of an open chain are exponentially close to each other is also a consequence of this broken symmetry. It is generally expected that the breaking of a discrete symmetry in the ground state leads to an excitation gap since Goldstone bosons do not appear. Excitations of the model can then be thought of as some sort of (hidden) domain walls, separating regions with different ground states. This picture was made more explicit by Elstner and Mikeska [11], who used spin-zero defects [12] to disorder the antiferromagnetic state. The spin-zero defects are in fact solitons. One of the main goals of this paper is to further examine this problem.

We will use numerical and analytical methods to study the low-lying excitations in the $\beta = 1/3$ case. Beside the fact that the ground state of the VBS model can be constructed analytically, there is another good reason to focus on this model. In a recent study of the general bilinear–biquadratic model of (1), we observed [6] that the convergence of various finite-size estimates to their thermodynamic limit is extremely fast in the close vicinity of $\beta = 1/3$. This is certainly not true for general β . Moving away from $\beta = 1/3$, finite-size corrections become stronger and one must consider longer and longer chains in order to see the real asymptotic behaviour. The rapid convergence at the VBS point may not be very surprising if we remember that at this point in the ground state only first-neighbour valence bonds are present and the ground-state energy density becomes independent of the chain length. Although the excited states do show some dependence on N , this is found to be exponentially small for the most relevant levels. Therefore, extrapolation from finite-size calculations allows one to draw quite reliable conclusions about the spectrum, and it can be compared directly to the analytical (variational) results.

After a detailed numerical analysis of the spectrum, we will study trial wavefunctions for the elementary excitations and illustrate their solitonic nature. Since the Haldane phase at $\beta = 0$ is believed to be in the same universality class as the VBS model at $\beta = 1/3$, our finding should be qualitatively correct for the usual HAF.

The layout of the paper is as follows. In section 2 we present our numerical results. Section 3 contains the analysis of two seemingly different trial wavefunctions and their equivalence is shown. The elementary excitations are argued to be triplet bonds in the VBS structure. In section 4, we recall the non-local unitary transformation of Kennedy and Tasaki. In section 5 the trial wavefunctions for the excitations are studied further using this transformation. Thus their domain wall nature becomes explicit. Finally, in section 6 we summarize our results.

2. Numerical results

Our first aim is to study the excitation spectrum of the VBS model numerically, using a periodic boundary condition. The symmetry properties of the Hamiltonian in (1) allow us to classify the eigenstates according to their total spin S_T , its component along the z axis S_T^z , and the momentum $k = 2\pi l/N$ (l integer) of the states, where N is the length of the chain. We computed several low-lying eigenvalues of the Hamiltonian for each possible value of k , using a Lánczos algorithm, and also determined the total spin of the states. Chains with an even number of sites up to $N = 16$ were considered.

Figure 1 shows the six lowest eigenvalues for all k in our longest chain with $N = 16$. For some of the energies the total spin quantum number S_T is also given. It is seen that, in full agreement with all previous results [2], the lowest excited state (denoted by A) is an $S_T = 1$ state with momentum $k = \pi$. Moreover, in the whole range $|k| \gtrsim \pi/2$ the lowest-energy excited states have the same total spin $S_T = 1$. In the thermodynamic limit, these states, as a function of k , seem to form a continuous branch of excitations. In fact, according to the general theorem we proved in [6], an excitation with $S_T \geq 1$ cannot remain isolated in the $N \rightarrow \infty$ limit.

On the other hand, near $k = \pi$, the energies of the next-higher-lying excitations are situated at a distance from the triplet branch that is much greater than their average energy difference from each other. This behaviour indicates that in the infinite-chain limit, at least near $k = \pi$, the lowest triplet excitations do not belong to a continuum. The existence of such a discrete branch below the higher-lying continuum seems to be another characteristic

feature of the non-integrable integer-spin models. Unlike the integrable spin models and general spin models of half-integer S , the lowest-lying excitations in the Haldane phase are real one-particle spin-1 excitations. They cannot be decomposed into $S = 1/2$ solitons.

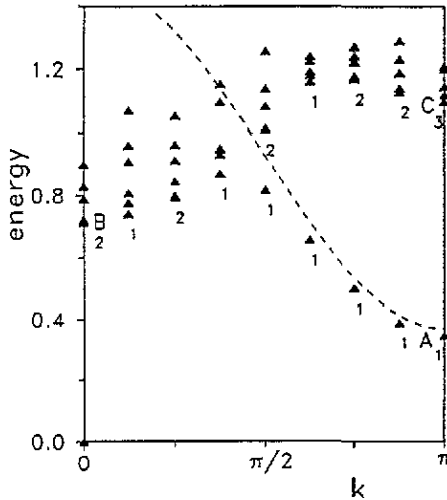


Figure 1. Low-lying eigenvalues of the vbs model plotted against momentum k , for a chain with $N = 16$ sites. Labels denote the total spin S_T of the states. The broken curve shows the energy of the trial state with the moving hidden soliton.

Above the triplet branch, the higher-lying excitations of the vbs model seem to be ‘dense’ for all k , supposedly forming a continuum. They probably cannot be described by a single parameter. For $N = 16$, the triplet branch merges into this continuum somewhere below $k \sim \pi/2$. Near $k = 0$ there is no sign of a discrete branch; here, the lowest-lying excitations are thought to belong to the continuum.

There is another remarkable feature that can be observed in our finite-chain calculation. The gap Δ_B to the lowest excited state of the $k = 0$ subspace is approximately twice the singlet–triplet gap Δ_A at $k = \pi$. The same property was observed by Takahashi [13] for the pure Heisenberg chain $\beta = 0$. Similarly, the gap Δ_C between the ground state and the second excited state in the $k = \pi$ sector seems to be three times as large as the singlet–triplet gap. It is also noteworthy that state B (the lowest $k = 0$ excited state) is a quintuplet ($S_T = 2$) state and C (the second lowest $k = \pi$ excited state) is a state with $S_T = 3$. The physical picture behind such a behaviour is simple. The excitations near $k = 0$ can be composed of two low-lying excitations near $k = \pi$ and, similarly, three excitations near $k = \pi$ can be combined to give another excitation near $k = \pi$.

Whether or not the spectrum has this property in the $N \rightarrow \infty$ limit was tested by extrapolating the finite-size calculations to infinitely long chains. In figure 2 the gaps Δ_A , Δ_B and Δ_C are plotted as a function of $1/N$. The convergence to the thermodynamic limit is very fast, especially for Δ_A . Using standard extrapolation methods, the limiting values of the three quantities are $\Delta_A = 0.350\,124 \pm 10^{-6}$, $\Delta_B = 0.71 \pm 0.01$ and $\Delta_C = 1.09 \pm 0.03$, respectively. As is seen, the ratios give the anticipated values 1 : 2 : 3 within an error of 4%.

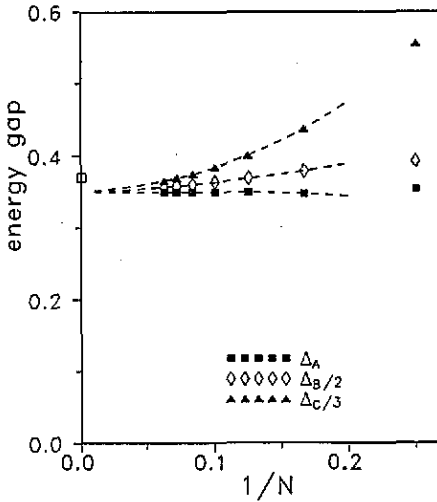


Figure 2. Energy gaps Δ_A , $\Delta_B/2$ and $\Delta_C/3$ plotted against $1/N$. Broken curves indicate the suggested large- N behaviour. \square shows the energy of the trial wavefunction at $k = \pi$.

This numerical calculation supports rather convincingly the idea that the elementary excitations of the model form a discrete triplet branch, which is separated from the multi-particle continuum in a wide range around $k = \pi$. Analysing the lower boundary of this multi-particle continuum, it seems very likely that the two-particle states near $k = 0$ are essentially *scattering* states of two elementary excitations. The energy and momentum of such a multi-particle state is then simply the sum of the energies and momenta, respectively, of the two particles. The situation is similar for the three-particle states near $k = \pi$. In the numerical calculation there does not seem to be any sign of bound states below the scattering continuum.

3. Trial wavefunctions for the elementary excitations

In this section we will study the elementary excitations of the VBS model analytically. We will see that it is possible to reproduce the dispersion relation of the discrete triplet branch quite precisely by assuming simple trial wavefunctions. It will be argued that the elementary excitations are (hidden) solitons that destroy the hidden order of the ground state.

First, we recall the form of the ground-state wavefunction. As was mentioned in section 1, the ground state of the VBS model can be constructed analytically using nearest-neighbour valence bonds. For this, an $S = 1$ operator will be composed of two $S = 1/2$ operators. Taking the tensor product of the two spin-1/2 spaces, a new orthogonal basis at site i [3] is constructed in the form

$$\psi_{\alpha\beta}^i = [\psi_\alpha \otimes \psi_\beta + \psi_\beta \otimes \psi_\alpha] / \sqrt{2} \quad (4)$$

where ψ_α and ψ_β represent the eigenstates of the two spin-1/2 operators and the greek indices take the values \uparrow and \downarrow . There are three independent symmetric combinations corresponding to the three eigenstates of the spin-1 operator, $|+\rangle_i$, $|0\rangle_i$, and $|-\rangle_i$ with $S_z^i = 1, 0$ and -1 , respectively,

$$|+\rangle_i = \psi_{\uparrow\uparrow}^i / \sqrt{2} \quad |0\rangle_i = \psi_{\uparrow\downarrow}^i \equiv \psi_{\downarrow\uparrow}^i \quad |-\rangle_i = \psi_{\downarrow\downarrow}^i / \sqrt{2}. \quad (5)$$

The fourth orthogonal state that completes the basis is the antisymmetric combination corresponding to an $S = 0$ state at site i . This configuration will be excluded.

The ground-state wavefunction of an open chain of length N can be written in terms of these states as [3]

$$\Omega(\alpha_1, \beta_N) = \psi_{\alpha_1\beta_1}^1 \varepsilon^{\beta_1\alpha_2} \psi_{\alpha_2\beta_2}^2 \varepsilon^{\beta_2\alpha_3} \dots \psi_{\alpha_i\beta_i}^i \varepsilon^{\beta_i\alpha_{i+1}} \dots \psi_{\alpha_N\beta_N}^N. \tag{6}$$

Here and in what follows summation is over repeated indices; $\varepsilon^{\alpha\beta}$ is an antisymmetric tensor with $\varepsilon^{\uparrow\downarrow} = -\varepsilon^{\downarrow\uparrow} = 1$. At both ends of the chain there is a loose spin-1/2 degree of freedom, denoted by α_1 and β_N . Since both can assume any of the two eigenstates independently, the ground state is fourfold degenerate. Three of these states constitute the three components of a spin triplet, while the fourth state is a spin singlet. It was shown, however, that these four ground states converge to the same infinite volume limit as $N \rightarrow \infty$.

A unique ground state can be formed even for finite N in the case of a periodic boundary condition by antisymmetrizing the two loose end-spins. The ground-state wavefunction can be written as

$$\Omega = \Omega(\alpha_1, \beta_N) \varepsilon^{\beta_N\alpha_1}. \tag{7}$$

Note that these states are not normalized: $\|\Omega(\alpha_1, \beta_N)\|^2 = \frac{1}{2}3^N + \mathcal{O}(1)$ and $\|\Omega\|^2 = 3^N + \mathcal{O}(1)$.

The term Ω has the interesting property that the configurations appearing in Ω look, in the conventional S^z representation, like

$$\dots 0 + 0 \dots 0 - 0 \dots 0 + 0 \dots 0 - 0 \dots \tag{8}$$

i.e. each + is followed by a - with an arbitrary number of 0 states between, and vice versa. This is nothing but a dilute spin-1/2 Néel antiferromagnet, where the 0s represent a background and the + and - states denote the two possible degrees of freedom of a spin-1/2 particle. As is seen, the hidden Néel order is perfect for the VBS ground state. For this case the string order parameter of den Nijs and Rommelse is [8] $O_{\text{string}}^\alpha(H_{\text{VBS}}) = \frac{4}{9}$, $\alpha = x, y, z$. Moving away from the VBS point, quantum fluctuations begin to destroy the above structure of Ω . However, the hidden long-range order, characterized by $O_{\text{string}}^\alpha > 0$, $\alpha = x, y, z$, is expected to persist in a wide region, in the whole Haldane phase [9].

As for the excited states of the VBS model our knowledge is much less accurate, since the eigenfunctions cannot be constructed in a similarly rigorous way. Recently, however, two seemingly rather different trial wavefunctions were proposed to describe elementary excitations in the model. Arovas and co-workers [14] proposed the form

$$|k\rangle = N^{-1/2} \sum_{j=1}^N e^{ikj} S_j^\mu |\Omega\rangle \quad \mu = z, +, - \tag{9}$$

and obtained

$$\epsilon(k) = \frac{\langle k | H_{\text{VBS}} | k \rangle}{\langle k | k \rangle} = \frac{25 + 15 \cos(k)}{27} \tag{10}$$

for the dispersion relation of the excitations. As is seen from figure 2, the variational *ansatz* yields an upper bound $\Delta_A \leq \frac{10}{27} = 0.3704$, very close to the real excitation gap obtained from the finite-size calculation at $k = \pi$.

The dispersion relation (10) is plotted in figure 1 with a broken curve. Comparison with the numerical results suggest that the trial wavefunction $|k\rangle$ gives a reasonable description of the elementary excitations not only at $k = \pi$, but in a large region of the Brillouin zone, in the range $|k| \gtrsim \pi/2$. Below that, in the region near $k = 0$, the two-particle scattering continuum dominates the spectrum.

Looking at the form of the trial wavefunction in (9), one is tempted to interpret the elementary excitations as *magnons*. Note, however, that although these 'magnons' would not destroy a conventional long-range order, they do destroy the hidden order. This is directly seen if we use, for example, the $\mu = +$ component in (9). In $S_j^+ \Omega$ only those configurations appear that look like

$$\dots 0 - 0 \dots 0 + 0 \dots 0 + 0 \dots 0 - 0 \dots 0 + 0 \dots \quad (11)$$

i.e. the Néel order of the non-zero components is broken at one point. In the dilute antiferromagnetic picture this is nothing else but a usual antiferromagnetic soliton embedded in the background of 0s. Such a soliton, unlike a magnon, destroys the long-range order, in this case the *hidden* antiferromagnetic order corresponding to O_{string}^z .

The solitonic nature of $S_j^z \Omega$ is much less obvious at first sight, since in this case the hidden Néel order of (8) seems to remain intact. However, as will be illustrated in section 5, now the hidden order in the transverse directions (i.e. O_{string}^x and O_{string}^y) will be destroyed.

In an alternative approach Knabe [15] proposed the following construction for the elementary excitations. Let us retain the valence-bond structure of Ω for every bond except that between sites j and $j + 1$, where the two spin-1/2 degrees of freedom β_j and α_{j+1} are symmetrized to form a triplet bond, instead of the antisymmetrized singlet bond.

To make this construction more explicit, divide the sites of the chain into two sets: $\mathcal{L} = \{1, 2, \dots, j\}$ and $\mathcal{R} = \{j + 1, j + 2, \dots, N\}$. We define first the states $\Phi_j^{\beta_j, \alpha_{j+1}}(\alpha_1, \beta_N)$, with $\beta_j, \alpha_{j+1} = \uparrow, \downarrow$ and $1 \leq j < N$, as explicit tensor products of two arbitrary ground states, one on \mathcal{L} and the other on \mathcal{R} , respectively, as

$$\Phi_j^{\beta_j, \alpha_{j+1}}(\alpha_1, \beta_N) = \Omega_{\mathcal{L}}(\alpha_1, \beta_j) \otimes \Omega_{\mathcal{R}}(\alpha_{j+1}, \beta_N). \quad (12)$$

Obviously, the ground state of the full chain can be obtained by antisymmetrizing with respect to α_j and β_{j+1} , i.e. by connecting the \mathcal{L} and \mathcal{R} sides with a singlet valence bond:

$$\Omega(\alpha_1, \beta_N) = \Phi_j^{\uparrow\downarrow}(\alpha_1, \beta_N) - \Phi_j^{\downarrow\uparrow}(\alpha_1, \beta_N). \quad (13)$$

On the other hand, *symmetrization* with respect to α_j and β_{j+1} defines three new states:

$$\Phi_j^+(\alpha_1, \beta_N) = \Phi_j^{\uparrow\uparrow}(\alpha_1, \beta_N) \quad (14)$$

$$\Phi_j^0(\alpha_1, \beta_N) = \frac{1}{\sqrt{2}}[\Phi_j^{\uparrow\downarrow}(\alpha_1, \beta_N) + \Phi_j^{\downarrow\uparrow}(\alpha_1, \beta_N)] \quad (15)$$

$$\Phi_j^-(\alpha_1, \beta_N) = \Phi_j^{\downarrow\downarrow}(\alpha_1, \beta_N). \quad (16)$$

In these states the singlet valence bond between sites j and $j + 1$ is substituted by a triplet bond. This adds an extra spin-1 degree of freedom to the two free spin-1/2 variables in the ground states of the *open* chain. The factor $1/\sqrt{2}$ is introduced in Φ_j^0 to ensure that the states have the same norm, $\|\Phi_j^a(\alpha_1, \beta_N)\|^2 = \frac{1}{4}3^N + \mathcal{O}(1)$, $a = +, 0, -$, as $N \rightarrow \infty$.

In the case of periodic boundary condition, the two loose spin-1/2 degrees of freedom at the chain ends should again be contracted with an ε tensor. This defines the functions

$$\Phi_j^a = \Phi_j^a(\alpha_1, \beta_N) \varepsilon^{\beta_N, \alpha_1} \quad a = +, 0, - \quad (17)$$

for $1 \leq j \leq N-1$. The state Φ_N^a , in which the spin-1 bond connects the last and first sites, N and 1 , is defined analogously. Unlike the case of an open boundary condition, now the total spin of the three states Φ_j^a , $a = +, 0, -$, is necessarily $S_T = 1$ with $S_T^z = +1, 0, -1$, respectively, since all the other antisymmetrized bonds have zero spin.

These states again have a soliton-like nature, just as in the other approach mentioned above. The term Φ_j^+ , for example, can be explicitly written as

$$\Phi_j^+ = \dots \varepsilon^{\beta_j - 2\alpha_{j-1}} \psi_{\alpha_{j-1}\beta_{j-1}}^{j-1} \varepsilon^{\beta_{j-1}\alpha_j} \psi_{\alpha_j\uparrow}^j \psi_{\uparrow\beta_{j+1}}^{j+1} \varepsilon^{\beta_{j+1}\alpha_{j+2}} \psi_{\alpha_{j+2}\beta_{j+2}}^{j+2} \varepsilon^{\beta_{j+2}\alpha_{j+3}} \dots \quad (18)$$

In each non-zero configuration the subscripts β_i and α_{i+1} are antiparallel except for $i = j$, for which $\beta_j = \alpha_{j+1} = \uparrow$. Transforming this into the standard S_z representation, the nearest non-zero spin states on the left- and right-hand side of the triplet bond are necessarily $+$ states. Otherwise the Néel order of the $+$ and $-$ states is complete on both sides.

As a variational *ansatz*, Knabe [15] analysed a general linear combination of the Φ_j^a states, $\sum_{j=1}^N c_j \Phi_j^a$ and found that the energy is minimized if $c_j = (-1)^j$. For the primary gap of the model he obtained an upper bound in the form $\Delta_A \leq \frac{5}{14} \approx 0.3571$. Correcting a small obvious mistake in the numerics of his paper, the correct upper bound is $10/27 \approx 0.3704$, exactly as in [14].

It is quite straightforward to generalize this calculation to arbitrary momentum k . Looking for translationally invariant trial wavefunctions, we define

$$\Phi^a(k) = \sum_{j=1}^N e^{ikj} \Phi_j^a \quad a = +, 0, -. \quad (19)$$

Knabe's wavefunction corresponds to $k = \pi$. With our definition of the (unnormalized) trial wavefunctions Φ_j^a , $a = +, 0, -$, Knabe's results can be re-expressed in the following form:

$$\langle \Phi_j^a | \Phi_{j'}^a \rangle = \frac{1}{2} 3^N \left(-\frac{1}{3}\right)^{|j-j'|} + \mathcal{O}(1) \quad (20)$$

and

$$\langle \Phi_j^a | H_{\text{VBS}} | \Phi_{j'}^a \rangle = \delta_{jj'} \frac{10}{27} 3^N + \mathcal{O}(1). \quad (21)$$

Using these results, it is now straightforward to calculate the normalization of the translationally invariant states $\Phi^a(k)$ defined by (19) and the expectation value of the energy in these states. In the thermodynamic limit we get

$$\langle \Phi^a(k) | \Phi^a(k) \rangle = \sum_{j, j'=0}^N e^{ik(j'-j)} \langle \Phi_j^a | \Phi_{j'}^a \rangle = N \frac{1}{2} 3^N \sum_{r=0}^N e^{ikr} \left(-\frac{1}{3}\right)^r = \frac{2}{5 + 3 \cos(k)} N 3^N \quad (22)$$

and

$$\langle \Phi^a(k) | H_{\text{VBS}} | \Phi^a(k) \rangle = \sum_{j, j'=0}^N e^{ik(j'-j)} \langle \Phi_j^a | H_{\text{VBS}} | \Phi_{j'}^a \rangle = \frac{10}{27} N 3^N \quad (23)$$

whence the dispersion of the excitations is again

$$\epsilon(k) = \frac{\langle \Phi^a(k) | H_{\text{VBS}} | \Phi^a(k) \rangle}{\langle \Phi^a(k) | \Phi^a(k) \rangle} = \frac{25 + 15 \cos(k)}{27}. \quad (24)$$

This dispersion is exactly the same as that obtained by Arovas and co-workers in (9). Despite the different forms of the wavefunctions, the identical result for the dispersion relation indicates a deep connection between the two approximations. In fact, it is not too difficult to show that $S_j^\mu |\Omega\rangle$ can be expressed in a simple form with our Φ_j^a configurations:

$$S_j^z |\Omega\rangle = \frac{1}{\sqrt{2}} (\Phi_j^0 - \Phi_{j-1}^0) \quad (25)$$

$$S_j^\pm |\Omega\rangle = \mp (\Phi_j^\pm - \Phi_{j-1}^\pm) \quad (26)$$

therefore $|k\rangle$ differs from $\Phi^\mu(k)$ in a constant factor only, which is cancelled when the expectation value of the energy is taken.

One may ask the following question: which construction of the above two should now be considered as the elementary excitation? Equations (25) and (26) show that $S_j^\mu |\Omega\rangle$ is a simple linear combination of the Φ_j^a configurations. The reverse, however, is not true: Φ_j^a cannot be expressed with $S_j^\mu |\Omega\rangle$ in a similarly simple way. Therefore, one should conclude that the elementary excitations are in fact the moving triplet bonds.

4. The Kennedy–Tasaki transformation

A better picture of the above described elementary excitations of the VBS model can be obtained by using the non-local unitary transformation U of Kennedy and Tasaki [10]. This transforms the antiferromagnetic Hamiltonian into a ferromagnetic-like model and makes explicit the $Z_2 \times Z_2$ symmetry breaking in the ground state. First we recall some features of this transformation, then show that the above trial wavefunctions transform under U into simple explicit domain walls. A small inconvenience, arising from the non-local character of the transformation, is that it can only be used conveniently on chains with *open* boundary conditions. Note, however, that we do not seek exact solutions but variational results only, so the boundary condition will have no relevance for long enough chains.

We define the unitary U in the usual way [10]: let $|s\rangle = |s_1, s_2, \dots, s_N\rangle$ denote a basis state in the S^z representation, where $s_i = +, 0, -$ stands for the eigenvalues $+1, 0, -1$, respectively of S_i^z . Introducing new variables by

$$\bar{s}_i = \exp\left(i\pi \sum_{l=1}^{i-1} s_l\right) s_i \quad (27)$$

the spin configurations can be given as $|\bar{s}\rangle = |\bar{s}_1, \bar{s}_2, \dots, \bar{s}_N\rangle$. Note that in $|\bar{s}\rangle$ all the 0s of $|s\rangle$ remain unchanged, while a $+$ or $-$ at site i is flipped or remains unchanged, depending on whether the number of $+$ and $-$ on sites $1 \leq l < i$ is odd or even. The unitary U is then defined by

$$U|s\rangle = (-1)^{M(s)} |\bar{s}\rangle \quad (28)$$

where $M(s)$ denotes the number of odd sites i on which $s_i = 0$.

Let us consider now the VBS Hamiltonian. It can be shown [10] that \tilde{h}_j , $j = 1, \dots, N - 1$, transforms under U in a relatively simple (local) way into

$$\tilde{h}_j = U h_j U^{-1} = \frac{1}{6} \begin{pmatrix} | + & + \rangle \\ | + & 0 \rangle \\ | 0 & + \rangle \\ | + & - \rangle \\ | 0 & 0 \rangle \\ | - & + \rangle \\ | 0 & - \rangle \\ | - & 0 \rangle \\ | - & - \rangle \end{pmatrix} \begin{pmatrix} 1 & & & -2 & & & & & 1 \\ & 3 & -3 & & & & & & \\ & -3 & 3 & & & & & & \\ & & & 6 & & & & & \\ -2 & & & & 4 & & & & -2 \\ & & & & & 6 & & & \\ & & & & & & 3 & -3 & \\ & & & & & & -3 & 3 & \\ 1 & & & -2 & & & & & 1 \end{pmatrix}. \tag{29}$$

This, however, does not hold for h_N , i.e. for the term that couples the last and the first spins of the chain; $\tilde{h}_N = U h_N U^{-1}$ cannot be written in a similar form, moreover it does not remain local either. This problem can, however, be avoided if we switch to open boundary conditions. In this case \tilde{H}_{VBS} is simply

$$\tilde{H}_{\text{VBS}} = U H_{\text{VBS}} U^{-1} = \sum_{j=1}^{N-1} \tilde{h}_j. \tag{30}$$

The diagonalization of the above two-site Hamiltonian \tilde{h}_j shows that its ground-state sector with zero energy is four dimensional and is spanned by the states $\phi_\nu \otimes \phi_\nu$, $\nu = 1, 2, 3, 4$ (here no summation is meant over ν), where the single-site states are

$$\phi_1 = (|0\rangle + \sqrt{2}|+\rangle)/\sqrt{3} \tag{31}$$

$$\phi_2 = (|0\rangle - \sqrt{2}|+\rangle)/\sqrt{3} \tag{32}$$

$$\phi_3 = (|0\rangle + \sqrt{2}|-\rangle)/\sqrt{3} \tag{33}$$

$$\phi_4 = (|0\rangle - \sqrt{2}|-\rangle)/\sqrt{3}. \tag{34}$$

Note that this basis is not orthogonal, since $|\langle \phi_{\nu'} | \phi_\nu \rangle| = 1/3$, $\nu' \neq \nu$.

The ground states of an open chain with N sites can simply be written as the tensor product of the above-introduced single-site states:

$$\Psi_\nu = \phi_\nu^1 \otimes \phi_\nu^2 \otimes \dots \otimes \phi_\nu^{N-1} \otimes \phi_\nu^N \quad \nu = 1, 2, 3, 4. \tag{35}$$

These wavefunctions and the ground-state wavefunctions described in (6) can be easily related. On an L -site lattice any linear combinations of the Ψ_ν are ground states. Such a linear combination is obtained if U acts directly on the ground state $\Omega(\alpha_1, \beta_L)$ of H_{VBS} . For all the configurations in $\Omega(\alpha_1, \beta_L)$, the value of α_1 decides unequivocally the sign of the first non-zero spin (if $\alpha_1 = \uparrow$ then it should be a $+$) and then for a given value of L , β_L fixes the parity of the total number of non-zero spins. Using these two observations, the following relations can easily be worked out:

$$U \Omega(\uparrow, \uparrow) = (-1)^{1+L+[L/2]} (3)^{L/2-\frac{1}{2}} (\Psi_1 - \Psi_2) \tag{36}$$

$$U \Omega(\uparrow, \downarrow) = (-1)^{1+[L/2]} (3)^{L/2-\frac{1}{2}} (\Psi_1 + \Psi_2) \tag{37}$$

$$U \Omega(\downarrow, \uparrow) = (-1)^{L+[L/2]} (3)^{L/2-\frac{1}{2}} (\Psi_3 + \Psi_4) \tag{38}$$

$$U \Omega(\downarrow, \downarrow) = (-1)^{[L/2]} (3)^{L/2-\frac{1}{2}} (\Psi_3 - \Psi_4) \tag{39}$$

where $[L/2]$ denotes the integer part of $L/2$.

It can be shown rigorously that the four states in (35) remain the only ground states as $N \rightarrow \infty$, and they converge to four *different* infinite-volume ground states. Note that the ground-state degeneracy of the original and transformed Hamiltonians differ in the infinite-volume limit. This is a consequence of the non-locality of U .

The states in (35) have long-range order reflecting the spontaneous breaking of a $Z_2 \times Z_2$ symmetry, the only explicit (local) symmetry of \tilde{H}_{VBS} . Introducing the ferromagnetic order parameter of the transformed system

$$O_{\text{ferro}}^\alpha(\tilde{H}) = \lim_{|i-j| \rightarrow \infty} \tilde{H} \langle S_i^\alpha S_j^\alpha \rangle_{\tilde{H}} \quad \alpha = x, y, z \quad (40)$$

one obtains that

$$O_{\text{ferro}}^\alpha(\tilde{H}) = \tilde{H} \langle S_i^\alpha \rangle_{\tilde{H}}^2 = \frac{4}{9} \quad \alpha = x, z. \quad (41)$$

While $\tilde{H} \langle S_i^z \rangle_{\tilde{H}} = +\frac{2}{3}$ for Ψ_1 and Ψ_2 , we find $\tilde{H} \langle S_i^z \rangle_{\tilde{H}} = -\frac{2}{3}$ for Ψ_3 and Ψ_4 . Similarly, $\tilde{H} \langle S_i^x \rangle_{\tilde{H}} = +\frac{2}{3}$ for Ψ_1 and Ψ_3 and $\tilde{H} \langle S_i^x \rangle_{\tilde{H}} = -\frac{2}{3}$ for Ψ_2 and Ψ_4 . The appearance of the long-range order in the transformed Hamiltonian corresponds to a non-vanishing value of the string order parameter in the original system, since by the equivalence

$$O_{\text{string}}^\alpha(H) = O_{\text{ferro}}^\alpha(\tilde{H}) \quad \alpha = x, z \quad (42)$$

the string order transforms into a ferromagnetic order under U [10]. This equivalence does not hold for the y component.

5. Solitons in the Kennedy–Tasaki transformation

Our aim now is to show how our soliton configurations Φ_j^a , $a = +, 0, -$ transform under the unitary transformation. It will be found that in the transformed model they are explicit domain walls separating regions with different ground states Ψ_ν . Since we work now with open boundary conditions, the two loose spin-1/2 variables at the left and right chain ends should be retained explicitly.

For this purpose, we cut the chain into \mathcal{L} and \mathcal{R} parts as in section 3 and define new unitary operators. Since a configuration $|s\rangle$ can be written as an explicit tensor product of the left and right states

$$|s_1, s_2, \dots, s_N\rangle = |s_1, s_2, \dots, s_j\rangle \otimes |s_{j+1}, s_{j+2}, \dots, s_N\rangle \quad (43)$$

the action of U on $|s\rangle$ can be given in the form

$$U|s_1, s_2, \dots, s_N\rangle = U_j^{\mathcal{L}}|s_1, s_2, \dots, s_j\rangle \otimes U_j^{\mathcal{R}}|s_{j+1}, s_{j+2}, \dots, s_N\rangle. \quad (44)$$

Here

$$U_j^{\mathcal{L}}|s_1, s_2, \dots, s_j\rangle = (-1)^{M_{\mathcal{L}}(s)} |\bar{s}_1, \bar{s}_2, \dots, \bar{s}_j\rangle \quad (45)$$

$$U_j^{\mathcal{R}}|s_{j+1}, s_{j+2}, \dots, s_N\rangle = (-1)^{M_{\mathcal{R}}(s)} |\bar{s}_{j+1}, \bar{s}_{j+2}, \dots, \bar{s}_N\rangle \quad (46)$$

with $|\bar{s}\rangle$ defined by (27); $M_{\mathcal{L}}(s)$ ($M_{\mathcal{R}}(s)$) is the number of odd sites for which $s_i = 0$ and $i \in \mathcal{L}$ ($i \in \mathcal{R}$). Obviously $M_{\mathcal{L}}(s) + M_{\mathcal{R}}(s) = M(s)$.

It is seen that in general the effect of $U_j^{\mathcal{R}}$ on $|s_{j+1}, s_{j+2}, \dots, s_N\rangle$ cannot be calculated without some explicit knowledge of the configuration on \mathcal{L} since, for example, the first non-zero spin of \mathcal{R} is flipped according to whether the parity of the number of non-zero spins of \mathcal{L} is even or odd. Therefore, we define another unitary $V_j^{\mathcal{R}}$, that will be independent of \mathcal{L} , in the following way:

$$V_j^{\mathcal{R}}|s_{j+1}, s_{j+2}, \dots, s_N\rangle = (-1)^{K_{\mathcal{R}}(s)}|\bar{s}_{j+1}, \bar{s}_{j+2}, \dots, \bar{s}_N\rangle \tag{47}$$

where

$$\bar{s}_i = \exp\left(i\pi \sum_{l=j+1}^{i-1} s_l\right)s_i \quad i \geq j + 1 \tag{48}$$

and $K_{\mathcal{R}}(s)$ is the number of sites i for which $i - j$ is odd and $s_i = 0$. Note that the definition of $V_j^{\mathcal{R}}$ is nothing else but that of U , if the sites of the chain are relabelled as $i \rightarrow i - j$. To illustrate the above definitions, compare the following examples:

$$\begin{aligned} | + 0 + - 0 \rangle \otimes U_5^{\mathcal{R}} | - 0 0 - + + 0 \rangle &= - | + 0 + - 0 \rangle \otimes | + 0 0 - - + 0 \rangle \\ | + 0 + - 0 \rangle \otimes V_5^{\mathcal{R}} | - 0 0 - + + 0 \rangle &= | + 0 + - 0 \rangle \otimes | - 0 0 + + - 0 \rangle \\ | + 0 + - 0 - \rangle \otimes U_6^{\mathcal{R}} | 0 0 - + + 0 \rangle &= - | + 0 + - 0 - \rangle \otimes | 0 0 - - + 0 \rangle \\ | + 0 + - 0 - \rangle \otimes V_6^{\mathcal{R}} | 0 0 - + + 0 \rangle &= - | + 0 + - 0 - \rangle \otimes | 0 0 - - + 0 \rangle. \end{aligned}$$

It is easy to see that in general $U_j^{\mathcal{R}}$ can be expressed by $V_j^{\mathcal{R}}$ as

$$U_j^{\mathcal{R}} = p(s)P(s)V_j^{\mathcal{R}} \tag{49}$$

where $p(s) = \pm 1$ is a sign factor and $P(s)$ is either the identity operator or a general spin-flip $s_i \rightarrow -s_i, j + 1 \leq i \leq N$, on \mathcal{R} . To be more specific, let us introduce the notation $Q_{\mathcal{L}}(s)$ for the number of sites i ($i \in \mathcal{L}$) for which $s_i = \pm 1$, and similarly introduce $Q_{\mathcal{R}}(s)$ for $i \in \mathcal{R}$. For the operator P , we simply get

$$P(s) = \begin{cases} \text{identity} & Q_{\mathcal{L}}(s) = \text{even} \\ \text{spin-flip} & Q_{\mathcal{L}}(s) = \text{odd}. \end{cases} \tag{50}$$

As for the sign factor p , it is trivially $+1$ if $j = \text{even}$, while for $j = \text{odd}$ it is

$$p(s) = (-1)^{M_{\mathcal{R}}(s) - K_{\mathcal{R}}(s)} = (-1)^{M_{\mathcal{R}}(s) + K_{\mathcal{R}}(s)} = (-1)^{N - j - Q_{\mathcal{R}}(s)} = -(-1)^{N - Q_{\mathcal{R}}(s)} \tag{51}$$

since for odd j , $K_{\mathcal{R}}(s)$ counts the 0s on even sites and thus $M_{\mathcal{R}}(s) + K_{\mathcal{R}}(s)$ is the total number of 0s on \mathcal{R} .

Let us consider now the states $\Phi_j^{\beta_j, \alpha_{j+1}}(\alpha_1, \beta_N), \beta_j, \alpha_{j+1} = \uparrow, \downarrow$, where the valence bond between sites j and $j + 1$ is simply removed. From (12) and (44)

$$U \Phi_j^{\beta_j, \alpha_{j+1}}(\alpha_1, \beta_N) = U_j^{\mathcal{L}} \Omega_{\mathcal{L}}(\alpha_1, \beta_j) \otimes U_j^{\mathcal{R}} \Omega_{\mathcal{R}}(\alpha_{j+1}, \beta_N). \tag{52}$$

Then, using (49) we obtain

$$U \Phi_j^{\beta_j, \alpha_{j+1}}(\alpha_1, \beta_N) = U_j^{\mathcal{L}} \Omega_{\mathcal{L}}(\alpha_1, \beta_j) \otimes p P V_j^{\mathcal{R}} \Omega_{\mathcal{R}}(\alpha_{j+1}, \beta_N). \tag{53}$$

The expressions for $U_j^{\mathcal{L}}\Omega_{\mathcal{L}}(\alpha_1, \beta_j)$ and $V_j^{\mathcal{R}}\Omega_{\mathcal{R}}(\alpha_{j+1}, \beta_N)$ can be read off directly from (36)–(39), using the fact that the number of sites in the left part is $L = j$, while it is $L = N - j$ in the right part. Care has to be taken in the proper account of p and P . Remember that these depend on the actual configurations $\{s\}$. However, fixing α_1 and β_j , the parity of $Q_{\mathcal{L}}(s)$ is uniquely determined for all the possible configurations in $\Omega_{\mathcal{L}}(\alpha_1, \beta_j)$. Without any loss of generality we will fix the leftmost spin-1/2 variable to $\alpha_1 = \uparrow$ and suppose that $N = \text{even}$. Then $Q_{\mathcal{L}}(s) = \text{odd}$ and thus P is a spin-flip (compare with (50)) if and only if $\beta_j = \uparrow$. Similarly, the parity of $Q_{\mathcal{R}}(s)$ is uniquely determined by α_{j+1} and β_N . From (51) we easily get

$$P = \begin{cases} 1 & j = \text{even} \\ -(-1)^{\delta_{\alpha_{j+1}, \beta_N}} & j = \text{odd}. \end{cases} \quad (54)$$

Using the above results and the fact that a spin flip transforms $\Psi_1 \rightarrow \Psi_3$, $\Psi_2 \rightarrow \Psi_4$ and vice versa, one straightforwardly obtains the following relations:

$$U\Phi_j^{\uparrow\uparrow}(\uparrow, \uparrow) = (-)^j(-3)^{N/2}(1/4)(\Psi_1^{\mathcal{L}} - \Psi_2^{\mathcal{L}}) \otimes (\Psi_3^{\mathcal{R}} - \Psi_4^{\mathcal{R}}) \quad (55)$$

$$U\Phi_j^{\uparrow\downarrow}(\uparrow, \uparrow) = -(-3)^{N/2}(1/4)(\Psi_1^{\mathcal{L}} - \Psi_2^{\mathcal{L}}) \otimes (\Psi_1^{\mathcal{R}} + \Psi_2^{\mathcal{R}}) \quad (56)$$

$$U\Phi_j^{\downarrow\uparrow}(\uparrow, \uparrow) = (-3)^{N/2}(1/4)(\Psi_1^{\mathcal{L}} + \Psi_2^{\mathcal{L}}) \otimes (\Psi_1^{\mathcal{R}} - \Psi_2^{\mathcal{R}}) \quad (57)$$

$$U\Phi_j^{\downarrow\downarrow}(\uparrow, \uparrow) = -(-)^j(-3)^{N/2}(1/4)(\Psi_1^{\mathcal{L}} + \Psi_2^{\mathcal{L}}) \otimes (\Psi_3^{\mathcal{R}} + \Psi_4^{\mathcal{R}}) \quad (58)$$

$$U\Phi_j^{\uparrow\uparrow}(\uparrow, \downarrow) = (-)^j(-3)^{N/2}(1/4)(\Psi_1^{\mathcal{L}} - \Psi_2^{\mathcal{L}}) \otimes (\Psi_3^{\mathcal{R}} + \Psi_4^{\mathcal{R}}) \quad (59)$$

$$U\Phi_j^{\uparrow\downarrow}(\uparrow, \downarrow) = -(-3)^{N/2}(1/4)(\Psi_1^{\mathcal{L}} - \Psi_2^{\mathcal{L}}) \otimes (\Psi_1^{\mathcal{R}} - \Psi_2^{\mathcal{R}}) \quad (60)$$

$$U\Phi_j^{\downarrow\uparrow}(\uparrow, \downarrow) = (-3)^{N/2}(1/4)(\Psi_1^{\mathcal{L}} + \Psi_2^{\mathcal{L}}) \otimes (\Psi_1^{\mathcal{R}} + \Psi_2^{\mathcal{R}}) \quad (61)$$

$$U\Phi_j^{\downarrow\downarrow}(\uparrow, \downarrow) = -(-)^j(-3)^{N/2}(1/4)(\Psi_1^{\mathcal{L}} + \Psi_2^{\mathcal{L}}) \otimes (\Psi_3^{\mathcal{R}} - \Psi_4^{\mathcal{R}}) \quad (62)$$

where the superscript \mathcal{L} (\mathcal{R}) indicates that the wavefunction $\Psi^{\mathcal{L}}$ ($\Psi^{\mathcal{R}}$) refers to the left (right) part of the chain.

Let us insert now the triplet bond in place of the missing valence bond, i.e. symmetrize with respect to the superscripts of $\Phi_j^{\beta_j, \alpha_{j+1}}$. Recalling (14)–(16), we find

$$U\Phi_j^+(\uparrow, \uparrow) = (-)^j(-3)^{N/2}(1/4)(\Psi_1^{\mathcal{L}} \otimes \Psi_3^{\mathcal{R}} - \Psi_2^{\mathcal{L}} \otimes \Psi_3^{\mathcal{R}} - \Psi_1^{\mathcal{L}} \otimes \Psi_4^{\mathcal{R}} + \Psi_2^{\mathcal{L}} \otimes \Psi_4^{\mathcal{R}}) \quad (63)$$

$$U\Phi_j^0(\uparrow, \uparrow) = (-3)^{N/2}(1/2\sqrt{2})(\Psi_2^{\mathcal{L}} \otimes \Psi_1^{\mathcal{R}} - \Psi_1^{\mathcal{L}} \otimes \Psi_2^{\mathcal{R}}) \quad (64)$$

$$U\Phi_j^-(\uparrow, \uparrow) = -(-)^j(-3)^{N/2}(1/4)(\Psi_1^{\mathcal{L}} \otimes \Psi_3^{\mathcal{R}} + \Psi_2^{\mathcal{L}} \otimes \Psi_3^{\mathcal{R}} + \Psi_1^{\mathcal{L}} \otimes \Psi_4^{\mathcal{R}} + \Psi_2^{\mathcal{L}} \otimes \Psi_4^{\mathcal{R}}) \quad (65)$$

$$U\Phi_j^+(\uparrow, \downarrow) = (-)^j(-3)^{N/2}(1/4)(\Psi_1^{\mathcal{L}} \otimes \Psi_3^{\mathcal{R}} - \Psi_2^{\mathcal{L}} \otimes \Psi_3^{\mathcal{R}} + \Psi_1^{\mathcal{L}} \otimes \Psi_4^{\mathcal{R}} - \Psi_2^{\mathcal{L}} \otimes \Psi_4^{\mathcal{R}}) \quad (66)$$

$$U\Phi_j^0(\uparrow, \downarrow) = (-3)^{N/2}(1/2\sqrt{2})(\Psi_2^{\mathcal{L}} \otimes \Psi_1^{\mathcal{R}} + \Psi_1^{\mathcal{L}} \otimes \Psi_2^{\mathcal{R}}) \quad (67)$$

$$U\Phi_j^-(\uparrow, \downarrow) = -(-)^j(-3)^{N/2}(1/4)(\Psi_1^{\mathcal{L}} \otimes \Psi_3^{\mathcal{R}} + \Psi_2^{\mathcal{L}} \otimes \Psi_3^{\mathcal{R}} - \Psi_1^{\mathcal{L}} \otimes \Psi_4^{\mathcal{R}} - \Psi_2^{\mathcal{L}} \otimes \Psi_4^{\mathcal{R}}). \quad (68)$$

What we obtained is nothing else but a linear combination of the simplest domain walls $\Psi_\nu^L \otimes \Psi_{\nu'}^R$, $\nu \neq \nu'$, between sites j and $j + 1$. By virtue of the $SU(2)$ symmetry of H_{VBS} and the open boundary condition, it is possible to consider some linear combinations of the above states in order to get the simplest forms on the right-hand sides, for example

$$U(\Phi_j^+(\uparrow, \downarrow) + \Phi_j^+(\uparrow, \uparrow) - \Phi_j^-(\uparrow, \downarrow) - \Phi_j^-(\uparrow, \uparrow)) = (-)^j (-3)^{N/2} \Psi_1^L \otimes \Psi_3^R \tag{69}$$

$$U(\Phi_j^+(\uparrow, \downarrow) - \Phi_j^+(\uparrow, \uparrow) + \Phi_j^-(\uparrow, \downarrow) - \Phi_j^-(\uparrow, \uparrow)) = (-)^j (-3)^{N/2} \Psi_1^L \otimes \Psi_4^R \tag{70}$$

$$U(\Phi_j^0(\uparrow, \downarrow) - \Phi_j^0(\uparrow, \uparrow)) = (1/\sqrt{2})(-3)^{N/2} \Psi_1^L \otimes \Psi_2^R. \tag{71}$$

Three other similar linear combinations can be composed with $\Psi_2^L \otimes \Psi_\nu^R$, $\nu = 1, 3, 4$, on the right-hand side. These final forms clearly demonstrate the solitonic nature of our trial wavefunctions. Note that in accordance with the three degrees of freedom of such a spin-1 soliton, there are three kinds of domain walls. For $\Psi_1^L \otimes \Psi_3^R$ ($\Psi_2^L \otimes \Psi_4^R$) only $\bar{H}\langle S_i^z \rangle_{\bar{H}}$ changes sign as we move from the left region to the right; $\bar{H}\langle S_i^x \rangle_{\bar{H}}$ does not change. The situation is just the opposite for $\Psi_1^L \otimes \Psi_2^R$ ($\Psi_2^L \otimes \Psi_1^R$). Here only $\bar{H}\langle S_i^x \rangle_{\bar{H}}$ flips. Then for $\Psi_1^L \otimes \Psi_4^R$ ($\Psi_2^L \otimes \Psi_3^R$) the expectation values of the magnetization in both directions change sign.

Now it is easy to see how Φ_j^0 (or $S_j^z \Omega$, recalling (25)) destroys the hidden order O_{string}^x (and by symmetry O_{string}^y) which was anticipated in section 3. For definiteness, we fix the boundary spins $\alpha_1 = \uparrow$, $\beta_N = \uparrow$ (other choices can be worked out similarly) and consider the expectation value

$$\frac{\langle \Phi_j^0(\uparrow, \uparrow) | \sigma_{n,m}^x | \Phi_j^0(\uparrow, \uparrow) \rangle}{\| \Phi_j^0(\uparrow, \uparrow) \|^2} \tag{72}$$

In the case when $j < n$ or $j > m$, i.e. n and m are in the same domain, the domain wall has no effect and the expectation value is $4/9$. On the other hand, when $n < j < m$, it is straightforward to obtain, using the Kennedy–Tasaki transformation, the following result in the thermodynamic limit:

$$\begin{aligned} \frac{\langle \Phi_j^0(\uparrow, \uparrow) | \sigma_{n,m}^x | \Phi_j^0(\uparrow, \uparrow) \rangle}{\| \Phi_j^0(\uparrow, \uparrow) \|^2} &= \frac{\langle U \Phi_j^0(\uparrow, \uparrow) | S_n^x S_m^x | U \Phi_j^0(\uparrow, \uparrow) \rangle}{\| U \Phi_j^0(\uparrow, \uparrow) \|^2} \\ &= \frac{\langle \Psi_2^L \otimes \Psi_1^R - \Psi_1^L \otimes \Psi_2^R | S_n^x S_m^x | \Psi_2^L \otimes \Psi_1^R - \Psi_1^L \otimes \Psi_2^R \rangle}{\| \Psi_2^L \otimes \Psi_1^R - \Psi_1^L \otimes \Psi_2^R \|^2} = -\frac{4}{9} \end{aligned} \tag{73}$$

where we used (64) and the asymptotic orthogonality of the different ground states $|\langle \Psi_{\nu'} | \Psi_\nu \rangle| \rightarrow 0$ ($\nu' \neq \nu$) if $N \rightarrow \infty$. In fact, the presence of the domain wall flips the expectation value of $\sigma_{n,m}^x$.

Finally, we show that in this formalism the dispersion relation of (10) can be obtained in a very elegant way. We can start, for example, from the trial wavefunction

$$|k\rangle = \sum_{j=1}^{N-1} e^{ikj} |j\rangle \tag{74}$$

with $|j\rangle = \phi_1^j \otimes \phi_2^j \otimes \dots \otimes \phi_1^j \otimes \phi_2^{j+1} \otimes \phi_2^{j+2} \otimes \dots \otimes \phi_2^N$. In this form k is a variational parameter rather than a momentum, because of the open boundary condition. In the thermodynamic

limit, however, the boundary condition should not matter (although it might bring a constant momentum shift q in the final result, since we have the freedom to redefine $|j\rangle$ with for example an arbitrary phase factor $|j\rangle \rightarrow e^{iqj}|j\rangle$), and the variational energy as a function of k is in fact the dispersion of the excitations in this simplest domain wall approach.

The computation would proceed similarly to that in the previous section. As we have seen there, the important quantities are $\langle j|j'\rangle$ and $\langle j|\tilde{H}_{\text{VBS}}|j'\rangle$. However, in this case they are trivial because of the tensor product form. A straightforward calculation gives

$$\langle j|j'\rangle = \left(-\frac{1}{3}\right)^{|j-j'|} \quad (75)$$

where we used the fact that $\langle \phi_1|\phi_1\rangle = \langle \phi_2|\phi_2\rangle = 1$ and $\langle \phi_1|\phi_2\rangle = -1/3$ and in a similarly simple way

$$\langle j|\tilde{H}_{\text{VBS}}|j'\rangle = \delta_{j,j'} \langle \phi_1 \otimes \phi_2 | \tilde{h}_j | \phi_1 \otimes \phi_2 \rangle = \delta_{j,j'} \frac{20}{27} \quad (76)$$

which is easily obtained from the explicit form of the two-site Hamiltonian \tilde{h}_j . Apart from a factor of $3^N/2$ these results are identical to those in (20) and (21). Therefore, they also lead to the same dispersion $\epsilon(k)$.

6. Conclusions

In summary, we studied the elementary excitations in the valence-bond point of the $S = 1$ bilinear–biquadratic model. Numerical calculations on finite-size systems were used to predict the spectrum in the thermodynamic limit. The lowest-lying excited states above the $k = 0$ singlet ground state form a discrete triplet branch with a minimum at $k = \pi$. Near this minimum this branch is separated from the higher-lying scattering continuum. The energy needed to excite the lowest $k = 0$ excitation was found to be twice the gap value at $k = \pi$. Similarly, the energy of the next lowest excitation at $k = \pi$ is three times the gap value. These excitations belong to the continuum and can be interpreted as being composed of two or three $S = 1$ elementary excitations.

Comparison with the numerical results show that the separate branch of excitations can be reasonably described with a trial wavefunction, where one singlet bond is replaced by a moving triplet bond. In the representation where the configurations are given in terms of the S^z eigenstates of the spins, a triplet bond in the sea of singlet bonds has a solitonic character. In the dilute system of $+$ and $-$ spin states there is a single domain wall. While this feature is hidden in the usual valence-bond description, it becomes apparent when the non-local Kennedy–Tasaki transformation is used. We have shown that the approximate wavefunctions of the excited states transform into explicit domain walls in the transformed system.

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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] Affleck I, Kennedy T, Lieb E H and Tasaki H 1987 *Phys. Rev. Lett.* **59** 799; 1988 *Commun. Math. Phys.* **115** 477
- [4] Affleck I and Lieb E H 1986 *Lett. Math. Phys.* **12** 57
- [5] Kolb M 1985 *Phys. Rev. B* **31** 7494
- [6] Fáth G and Sólyom J 1993 *Phys. Rev. B* **47** 872
- [7] Faddeev L D and Takhtajan L A 1981 *Phys. Lett.* **85A** 375
Takhtajan L A 1982 *Phys. Lett.* **87A** 479
- [8] den Nijs M and Rommelse K 1989 *Phys. Rev. B* **40** 4709
- [9] Girvin S M and Arovas D P 1989 *Phys. Scr. T* **27** 156
Hatsugai Y and Kohmoto M 1991 *Phys. Rev. B* **44** 11789
Alcaraz F C and Hatsugai Y 1992 *Phys. Rev. B* **46** 13914
- [10] Kennedy T and Tasaki H 1992 *Phys. Rev. B* **45** 304; 1992 *Commun. Math. Phys.* **147** 431
- [11] Elstner N and Mikeska H-J 1992 *Z. Phys. B* **89** 321
- [12] Gomez-Santos G 1989 *Phys. Rev. Lett.* **63** 790
- [13] Takahashi M 1989 *Phys. Rev. Lett.* **62** 2313
- [14] Arovas D P, Auerbach A and Haldane F D M 1988 *Phys. Rev. Lett.* **60** 531
- [15] Knabe S 1988 *J. Stat. Phys.* **52** 627