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Hidden symmetry breaking in a generalized valence-bond solid model

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Abstract. A 'boson' representation for the ground state of the generalized valence-bond solid model is derived. The relation between this expression and the matrix-product representation of Klümper *et al* is discussed. It is shown that the hidden $Z_2 \times Z_2$ -symmetry is partially broken in this model. Elementary excitations of this system have a topological nature similar to that in the Affleck, Kennedy, Lieb and Tasaki model.

1. Introduction

Since Haldane [1, 2] predicted the peculiar behaviour of the Heisenberg chain with respect to the value of its spin S , one-dimensional spin systems with an integer spin have attracted great interest among many researchers (see [3] for a review). For the $S = 1$ chain at least, our qualitative understanding of the massive (or disordered) behaviour has deepened through the work of Affleck, Kennedy, Lieb and Tasaki (AKLT) [4]. They constructed an exact ground state called the valence-bond solid (VBS) state for a special bilinear-biquadratic Hamiltonian (AKLT model). They also showed that: (i) the infinite-volume ground state is unique; and (ii) the (ordinary) correlation functions decay exponentially with a correlation length $1/\ln 3$.

Further progress has been achieved by den Nijs and Rommels [5] and by Tasaki [6]. They have found that although there is no ordinary long-range order (LRO) in the ground state of the AKLT model, it has a special type of long-range order, i.e., *the string order*, which can be measured by the so-called string-order parameter. Numerical calculations suggest that the string order exists at the Heisenberg point as well as at the AKLT point [7, 8]. Now it is believed that the string LRO exists in a wide class of $S = 1$ chains with anisotropy.

On the other hand, we can construct exact ground states for $S = 1$ chains with the z -axis anisotropy in the same manner as in the AKLT. One way is to replace the $su(2)$ -projection operator of the AKLT model by the $U_q(su(2))$ -projector [9, 10] (for other deformed spin chains, see [11]). The quantum group was originally introduced independently by Drinfeld [12] and Jimbo [13] in the context of integrable systems. One of the crucial differences between $su(2)$ and $U_q(su(2))$ is the asymmetric *co-product*. Under this rule, the ordinary Clebsch–Gordan decomposition enjoys the one-parameter deformation by $q = e^\lambda$. Replacing the 'projection onto the $S = 2$ representation' by the 'projection onto the $J = 2$

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representation of $U_q(su(2))$ ' as

$$\frac{1}{[2]_q[3]_q[4]_q} \left(C - \left[\frac{1}{2} \right]_q \right) \left(C - \left[\frac{3}{2} \right]_q \right)$$

for the Casimir operator C defined by (7) (see section 2 for the meaning of the notation $[n]_q$), we can construct the q -analogue of the VBS state as an exact ground state of the deformed AKLT model [10]

$$\begin{aligned} \mathcal{H} = & \frac{[2]}{[3][4]} \sum_i \left\{ [3] S_i \cdot S_{i+1} + (S_i \cdot S_{i+1})^2 + \frac{[4]}{[2]} + a(q)^2 \frac{[4]}{[2]} S_i^z S_{i+1}^z \right. \\ & + \frac{1}{2} a(q) ([2] + [4]) (S_i^z - S_{i+1}^z) + \frac{1}{2} a(q)^2 (5[3] - 1) ((S_i^z)^2 + (S_{i+1}^z)^2) \\ & + \frac{1}{2} a(q) [2]^3 S_i^z S_{i+1}^z (S_i^z - S_{i+1}^z) - \frac{1}{2} a(q)^2 \frac{[4]}{[2]} ((S_i^z)^2 + (S_{i+1}^z)^2)^2 \\ & - \frac{1}{2} (q^{1/2} - q^{-1/2})^2 \frac{[4]}{[2]} \{ (S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+), S_i^z S_{i+1}^z \}_{\text{sym}} \\ & \left. + \frac{1}{4} [2]^2 a(q) \{ (S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+), (S_i^z - S_{i+1}^z) \}_{\text{sym}} \right\} \quad (1) \end{aligned}$$

with $a(q) = (q - q^{-1})/2$ and $\{A, B\}_{\text{sym}} \equiv (AB + BA)/2$ (it is constructed by representing C in terms of the $su(2)$ -operators). It should be remarked that it is invariant under the rotation about the z -axis ($U(1)$ -symmetry) and a simultaneous operation $S_i^z \rightarrow -S_i^z$, $q \rightarrow q^{-1}$ (the latter symmetry can be regarded as a generalization of the ordinary Z_2 -symmetry and this is quite natural in view of the $U_q(su(2))$).

Klümper *et al* constructed its ground state as a matrix product (MP) by tuning the parameters and showed that the ordinary correlation is short ranged for generic values of q . However, nobody has studied explicitly the relation between their MP construction and the conventional valence-bond construction [14]. It is also an open question as to whether there exists a hidden symmetry in this system. In this paper, we shall clarify these points.

The present paper is organized as follows. In section 2, we introduce the so-called q -Schwinger realization of $U_q(su(2))$ and construct the boson representation of the q -VBS state using it. From this bosonic expression, we can *rederive* the MP ground state (MPG) of Klümper *et al* in such a manner that the edge degrees of freedom are manifest and clarify its relation to the valence-bond-type models. Section 3 is devoted to a discussion of the hidden symmetry. There, we formally introduce the Kennedy–Tasaki transformation [15, 16] and calculate the string correlation functions both in the x - and z -directions. The effect of the deformation parameter q on various quantities is also discussed. In section 4, we calculate an approximate energy spectrum using the single-mode approximation (SMA) and discuss its properties. In the appendices, a generalization of the MP construction to higher S systems and the outline of the proof of the infinite-volume uniqueness are given (proof of the uniqueness for the case of a *finite* periodic chain is given in [10]).

2. q -boson representation of the q -VBS state

The quantum group $U_q(su(2))$ is defined by the three elements $\{J^+, J^-, J^3\}$ satisfying the following relations [12, 13]:

$$[J^+, J^-] = [2J^3]_q \quad \text{and} \quad q^{J^3} J^\pm q^{-J^3} = q^{\pm 1} J^\pm. \quad (2)$$

$[X]_q$ is the q -integer defined by

$$[X]_q \equiv \frac{q^X - q^{-X}}{q - q^{-1}} = \frac{\sinh(X\lambda)}{\sinh \lambda} \tag{3}$$

where we have parametrized q as e^λ . As in the ordinary $su(2)$ ($q = 1$) case, there is a bosonic construction of $U_q(su(2))$. While $su(2)$ -algebra is realized by the well known Schwinger construction using two independent bosons (each corresponds to \uparrow -spin and \downarrow -spin), $U_q(su(2))$ is realized by the so-called q -deformed bosons [17–19].

To construct $U_q(su(2))$, let us introduce two independent q -bosons, a and b , whose commutation relations are given by

$$aa^\dagger - qa^\dagger a = q^{-N_a} \quad bb^\dagger - qb^\dagger b = q^{-N_b} \tag{4a}$$

$$[N_a, a] = -a \quad [N_a, a^\dagger] = a^\dagger \tag{4b}$$

$$[N_b, b] = -b \quad [N_b, b^\dagger] = b^\dagger \tag{4c}$$

$$\text{otherwise } 0. \tag{4d}$$

It is important to note that the number operator N_a (N_b) is different from $a^\dagger a$ ($b^\dagger b$) when $q \neq 1$. The formal relation between them is

$$a^\dagger a = [N_a]_q.$$

Then, $U_q(su(2))$ is realized through the following relations:

$$J^+ = a^\dagger b \quad J^- = b^\dagger a \quad J^3 = \frac{1}{2}(N_a - N_b). \tag{5}$$

We can readily check that they, in fact, satisfy the defining relations of $U_q(su(2))$. The basis of the $(2j + 1)$ -dimensional representation of $U_q(su(2))$ is given by

$$|j, m\rangle = \frac{(a^\dagger)^{j+m} (b^\dagger)^{j-m}}{\sqrt{[j+m]_q!} \sqrt{[j-m]_q!}} |0\rangle \quad (m = -j, \dots, j) \tag{6}$$

where $[N]!$ is the q -factorial defined by $[N]! \equiv [N]_q [N-1]_q \dots [2]_q [1]_q$. To avoid confusion, we denote the vacuum by $|0\rangle$ and distinguish it from $|j, 0\rangle$ in the following. All the above $(2j + 1)$ states are eigenstates of the Casimir operator

$$C = [J^3 + \frac{1}{2}]_q^2 + J^- J^+ \tag{7}$$

with the eigenvalue $[j + \frac{1}{2}]_q^2$. The ‘spin’- j is the eigenvalue of $J = (N_a + N_b)/2$ as in the $su(2)$ case. That is, the three-dimensional representation relevant to our problem is constructed using two bosons ($N_a + N_b = 2$). For brevity, we abbreviate the symbol for q -integer $[]_q$ as $[]$ in the following.

Next, we derive the ‘ q -boson representation’ of the q -VBS state which is the analogue of the following bosonic representation found by Arovas *et al* [14] in the ordinary isotropic case:

$$\prod_i (a_i^\dagger b_{i+1}^\dagger - b_i^\dagger a_{i+1}^\dagger) |0\rangle_1 \otimes \dots \otimes |0\rangle_L. \tag{8}$$

Since $(a_i^\dagger b_{i+1}^\dagger - q b_i^\dagger a_{i+1}^\dagger)$ creates a $j = 0$ state out of two $j = \frac{1}{2}$ representations, we may naively write $\prod (a_i^\dagger b_{i+1}^\dagger - q b_i^\dagger a_{i+1}^\dagger) |0\rangle$. However, this expression is incorrect owing to the asymmetry of the co-product. To get a correct answer, we proceed as follows.

We seek the valence-bond operator of the following form:

$$\mathcal{O}_{\text{VB}}(i, i+1) = f_2(a_i^\dagger, b_i^\dagger, a_{i+1}^\dagger, b_{i+1}^\dagger) = a_i^\dagger b_{i+1}^\dagger - \alpha b_i^\dagger a_{i+1}^\dagger + \beta a_i^\dagger a_{i+1}^\dagger + \gamma b_i^\dagger b_{i+1}^\dagger.$$

Making the requirement that the four states $a_i^\dagger \mathcal{O}_{\text{VB}}(i, i+1) a_{i+1}^\dagger$, $a_i^\dagger \mathcal{O}_{\text{VB}}(i, i+1) b_{i+1}^\dagger$, $b_i^\dagger \mathcal{O}_{\text{VB}}(i, i+1) a_{i+1}^\dagger$ and $b_i^\dagger \mathcal{O}_{\text{VB}}(i, i+1) b_{i+1}^\dagger$ have no projection onto the $V(2)$ ($j = 2$ representation of $Uq(\mathfrak{su}(2))$), we can fix $\alpha = q^2$ and $\beta = \gamma = 0$. For convenience, we use

$$\mathcal{O}_{\text{VB}}(i, i+1) = q^{-1} a_i^\dagger b_{i+1}^\dagger - q b_i^\dagger a_{i+1}^\dagger \quad (9)$$

as the valence-bond operator. Using this, the q -VBS state is written in terms of the product of the valence-bond operators

$$|q\text{-VBS}(L)\rangle = (a_1^\dagger)^{2-m} (b_1^\dagger)^{m-1} \prod_{i=1}^{L-1} (q^{-1} a_i^\dagger b_{i+1}^\dagger - q b_i^\dagger a_{i+1}^\dagger) (a_L^\dagger)^{n-1} (b_L^\dagger)^{2-n} |0\rangle_1 \otimes \cdots \otimes |0\rangle_L. \quad (10)$$

As expected, the $q \rightarrow 1$ limit recovers the well known Schwinger boson representation of the ordinary VBS state [9, 10]. The ground states are fourfold degenerate, corresponding to the four degrees of freedom ($m, n = 1, 2$) of the left- and right-edge states. Let us express these four states in terms of 2×2 matrices and derive the matrix representation of the q -VBS state [9, 10]

First, we consider the situation of adding a single site to the L -site q -VBS state (namely the q -VBS state defined on a lattice of length L) to make the new $(L+1)$ -site q -VBS state. Let us express the L -site VBS state as the following 2×2 matrix ($\uparrow\downarrow$ denotes the edge states at both ends):

$$\begin{aligned} \Psi_{\text{VBS}}(L) &= \begin{pmatrix} \psi_{\text{VBS}}(L; \uparrow\downarrow) & \psi_{\text{VBS}}(L; \uparrow\uparrow) \\ \psi_{\text{VBS}}(L; \downarrow\downarrow) & \psi_{\text{VBS}}(L; \downarrow\uparrow) \end{pmatrix} \\ &= \begin{pmatrix} a_1^\dagger \mathcal{O}_{\text{VB}}(L) b_L^\dagger \otimes |0\rangle_k & a_1^\dagger \mathcal{O}_{\text{VB}}(L) a_L^\dagger \otimes |0\rangle_k \\ b_1^\dagger \mathcal{O}_{\text{VB}}(L) b_L^\dagger \otimes |0\rangle_k & b_1^\dagger \mathcal{O}_{\text{VB}}(L) a_L^\dagger \otimes |0\rangle_k \end{pmatrix} \end{aligned}$$

where $\mathcal{O}_{\text{VB}}(L) = \prod_{i=1}^{L-1} (q^{-1} a_i^\dagger b_{i+1}^\dagger - q b_i^\dagger a_{i+1}^\dagger)$. To write the q -boson at the right edge explicitly, $\psi_{\text{VBS}}(L; \uparrow\downarrow) = \psi_{\text{VBS}}(L; \uparrow b_L^\dagger)$ etc. Then we can easily verify that

$$\Psi_{\text{VBS}}(L+1) = \Psi_{\text{VBS}}(L) \otimes g_{L+1} \quad (11)$$

where g is the following 2×2 matrix:

$$g_i = \begin{pmatrix} -q a_i^\dagger b_i^\dagger |0\rangle_i & -q (a_i^\dagger)^2 |0\rangle_i \\ q^{-1} (b_i^\dagger)^2 |0\rangle_i & q^{-1} a_i^\dagger b_i^\dagger |0\rangle_i \end{pmatrix}. \quad (12)$$

From these equations, it can easily be seen that there is a close analogy between the g -matrix construction and the transfer matrix in one-dimensional (not two-dimensional!) classical statistical systems. In both formalisms, the action of a matrix increases the system size by

one. However, while the latter spin states on lattice sites play the role of matrix-indices, the indices of the g -matrices correspond to the *edge states* in the former.

Note that g_i is written only in terms of the q -bosons of the i -site. We can also express it by the states of $U_q(su(2))$

$$g_i = \begin{pmatrix} -q|0\rangle_i & -q\sqrt{[2]}|1\rangle_i \\ q^{-1}\sqrt{[2]}|-1\rangle_i & q^{-1}|0\rangle_i \end{pmatrix}.$$

This is nothing but the matrix found by Klümper *et al* [9, 10] (except that we choose slightly different coefficients). Using this matrix, the q -VBS state is given by the matrix product

$$\Psi_{\text{VBS}}(L) = g_{\text{start}} \otimes g_2 \otimes \cdots \otimes g_L \tag{13}$$

where g_{start} is

$$g_{\text{start}} = \begin{pmatrix} a_1^\dagger b_1^\dagger |0\rangle_1 & (a_1^\dagger)^2 |0\rangle_1 \\ (b_1^\dagger)^2 |0\rangle_1 & a_1^\dagger b_1^\dagger |0\rangle_1 \end{pmatrix}$$

(note that the action of the above g -matrix is not defined for a single-site state) and each element on the RHS corresponds to one of the four degenerate ground states. Namely, the VBS state with an open boundary condition is naturally incorporated into the matrix construction.

For a chain with a periodic boundary condition, we obtain the following expression for the g -matrix:

$$\begin{aligned} \psi_{\text{VBS}}(L) &= \prod_{i=1}^L (q^{-1} a_i^\dagger b_{i+1}^\dagger - q b_i^\dagger a_{i+1}^\dagger) |0\rangle_1 \otimes \cdots \otimes |0\rangle_L \\ &= \text{Tr}(g_1 \otimes g_2 \cdots \otimes g_L) \end{aligned} \tag{14}$$

where $a_{L+1} = a_1, b_{L+1} = b_1$.

It is easy to generalize the above matrix-product construction to the extended VBS-type ($q = 1$) states (inhomogeneous, intermediate-VBS etc) [20,21]. In appendix A, we shall discuss this point in some detail. It may be worth mentioning that we can represent the VBS states using the matrix-product form though it cannot be expressed by a simple direct-product form. Furthermore, the g -matrix contains states of a single site while the valence-bond operator contains the bosons of the two adjacent sites. This fact enables us to calculate the expectation values rather easily.

3. Hidden symmetry in the q -VBS state

As mentioned in section 1, the ground state of the AKLT model has short-ranged correlations and seems to have no order. However, as was pointed out by den Nijs and Rommels and by Tasaki [5, 6], there is a kind of *hidden* antiferromagnetic order. That is, its S^z -configuration has a generalized Néel order with randomly inserted zeros. This kind of order can be observed not by the ordinary staggered correlators but by the *string-correlation functions* [5, 6]. Furthermore, Kennedy and Tasaki [15, 16] demonstrated that a wide class of models, including the VBS model, exhibit a *discrete* $Z_2 \times Z_2$ symmetry through the non-local unitary transformation and related the breakdown of this symmetry to a non-vanishing

string order [15, 16]. In this section, we calculate the ordinary two-point functions and the string correlations to discuss the relation with the hidden symmetry breaking.

In order to discuss the S^z -configuration, it is convenient to use the matrix-representation of the q -VBS state. First, we rewrite the definition of the g -matrix (11) as follows

$$\Psi_{\text{VBS}}(L+1) = \begin{pmatrix} \psi_{\text{VBS}}(L; S_{\text{tot}}^z = 0) & \psi_{\text{VBS}}(L; S_{\text{tot}}^z = 1) \\ \psi_{\text{VBS}}(L; S_{\text{tot}}^z = -1) & \psi_{\text{VBS}}(L; S_{\text{tot}}^z = 0) \end{pmatrix} \\ \times \begin{pmatrix} -q|0\rangle_{L+1} & -q\sqrt{[2]}|1\rangle_{L+1} \\ q^{-1}\sqrt{[2]}|-1\rangle_{L+1} & q^{-1}|0\rangle_{L+1} \end{pmatrix} \quad (15)$$

where S_{tot}^z denotes $\sum_{k=1}^L S_k^z$. From the above expression, we can find a remarkable feature of the VBS-type states. That is, when we construct the configuration of the VBS state from the left, the value of S_i^z is determined only by the sum of the S_k^z 's sitting to the left of the site i . This reminds us of the Markov process. The situation can be seen more clearly using the following pictorial representation. If we notice that $\sum_{k=1}^{i-1} S_k^z$ always (i.e. for all i) takes the values $-1, 0$ or 1 , we can depict the S^z -configuration by the steps going upward and downward between level 0 ($\sum S_k^z = 0$) and level 1 ($\sum S_k^z = 1$) (when the left-edge state = \uparrow) or level (-1) and level 0 (when the left-edge state = \downarrow). Such a feature of the VBS state was first noticed by den Nijs and Rommels, who named it 'the disordered flat phase' [5]. What the g -matrix formalism tells us is that the S_i^z -value of a given site i ('height' of the steps) depends *only* on the 'level' between site $(i-1)$ and site i . Nachtergaele *et al* [22, 23] discussed the massive behaviour of the states which possess such a 'Markov-like' property.

From the above argument, it is obvious that string order also exists in our model. That is, only the downward (upward) steps are allowed when the last level is 1 (-1). This rule excludes configurations like $(\dots, -1, 0, 0, -1, \dots)$ or $(\dots, 1, 0, 1, \dots)$. Hence, we may expect the non-vanishing string-order parameter, at least in the z -direction. It is interesting to see which S^z -value is most probable in this ground state. It can be seen by calculating $\langle P(S^z = m) \rangle$ (projection operator onto $S^z = m$ state). The results are

$$\text{Prob}(S^z = \pm 1) = \frac{1}{[3]} \quad \text{Prob}(S^z = 0) = \frac{q^2 - 1 + q^{-2}}{[3]}. \quad (16)$$

Namely, the probability of finding non-zero (± 1) S^z -values decreases as we move away from $q = 1$ ($su(2)$). The $(00\dots 00)$ configuration especially dominates in the $q \rightarrow 0$ or ∞ limit, as can be seen from the boson representation of q -VBS.

Next, we formally introduce the Kennedy–Tasaki transformation in our model. As mentioned earlier, if we identify $|j, m\rangle$ (rep. basis of $U_q(su(2))$) with $|S, S^z\rangle$ (those of $su(2)$), the following relations hold for the $j = 1$ representation:

$$S^\pm = \sqrt{\frac{2}{[2]}} J^\pm \quad S^z = J^3. \quad (17)$$

Using these, we can define the following generalized Kennedy–Tasaki transformation

$$U = \prod_{j=1}^L \exp \left\{ i\pi \left(\sum_{k=1}^{j-1} J_k^3 \right) \frac{J_j^+ + J_j^-}{\sqrt{2[2]}} \right\} \quad (18)$$

in our anisotropic q -VBS state. Of course, our argument is essentially based on the S - J relations; this expression is valid only for the $S = 1$ (or $j = 1$) case. Using the formal definition

$$J^x \equiv \frac{1}{\sqrt{2[2]}}(J^+ + J^-) = S^x$$

we can easily derive the well known formulae [15, 21]

$$\begin{aligned} U S_j^x U^{-1} &= S_j^x \exp \left[i\pi \sum_{k=j+1}^L S_k^x \right] \equiv V_j^x \\ U S_j^z U^{-1} &= \exp \left[i\pi \sum_{k=1}^{j-1} S_k^z \right] S_j^z \equiv V_j^z \\ U S_j^y U^{-1} &= \exp \left[i\pi \sum_{k=1}^{j-1} S_k^z \right] S_j^y \exp \left[i\pi \sum_{l=j+1}^L S_l^x \right]. \end{aligned} \tag{19}$$

Using these relations, we can verify that the transformed Hamiltonian $U^{-1}\mathcal{H}U$ is invariant under: (i) $S^x \rightarrow -S^x$; and (ii) the simultaneous transformation $S^z \rightarrow -S^z, q \rightarrow q^{-1}$. That is, $U^{-1}\mathcal{H}U$ has a generalized $Z_2 \times Z_2$ symmetry. To see how the Kennedy–Tasaki transformation works, we have only to compute the probability distribution (16) for the transformed state $U|q$ -VBS (it is calculated using the method described in appendix B)

$$\text{Prob}(+1), \text{Prob}(0), \text{Prob}(-1) = \begin{cases} \left(\frac{2}{[3]}, \frac{q^2 - 1 + q^{-2}}{[3]}, 0 \right) & \text{if the left edge is } \uparrow \\ \left(0, \frac{q^2 - 1 + q^{-2}}{[3]}, \frac{2}{[3]} \right) & \text{if the left edge is } \downarrow. \end{cases} \tag{20}$$

This implies that the Kennedy–Tasaki transformation converts the q -VBS state into a ‘ferromagnetic’ state as in the VBS case except that the ‘magnetization’ shrinks.

To investigate the breakdown of this hidden $Z_2 \times Z_2$ symmetry, we calculate: (i) two-point correlators; (ii) string correlators $\langle V_i^\alpha V_j^\alpha \rangle$ ($\alpha = x$ or z); and (iii) a one-point function of the string variables V_i^α . Now that we have the boson representation of the q -VBS state, it is possible to calculate these quantities straightforwardly. However, there is a more elegant way of computing various quantities [10]. This method is briefly reviewed in appendix B.

First, we calculate the norm of the VBS state $\langle \text{VBS}; \alpha, \beta | \text{VBS}; \alpha, \beta \rangle$. Using the tensorial method, the calculation reduces to evaluating the products of the 4×4 matrices

$$\langle \text{VBS}; \alpha, \beta | \text{VBS}; \alpha, \beta \rangle = (G^{\text{start}}(G)^{L-1})_{i,j} \quad (i, j = 1 \text{ or } 4)$$

where the matrices G and G^{start} are defined as

$$G^z = \begin{pmatrix} q^2 & 0 & 0 & q^2[2] \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ q^{-2}[2] & 0 & 0 & q^{-2} \end{pmatrix} \quad G^x = \begin{pmatrix} 1 & 0 & 0 & [2] \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ [2] & 0 & 0 & 1 \end{pmatrix}. \tag{21}$$

Thus, we get

$$\langle q\text{-VBS} | q\text{-VBS} \rangle = \frac{1}{[2]} \begin{pmatrix} q^{-2}(q[3]^L + q^{-1}(-1)^L) & [3]^L - (-1)^L \\ [3]^L - (-1)^L & q^2(q^{-1}[3]^L + q(-1)^L) \end{pmatrix}. \tag{22}$$

To evaluate the two-point functions and the string correlators (the two-point function of the *non-local* string operators V_i^α), we need two other types of matrix

$$\begin{aligned}
 G^{S^x} &= \sqrt{\frac{[2]}{2}} \begin{pmatrix} 0 & q^2 & q^2 & 0 \\ -1 & 0 & 0 & -1 \\ -1 & 0 & 0 & -1 \\ 0 & q^{-2} & q^{-2} & 0 \end{pmatrix} & G^{S^z} &= \begin{pmatrix} 0 & 0 & 0 & q^2[2] \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -q^{-2}[2] & 0 & 0 & 0 \end{pmatrix} \\
 G_{\text{string}}^x &= \begin{pmatrix} -q^2 & 0 & 0 & 0 \\ 0 & 1 & [2] & 0 \\ 0 & [2] & 1 & 0 \\ 0 & 0 & 0 & -q^{-2} \end{pmatrix} & G_{\text{string}}^z &= \begin{pmatrix} q^2 & 0 & 0 & -q^2[2] \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ -q^{-2}[2] & 0 & 0 & q^{-2} \end{pmatrix}.
 \end{aligned}$$

In terms of the above matrices, for example, $\langle q\text{-VBS} | S_i^\alpha \prod_{k=i+1}^{j-1} \exp(i\pi S_k^\alpha) S_j^\alpha | q\text{-VBS} \rangle$ are simply expressed as

$$(G^{\text{start}}(G)^{i-2} G^{S^\alpha} (G_{\text{string}}^\alpha)^{i-j-1} G^{S^\alpha} (G)^{L-j})_{m,n}.$$

Although we can compute them for an arbitrary i, j, L , the final expressions are very lengthy and complicated. Hence, we will show only the asymptotic ($i, j, L \rightarrow \infty$ while $|i - j| = \text{fixed}$) form

$$\langle S_i^z S_j^z \rangle = \frac{[2]^2}{[3]} \left(\frac{-1}{[3]} \right)^{|i-j|} \tag{23a}$$

$$\langle S_i^x S_j^x \rangle = \frac{q^3 + 2 + q^{-3}}{[3]} \left(\frac{-1}{[3]} \right)^{|i-j|}. \tag{23b}$$

From the above results, we can readily see that $q = \pm i$ ($[3] = -1$) are special points where damping factors disappear. They correspond to the ‘critical point’, found by Klümper *et al* [9, 10], where the model (1) reduces to the (integrable) 19-vertex model. Furthermore, at these points, the ground-state uniqueness does not hold (see appendix B). For later convenience, we also calculate the static structure factors $\langle S^\alpha(k) S^\alpha(-k) \rangle$ ($S^\alpha(k)$ is a Fourier transform of S_j^α).

$$\langle S^z(k) S^z(-k) \rangle = \frac{2[4]}{[2]} \frac{1 - \cos k}{(1 + [3]^2) + 2[3] \cos k}. \tag{24}$$

The string correlation functions in the z -direction are

$$\begin{aligned}
 \langle q\text{-VBS} | S_i^z \prod_{k=i+1}^{j-1} \exp(i\pi S_k^z) S_j^z | q\text{-VBS} \rangle \\
 = \left\{ - \left(\frac{2}{[3]} \right)^2 + (q - q^{-1})(-1)^{i-j} \exp(-\ln[3]|i - j|) \right\} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \tag{25}
 \end{aligned}$$

$$\langle q\text{-VBS} | \prod_{k=1}^{i-1} \exp(i\pi S_k^z) S_i^z | q\text{-VBS} \rangle = \frac{2}{[3]} \begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix}. \tag{26}$$

This clearly shows that the string order exists in the z -direction as expected. If we take $q \rightarrow 0$ or $q \rightarrow \infty$ limits in the above result, we obtain $\langle V_i^z V_j^z \rangle = 0$, which is consistent with the fact that only $00 \cdots 00$ (i.e., the large- D -phase-like situation) is allowed in these limits.

Owing to the lack of rotational symmetry, it is convenient to use the periodic boundary condition in calculating the string correlation function in the x -direction. The calculation is as before. The result is

$$\langle q\text{-VBS} | S_i^x \prod_{k=i+1}^{j-1} \exp(i\pi S_k^z) S_j^x | q\text{-VBS} \rangle_{\text{PBC}} = -\frac{1}{[2][3]^2} \left\{ \frac{[8]}{[4]} + 2[2] + \frac{[4]}{[2]} \right\} \left(\frac{1+[2]}{[3]} \right)^{|i-j|-1}. \quad (27)$$

Since $(1+[2])/[3] < 1$ for real q , it vanishes as $|i-j| \rightarrow \infty$. That is, the Z_2 -symmetry which corresponds to the rotation about the z -axis by π is *unbroken*. Of course, it becomes non-vanishing ($-4/9$) in the $q \rightarrow 1$ limit. Here, we emphasize that any small finite value of $|q-1|$ destroys the string order in the x -direction in our model.

The above results suggest that the $Z_2 \times Z_2$ symmetry is broken only *partially*, though the ground state has all the other properties that the Haldane systems are expected to have, namely, the unique infinite-volume ground state, the excitation gap and the non-existence of the ordinary Néel order. In this sense, systems with a breakdown of $Z_2 \times Z_2$ symmetry may belong to a subclass of the whole Haldane systems.

4. Approximate excitation spectra

From the results in the preceding section, we may also expect massive excitations for our generalized VBS model. Since it is difficult to get exact excited states for it, we have to be satisfied with some approximate calculations. The SMA is one of the most standard methods for evaluating an upper bound of the true spectrum. Using this method, Arovas *et al* [14] obtained the approximate spectrum for the $S=1$ VBS model.

To do this, we first calculate the action of S_j^\pm , S_j^z on the q -VBS state. Using the relations

$$S_j^+ = \sqrt{\frac{2}{[2]}} a_j^\dagger b_j \quad S_j^- = \sqrt{\frac{2}{[2]}} b_j^\dagger a_j \quad S_j^z = \frac{1}{2}(N_j^a - N_j^b)$$

and the commutation relations (4a)–(4c), we easily obtain

$$\begin{aligned} S_j^+ |q\text{-VBS}\rangle &= (\cdots) \sqrt{\frac{2}{[2]}} a_{j-1}^\dagger a_j^\dagger (q^{-2} a_j^\dagger b_{j+1}^\dagger - q^{-1} b_j^\dagger a_{j+1}^\dagger) (\cdots) |0\rangle \\ &\quad - (\cdots) \sqrt{\frac{2}{[2]}} (q a_{j-1}^\dagger b_j^\dagger - q^2 b_{j-1}^\dagger a_j^\dagger) a_j^\dagger a_{j+1}^\dagger (\cdots) |0\rangle \end{aligned} \quad (28)$$

$$\begin{aligned} S_j^- |q\text{-VBS}\rangle &= -(\cdots) \sqrt{\frac{2}{[2]}} b_{j-1}^\dagger b_j^\dagger (q^{-1} a_j^\dagger b_{j+1}^\dagger - q^2 b_j^\dagger a_{j+1}^\dagger) (\cdots) |0\rangle \\ &\quad + (\cdots) \sqrt{\frac{2}{[2]}} (q^{-2} a_{j-1}^\dagger b_j^\dagger - q b_{j-1}^\dagger a_j^\dagger) b_j^\dagger b_{j+1}^\dagger (\cdots) |0\rangle \end{aligned} \quad (29)$$

$$\begin{aligned} S_j^z |q\text{-VBS}\rangle &= -(\cdots) \frac{1}{2} (q^{-1} a_{j-1}^\dagger b_j^\dagger + q b_{j-1}^\dagger a_j^\dagger) (q^{-1} a_j^\dagger b_{j+1}^\dagger - q b_j^\dagger a_{j+1}^\dagger) (\cdots) |0\rangle \\ &\quad + (\cdots) \frac{1}{2} (q^{-1} a_{j-1}^\dagger b_j^\dagger - q b_{j-1}^\dagger a_j^\dagger) (q^{-1} a_j^\dagger b_{j+1}^\dagger + q b_j^\dagger a_{j+1}^\dagger) (\cdots) |0\rangle \end{aligned} \quad (30)$$

where (\dots) denotes the product of the q -valence-bond operators. As in the ordinary VBS case, S_j^\pm and S_j^z destroy the valence-bond structure *locally*. Such defects were called 'crackions' by Knabe [24]. Such configurations can also be treated by the matrix formalism.

In the SMA, the following inequality holds for the true spectrum:

$$\omega(k) \leq \omega_{\text{SMA}}(k) \quad (31)$$

where

$$\omega_{\text{SMA}}(k) \equiv - \frac{\langle \text{GS} | [[\mathcal{H}, S^i(k)], S^i(-k)] | \text{GS} \rangle}{2 \langle \text{GS} | S^i(k) S^i(-k) | \text{GS} \rangle}. \quad (32)$$

The evaluation of the RHS of equation (32) is lengthy but straightforward and we finally arrive at

$$\omega_{\text{SMA}}^z(k) = \frac{[2]^4 [5]}{2[3]^3 [4]^2} \{ (1 + [3]^2) + 2[3] \cos k \}. \quad (33)$$

The $q \rightarrow 1$ limit of this expression agrees with the known results [14]. The Haldane gap for the z -mode is given by

$$\Delta_{\text{H}}^z = \frac{[2]^2 [5]}{2[3]^3} \left(> \frac{10}{27} \right). \quad (34)$$

This suggests that the 'mass' of a magnon increases by the q -deformation (for a real value of q). The limits $q \rightarrow 0$ and $q \rightarrow \infty$ are subtle. As shown in [10], the 'kinetic term' is absent from \mathcal{H} in this limit and, hence, $\omega(k)$ is independent of k .

Although the action of the magnon operators S_i^\pm on the classical Néel state is quite simple and manifest, it is obscured in the VBS state owing to its liquid-like nature. However, as pointed out by Fáth and Sólyom [25], the kink nature of the isolated magnon (or equivalently 'crackion') is revealed through the Kennedy–Tasaki transformation.

First, we note

$$\langle q\text{-VBS} | S_i^\mp U^{-1} S_j^z U S_i^\pm | q\text{-VBS} \rangle = \langle q\text{-VBS} | S_i^\mp V_j^z S_i^\pm | q\text{-VBS} \rangle.$$

Using the matrix-formalism, the evaluation of the RHS is easy and we get

$$\left\langle \prod_{k=1}^{j-1} \exp(i\pi S_k^z) S_j^z \right\rangle_{1\text{-magnon}} = \pm \frac{2}{[3]} \begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix} \quad (35)$$

where we choose $+$ if $i < j$ and $-$ if $i > j$, i.e., after the Kennedy–Tasaki transformation, a kink at the magnon position becomes visible. In the original S^z -configuration, it appears as a domain wall $(0, -1, 0, 1, 0, 0, 1, -1, 0)$ etc for the string order. Such a topological excitation is responsible for the destruction of the hidden order.

5. Summary and discussion

Using the q -Schwinger realization of $U_q(su(2))$, we have constructed the ‘bosonic’ representation of the q -VBS state. Of course, the matrix-product ground state (MPG) can be constructed independently of the bosonic representation and the MPG does not always have a corresponding expression in terms of (Schwinger-type) bosons. However, in order to obtain a physical meaning for the MPG and see how it is natural for the valence-bond-type states, it would be important to investigate the relation between the two types of construction for special cases. Moreover, it is known [16] that the edge states (which are manifest in the ‘Schwinger-boson’ representation) have an important meaning in the discussion of the hidden-symmetry breaking. It has a simple expression similar to the Schwinger boson representation of the ordinary VBS state found by Arovas *et al* except that the coefficients of the ‘valence-bond’ operator are deformed. In this representation, the edge state is manifest.

Then, we have derived the MP representation, where the valence-bond operator is inserted when we contract matrix indices. The four entries of the g -matrix correspond to the four edge states of the (q -)AKLT model with free ends. Our method provides a very simple way to obtain the MP representation for a wide class of valence-bond-type states including the completely dimerized state. The MP representation is also useful in calculating quantities which are difficult to evaluate by the coherent-state method. Another possible application of it is to construct anisotropic VBS-type states for higher values of S . Once we obtain a matrix representation of a given (isotropic) VBS-type state, we can get its anisotropic version by modifying the weights (see appendix A). Changing the weights corresponds to changing the ‘particle’ concentration without destroying the string order, as we have seen in section 3.

We calculated the string-order parameters using the matrix formalism and found that the string LRO does not exist in the x -direction, whereas it does in the z -direction as expected. In the context of the hidden $Z_2 \times Z_2$ -breaking picture, this means that only a single Z_2 -symmetry is broken in our model, however small the deformation is. That is, our $S = 1$ model has a unique disordered ground state with a gap, while the hidden symmetry is only partially broken.

An approximate excitation spectrum is given using the SMA. Within this approximation, the gap increases both in the z -directions by the q -deformation. Excitations are created by breaking the valence bonds *locally*, analogously to the ordinary VBS case. They have a topological character, namely, they behave like kinks for the string variables. Such excitation reduces the string order at finite temperatures.

After we finished this work, we discovered that M T Batchelor and C M Yung are also discussing the q -deformation of the VBS-type models [26].

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Appendix A. g -matrix for general VBS-type states

In this appendix, we discuss the matrix-representation of section 3 in more detail. As mentioned there, the indices of the ‘ g ’-matrix correspond to the edge states at both ends. The essential fact of this construction is that contraction of the matrix indices yields the valence-bond operators. In the following, we restrict ourselves to the $q = 1$ ($su(2)$) case.

For example, we consider first a spin- S VBS state [14–27]. In this case, the edge states consist of $(S + 1)$ -states $\sqrt{{}_S C_{p-1}} (a^\dagger)^{S-p+1} (b^\dagger)^{p-1}$ ($p = 1, \dots, S + 1$) (we have multiplied the numerical factor for later convenience). Correspondingly, the ‘ g -matrix’ is an $(S + 1) \times (S + 1)$ -matrix. Just as in the $S = 1$ case, the elements of g are determined so that the valence-bond operator $(a_i^\dagger b_{i+1}^\dagger - b_i^\dagger a_{i+1}^\dagger)^S$ may appear when we contract the matrix indices. The results are

$$(g_i)_{mn} = (-1)^{S-m+1} \sqrt{{}_S C_{m-1} \times {}_S C_{n-1}} (a_i^\dagger)^{S-m+n} (b_i^\dagger)^{S+m-n} |0\rangle_i \quad (\text{A.1})$$

and

$$(g_1^{\text{start}})_{mn} = \sqrt{{}_S C_{m-1} \times {}_S C_{n-1}} (a_1^\dagger)^{S-m+n} (b_1^\dagger)^{S+m-n} |0\rangle_1. \quad (\text{A.2})$$

To be concrete, the g_i for the $S = 2$ case is given as

$$g_i = \begin{pmatrix} 2|0\rangle_i & 2\sqrt{3}|1\rangle_i & 2\sqrt{6}|2\rangle_i \\ -2\sqrt{3}|-1\rangle_i & -4|0\rangle_i & -2\sqrt{3}|1\rangle_i \\ 2\sqrt{6}|-2\rangle_i & 2\sqrt{3}|-1\rangle_i & 2|0\rangle_i \end{pmatrix}.$$

In a similar way, we obtain the matrix representation of the ‘intermediate- D VBS state’ discussed by Oshikawa [21]

$$|\text{int-}DVBS; L\rangle = (a_1^\dagger)^p (b_1^\dagger)^{S-d-p} \prod_{i=1}^{L-1} (a_i^\dagger b_i^\dagger)^d (a_i^\dagger b_{i+1}^\dagger - b_i^\dagger a_{i+1}^\dagger)^{S-d} (a_L^\dagger)^{q+d} (b_L^\dagger)^{S-q} |0\rangle_1 \otimes \dots \otimes |0\rangle_L. \quad (\text{A.3})$$

It is expressed in the following $((S - d + 1)$ -dimensional) matrix form:

$$|\text{int-}DVBS; L\rangle = g^{\text{start}} \otimes g_1^{\text{int-D}} \otimes \dots \otimes g_L^{\text{int-D}} \quad (\text{A.4})$$

where

$$(g_i^{\text{int-D}})_{mn} = (-1)^{S-d-m+1} {}_{S-d} C_{m-1} (a_i^\dagger)^{S-m+n} (b_i^\dagger)^{S+m-n} |0\rangle_i \quad (\text{A.5})$$

and

$$(g^{\text{start}})_{mn} = (a_1^\dagger)^{S-m+n} (b_1^\dagger)^{S+m-n} |0\rangle_1. \quad (\text{A.6})$$

The inhomogeneous VBS state discussed by Arovas *et al* [14] and Freitag *et al* [20] has the g -matrix (The following example is the $S = 3/2$ case)

$$g_{i,i+1} = \begin{pmatrix} -a_i^\dagger (a_i^\dagger b_{i+1}^\dagger - b_i^\dagger a_{i+1}^\dagger)^2 b_{i+1}^\dagger |0\rangle_i \otimes |0\rangle_{i+1} & -a_i^\dagger (a_i^\dagger b_{i+1}^\dagger - b_i^\dagger a_{i+1}^\dagger)^2 a_{i+1}^\dagger |0\rangle_i \otimes |0\rangle_{i+1} \\ b_i^\dagger (a_i^\dagger b_{i+1}^\dagger - b_i^\dagger a_{i+1}^\dagger)^2 b_{i+1}^\dagger |0\rangle_i \otimes |0\rangle_{i+1} & b_i^\dagger (a_i^\dagger b_{i+1}^\dagger - b_i^\dagger a_{i+1}^\dagger)^2 a_{i+1}^\dagger |0\rangle_i \otimes |0\rangle_{i+1} \end{pmatrix}. \quad (\text{A.7})$$

In this case, the g -matrix consists of the two-site state. Of course, we can construct g 's which consist of a single site using rectangular matrices.

Combining these expressions with the tensorial method used by Klümper *et al*, we can easily evaluate the ordinary two-point functions, the string correlation functions etc. These results will be reported elsewhere.

Appendix B. A method of calculating expectation values

In this appendix, we briefly review the method of calculating expectation values with respect to the VBS-type states [10]. For our purpose, we extend the result of [10] to the case of an open chain.

As we have seen, the VBS-type states are simply expressed using the g -matrices as

$$|\text{VBS}; \alpha, \beta\rangle = [g^{\text{start}} \otimes g_2 \otimes \cdots \otimes g_L]_{\alpha, \beta}.$$

In the above expression, it is important that the matrix g is written in terms of local operators (usually those of a single site). We are interested in expectation values of the following type:

$$\langle \mathcal{A}_i \rangle_{\alpha, \beta} = \langle \text{VBS}; \alpha, \beta | \mathcal{A}_i | \text{VBS}; \alpha, \beta \rangle.$$

If we rewrite the RHS using the elements of g and introduce the following G -matrix whose entries are c -numbers:

$$G_{(m_{j-1}, n_{j-1}), (m_j, n_j)} \equiv g_j^\dagger(m_{j-1}, m_j) g_j(n_{j-1}, n_j) \quad (\text{B.1})$$

and

$$G_{(m_{i-1}, n_{i-1}), (m_i, n_i)}^A \equiv g_i^\dagger(m_{i-1}, m_i) \mathcal{A}_i g_i(n_{i-1}, n_i) \quad (\text{B.2})$$

we can express the desired quantity as follows

$$\begin{aligned} \langle \mathcal{A}_i \rangle_{\uparrow\downarrow} &= (M_{\mathcal{A}})_{1,1} & \langle \mathcal{A}_i \rangle_{\uparrow\uparrow} &= (M_{\mathcal{A}})_{1,4} \\ \langle \mathcal{A}_i \rangle_{\downarrow\downarrow} &= (M_{\mathcal{A}})_{4,1} & \langle \mathcal{A}_i \rangle_{\downarrow\uparrow} &= (M_{\mathcal{A}})_{4,4}. \end{aligned}$$

In the above equation, the 4×4 matrix $M_{\mathcal{A}}$ is defined by

$$M_{\mathcal{A}} = G^{\text{start}} (G)^{i-2} G^A (G)^{L-i} \quad (\text{B.3})$$

and we have adopted the lexicographical ordering for the double (tensorial) indices of G to regard it as an ordinary matrix. For the case of a periodic boundary condition, we take a trace of $M_{\mathcal{A}}$.

Using the above results, we can readily give a proof for the uniqueness of the ground state. Essentially, the proof goes is as in [4].

First, we show that an arbitrary *finite*-volume ground state $|\varphi; L\rangle$ of an open chain is expanded by the four q -VBS states (10), i.e.

$$|\varphi; L\rangle = \sum_{\alpha\beta=1}^2 A_{\alpha\beta} |q\text{-VBS}; L; \alpha, \beta\rangle. \quad (\text{B.4})$$

This is proved by Klümper *et al* and we refer the reader to the appendix of [10] for the detail. It is important to note that the proof breaks down for $q = \pm i$.

To prove the *infinite*-volume uniqueness, we show the following equality:

$$\begin{aligned} \lim_{L, i \rightarrow \infty} \frac{\langle q\text{-VBS}; L; \alpha\beta | \mathcal{A} | q\text{-VBS}; L; \gamma\delta \rangle}{\| |q\text{-VBS}; L; \alpha\beta \rangle \| \| |q\text{-VBS}; L; \gamma\delta \rangle \|} \\ = \delta_{\alpha\gamma} \delta_{\beta\delta} \frac{\sum_{\mu, \nu=1}^2 \langle q\text{-VBS}; L; \mu\nu | \mathcal{A} | q\text{-VBS}; L; \mu\nu \rangle q^{\mu-3\nu}}{\sum_{\mu, \nu=1}^2 \langle q\text{-VBS}; L; \mu\nu | q\text{-VBS}; L; \mu\nu \rangle q^{\mu-3\nu}}. \end{aligned} \quad (\text{B.5})$$

The proof is straightforward. Using the matrix formalism and

$$\lim_{n \rightarrow \infty} \left(\frac{1}{[3]} G \right)_{(i,j)(k,l)}^n = \frac{1}{[2]} \delta_{i,j} \delta_{k,l} q^{-3i+k+3}$$

the numerator of the LHS of equation (B.5) can be rewritten as

$$\delta_{\alpha\gamma} \delta_{\beta\delta} \left(\frac{1}{[2]} \right)^2 [3]^{L-i-1} \{ [\alpha]! [2-\alpha]! + q^{-3} [\alpha-1]! [3-\alpha]! \} q^{\beta+3} \\ \times \sum_{m_1, m_{l+1}} \langle q\text{-VBS}; l; m_1, m_{l+1} | \mathcal{A} | q\text{-VBS}; l; m_1, m_{l+1} \rangle q^{m_1 - 3m_{l+1}}.$$

Thus the equality is proved. We define the infinite-volume ground state by the RHS of (B.5) and denote it by $\omega(\mathcal{A})$.

Using the above two facts, we can prove the desired theorem stating that the infinite-volume ground state ρ which satisfies $\rho(h_{i,i+1}) = 0$ is indeed equal to the ground state ω defined above. The reader is referred to [4] for the details of the proof. It may be worth mentioning that for $q = \pm i$, the above theorem of the uniqueness breaks down and in fact we have degenerate ground states [10]. We can also extend the theorem to more general matrix-product states as discussed by Klümper *et al.* For generic values of parameters, these models have a unique $S_{\text{tot}}^z = 0$ ground state in the infinite-volume limit.

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