# Hidden $Z_2$*$Z_2$ symmetry in quantum spin chains with arbitrary integer spin



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# Hidden $Z_2 \times Z_2$ symmetry in quantum spin chains with arbitrary integer spin

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**Abstract.** We study integer $S > 1$ spin chains. We extend the Kennedy–Tasaki non-local unitary transformation for $S = 1$ to arbitrary integer $S$. We show the main results of Kennedy and Tasaki are maintained for $S > 1$: Heisenberg-type Hamiltonians are transformed to Hamiltonians of nearest-neighbour interactions with $Z_2 \times Z_2$ symmetry, and the den Nijs–Rommelse string observables are transformed to the ferromagnetic correlation observables. We assert that in general values of integer $S$ there exist several phases with the hidden $Z_2 \times Z_2$ symmetry breaking. The den Nijs–Rommelse string order parameters, which measure the hidden $Z_2 \times Z_2$ symmetry breaking, are calculated explicitly for several variants of the VBS-type states. In the standard VBS state, the hidden $Z_2 \times Z_2$ symmetry breaks down when $S$ is odd but remains unbroken when $S$ is even. Our results for partially dimerized VBS states suggest that the hidden $Z_2 \times Z_2$ symmetry breaking can be used to detect the successive dimerization transitions predicted by Affleck and Haldane. Some new anisotropic VBS-type states are investigated. The result suggests that there are successive phase transitions when we increase the uniaxial anisotropy in a Heisenberg-type model. Other new VBS-type states with long-range order are considered, and their relevance to the phase diagram of the Heisenberg $XXZ$ model and the magnetization process of antiferromagnets is investigated. We introduce an extended string order parameter which possesses a characteristic behaviour in the partially dimerized VBS states.

## 1. Introduction

Haldane [1] was the first to predict the qualitative difference between integer-$S$ and half-integer-$S$ spin chains. He argued that, when $S$ is an integer, the spin-$S$ quantum Heisenberg antiferromagnetic chain has a unique disordered ground state with a finite excitation gap, while the same model has no excitation gap when $S$ is a half integer. Although his prediction was based on large-$S$ arguments, it has been confirmed for $S = 1$ by experimental, numerical and theoretical studies (for a review, see [2]).

Furthermore, deeper insight into the mechanism of Haldane-gap phenomena has been derived from the work of Affleck and co-workers [3], who constructed the valence-bond-solid (VBS) states and the Hamiltonians leading to them. The VBS models, though different from the standard Heisenberg models, are examples of

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integer-$S$ quantum antiferromagnetic chains with most of the properties Haldane predicted.

It has been observed that the $S = 1$ VBS model has two non-standard properties. First, the $S = 1$ VBS state has a hidden antiferromagnetic order, i.e. in the standard $S^z$-basis representation of the VBS state, non-zero spins must alternate between $+1$ and $-1$. Second, the VBS states on a finite open chain have two almost-free $S = \frac{1}{2}$ degrees of freedom at the ends of the chain; thus they are fourfold degenerate.

These two properties are not specific to the solvable VBS model, but turned out to be common characteristics in the Haldane phase, which includes the Heisenberg point. Den Nijs and Rommelse [4] argued that the Haldane phase is characterized by the hidden antiferromagnetic order, which can be measured by the string order parameters

$$O^{\alpha}_{\text{string}}(H) = -\lim_{|k-j|\to\infty} \langle S^{\alpha}_j \exp\left(i\pi \textstyle\sum_{l=j+1}^{k-1} S^{\alpha}_l\right) S^{\alpha}_k \rangle_H \tag{1}$$

where $\alpha = x, y$ or $z$ (see also [5]). Numerical calculations [6] confirmed their prediction. On the other hand, Kennedy [7] pointed out that $S = 1$ systems in the Haldane phase defined on a finite open chain have four nearly-degenerate states of lowest energies, and they are separated from the other states by a finite Haldane gap.

We can naturally understand these two characteristic features as consequences of a hidden $Z_2 \times Z_2$ symmetry breaking. Kennedy and Tasaki [8] introduced a non-local unitary transformation, which reveals the hidden $Z_2 \times Z_2$ symmetry in the following sense. The transformation converts $S = 1$ Heisenberg-type antiferromagnetic models into models of local interactions with $Z_2 \times Z_2$ symmetry, and the den Nijs–Rommelse string observable into the ferromagnetic correlation observable. The hidden $Z_2 \times Z_2$ symmetry is completely broken in the Haldane phase but is partly broken or unbroken in the other phases.

Thus the notion of the hidden $Z_2 \times Z_2$ symmetry shed light on the understanding of the ground-state properties of the $S = 1$ quantum antiferromagnetic chains. Since Haldane's original prediction was universal for all integer $S$, one may ask whether there is a similar mechanism for higher values of $S$. The purpose of the present paper is to extend the notion of the hidden $Z_2 \times Z_2$ symmetry to the spin chains with higher values of $S$, and investigate their ground states on the basis of this symmetry.

We show that the Kennedy–Tasaki unitary transformation can be written in a compact operator form and can be extended to spin chains with arbitrary integer $S$. As in the $S = 1$ spin chains, the Heisenberg-type models are transformed into models of local interactions with a $Z_2 \times Z_2$ symmetry, and the den Nijs–Rommelse string order parameters are converted into the ferromagnetic order parameters.

We evaluate the string order parameters explicitly in several variants of the VBS states. The results for the standard VBS states suggest that, in the Haldane phase, the hidden $Z_2 \times Z_2$ symmetry is completely broken when $S$ is an odd integer, but remains unbroken when $S$ is an even integer. The results for partially dimerized VBS states suggest that the notion of the hidden $Z_2 \times Z_2$ symmetry breaking can be used to detect the successive dimerization transitions predicted by Affleck and Haldane [9].

We construct new VBS-type states, which we will call intermediate-$D$ VBS states, and evaluate the string order parameters in these states. The results suggest that the Heisenberg model with uniaxial anisotropy for an integer $S$ undergoes $S$ successive phase transitions when the uniaxial anisotropy parameter $D$ is varied. We also construct other new VBS-type states with long-range order and discuss their properties.

We introduce extended string order parameters characterized by an angle parameter $\theta$. The extended order parameters reduce to the original den Nijs–Rommelse ones when $\theta = \pi$. We evaluate the extended string order parameters in the various VBS-type states for integer and half-integer $S$. We find characteristic behaviour in the location of the zero points of the extended string order parameters in partially dimerized VBS states.

The organization of the present paper is as follows. In section 2, we show the compact operator form of the Kennedy–Tasaki unitary transformation. In section 3, we give a method to evaluate the string order parameters in the spin-$S$ VBS states, and investigate the hidden symmetry breaking in these states. In section 4, we evaluate the string order parameters in partially dimerized VBS states and discuss their relevance to the successive dimerization transitions. In section 5, we construct new VBS-type states with anisotropy. Our analysis leads us to conjecture the existence of new phase transitions in Heisenberg models with uniaxial anisotropy. In section 6, we construct novel VBS-type states with long-range order and study their properties. In section 7, we introduce an extension of the den Nijs–Rommelse string order parameters and evaluate these order parameters in various VBS-type states.

## 2. Non-local unitary transformation for arbitrary integer $S$

The $S = 1$ VBS state has a hidden antiferromagnetic order [4,5]. In the standard $S^z$-basis representation of the VBS state, non-zero spins must alternate between $+1$ and $-1$. An example of an allowed configuration is $(+-000+0-+-+0000-0+)$. Other ground states of the $S = 1$ spin chains in the Haldane phase also have similar (but not perfect) hidden antiferromagnetic order. Kennedy and Tasaki [8] defined a non-local unitary transformation which reveals a hidden $Z_2 \times Z_2$ symmetry breaking in the systems with such hidden antiferromagnetic order. Their unitary transformation $U$ is defined in the following way. In the $S^z$-basis representation, we move to the right from the left end of the chain, looking for non-zero spins. The first non-zero spin is left unchanged, the second is flipped, the third is left unchanged, the fourth is flipped, and so on. Finally, we multiply the state vector with the factor $(-1)^{N(\sigma)}$ where $N(\sigma)$ is the number of odd sites on which there is a 0. A few examples of the action of $U$ are as follows:

$$(0+-000+00-+-00) \to (0++000+00+++00)$$
$$(+0+-000+---+000) \to -(+0--000---++000).$$

In particular, we see that the $S = 1$ VBS states are transformed to the states containing only 0 and $+1$ or only 0 and $-1$.

The hidden antiferromagnetic order found in the $S = 1$ VBS state gave a hint to the construction of the Kennedy–Tasaki unitary transformation. On the other hand, the $S > 1$ VBS states are expected to possess more complicated hidden structure. Hence we shall formally extend the Kennedy–Tasaki unitary transformation to the $S > 1$ spin chains.

Throughout this section, $S$ denotes an arbitrary integer. First, we define a unitary transformation $V$ by

$$V = V^{-1} = \prod_{j<k} \exp(\mathrm{i}\pi S_j^z S_k^x) \tag{2}$$

which will turn out to be equivalent to $U$ of Kennedy and Tasaki for $S = 1$.

A little calculation shows that the factors in $V$ commute with each other:

$$[\exp(i\pi S_j^z S_k^x), \exp(i\pi S_l^z S_m^x)] = 0 \tag{3}$$

where $j < k$ and $l < m$. Thus we can arbitrarily order the factors in $V$.

Let us consider the $S = 1$ case. In the standard $S^z$-basis representation, from

$$\exp(i\pi S^x) = \begin{pmatrix} 0 & 0 & -1 \\ 0 & -1 & 0 \\ -1 & 0 & 0 \end{pmatrix}$$

we see that $\exp(i\pi S_i^z S_j^x)$ does not change the state when $S_i^z = 0$, but flips the spin at site $j$ and multiplies the state vector with the phase factor $(-1)$ when $S_i^z = \pm 1$. A little calculation shows that $U = (-1)^{L/2} V$ for $S = 1$ chains when the number of sites $L$ is even. (This argument is given by Tasaki [10].)

Now we consider general cases of integral $S$ and calculate the transformation of spin operators by $V$. After some calculations, we find

$$\begin{aligned} V S_j^x V^{-1} &= S_j^x \exp\left(i\pi \textstyle\sum_{k=j+1}^{L} S_k^x\right) \\ V S_j^y V^{-1} &= \exp\left(i\pi \textstyle\sum_{k=1}^{j-1} S_k^z\right) S_j^y \exp\left(i\pi \textstyle\sum_{k=j+1}^{L} S_k^x\right) \\ V S_j^z V^{-1} &= \exp\left(i\pi \textstyle\sum_{k=1}^{j-1} S_k^z\right) S_j^z \end{aligned} \tag{4}$$

where we made use of the commutation relations between spin operators.

This is the same form as the result for $S = 1$ in [8]. Moreover, having used only the commutation relations of the spin operators, we have extended the unitary transformation to arbitrary integer-$S$ spin chains.

We can show that a wide class of Hamiltonians, which contain only polynomials of the operators $S_i^\alpha S_{i+1}^\alpha$ and $(S_i^\alpha)^2$, are transformed to Hamiltonians of local interactions with a $Z_2 \times Z_2$ symmetry. For example, if we have the Hamiltonian

$$H = \sum_j S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \lambda S_j^z S_{j+1}^z + D(S_j^z)^2 \tag{5}$$

its transformation is

$$\begin{aligned} \tilde{H} = V H V^{-1} = \sum_j & S_j^x \exp(i\pi S_{j+1}^x) S_{j+1}^x + S_j^y \exp[i\pi(S_j^z + S_{j+1}^x)] S_{j+1}^y \\ & + \lambda S_j^z \exp(i\pi S_j^z) S_{j+1}^z + D(S_j^z)^2. \end{aligned}$$

We see that this has a $Z_2 \times Z_2$ symmetry, i.e. it is invariant under the rotation of all sites about the $x$, $y$ or $z$ axis by angle $\pi$. Among the other important examples are the VBS Hamiltonians, which only contain polynomials of $\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1}$.

To measure the $Z_2 \times Z_2$ symmetry breaking in the transformed system, we consider the den Nijs–Rommelse string order parameters defined by

$$\begin{aligned} O_{\text{string}}^z(H) &= \lim_{|k-j|\to\infty} \left\langle S_j^z \exp\left(i\pi \textstyle\sum_{l=j}^{k-1} S_l^z\right) S_k^z \right\rangle_H \\ O_{\text{string}}^x(H) &= \lim_{|k-j|\to\infty} \left\langle S_j^x \exp\left(i\pi \textstyle\sum_{l=j+1}^{k} S_l^x\right) S_k^x \right\rangle_H \end{aligned}$$

where $\langle\rangle_H$ denotes the expectation value in the ground state of the Hamiltonian $H$. The transformation of the string observables leads to

$$O^{\alpha}_{\text{string}}(H) = O^{\alpha}_{\text{ferro}}(\tilde{H}) = \lim_{|k-j|\to\infty} \langle S^{\alpha}_j S^{\alpha}_k \rangle_{\tilde{H}} \qquad \alpha = z, x \tag{6}$$

which means the string order parameters measure the hidden symmetry breaking for an arbitrary integer $S$.

We remark that, although our definition of the string order parameters and our representation of the transformed Hamiltonian seem different from those in [8], they are equivalent for $S = 1$ because $\exp(i\pi S^{\alpha})S^{\alpha} = -S^{\alpha}$.

We finally note that, when $S$ is a half integer, the unitary transformation defined by (2) does not transform standard Hamiltonians like (5) into Hamiltonians of local interactions. The technical reason for this is that the factor $\exp(2i\pi S^z_j S^x_k)$, which appears in the calculation, is equal to 1 only when $S$ is an integer. Here we again see a difference between integer-$S$ and half-integer-$S$ spin chains.

## 3. Hidden $Z_2 \times Z_2$ symmetry breaking in the VBS states

To see whether or not the hidden $Z_2 \times Z_2$ symmetry discussed in the previous section is broken, we explicitly calculate the string order parameters in several VBS-type states of integer $S$ spin chains.

In this section, we consider the standard (translationally invariant) VBS state for integer $S$. The VBS states are the exact ground states of certain Hamiltonians [3] and are expected to represent the ground states accompanied by the Haldane gap. Using the Schwinger boson representation [11], the VBS state on a finite chain with $L$ sites is represented as

$$|\text{VBS}(p,q)\rangle = (a^{\dagger}_1)^p (b^{\dagger}_1)^{S-p} (a^{\dagger}_L)^q (b^{\dagger}_L)^{S-q} \prod_{j=1}^{L-1} (a^{\dagger}_j b^{\dagger}_{j+1} - b^{\dagger}_j a^{\dagger}_{j+1})^S |0\rangle \tag{7}$$

where $0 \leqslant p, q \leqslant S$. Here the $a^{\dagger}_i$ and $b^{\dagger}_j$ are mutually independent boson creation operators, which satisfy the commutation relations $[a_i, a^{\dagger}_j] = [b_i, b^{\dagger}_j] = \delta_{ij}$ with all the other commutators vanishing, and $|0\rangle$ is the vacuum with respect to bosons, namely $a_i|0\rangle = b_j|0\rangle = 0$. Spin operators are represented by the boson operators as

$$S^z_i = \frac{a^{\dagger}_i a_i - b^{\dagger}_i b_i}{2} \qquad S^x_i = \frac{a^{\dagger}_i b_i + b^{\dagger}_i a_i}{2} \qquad S^y_i = \frac{a^{\dagger}_i b_i - b^{\dagger}_i a_i}{2i}.$$

The meaning of the Schwinger boson representation is as follows. One can get a spin $S$ variable by symmetrizing $2S$ spin-$\frac{1}{2}$ variables; $a^{\dagger}_i$ ($b^{\dagger}_i$) increases the number of up (down) spin-$\frac{1}{2}$ variables under symmetrization. In particular, $(a^{\dagger}_i b^{\dagger}_{i+1} - b^{\dagger}_i a^{\dagger}_{i+1})$ creates the valence bond on the sites $i$ and $i+1$.

The integers $p$ and $q$ represent the spin-$\frac{S}{2}$ degrees of freedom at the ends of the chain. The VBS states with any $p, q$ satisfying $0 \leqslant p, q \leqslant S$ are the ground states of the VBS Hamiltonian; hence they are $(S+1)^2$-fold degenerate. An important feature

of the VBS states (7) is that when $L \to \infty$ these two degrees of freedom at both ends can be regarded as free spin-$\frac{S}{2}$ variables. In fact

$$\lim_{L\to\infty} \langle \mathrm{VBS}(p,q)|\mathrm{VBS}(r,s)\rangle = C(L)[p!(S-p)!q!(S-q)!\delta_{p,r}\delta_{q,s} + \mathrm{O}(\mathrm{e}^{-aL})] \quad (8)$$

where $a$ is some positive constant. This property, which we will call the decoupling property of the VBS states, is proved in the appendix.

Now we move on to the evaluation of the string order parameters. Since we have $\mathrm{O}^z_{\mathrm{string}} = \mathrm{O}^x_{\mathrm{string}}$ by the rotational invariance of the VBS state, it is sufficient to evaluate $\mathrm{O}^z_{\mathrm{string}}$ only.

To avoid complications with the degrees of freedom at the ends, we evaluate the expectation value of the string observable in the VBS state $|VBS\rangle$ on a periodic chain. After taking the limit $L \to \infty$, the boundary condition does not affect the result. Although we eliminated the degrees of freedom at the ends, the decoupling property of the VBS states on a finite open chain will play an important role, as we will show later.

First, we apply the string operator $\exp(\mathrm{i}\pi \sum_{l=j}^{k-1} S^z_l)$ to $|\mathrm{VBS}\rangle$. The action of the string operator is to rotate the spins at sites $j, j+1, \cdots, k-1$ about the $z$ axis by an angle $\pi$; thus the valence bonds at $(j-1, j)$ and $(k-1, k)$ are twisted while all the other valence bonds remain unchanged. The twisted VBS state in the Schwinger boson representation is

$$\begin{aligned}\exp(\mathrm{i}\pi \textstyle\sum_{l=j+1}^{k-1} S^z_l)|\mathrm{VBS}\rangle = {} & \textstyle\prod_{1\leqslant l<(j-1)}(a^\dagger_l b^\dagger_{l+1} - b^\dagger_l a^\dagger_{l+1})^S \\ & \times (\mathrm{e}^{-\mathrm{i}\pi/2} a^\dagger_{j-1} b^\dagger_j - \mathrm{e}^{\mathrm{i}\pi/2} b^\dagger_{j-1} a^\dagger_j)^S \\ & \times \prod_{j\leqslant l<(k-1)} (a^\dagger_l b^\dagger_{l+1} - b^\dagger_l a^\dagger_{l+1})^S (\mathrm{e}^{\mathrm{i}\pi/2} a^\dagger_{k-1} b^\dagger_k - \mathrm{e}^{-\mathrm{i}\pi/2} b^\dagger_{k-1} a^\dagger_k)^S \\ & \times \prod_{k\leqslant l\leqslant L} (a^\dagger_l b^\dagger_{l+1} - b^\dagger_l a^\dagger_{l+1})^S |0\rangle\end{aligned}$$

where $a^\dagger_{L+1} = a^\dagger_1$, $b^\dagger_{L+1} = b^\dagger_1$.

Next, we evaluate the matrix element of $S^z_j S^z_k$ between the original VBS state and the twisted one. Each of the regions $k+1, k+2, \cdots, L, 1, 2, \cdots, j-1$ and $j+1, j+2, \cdots, k-1$ can be regarded as a finite chain. Applying the decoupling property (8) to these two regions, we get

$$\mathrm{O}^z_{\mathrm{string}} = \lim_{|k-j|\to\infty} \langle VBS|S^z_j \exp(\mathrm{i}\pi \textstyle\sum_{l=j}^{k-1} S^z_l) S^z_k |VBS\rangle = |f_S(-1)|^2$$

where

$$\begin{aligned} f_S(w) = {} & \frac{1}{N}\langle 0|(a_1 b_2 - b_1 a_2)^S (a_2 b_3 - b_2 a_3)^S \frac{a^\dagger_2 a_2 - b^\dagger_2 b_2}{2} \\ & \times (a^\dagger_1 b^\dagger_2 - w b^\dagger_1 a^\dagger_2)^S (a^\dagger_2 b^\dagger_3 - b^\dagger_2 a^\dagger_3)^S |0\rangle \end{aligned}$$

$$N = \langle 0|(a_1 b_2 - b_1 a_2)^S (a_2 b_3 - b_2 a_3)^S (a^\dagger_1 b^\dagger_2 - b^\dagger_1 a^\dagger_2)^S (a^\dagger_2 b^\dagger_3 - b^\dagger_2 a^\dagger_3)^S |0\rangle.$$

We have thus reduced the problem of finding the string order parameter to a three-site problem. Detailed analysis will be given in the next section. Here we show only the result:

$$\mathrm{O}^z_{\mathrm{string}} = \left(\frac{S+1}{S+2}\right)^2 \delta_{S,\mathrm{odd}}$$

where $\delta_{n,\text{odd}}$ is equal to 1 if $n$ is an odd integer and 0 otherwise. This is consistent with the known result [4] for $S = 1$. Moreover, we have found that for an odd integer $S$ the VBS states break the hidden $Z_2 \times Z_2$ symmetry, but for an even integer $S$ they do not. (Tasaki [10] independently evaluated the den Nijs–Rommelse string order parameters in these states and reached a similar conclusion.) This difference between even and odd integer $S$ may not lead to an essential difference in physical properties. In the following sections, however, we will show that the hidden symmetry breaking can be a measure of certain phase transitions in the ground state of quantum spin chains.

In $S = 1$ spin chains, the hidden $Z_2 \times Z_2$ symmetry breaking implies the fourfold near degeneracy in the ground states of a finite open chain. This degeneracy corresponds to the existence of spin-$\frac{1}{2}$ degrees of freedom at the ends of the chain [8]. It would be worthwhile to see such degeneracy in the higher-$S$ cases. We evaluate the magnetization in the transformed system of the VBS state on an open chain. Similar arguments as in the evaluation of the string order parameter lead to

$$\lim_{j\to\infty} \langle \text{VBS}(p,q)|VS_j^z V^{-1}|\text{VBS}(p,q)\rangle = (-1)^p \frac{S+1}{S+2}\delta_{S,\text{odd}}.$$

We have $O^z_{\text{string}} = |\langle VS^zV^{-1}\rangle|^2$ as expected. The factor $(-1)^p$ indicates that the spin-$\frac{S}{2}$ degree of freedom at the left end of the chain just corresponds to the magnetization in the transformed system $\langle VS^zV^{-1}\rangle$, as in the $S = 1$ spin chains. Similar arguments show that the other spin-$\frac{S}{2}$ degree of freedom at the right end of the chain corresponds to $\langle VS^xV^{-1}\rangle$.

However, since our hidden symmetry is always $Z_2 \times Z_2$, the ground states which break the hidden symmetry can be divided into only four classes. For $S = 1$, the fourfold degeneracy implied by hidden $Z_2 \times Z_2$ symmetry breaking just corresponds to the fourfold degeneracy of the VBS states on a finite open chain. In contrast, for $S > 1$, the hidden $Z_2 \times Z_2$ symmetry cannot completely specify each of the $(S+1)^2$-fold degenerate ground states of the VBS model. This fact suggests the possibility that there is another hidden symmetry, but we still do not know any such extended symmetries.

Finally, we note a simple reason why the hidden $Z_2 \times Z_2$ symmetry cannot be broken in the VBS states when $S$ is even. If the hidden $Z_2 \times Z_2$ symmetry is completely broken, the ground states should be classified into four sectors. On the other hand, there are $(S+1)^2$-fold degenerate ground states and $(S+1)^2$ cannot be divided by four; they cannot be classified into four equivalent sectors.

## 4. Application to dimerization transitions

Affleck and Haldane [9] studied a dimerization transition problem in quantum antiferromagnetic chains. For example, consider the following Hamiltonian:

$$H = \sum_i [1 + \epsilon(-1)^i] S_i \cdot S_{i+1}. \tag{9}$$

When $\epsilon = \pm 1$, the Hamiltonian becomes a sum of independent two-spin interactions, and the ground state of the Hamiltonian is completely dimerized. When $\epsilon = 0$

the Hamiltonian is the standard Heisenberg antiferromagnetic Hamiltonian, and the ground state is expected to be in the massive Haldane phase if $S$ is an integer, or in a massless phase if $S$ is a half integer.

Affleck and Haldane argued that there are (at least) $2S$ massless phase transition points separating $2S+1$ massive phases when $\epsilon$ is varied from $-1$ to $+1$. Besides their original field-theoretical arguments, there is also a VBS picture for these transitions [12]. Each of the $2S+1$ massive phases can be represented by the $(n,m)$-VBS state which is a VBS-type state with $n$ valence bonds between sites $2i$ and $2i+1$, and $m$ valence bonds between $2i+1$ and $2i+2$. Obviously $n+m=2S$ must be satisfied. An example is given in figure 1.

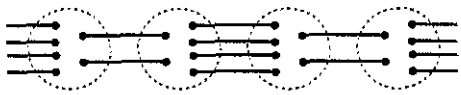

**Figure 1.** Partially dimerized VBS state with $n=2$ and $m=4$ ($S=3$). A full line denotes a valence bond (a singlet of two spin-$\frac{1}{2}$ variables). A broken circle represents the symmetrization of spin-$\frac{1}{2}$ variables at each site.

The Schwinger boson representation of the $(n,m)$-VBS state is as follows:

$$|nm\mathrm{VBS}\rangle = \prod_j (a_{2j}^\dagger b_{2j+1}^\dagger - b_{2j}^\dagger a_{2j+1}^\dagger)^n (a_{2j+1}^\dagger b_{2j+2}^\dagger - b_{2j+1}^\dagger a_{2j+2}^\dagger)^m |0\rangle \tag{10}$$

where the degrees of freedom at both ends are neglected (cf equation (7)). This VBS picture also supports the existence of $2S$ phase-transition points.

Here we apply the notion of the hidden $Z_2 \times Z_2$ symmetry to the successive dimerization transitions for integer $S$. To do this, we evaluate the string order parameters in the $(n,m)$-VBS states. If there is bond alternation, a variety of order parameters exist. For simplicity, we consider only

$$O_{\mathrm{string}}^z = \lim_{(k-j)\to\infty} \langle S_{2j+1}^z \exp\left(i\pi \textstyle\sum_{l=2j+1}^{2k} S_l^z\right) S_{2k+1}^z \rangle .$$

Following the method described in the previous section, we have

$$O_{\mathrm{string}}^z = |f_{n,m}(-1)|^2$$

where

$$f_{n,m}(w) = \frac{1}{N}\langle 0|(a_1 b_2 - b_1 a_2)^n (a_2 b_3 - b_2 a_3)^m \frac{a_2^\dagger a_2 - b_2^\dagger b_2}{2} \times (a_1^\dagger b_2^\dagger - w b_1^\dagger a_2^\dagger)^n (a_2^\dagger b_3^\dagger - b_2^\dagger a_3^\dagger)^m |0\rangle$$

$$N = \langle 0|(a_1 b_2 - b_1 a_2)^n (a_2 b_3 - b_2 a_3)^m (a_1^\dagger b_2^\dagger - b_1^\dagger a_2^\dagger)^n (a_2^\dagger b_3^\dagger - b_2^\dagger a_3^\dagger)^m |0\rangle .$$

We have used the decoupling property of the $(n,m)$-VBS states similar to (8) (see the appendix.) Straightforward calculations show

$$f_{n,m}(w) = \frac{n+m+2}{2(n+2)(n+1)} \sum_{k=0}^{n} (2k-n) w^k . \tag{11}$$

We immediately get

$$O^z_{\text{string}} = |f_{n,m}(-1)|^2 = \left(\frac{m+n+2}{2(n+2)}\right)^2 \delta_{n,\text{odd}}. \tag{12}$$

We note that, since $f_S(w) = f_{S,S}(w)$, this includes the result in the previous section.

We found that $(n, m)$-VBS states with odd $n$ and $m$ break the hidden $Z_2 \times Z_2$ symmetry, but for even $n$ and $m$ they do not. Hence we expect that the successive dimerization transitions separate these two kinds of states, i.e. the hidden-symmetry broken and unbroken phases appear alternatingly when the dimerization proceeds. Our result gives one more support for the existence of the successive dimerization transition.

However, our hidden-symmetry argument is not perfectly successful in the following points. Our argument can only classify phases into two groups, namely, symmetry broken and unbroken phases. Moreover, though Affleck and Haldane predict successive dimerization transition both for integer $S$ and half-integer $S$, our hidden $Z_2 \times Z_2$ symmetry argument can be applied only to integer $S$. We will however show an approach to complement this defect in section 7.

Finally we note that the validity of the VBS picture and our arguments for the model (9) is not yet established, because the VBS Hamiltonians are different from (9). We expect them to be valid, however, from the consistency with the field-theoretical prediction [9] (see also [13].)

## 5. Application to anisotropic states

The $S = 1$ quantum spin chains with the simple anisotropic Hamiltonian (5) have been studied intensively. Figure 2 shows the expected phase diagram of the ground state of the Hamiltonian (5) for $S = 1$.

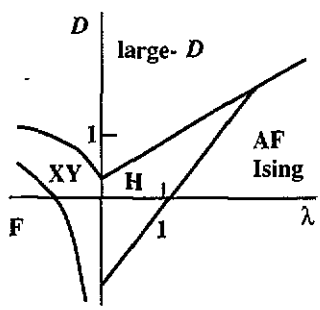


**Figure 2.** Qualitative phase diagram of the $S = 1$ Hamiltonian (5). H denotes the Haldane phase, and F denotes the ferromagnetic phase.

Here we concentrate on the region $\lambda > 0$, in which there are three phases: a large-$D$ phase, a Haldane phase and an antiferromagnetic (AF) Ising phase. When the uniaxial anisotropy $D$ is large enough, the ground state is dominated by zeros in the standard $S^z$-basis representation, because $\pm 1$ terms are suppressed; such states

belong to the large-$D$ phase. When the anisotropic coupling $\lambda$ is large enough, the Hamiltonian resembles the one-dimensional AF Ising Hamiltonian, and hence the ground state has a Néel order; such states belong to the AF Ising phase. Finally, in the Haldane phase, which includes the Heisenberg point ($D = 0, \lambda = 1$), the properties found for the VBS state are expected to appear.

Den Nijs and Rommelse [4], Tasaki [5], and Kennedy and Tasaki [8] argued that these phases are distinguished by the string order parameters or the hidden-symmetry breaking. For example, although the large-$D$ phase and the Haldane phase cannot be classified by the correlations of local observables, they are specified by the hidden $Z_2 \times Z_2$ symmetry. In the Haldane phase the symmetry is completely broken, while in the large-$D$ phase it is not broken at all.

In this section, we concentrate on the integer-$S$ spin chains, and construct new anisotropic VBS-type states, which we call intermediate-$D$ VBS states. Then we evaluate the string order parameters in these states.

We construct the intermediate-$D$ VBS states as follows. Let $n$ and $d$ be such integers that $S = n + d$. At each site there are $d$ pairs of up and down spin. The nearest-neighbour sites are connected by $n$ valence bonds. There are $2(n+d)$ spin-$\frac{1}{2}$ variables at each site. We symmetrize these spin-$\frac{1}{2}$ variables at each site to obtain the intermediate-$D$ VBS state with spin $S$.

An example of the intermediate-$D$ VBS states is illustrated in figure 3.

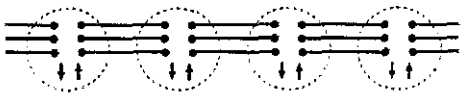

**Figure 3.** Intermediate-$D$ VBS state with $n = 3$ and $d = 1$ ($S = 4$). An up (down) arrow denotes an up (down) spin-$\frac{1}{2}$ (cf figure 1).

Using the Schwinger boson representation, these states can be written as

$$|\mathrm{i}D\mathrm{VBS}(p,q)\rangle = (a_1^\dagger)^p (b_1^\dagger)^{n-p} (a_L^\dagger)^{q+d} (b_L^\dagger)^{n-q+d} \prod_{j=1}^{L-1} (a_j^\dagger b_j^\dagger)^d (a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger)^n |0\rangle \tag{13}$$

where $p$ and $q$ satisfy $0 \leqslant p, q \leqslant n$, and represent the spin-$\frac{n}{2}$-like degree of freedom at both ends (cf equation (7)). These states are no longer invariant under arbitrary rotation but are invariant only for the rotation about the $z$ axis by an arbitrary angle or the rotation about an axis perpendicular to the $z$ axis by an angle $\pi$.

We can also construct a Hamiltonian which has the intermediate-$D$ VBS states (13) as the ground states as follows:

$$H = \sum_i P(S_{i,i+1} > n + 2d) + P((S_i^z)^2 > n^2). \tag{14}$$

Here $P$ represents the projection operator defined by

$$P(S_{i,i+1} > S_c) = \begin{cases} 1 & \text{when } (S_i + S_{i+1})^2 > S_c(S_c+1) \\ 0 & \text{otherwise} \end{cases}$$

$$P((S_i^z)^2 > n^2) = \begin{cases} 1 & \text{when } (S_i^z)^2 > n^2 \\ 0 & \text{otherwise} \end{cases}$$

where $S_c$ is an arbitrary integer.

We can prove that there are no other ground states of (14) than (13), following the method of Kennedy and co-workers [14]. Here we briefly describe the proof. First, the ground-state energy is greater than or equal to zero, because the Hamiltonian is the sum of the projection operators. Next, the existence of the intermediate-$D$ VBS states (13) implies that the ground-state energy is exactly zero. As a consequence, the ground state must belong to the zero-eigenvalue of each projection operator. On the other hand, any state of a chain with spin $S$ can be identified, in the Schwinger boson representation, with a polynomial of $a_i^\dagger, b_j^\dagger$ which is of degree $2S$ for each $a_i^\dagger$ and $b_i^\dagger$. We can show that the polynomial which represents a zero eigenstate of $P(S_{i,i+1} > n + 2d)$ must contain a factor $(a_i^\dagger b_{i+1}^\dagger - b_i^\dagger a_{i+1}^\dagger)^n$, and the polynomial which represents a zero eigenstate of $P((S_i^z)^2 > n^2)$ must contain a factor $(a_i^\dagger b_i^\dagger)^d$. We can conclude, from the unique factorizability of polynomials, that the ground states of the Hamiltonian (14) must be the intermediate-$D$ VBS states (13).

Now we move on to the evaluation of the string order parameters in these intermediate-$D$ VBS states. The method described in the previous sections is also useful here. However, the decoupling property must be modified for these states due to the lack of the full rotational invariance (see the appendix for more details). Let us write the decoupling property in the following form:

$$\langle \mathrm{i}D\mathrm{VBS}(p', q')|\mathrm{i}D\mathrm{VBS}(p, q)\rangle \sim C(L)\delta_{p',p}\delta_{q',q}g(p)g(q) \qquad L \to \infty.$$

We determine the 'metric' $g(p)$ by means of a self-consistency condition. Let $L$ be so large that the two spin-$\frac{n}{2}$-like degrees of freedom decouple completely. Suppose we obtain $g(p)$ in such case. We add one more site to the chain, and construct the state of the same type with $L + 1$ sites. The new metric $g(p)$ can be determined from the previous metric $g(p)$, and they must be equal up to a constant factor. From this self-consistency condition we find that $g(q)$ must be an eigenvector of the $(n + 1) \times (n + 1)$ matrix:

$$M_{q,r} = \frac{(n + d + q - r)!(n + d + r - q)!}{[r!(n - r)!]^2}.$$

By definition, $g(q)$ must be positive, and the matrix $M_{q,r}$ has a unique positive eigenvector according to the Perron–Frobenius theorem. We can therefore determine $g(q)$ uniquely from the consistency condition.

Once we get $g(q)$, we can calculate the string order parameters $\mathrm{O}^z_{\mathrm{string}}$ and $\mathrm{O}^x_{\mathrm{string}}$. After some calculation, we get

$$\mathrm{O}^z_{\mathrm{string}} = |f^{(D)}_{n,d}(-1)|^2 \tag{15}$$

where

$$f^{(D)}_{n,d}(w) = \frac{1}{N}\sum_{k=0}^{n}\sum_{l=0}^{n}\left(\frac{1}{k!(n-k)!l!(n-l)!}\right)^2 g(k)g(l) \times (n + d + k - l)!(n + d + l - k)!(k - l)w^k \tag{16}$$

$$N = \sum_{k=0}^{n}\sum_{l=0}^{n}\left(\frac{1}{k!(n-k)!l!(n-l)!}\right)^2 g(k)g(l)(n + d + k - l)!(n + d + l - k)!$$

and

$$O^{x}_{\text{string}} = \delta_{n,\text{odd}} \left[ \frac{1}{N} \frac{g((n+1)/2)}{\{[(n+1)/2]![(n-1)/2]!\}^2} \sum_{l=0}^{n} \left( \frac{1}{l!(n-l)!} \right)^2 \times [\tfrac{1}{2}(n+1)+d+l]![\tfrac{1}{2}(n+1)+d+n-l]! \right]^2 . \tag{17}$$

We immediately see that $O^{x}_{\text{string}}$ vanishes if $n$ is even but does not vanish if $n$ is odd. Furthermore, we see that $O^{z}_{\text{string}}$ vanishes if $n$ is even, because of the symmetry $g(n-q) = g(q)$ which is implied by the invariance under rotation about the $x$ axis by an angle $\pi$. Although we have no rigorous argument, $O^{z}_{\text{string}}$ is expected to be non-vanishing for an odd $n$ in general; numerical calculations for some values of $n$ and $d$ support this conjecture.

Therefore we have shown that the hidden $Z_2 \times Z_2$ symmetry is completely broken in the intermediate-$D$ VBS states when the number of valence bond $n$ is odd, but remains unbroken when $n$ is even. The fact that the hidden $Z_2 \times Z_2$ symmetry breaking depends on the parity of the number of the valence bond, has been found in the intermediate-$D$ VBS states, as well as in partially dimerized VBS states. We can understand this by the argument given in the end of section 3.

The above result suggests the following picture for the ground-state phase diagram of the Hamiltonian (5) with an integer $S > 1$. When we move to the $D \to \infty$ limit from the Heisenberg point ($D = 0, \lambda = 1$), several phases which are represented by the intermediate-$D$ VBS states appear. Phase transitions between these phases are accompanied by a change in the hidden symmetry. A part of the expected phase diagram in the Hamiltonian (5) is shown in figure 4.

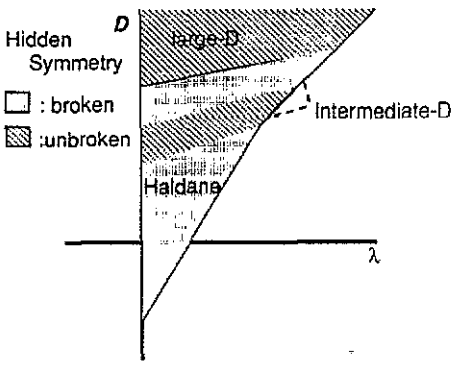


**Figure 4.** Conjectured phase diagram of the Hamiltonian (5) for $S = 3$. Only the regions with specified hidden symmetry is considered here.

Our conjecture implies a different phase diagram from that in the bosonization approach [15].

We remark that, as we noted in the previous section, the discrepancy of the VBS-type Hamiltonians from the standard Hamiltonian (5) makes our arguments weak. However, the successive phase transitions are likely to exist, at least when we modify the form of the uniaxial anisotropy. Here we present an $S = 2$ model which

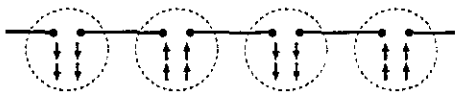

**Figure 5.** Antiferromagnetic Ising-VBS state. The figure shows the ground state of the $S = 3$ Hamiltonian (19). An up (down) arrow denotes an up (down) spin $\frac{1}{2}$ (cf figure 1).

probably undergoes two successive phase transitions when we change the strength of the uniaxial anisotropy.

We consider the $S = 2$ model with Hamiltonian

$$H = \sum_j \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} + D'(\tfrac{2}{3}S_i^z)^{2n}. \tag{18}$$

For $n = 1$, this reduces to the standard Hamiltonian (5) with $\lambda = 0, D = 4D'/9$.

When $n$ is sufficiently large, the uniaxial anisotropy term $D'(\frac{2}{3}S_i^z)^{2n}$ suppresses the $\pm 2$ terms in the $S^z$ basis, but does not affect the $\pm 1$ terms. We can then identify the ground state of the chain with the ground state of some $S = 1$ spin chains, by identifying $0, \pm 1$ for $S = 2$ with $0, \pm 1$ for $S = 1$ in the $S^z$-basis representation.

In this identification, the spin operators for $S = 2$ are replaced by $S = 1$ spin operators as follows:

$$S^z \to S^z \qquad S^{x,y} \to \sqrt{3}S^{x,y}.$$

Hence the $S = 2$ Hamiltonian (18) is equivalent to the $S = 1$ Hamiltonian (5) with $\lambda = \frac{1}{3}, D = 0$, whose ground state is expected to be in the $S = 1$ Haldane phase. Therefore the den Nijs–Rommelse string order parameter $O^{\alpha}_{\text{string}}$ does not vanish and the hidden $Z_2 \times Z_2$ symmetry is broken at this point.

On the other hand, when we move to the $D' \to \infty$ region for any finite $n$, the site spin states $\pm 1$ and $\pm 2$ are inaccessible, and we have the large-$D$ phase which does not break the hidden $Z_2 \times Z_2$ symmetry at all.

We conclude that, for sufficiently large $n$, as $D'$ increases from 0, there must be two phase transitions separating different characters for the hidden $Z_2 \times Z_2$ symmetry. (Here we adopt the plausibility argument that the hidden $Z_2 \times Z_2$ symmetry is not broken in the $S = 2$ Heisenberg point ($D' = 0$).)

It is also possible to construct similar models for higher $S$, and discuss the phase diagram of spin-$S$ chains referring to the phase diagram of the spin $1, 2, \cdots, S-1$ chains. However we do not investigate them here, because the phase diagram of the $S \geqslant 2$ chains are not yet established.

## 6. VBS-type states with long-range order

In this section, we construct new VBS-type states with a long-range order and evaluate the string order parameters in these states.

First, we construct antiferromagnetic (AF) Ising-VBS states, which have a long-range Néel order as well as the VBS structure, by symmetrizing the valence bonds and Néel ordered spin-$\frac{1}{2}$ terms. Figure 5 shows an example, which is the ground state of the Hamiltonian

$$H = \sum_j P(S_{j,j+1} = 6) + P((S_j^z + S_{j+1}^z)^2 > 1) + P((S_j^z)^2 = 0) \tag{19}$$

for $S = 3$.

The generalization of this model is not straightforward. We have not yet obtained the Hamiltonian that gives rise to an arbitrary Ising-VBS state as the unique ground state.

There are $[S+\frac{1}{2}]$ (here $[x]$ denotes the maximum integer which does not exceed $x$) types of AF Ising-VBS states, including the completely Néel ordered state. We expect that these states would represent certain aspects of the ground state of the more realistic Hamiltonian (5). When we increase the value of $\lambda$ in (5) from the Heisenberg point ($D = 0$, $\lambda = 1$), phases represented by these AF Ising-VBS states might appear through successive phase transitions.

However, even for an integer $S$, our hidden symmetry arguments cannot describe such successive phase transitions. Of course, when we move from the Haldane phase (which might be represented by the standard VBS state) to the phase which is represented by the first AF Ising-VBS state, there is a change in the explicit $Z_2$ symmetry and we thus expect a phase transition. On the other hand, Af Ising-VBS states with different numbers of the valence bonds have no difference either in the apparent $Z_2$ symmetry or in the hidden $Z_2 \times Z_2$ symmetry breaking; in any AF Ising-VBS state, the string order parameter $O^z_{\text{string}}$ does not vanish in general because of the Néel order, and $O^x_{\text{string}}$ vanishes because the Ising-VBS state is not invariant under the rotation about $x$ axis by an angle $\pi$. Thus in any AF Ising-VBS phase, the hidden $Z_2 \times Z_2$ symmetry is partially broken.

In addition, we can also construct ferromagnetic (F) Ising-VBS states, which have ferromagnetic long-range order as well as the VBS structure, by symmetrizing valence bonds and ordered spin-$\frac{1}{2}$ terms. An example of such states is shown in figure 6.

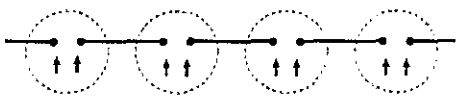

**Figure 6.** Ferromagnetic Ising-VBS state.

These states may represent the ground states which appear in a magnetization process of a quantum antiferromagnet. For example, let us suppose that we increase the strength of the magnetic field $B$ from 0 in the Hamiltonian

$$H = \sum_i S_i \cdot S_{i+1} + D(S_i^x)^2 - BS_i^z. \tag{20}$$

An intuitive VBS picture suggests that the successive phase transitions take place in the magnetization process of $S > 1$ quantum antiferromagnets. However, even for an integer $S$, the F Ising-VBS states with a different number of valence bonds have common properties concerning the hidden $Z_2 \times Z_2$ symmetry; the hidden $Z_2 \times Z_2$ symmetry argument cannot account for such successive phase transitions, as in the case of AF Ising-VBS states. (For the present studies on the magnetization process of $S = 1$ quantum antiferromagnets, see [16]. Affleck [17] studied the problem using large-$S$ field-theory mapping. Successive phase transitions are not predicted there.)

It is remarked here that the F Ising-VBS states have not only a long-range ferromagnetic order but also valence bonds which favour short-range antiferromagnetic order. Applying the method described in the previous sections,

we can calculate the nearest-neighbour and long-range correlations in these states and verify the above observation. For example, we consider an F Ising VBS state with a valence bond between the neighbouring sites, and an up spin-$\frac{1}{2}$ at each site. In this state, we find

$$\langle S_j^z S_{j+1}^z \rangle = -0.151\,92.$$

which implies the spin correlation is antiferromagnetic for every link.

Finally, we mention another candidate for VBS-type states. In $S = 1$ spin chains, there are $XY$ phases which are similar to the low-temperature phase of the two-dimensional classical $XY$ model (see figure 2). We might expect that, when $S > 1$, there are states in which $XY$ structure and the VBS structure coexist. However, we have not yet succeeded in constructing such states.

## 7. Extended string order parameters

We have investigated the integer-$S$ spin chains on the basis of the hidden $Z_2 \times Z_2$ symmetry. However, our hidden $Z_2 \times Z_2$ symmetry does not completely specify all possible states, and cannot be applied to half-integer $S$.

To search for a more general specification, we here investigate an extension of the den Nijs–Rommelse string order parameter. We define extended string order parameters, which are characterized by an angle parameter $\theta$ and reduce to the den Nijs–Rommelse ones at $\theta = \pi$, as follows:

$$O^{\alpha}_{\text{string}}(\theta) = \lim_{|k-j|\to\infty} \langle S_j^z \exp\left(i\theta \textstyle\sum_{j\leqslant l<k} S_l^z\right) S_k^z \rangle$$

where $\alpha = x, y, z$. We evaluate the extended string order parameter in several VBS-type states for integer $S$ and half-integer $S$.

We begin with the $(n, m)$-VBS states (10). As we did in section 4, we only consider the extended order parameter

$$O^{\alpha}_{\text{string}}(\theta) = \lim_{|k-j|\to\infty} \langle S_{2j+1}^z \exp\left(i\theta \textstyle\sum_{l=2j+1}^{2k} S_l^z\right) S_{2k+1}^z \rangle$$

in these states with a bond alternation. Replacing the twist angle $\pi$ with $\theta$, we can apply the method which we used to evaluate the den Nijs–Rommelse string order parameter in section 4. The result is

$$O^{\alpha}_{\text{string}} = |f_{n,m}(e^{i\theta})|^2$$

where $f_{n,m}(w)$ is given in (11). We see that, since $f_{n,m}(w)$ is an $n$th-order polynomial of $w$, $O^{\alpha}_{\text{string}}(\theta)$ does not vanish except (at most) at $n$ points. We can prove a stronger statement that $O^{\alpha}_{\text{string}}$ has exactly $n$ distinct zero points in $0 \leqslant \theta < 2\pi$ [18]. According to (11), we have to prove that the $n$th order polynomial $\sum_{k=0}^{n}(2k-n)z^k$ has $n$ simple zero points on the unit circle $|z| = 1$.

First we define the polynomials

$$P(z) = \sum_{k=0}^{n} z^k$$

$$Q(z) = \sum_{k=0}^{n}(2k-n)z^k.$$

A little calculation shows

$$\frac{\mathrm{d}}{\mathrm{d}\theta}|P(\mathrm{e}^{\mathrm{i}\theta})|^2 = \mathrm{i}\mathrm{e}^{-\mathrm{i}n\theta}P(\mathrm{e}^{\mathrm{i}\theta})Q(\mathrm{e}^{\mathrm{i}\theta}). \tag{21}$$

It is well known that $P(z)$ has $n$ simple zero points on the unit circle $|z| = 1$, namely $|P(\mathrm{e}^{\mathrm{i}\alpha_\nu})|^2 = 0$ $(0 < \alpha_1 < \alpha_2 < \cdots < \alpha_n < 2\pi)$. (To be concrete, $\alpha_\nu = [\nu/(n+1)]2\pi$.) According to the mean value theorem, there are $\beta_\nu$ satisfying $\alpha_\nu < \beta_\nu < \alpha_{\nu+1}$ (we define $\alpha_{n+1} = \alpha_1 + 2\pi$) and

$$\frac{\mathrm{d}}{\mathrm{d}\theta}|P(\mathrm{e}^{\mathrm{i}\beta_\nu})|^2 = 0.$$

From equation (21) and $P(\mathrm{e}^{\mathrm{i}\beta_\nu}) \neq 0$ we can see $Q(\mathrm{e}^{\mathrm{i}\beta_\nu}) = 0$, which completes the proof.

We note that one of the zero points is always $\theta = 0$ because $f_{n,m}(1) = 0$, and when $n$ is odd another one is $\theta = \pi$, which corresponds to the den Nijs–Rommelse string order parameter. We expect that the number of the zero points is an invariant characteristic of the phase which is represented by one of the $(n, m)$-VBS state. That is, all the phases appearing in the successive dimerization transitions are characterized by the number of zero points of $\mathrm{O}^{\alpha}_{\mathrm{string}}$. However, we have not found any hidden symmetry which corresponds to the extended order parameters.

Next, we move on to the intermediate-$D$ VBS state with $n$ valence bonds and $d$ pairs of up and down spin-$\frac{1}{2}$ terms symmetrized. In this state, we have $\mathrm{O}^{x}_{\mathrm{string}}(\theta) = \mathrm{O}^{y}_{\mathrm{string}}(\theta)$. First we consider $\mathrm{O}^{x}_{\mathrm{string}}(\theta)$. We see that $\mathrm{O}^{x}_{\mathrm{string}}(\theta)$ vanishes except at $\theta = \pi$, because the states are not invariant under rotation about the $x$ axis by $\theta \neq 0, \pi$. When $\theta = \pi$, we recover the den Nijs–Rommelse one, which we have already obtained in (17). We turn to the evaluation of $\mathrm{O}^{z}_{\mathrm{string}}(\theta)$. We find $\mathrm{O}^{z}_{\mathrm{string}}(\theta) = |f^{(D)}_{n,d}(e^{\mathrm{i}\theta})|^2$, where $f^{(D)}_{n,d}$ is given in (16). Let us see whether this string order parameter has a characteristic behaviour. For example, a numerical calculation of $\mathrm{O}^{z}_{\mathrm{string}}(\theta)$ shows that $\mathrm{O}^{z}_{\mathrm{string}}(\theta)$ has only the trivial zero point $\theta = 0$ in the $n = 3, d = 3$ intermediate-$D$ VBS state. Thus the number of zero points of $\mathrm{O}^{z}_{\mathrm{string}}$ does not distinguish different intermediate-$D$ VBS states in general, and our extension is not useful in distinguishing these states. Evaluation of the extended order parameter in the Ising-VBS states leads to a similar conclusion.

We note that the formulae for the string order parameters in (15) and (17) are valid even for half-integer $S$. Hence the den Nijs–Rommelse string order parameter $(\theta = \pi)$ distinguishes the intermediate-$D$ VBS states with odd $n$ from those with even $n$ for a half-integer $S$, as well as for an integer $S$.

Hatsugai [19] made a numerical study on the extended order parameters for $S = 1, 2$.

## 8. Conclusion

We found a compact operator representation for the Kennedy–Tasaki unitary transformation, and extended it to spin chains with arbitrary integer spin. Under this transformation, a wide class of Heisenberg-like Hamiltonians of spin chains with an integer spin were found to transform into Hamiltonians of local interactions with a $\mathrm{Z}_2 \times \mathrm{Z}_2$ symmetry.

It was also shown that the den Nijs–Rommelse string order parameter in the original system is equivalent to the ferromagnetic order parameter in the transformed system. Thus the non-vanishing string order parameter indicates the hidden $Z_2 \times Z_2$ symmetry breaking. We found also a method to evaluate the string order parameter in the VBS-type states.

In the partially dimerized VBS states, our analysis showed that the hidden $Z_2 \times Z_2$ symmetry is broken if the number of the valence bonds between the neighbouring sites is odd, and is unbroken otherwise. This result suggests that the $Z_2 \times Z_2$ symmetry broken and unbroken phases appear alternatingly when the dimerization proceeds.

We constructed a new type of anisotropic VBS-type states termed the intermediate-$D$ VBS states. We found that, in these states, the hidden $Z_2 \times Z_2$ symmetry is broken if the number of the valence bonds between the neighbouring sites is odd, and is unbroken otherwise. Hence we were led to the conjecture that the Heisenberg antiferromagnetic chain undergoes successive phase transitions when we change the strength of the uniaxial anisotropy.

Other new VBS-type states with long-range order were constructed. VBS-type states with ferromagnetic long-range order may represent phases which appear in the magnetization process of an antiferromagnetic chain. VBS-type states with antiferromagnetic long-range order may represent phases of the Heisenberg $XXZ$ chain. However, we could not distinguish these states with a different number of valence bonds with respect to the hidden $Z_2 \times Z_2$ symmetry.

We defined an extended string order parameter characterized by an angle parameter $\theta$. In the partially dimerized VBS states with $n$ valence bonds between a neighbouring site, this order parameter was found to have $n$ simple zero points in $0 \leqslant \theta < 2\pi$.

We therefore conclude that the notion of the hidden $Z_2 \times Z_2$ symmetry breaking is useful in discussing the phase structure of the quantum spin chains with an integer spin. Our analysis suggests rich phase structures for $S > 1$ chains previously undetected by other approaches. It should be noted, however, that for the states which are not of the VBS-type, our analysis cannot determine whether they break the hidden $Z_2 \times Z_2$ symmetry.

On the other hand, we could not distinguish several VBS-type states completely in terms of the hidden $Z_2 \times Z_2$ symmetry breaking. Hence there may be more unknown hidden structures in $S > 1$ chains. Our extension of the string order parameter is a candidate to detect such structures (see also [19]). Moreover, the large ground-state degeneracy of the VBS models with $S > 1$ suggests that there are higher hidden symmetries other than our $Z_2 \times Z_2$ symmetry. Investigation of such symmetries is an open problem to the future.

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## Appendix. Proof of the decoupling property

Here we outline a proof of the decoupling property (8) for the VBS states. Using the Weyl representation [11], we have

$$\langle \mathrm{VBS}(p,q)|\mathrm{VBS}(r,s)\rangle = \text{constant} \int \cdots \int \prod_{j=1}^{L} \mathrm{d}\Omega_j \, w_{p,r}(\Omega_1) \times \prod_{k=1}^{L-1} (1-\Omega_k \cdot \Omega_{k+1})^S w_{q,s}(\Omega_L)$$

where

$$\Omega = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$$
$$w_{p,r}(\Omega) = (\cos\tfrac{1}{2}\theta)^p (\sin\tfrac{1}{2}\theta)^r \mathrm{e}^{\frac{1}{2}\mathrm{i}\phi(p-r)}$$
$$\mathrm{d}\Omega = \frac{\sin\theta \mathrm{d}\theta \mathrm{d}\phi}{4\pi}.$$

As is emphasized in [11], this integral can be interpreted as a formula for a correlation in a one-dimensional classical statistical system. Hence the decoupling property is very natural from the physical point of view. In fact, we can prove it.

Let us consider the eigenfunction of the transfer integral

$$\psi_i(\Omega_x) = \mu_i \int \mathrm{d}\Omega_y \, K(\Omega_x, \Omega_y)\psi_i(\Omega_y).$$

The integral kernel $K(\Omega_x, \Omega_y) = (1-\Omega_x \cdot \Omega_y)^S$ is symmetric and positive except for the region with measure zero.

The mathematical properties of symmetric kernels defined on a finite space are well established [20]. Their eigenvalues are all real, and they have an orthogonal complete set of eigenfunctions. Furthermore, the eigenvalues $\mu_i$ must satisfy $\sum_i (\mu_i)^2 < \infty$. In particular, the eigenvalues never have non-zero values as their accumulation point.

We will call an eigenfunction which belongs to the maximum eigenvalue a maximum eigenfunction. We shall show that the maximum eigenfunction is positive and not degenerate, if the kernel is positive. Assume we have an eigenfunction $\psi(\Omega)$ which changes the sign. The maximum eigenfunction makes the functional

$$J[\psi] = \int \mathrm{d}\Omega_x \mathrm{d}\Omega_y \, K(\Omega_x, \Omega_y)\psi(\Omega_x)\psi(\Omega_y)$$

maximum under the constraint $\int \mathrm{d}\Omega |\psi(\Omega)|^2 = 1$. However, we can easily see that $J[\psi] < J[|\psi|]$ since $K$ is positive, and therefore $\psi(\Omega)$ cannot be a maximum

eigenfunction. Thus we see that the maximum eigenfunction must be non-negative. Then the eigenequation implies that it must be positive. Furthermore, the non-degeneracy follows from the fact that we can choose the orthogonal complete set of eigenfunctions and that two positive functions are never orthogonal with each other.

Hence our kernel $K$ has the unique maximum eigenfunction $\psi_1(\Omega)$. Moreover, there is finite difference $\delta\mu$ between the maximum eigenvalue and the second one, because there is no non-zero accumulation point of eigenvalues.

Thus we get

$$\langle \mathrm{VBS}(p,q)|VBS(r,s)\rangle = \text{constant} \times \int d\Omega_1 w_{p,r}(\Omega_1)\psi_1(\Omega_1) \times \int d\Omega_L w_{q,s}(\Omega_L)\psi_1(\Omega_L)(\mu_1)^L(1+O((\delta\mu)^{-L})).$$

This is the decoupling property of the VBS states. For the standard VBS states, the maximum eigenfunction is a constant function of $\Omega$ because of the rotational invariance. Hence the boundary degrees of freedom become normal spin-$\frac{S}{2}$ objects, namely

$$\langle \mathrm{VBS}(p,q)|\mathrm{VBS}(r,s)\rangle \sim \text{constant} \times \delta_{p,r}\delta_{q,s}p!(S-p)!q!(S-q)!.$$

We can apply similar arguments to the $(n,m)$-VBS states, the intermediate-$D$ VBS states and the Ising-VBS states; all these states have the decoupling property. However, for intermediate-$D$ or Ising-VBS states, the integral kernel no longer has rotational invariance. Hence the maximum eigenfunction is not the constant function, and the boundary degrees of freedom become different from the normal spin-$\frac{n}{2}$ objects with rotational invariance. (Here $n$ represents the number of the valence bonds.) We describe a method to determine the nature of the boundary degrees of freedom in section 5.

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