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Maximized string order parameters in the valence bond solid states of quantum integer spin chains

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Abstract

We propose a set of maximized string order parameters to describe the hidden topological order in the valence bond solid states of quantum integer spin- S chains. These optimized string order parameters involve spin-twist angles corresponding to Z_{S+1} rotations around z or x -axes, suggesting a hidden $Z_{S+1} \times Z_{S+1}$ symmetry. Our results also suggest that a local triplet excitation in the valence bond solid states carries a Z_{S+1} topological charge measured by these maximized string order parameters.

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(Some figures in this article are in colour only in the electronic version)

Determining order parameters is one of the most important issues in the study of strongly correlated systems. It is the basis of Landau theory in describing continuous phase transitions between different phases with spontaneous symmetry breaking. However, some novel phenomena or phases, for example, the fractional quantum Hall states and the Haldane gap phenomena in quantum integer-spin chains, are not amenable to such a description. In particular, to find an order parameter in a system with strong frustrations or quantum fluctuations is challenging and highly nontrivial [1, 2].

For quantum integer-spin antiferromagnetic Heisenberg chains, Haldane predicted that there is a finite excitation gap above the ground state [3]. To understand this intriguing conjecture, Affleck, Kennedy, Lieb and Tasaki (AKLT) proposed a set of exactly solvable quantum spin models whose ground states are the valence bond solid (VBS) states [4]. In the $S = 1$ VBS state, there is a hidden antiferromagnetic order which can be characterized by string order parameters (SOPs) [5]. Corresponding to this nonlocal string order, Kennedy and Tasaki showed that there is a hidden $Z_2 \times Z_2$ symmetry [6]. To reveal this symmetry clearly, they introduced a nonlocal unitary transformation to convert the VBS state to a 'diluted'

ferromagnetic state and showed that the ground state is four-fold degenerate if this symmetry is broken in an open chain.

For quantum integer-spin chains with $S > 1$, it is extremely difficult to find the corresponding nonlocal unitary transformation to convert the VBS state into a long-range ordered state. So far no one has succeeded along this direction. However, this is not the only approach for revealing a hidden topological symmetry. This hidden symmetry can also be identified from the non-local string order parameters of the ground state. So the extended SOPs with a twist angle $\theta = \pi/S$ were proposed to account for the hidden order in the VBS states [7, 8]. Actually, this kind of extended SOPs does not give a comprehensive description to the Haldane phase in these systems [9]. Recently, we have extended the $S = 1$ VBS (which is $SO(3)$ invariant) to the $SO(2n+1)$ symmetric system [10]. We find that these $SO(2n+1)$ symmetric matrix product states are the exact ground states of Hamiltonians of spin $S = n$ with either $SO(2n+1)$ or $SU(2)$ symmetry. Furthermore, we show that this system possesses a hidden topological $(Z_2 \times Z_2)^n$ symmetry and the ground state can be characterized by n -set of hidden antiferromagnetic orders. This study suggests that the topological order is generally more complicated than the θ -twisted SOP as previously studied in the VBS states. It motivates us to consider how to find proper SOPs to characterize the hidden topological order in the higher integer-spin VBS states [11].

In this paper, we will propose a systematical method to find the optimized SOPs in the VBS states. By generalizing the $S = 1$ den Nijs–Rommelse SOP to arbitrary integer spin- S VBS states, the corresponding hidden long-range order can be most comprehensively manifested by the maximal string correlation functions between two polynomial spin operators

$$A_j^\alpha = \sum_{n=0}^S a_n (S_j^\alpha)^n \quad (\alpha = x, y, z), \quad (1)$$

where a_n are the coefficients which maximize the string correlation function. We find that these maximized SOPs suggest a hidden $Z_{S+1} \times Z_{S+1}$ symmetry, in consistent with the degeneracy of the ground states in an open chain case. Moreover, our optimized SOPs measure a Z_{S+1} topological charge carried by a localized triplet excitation in the VBS state.

The AKLT Hamiltonian is defined by [4, 12]

$$H_{\text{AKLT}} = \sum_i \sum_{J=S+1}^{2S} K_J \mathcal{P}_J(i, i+1), \quad (2)$$

where $K_J > 0$ and $\mathcal{P}_J(i, i+1)$ is to project two spins at i and $i+1$ onto the subspace of the total spin J . This Hamiltonian can be written as a polynomial of $SU(2)$ invariant nearest-neighbor spin exchange interactions. The VBS state is the ground state of this Hamiltonian.

In the Schwinger boson representation, the spin operators are expressed by $S_i^+ = a_i^\dagger b_i$, $S_i^- = b_i^\dagger a_i$, $S_i^z = (a_i^\dagger a_i - b_i^\dagger b_i)/2$ with a local constraint $a_i^\dagger a_i + b_i^\dagger b_i = 2S$. The VBS state in a length- L periodic chain is then given by

$$|\text{VBS}\rangle = \prod_{i=1}^L (a_i^\dagger b_{i+1}^\dagger - b_i^\dagger a_{i+1}^\dagger)^S |\text{vac}\rangle. \quad (3)$$

In an open chain, the VBS states have effectively two spin- $S/2$ edge states at the two ends of the chain. In the thermodynamic limit, $L \rightarrow \infty$, the VBS states with different edge states are asymptotically orthogonal to each other, giving rise to $(S+1)^2$ -fold degenerate ground states.

The VBS state can also be represented in a matrix product form [8, 13, 14]. By using the binomial theorem, it can be shown that

$$|\text{VBS}\rangle = \sum_{\{m_i\}=-S}^S \text{Tr}(B^{[m_1]} \dots B^{[m_L]} |m_1 \dots m_L\rangle), \quad (4)$$

where $B^{[m]}$ is a $(S+1) \times (S+1)$ matrix defined by its matrix elements as

$$B^{[m]}(p, q) = (-1)^{S-p+1} \sqrt{(S+m)!(S-m)!} \sqrt{\binom{S}{p-1} \binom{S}{q-1}} \delta_{m, q-p}, \quad (5)$$

where $1 \leq p, q \leq S+1$.

The correlation function of the VBS state in the matrix product form can be evaluated using the transfer matrix method [8, 14]. To do this, let us first introduce the following $(S+1)^2 \times (S+1)^2$ transfer matrix:

$$G_P = \sum_{m, m'} \langle m' | \hat{P} | m \rangle (\bar{B}^{[m']} \otimes B^{[m]}), \quad (6)$$

where \hat{P} is a local operator acting on a single site and \bar{B} denotes the complex conjugate of B . For the identity operator $\hat{P} = I$, G_P is a Hermitian transfer matrix $G = \sum_m (\bar{B}^{[m]} \otimes B^{[m]})$. With these definitions, it is straightforward to show that the two-point spin correlation function can be expressed as

$$\langle S_i^z S_j^z \rangle = \lim_{L \rightarrow \infty} \frac{\text{Tr}[(G)^{L-j+i-1} G_S (G)^{j-i-1} G_S]}{\text{Tr}(G)^L}, \quad (7)$$

where

$$G_S = \sum_m m (\bar{B}^{[m]} \otimes B^{[m]}).$$

In the long distance limit, the two-point spin correlation function always decays exponentially with the distance between the sites i and j ,

$$\langle S_i^z S_j^z \rangle \sim \exp\left(-\frac{|j-i|}{\xi}\right), \quad (8)$$

where $\xi = 1/\ln(1+2/S)$ is the correlation length [12].

In order to describe the hidden topological order in the VBS states, let us introduce the following generalized string correlation function [8]:

$$\mathcal{O}_A^\alpha(\theta) = \lim_{|j-i| \rightarrow \infty} \left\langle (A_i^\alpha)^\dagger \prod_{k=i}^{j-1} e^{i\theta S_k^\alpha} A_j^\alpha \right\rangle, \quad (9)$$

where A_j^α is defined by equation (1). The value of a_0 in A_j^α can be fixed by demanding the expectation value of A_j^α to be zero, i.e., $a_0 = -\sum_{n=1}^S a_n \langle (S_j^\alpha)^n \rangle$.

Since the VBS state is spin $SU(2)$ rotational invariant, we need only to evaluate the z -component of the string correlation function $\mathcal{O}_A^z(\theta)$. Based on the transfer matrix technique, it can be shown that

$$\mathcal{O}_A^z(\theta) = \lim_{|j-i| \rightarrow \infty} \lim_{L \rightarrow \infty} \frac{\text{Tr}[(G)^{L-j+i-1} G_{A^\dagger} (G_O)^{j-i-1} G_A]}{\text{Tr}(G)^L}, \quad (10)$$

where G_O, G_{A^\dagger} and G_A are obtained by replacing operator \hat{P} in equation (6) by $\exp(i\theta S^z), (A^z)^\dagger \exp(i\theta S^z)$ and A^z , respectively. We emphasize that only G and G_O are Hermitian, while G_{A^\dagger} and G_A are not.

In the limit of $|j - i| \rightarrow \infty$ and $L \rightarrow \infty$, $\mathcal{O}_A^z(\theta)$ is determined purely by the largest eigenvalues and eigenvectors of G and $G_{\mathcal{O}}$. We find that equation (10) can be simplified as

$$\mathcal{O}_A^z(\theta) = \frac{1}{\lambda_{\max}^2} |\langle \lambda_{\max}^{\mathcal{O}} | G_A | \lambda_{\max} \rangle|^2, \quad (11)$$

where $|\lambda_{\max}\rangle$ and $|\lambda_{\max}^{\mathcal{O}}\rangle$ are the eigenvectors corresponding to the same largest eigenvalue of G and $G_{\mathcal{O}}$, respectively.

When $\theta = 0$, $\mathcal{O}_A^z(\theta)$ becomes the ordinary two-point correlation function. It vanishes because $|\lambda_{\max}^{\mathcal{O}}\rangle = |\lambda_{\max}\rangle$ for $\theta = 0$ and the vector $G_A |\lambda_{\max}\rangle$ is orthogonal to $|\lambda_{\max}\rangle$. If we fix the form of the operator A^z and tune the spin-twist angle θ , $\mathcal{O}_A^z(\theta)$ will reach its maximum only when the vector $G_A |\lambda_{\max}\rangle$ is parallel to the vector $|\lambda_{\max}^{\mathcal{O}}\rangle$. This means that in order to maximize the SOP, $|\lambda_{\max}^{\mathcal{O}}\rangle$ is orthogonal to $|\lambda_{\max}\rangle$, i.e., $\langle \lambda_{\max}^{\mathcal{O}} | \lambda_{\max} \rangle = 0$. For the VBS state, the eigenvectors $|\lambda_{\max}\rangle$ and $|\lambda_{\max}^{\mathcal{O}}\rangle$ can be readily calculated, we find that the orthogonality condition can be satisfied *if and only if* the following equation is satisfied:

$$1 + e^{i\theta} + e^{i2\theta} + \dots + e^{iS\theta} = 0. \quad (12)$$

Thus, the spin-twist angle corresponding to the maximal SOP is determined by

$$\theta = \frac{2n\pi}{S+1}, \quad (n = 1, \dots, S). \quad (13)$$

Importantly, these spin-twist angles correspond to a discrete symmetry group Z_{S+1} . Because of the spin SU(2) rotational symmetry, a similar maximal SOP can be found in terms of the x -component operators $\mathcal{O}_A^x(\theta)$. The spin-twist angles corresponding to the maximal $\mathcal{O}_A^x(\theta)$ are also given by equation (13).

In the conventional Landau theory, it is well known that the maximized order parameters fully characterize the symmetry of the low-temperature ordered phases, and these order parameters can also be used to describe the possible phase transitions as decreasing the temperature from the high-temperature disordered phases. When we generalize the similar rule to the present case, the maximal SOPs fully describe the hidden long-range order of the spin- S VBS states, suggesting that there exists a hidden $Z_{S+1} \times Z_{S+1}$ symmetry. In a finite open chain, this hidden $Z_{S+1} \times Z_{S+1}$ symmetry is broken in the ground states, leading to the spin- $\frac{S}{2}$ edge states with $(S+1)^2$ -fold degeneracy. We would like to emphasize that these spin- $\frac{S}{2}$ edge states are dictated by the underlying low-energy effective field theory, i.e., $O(3)$ nonlinear sigma model plus a topological term [15]. Moreover, the hidden $Z_{S+1} \times Z_{S+1}$ symmetry also incorporates the previous results given by Oshikawa [7]. For an odd integer S chain, the Z_{S+1} group has always a Z_2 subgroup with $\theta = \pi$. However, for an even integer S chain, a twist angle $\theta = \pi$ is always absent. This result explains why the hidden $Z_2 \times Z_2$ symmetry described by the den Nijs–Rommelse SOP is broken in the odd- S VBS states but not in the even- S ones [7].

Let us consider the hidden topological symmetries in the first few cases of the spin- S VBS states. For the $S = 1$ VBS state, we have $A_j^z = S_j^z$. The maximal eigenvalues of the transfer matrices G and $G_{\mathcal{O}}$ are equal to $\lambda_{\max} = 3$, and their eigenvectors are given by

$$|\lambda_{\max}\rangle = \frac{1}{\sqrt{2}}(1 \ 0 \ 0 \ 1)^T, \quad |\lambda_{\max}^{\mathcal{O}}\rangle = \frac{1}{\sqrt{2}}(e^{i\theta} \ 0 \ 0 \ 1)^T,$$

respectively. With a simple calculation, it can be shown that $\mathcal{O}_A^z(\theta) = (4/9) \sin^2(\theta/2)$, from which its maximal value corresponds to $\theta = \pi$. This result is fully consistent with the orthogonality condition. According to the nonlocal unitary transformation, the corresponding VBS state does exhibits a $Z_2 \times Z_2$ topological symmetry. Therefore, it is a reliable method of using the maximal SOPs to reveal the hidden symmetry.

Next let us consider the $S = 2$ VBS state, the maximal eigenvalues of the transfer matrices G and $G_{\mathcal{O}}$ is $\lambda_{\max} = 40$ and the corresponding eigenvectors are given by

$$\begin{aligned} |\lambda_{\max}\rangle &= \frac{1}{\sqrt{3}}(1 \ 0 \ 0 \ 0 \ 1 \ 0 \ 0 \ 0 \ 1)^T, \\ |\lambda_{\max}^{\mathcal{O}}\rangle &= \frac{1}{\sqrt{3}}(e^{2i\theta} \ 0 \ 0 \ 0 \ e^{i\theta} \ 0 \ 0 \ 0 \ 1)^T. \end{aligned}$$

When $\theta = 2\pi/3$ or $\theta = 4\pi/3$, the SOP (9) is maximal. From the condition that $G_A|\lambda_{\max}\rangle$ is parallel to $|\lambda_{\max}^{\mathcal{O}}\rangle$, we can find the corresponding optimal operators displaying the maximal string correlation function as the form

$$A_j^z = S_j^z \pm \frac{5\sqrt{3}i}{7}[(S_j^z)^2 - 2], \quad (14)$$

for $\theta = 2\pi/3$ and $\theta = 4\pi/3$, respectively. The maximal value of the SOPs is $\mathcal{O}_A^z(\theta) = 3$. In this nontrivial case, it is the linear combination of spin operator S_j^z and its spin quadrupole operator $(S_j^z)^2 - 2$ that exhibits the maximal hidden string order instead of the spin operator itself. The hidden topological symmetry in the $S = 2$ VBS state corresponds to the $Z_3 \times Z_3$ discrete symmetry.

For the $S = 3$ case, the spin-twist angles for the maximal SOPs are determined by $\theta = \pi/2, \pi, 3\pi/2$ from the orthogonality condition. Similar to the previous procedure, it is straightforward to show that the corresponding combinations of the spin operators are given by

$$A_j^z = S_j^z \pm \frac{15i}{67}[(S_j^z)^2 - 4] - \frac{7}{67}(S_j^z)^3 \quad (15)$$

for $\theta = \pi/2$ or $3\pi/2$, and

$$A_j^z = \frac{89\sqrt{2}}{67} \left[S_j^z - \frac{14}{89}(S_j^z)^3 \right] \quad (16)$$

for $\theta = \pi$. The maximal value of the SOPs is $\mathcal{O}_A^z(\theta) = 2592/4489$, and the corresponding hidden symmetry is $Z_4 \times Z_4$.

Accordingly, the above discussions can be readily extended to any higher integer spin- S VBS states. In addition to the VBS states, it can also be generalized to reveal the possible hidden topological order of arbitrary matrix product states. Thus, this is a systematic approach to analyze the hidden topological symmetry of matrix product states.

In fact, the topological property of the ground state can also be understood from its elementary excitations. For the AKLT model, to create an elementary excitation is to insert a triplet defect in the VBS ground state. This kind of excitation is called crackion [16]. Under the Kennedy–Tasaki unitary transformation for $S = 1$, a crackion is a kink linking two ferromagnetic ordered ground states from left to right. In higher- S systems, although the Kennedy–Tasaki unitary transformation does not transfer the VBS state to a ferromagnetic one, the kink or soliton-like feature of crackion can still be revealed by studying the string correlation function in the presence of a triplet defect [8]. An example of a crackion in the $S = 2$ VBS state is depicted in figure 1.

With the Schwinger boson representation, the wavefunction of a localized crackion between k and $k + 1$ sites can be constructed by replacing a singlet $(a_k^\dagger b_{k+1}^\dagger - b_k^\dagger a_{k+1}^\dagger)$ with one of the triplet operators T^a

$$T^1 = a_k^\dagger a_{k+1}^\dagger, \quad T^0 = a_k^\dagger b_{k+1}^\dagger + b_k^\dagger a_{k+1}^\dagger, \quad T^{-1} = b_k^\dagger b_{k+1}^\dagger.$$

The corresponding matrix product wavefunctions for these excitations are

$$|\psi_k^a\rangle = \sum_{\{m_i\}} \text{Tr}(B^{[m_1]} \dots C_a^{[m_k]} \dots B^{[m_L]}) |m_1 \dots m_L\rangle, \quad (17)$$

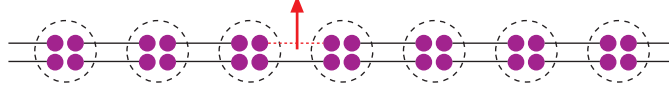


Figure 1. The schematic of a crackion excitation in a spin-2 VBS state. The solid lines represent the valence bond singlets. A dot represents a spin-1/2 Schwinger boson. The four bosons enclosed by each dashed circle form a spin-2 state. The arrow represents a crackion of local triplet defect.

where $C_a^{[m]}$ is defined by

$$\begin{pmatrix} C_1^{[m]}(p, q) \\ C_0^{[m]}(p, q) \\ C_{-1}^{[m]}(p, q) \end{pmatrix} = \frac{1}{S} (-1)^{S-p} \sqrt{(S+m)!(S-m)!} \\ \times \sqrt{\binom{S}{p-1} \binom{S}{q-1}} \begin{pmatrix} (S-q+1) \delta_{m,q-p+1} \\ (S-2q+2) \delta_{m,q-p} \\ (1-q) \delta_{m,q-p-1} \end{pmatrix}.$$

For one crackion in the string, it can be shown that the SOP in the thermodynamic limit is given by

$$\lim_{|j-i| \rightarrow \infty} \left\langle (A_i^z)^\dagger \prod_{k=i}^{j-1} e^{i\theta S_k^z} A_j^z \right\rangle_{\text{cr}} = \mathcal{O}_A^z(\theta) \frac{\langle \lambda_{\text{max}}^\mathcal{O} | G_\mathcal{O}^a | \lambda_{\text{max}}^\mathcal{O} \rangle}{\langle \lambda_{\text{max}} | G^a | \lambda_{\text{max}} \rangle}, \quad (18)$$

where $\mathcal{O}_A^z(\theta)$ is the maximized string order parameter without crackions. When replacing operator \hat{P} by $\exp(i\theta S^z)$ and I in the following crackion transfer matrix:

$$G_p^a = \sum_{m,m'} \langle m' | \hat{P} | m \rangle (\bar{C}_a^{[m']} \otimes C_a^{[m]}), \quad (19)$$

one obtains $G_\mathcal{O}^a$ and G^a , respectively. From these definitions, one can show that the ratio between $\langle \lambda_{\text{max}}^\mathcal{O} | G_\mathcal{O}^a | \lambda_{\text{max}}^\mathcal{O} \rangle$ and $\langle \lambda_{\text{max}} | G^a | \lambda_{\text{max}} \rangle$ is equal to $\exp(ia\theta)$ ($a = \pm 1, 0$) for the three kinds of crackions. If there are a few diluted crackions between i and j , the above result can be extended to

$$\lim_{|j-i| \rightarrow \infty} \left\langle (A_i^z)^\dagger \prod_{k=i}^{j-1} e^{i\theta S_k^z} A_j^z \right\rangle_{\text{cr}} = \mathcal{O}_A^z(\theta) \exp\left(i\theta \sum_{k=i}^j a_k\right), \quad (20)$$

where the phase factor $\exp(i\theta \sum_{k=i}^j a_k)$ counts the total number of crackions between i and j .

For the $S = 1$ VBS state, we have $\theta = \pi$ and the SOP alternates its sign according to the parity of $\sum_{k=i}^j a_k$, which can be interpreted as a Z_2 topological charge [8]. If we consider the SOP in the x -direction, a crackion with $a = 0$ also flips the sign. In a general spin- S case, the spin-twist angle of the maximized SOP is given by $\theta = 2\pi n/(S+1)$ ($n = 1, \dots, S$). Our optimized SOP suggests that the crackion carries a Z_{S+1} topological charge, in consistent with the hidden $Z_{S+1} \times Z_{S+1}$ symmetry argument.

In summary, we have shown that the hidden order in the VBS states can be characterized by the generalized den Nijs–Rommelse-type SOPs. The maximization of these SOPs automatically leads to spin-twist angles corresponding to Z_{S+1} rotations around z or x axes, suggesting the existence of a hidden $Z_{S+1} \times Z_{S+1}$ symmetry. In the presence of the crackion excitation, the maximized SOPs are shown to exhibit a Z_{S+1} topological charge. Recently, it was shown that the den Nijs–Rommelse SOP is an effective measure of the localizable entanglement in the $S = 1$ VBS state [17]. We believe that our maximized SOPs provide a natural extension of the den Nijs–Rommelse SOP and can be used to explore multipartite entanglement properties of arbitrary VBS states.

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