Novel Order Parameter to Characterize Valence-Bond-Solid States

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We propose an order parameter to characterize valence-bond-solid (VBS) states in quantum spin chains, given by the ground-state expectation value of a unitary operator appearing in the Lieb-Schultz-Mattis argument. We show that the order parameter changes the sign according to the configuration of the valence bonds. This allows us to determine the phase transition point in between different VBS states accurately. We demonstrate this theory in the bond-alternating Heisenberg chain and in the frustrated spin ladder.

\section{Introduction}

To study Haldane’s conjecture\cite{Haldane}, Affleck, Kennedy, Lieb and Tasaki proposed the valence-bond-solid (VBS) state, and showed that the ground state of the spin $S = 1$ Heisenberg chain is described approximately by the VBS state\cite{AKLT}. Since the spin configurations of the VBS state show the hidden antiferromagnetic order, den Nijs and Rommelse proposed the string order parameter (SOP) to characterize the $S = 1$ Haldane phase\cite{DenNijs},

\begin{equation}
\mathcal{O}_\text{string}^\alpha = -\lim_{|k-l| \to \infty} \langle \Psi_0 | S_k^\alpha \exp \left[ i \pi \sum_{j=k+1}^{l-1} S_j^\alpha \right] S_l^\alpha | \Psi_0 \rangle,
\end{equation}

where $\alpha = x, y, z$ and $| \Psi_0 \rangle$ means the ground state. Thus this order parameter enables us to detect the VBS state indirectly. The SOP was generalized to $S > 1$ cases by Oshikawa\cite{Oshikawa}.

On the other hand, Affleck and Lieb studied the Haldane’s conjecture by the Lieb-Schultz-Mattis (LSM) type argument\cite{AffleckLieb}. However, relation between the LSM argument and the VBS picture including the SOP has not been fully understood. In this paper, we show that the ground-state expectation value of a unitary operator appearing in the LSM argument, for a spin chain with length $L$,

\begin{equation}
z_L = \langle \Psi_0 | \exp \left[ \frac{2\pi}{L} \sum_{j=1}^{L} j S_j^z \right] | \Psi_0 \rangle,
\end{equation}

plays a role of an order parameter which detects VBS ground states directly, and that it can be applied to determination of phase boundaries in between different VBS states. We demonstrate this idea in the bond-alternating Heisenberg spin chains, and in the $S = 1/2$ two-leg frustrated ladder.
§2. Properties of the Order Parameter

2.1. The valence-bond-solid picture

According to the LSM argument, if the unique ground state $|\Psi_0\rangle$ and $U|\Psi_0\rangle$ with $U \equiv \exp{[2\pi i / L \sum_{j=1}^{L} J S_j^z]}$ are orthogonal ($z_L = 0$), there exists at least one eigenstate with energy of $O(L^{-1})$. Now we consider the overlap $z_L$ in the opposite situations such as the Haldane gap phase. In order to calculate $z_L$ explicitly in VBS states, we introduce the Schwinger boson representation for the spin operators:

$$S_j^+ = a_j^\dagger b_j, \quad S_j^- = b_j^\dagger a_j, \quad S_j^z = \frac{1}{2}(a_j^\dagger a_j - b_j^\dagger b_j), \quad S_j = \frac{1}{2}(a_j^\dagger a_j + b_j^\dagger b_j), \quad (2.1)$$

where these bosons satisfy the commutation relation $[a_i, a_j^\dagger] = [b_i, b_j^\dagger] = \delta_{ij}$ with all the other commutations vanishing. $a_j^\dagger$ ($b_j^\dagger$) increases the number of up (down) $S = 1/2$ variables under symmetrization. Then, a generalized VBS state in a periodic system is written as

$$|\Psi^{(m,n)}_{\text{VBS}}\rangle \equiv \frac{1}{\sqrt{\mathcal{N}}} \prod_{k=1}^{L/2} (B_{2k-1,2k}^\dagger)^m (B_{2k,2k+1}^\dagger)^n |\text{vac}\rangle, \quad (2.2)$$

where $B_{i,j}^\dagger \equiv a_i^\dagger b_j^\dagger - b_j^\dagger a_i^\dagger$, $\mathcal{N}$ is a normalization factor, and $|\text{vac}\rangle$ is the vacuum with respect to bosons. $m$ and $n$ are integers satisfying $m + n = 2S$. Using relations

$$U a_j^\dagger U^{-1} = a_j^\dagger e^{i\pi j / L} \quad \text{and} \quad U b_j^\dagger U^{-1} = b_j^\dagger e^{-i\pi j / L}, \quad (2.3)$$

a twisted valence bond $UB_{j,j+1}^\dagger U^{-1}$ for $1 \leq j \leq L - 1$, and that located at the boundary are calculated as follows,

$$UB_{j,j+1}^\dagger U^{-1} = e^{-i\pi / L} a_j^\dagger b_{j+1}^\dagger - e^{i\pi / L} b_j^\dagger a_{j+1}^\dagger, \quad (2.4)$$

In the latter case, a negative sign appears for each valence bond. Thus the asymptotic form of $z_L$ is given by

$$z_L = \langle \Psi^{(m,n)}_{\text{VBS}} | U | \Psi^{(m,n)}_{\text{VBS}} \rangle = (-1)^n [1 - O(1/L)]. \quad (2.5)$$

It turns out that $z_L$ changes its sign according to the number of valence bonds at the boundary. $z_L$ can be calculated in more detail by the matrix product formalism.

2.2. The sine-Gordon theory

Next, we consider $z_L$ from the viewpoint of a low energy effective theory. In general, the Lagrangian density of a spin chain is given by the sine-Gordon model,

$$\mathcal{L} = \frac{1}{2\pi K} \left[ \nabla \phi(x, \tau) \right]^2 - \frac{y_\phi}{2\pi \alpha^2} \cos \left[ \sqrt{2} \phi(x, \tau) \right], \quad (2.6)$$

where $\tau$ is the imaginary time, $\alpha$ is a short range cut off, and $K$ and $y_\phi$ are the parameters determined phenomenologically. In the gapped (gapless) region one has $y_\phi(l) \to \pm \infty$ ($y_\phi(l) \to 0$) for $l \to \infty$ under renormalization $\alpha \to e^l \alpha$. On the unstable
Gaussian fixed line \([y_\delta(0) = 0 \text{ with } K(0) < 4]\), a second-order “Gaussian transition” takes place between the two gapped states. In this formalism, the spin wave excitation created by \(U\) corresponds to the vertex operator \(\exp(i\sqrt{2}\phi)\), so that \(z_L\) is related to the ground-state expectation value of the nonlinear term as \(z_L \propto \langle \cos(\sqrt{2}\phi) \rangle\) and the three fixed points \(y_\delta = \pm \infty, 0\) correspond to \(z_\infty = \mp 1, 0\), respectively. Thus the Gaussian critical point can be identified by observing \(z_L = 0\).

§3. Application to Physical Systems

3.1. The bond-alternating Heisenberg chain

In the bond-alternating Heisenberg chain,

\[
\mathcal{H} = \sum_{j=1}^{L} \left[1 - \delta(-1)^j\right] S_j \cdot S_{j+1},
\]  

(3.1)

the VBS picture is considered to be realized approximately: The configuration of the valence bonds \((m,n)\) changes from \((0,2S)\) to \((2S,0)\) successively as \(\delta\) is increased from \(-1\) to \(1\), meaning the existence of \(2S\) quantum phase transitions. We calculate \(z_L\) for \(2S = 1, 2, 3, 4\) in a periodic system by the quantum Monte Carlo (QMC) method with the continuous-time loop algorithm, and confirmed that qualitative behavior of \(z_L\) agrees with our theory given in Sec. 2.

Next, we determine the successive dimerization transition points by observing \(z_L = 0\) with \(L\) up to 320. Extrapolation of the data has been done by the function \(\delta_c(L) = \delta_c(\infty) + A/L^2 + B/L^4 + C/L^6\). For \(S = \{1, 1\}, \{2, 0\}, S = 3/2, \{2, 1\}, \{3, 0\}\) and \(S = 2 \{2, 2\}, \{3, 1\}, \{4, 0\}\) cases, we obtain the transition points \(\delta_c = 0.25997(3), 0.43131(7), 0.1866(7), 0.5500(1)\), respectively, where ( ) denotes \(2\sigma\). The results are consistent with the previous estimates, but much more accurate: \(\delta_c = 0.2595(5)\) for the \(S = 1\) case by the QMC calculation for the susceptibility, and \(\delta_c = 0.2598, 0.4315, 0.1830, 0.5505\) obtained by the level-crossing method.

3.2. The spin-1/2 frustrated ladder

We discuss \(z_L\) in the \(S = 1/2\) two-leg ladder with frustration:

\[
\mathcal{H} = \sum_{j=1}^{L} [S_j \cdot S_{j+1} + T_j \cdot T_{j+1} + J_\perp S_j \cdot T_j + J_x(S_j \cdot T_{j+1} + T_j \cdot S_{j+1})],
\]  

(3.2)

where \(S_j\) and \(T_j\) denote \(S = 1/2\) operators at \(j\)-th site. In has been pointed out that there appears competition between a rung dimer phase \((J_x \ll J_\perp)\) and a Haldane phase \((J_\perp \ll J_x \leq 1)\), and that these two phases are identified by two distinct SOPs, \(O_{\text{odd}}, O_{\text{even}}\) given by Eq.(1.7), where \(S_j^\alpha\) is replaced by the following two types of composite spin operators:

\[
\tilde{S}_{\text{odd},j}^\alpha \equiv S_j^\alpha + T_j^\alpha, \quad \tilde{S}_{\text{even},j}^\alpha \equiv S_j^\alpha + T_{j+1}^\alpha.
\]  

(3.3)

Then, \(O_{\text{odd}} = 0\) and \(O_{\text{even}} \neq 0\) for the rung dimer phase, and \(O_{\text{odd}} \neq 0\) and \(O_{\text{even}} = 0\) for the Haldane phase. Instead of \(O_{\text{odd}}\) and \(O_{\text{even}}\), we introduce \(z_{\text{odd}}\) and \(z_{\text{even}}\) defined.
by Eq. (1.2) where $S_j^z$ is replaced by $\tilde{S}_{odd,j}^z$ and $\tilde{S}_{even,j}^z$. In Fig. 1, we show $z_{odd}$ and $z_{even}$ for $J_\perp = 1$ and $L = 14$ calculated by the exact diagonalization. We find that $|z_{odd}| \neq |z_{even}|$ in general, and $z_{odd}$ and $z_{even}$ have opposite signs. Especially, $z_{odd} = z_{even} = 0$ at the same point which corresponds to the dimer-Haldane phase boundary. This tells us that one of the two $z_L$ has enough information to describe this system, since $z_L$ characterizes the system by its magnitude and sign, while the SOPs give zero or finite value without changing the sign. Thus $z_L$ turns out to be a more rational order parameter to describe VBS states in a unified way. The properties of $z_L$ is also useful to determine the accurate phase boundary from numerical data of finite-size clusters.

§4. Summary

We have introduced $z_L$ given by Eq. (1.2) as an order parameter to characterize VBS states. The proposed order parameter changes its sign according to the configuration of valence bonds. This property enables us to determine the critical point between different VBS states by observing $z_L = 0$. We have demonstrated this theory for phase transitions in the bond-alternating Heisenberg chain, and in the frustrated spin ladder. Details of the present results will be published elsewhere.\[1]

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