Boundary effects to the entanglement entropy and two-site entanglement of the spin-1 valence-bond solid

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We investigate the von Neumann entropy of a block of subsystem for the valence-bond solid (VBS) state with general open boundary conditions. We show that the effect of the boundary on the von Neumann entropy decays exponentially fast in the distance between the subsystem considered and the boundary sites. Further, we show that as the size of the subsystem increases, its von Neumann entropy exponentially approaches the summation of the von Neumann entropies of the two ends, the exponent being related to the size. In contrast to critical systems, where boundary effects to the von Neumann entropy decay slowly, the boundary effects in a VBS, a non-critical system, decay very quickly. We also study the entanglement between two spins. Curiously, while the boundary operators decrease the von Neumann entropy of L spins, they increase the entanglement between two spins.

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I. INTRODUCTION

Recently much research has been undertaken to understand the subtle interplay between quantum entanglement and quantum criticality for spin systems[1,2,3,4,5,6,7,8,9]. Vidal et al. [4] showed that the entanglement between a block of contiguous spins and its complement in the ground state of the Ising model shows different behaviours for the gapped and gapless cases (critical and non-critical). The entanglement of the VBS ground state of the much-studied Affleck–Kennedy–Lieb–Tasaki (AKLT) model [10,11,12] is considered in Refs. 6, 7, and very recently Campos Venuti et al. studied this state’s long-distance entanglement property 8. The entanglement of the fermionic system was studied in Refs. [13,14].

While much theoretical work in this area has focused on periodic boundary conditions, the open boundary condition has also attracted recent attention [13,15]. Laflamme et al. [15] numerically studied the boundary effects in the critical scaling of entanglement entropy (von Neumann entropy of a block of spins) for the (gapless) 1D XXZ model, and found the entanglement entropy slowly decays away from the boundary with a power-law. This result can be interpreted as stating that in critical systems, the boundary effects to the entanglement entropy is quasi-long-ranged; i.e. there is a quasi-long-ranged entanglement between the boundaries and the subsystem in question. This agrees with the fact that entanglement entropy increases logarithmically with the size of the subsystem in critical systems [4,17]. By contrast, the entanglement entropy for non-critical systems saturates to a constant bound when the subsystem size is increased, implying that the entanglement in the bulk is short-ranged. It is this localised nature of the entanglement entropy around the block edges which gives rise to an area law [17,18] and makes ground states of gapped 1D systems particularly amenable to simulation through matrix product states (MPS) [19,20].

One might expect that boundary effects to the entanglement entropy also have different behaviours for critical and non-critical systems, and an interesting question then is whether the boundary effects to the entanglement entropy are short- or long-ranged, and what the exact behaviour of these are. This is one of the main motivations of this work: here we study the entanglement entropy of a VBS with general open boundary conditions. We will show that, in contrast with the critical XXZ chain, the boundary effect to the entanglement entropy in the VBS state is short-ranged. We will also show that the saturated bound for this state is the sum of von Neumann entropy of the two boundaries. Furthermore, it is not a constant (as is the case for a fixed boundary condition); it varies for different boundary conditions. This saturated bound in 1D state corresponds to the area law for higher-dimensional systems.

This model was originally studied by Affleck et al. in the context of the Haldane conjecture [11,12]. It has also been the focus of much renewed interest since its generalisation to MPS—which have been shown to efficiently simulate many 1D systems [19,20] and may be used as a variational set in density matrix renormalisation group (DMRG) calculations—[21,22] and the discovery that its analogue in 2D is a resource for universal quantum computation [23]. We hope that studying the boundary effect on the entanglement entropy will give some further insight into this model. Since the boundary effects to the block entanglement entropy decays fast, we expect the the DMRG method can be applied efficiently to this model.
II. DEFINITION OF THE VBS STATE

The spin-1 VBS state with general open boundary conditions (GOBC) [24] takes the form:

\[
|\text{VBS}⟩ = Q^p_L \prod_{k=-N_l+1}^{L+N_r-1} (a_k^+ b_{k+1}^+ - b_k^+ a_{k+1}^+) |\text{vac}⟩ \tag{1}
\]

where \( a_k^+, b_k^+ \) are bosonic operators, \( Q^p_L \) and \( Q^p_r \) are respectively the left and right boundary operators; \( p, q = \pm \) with \( Q^+_L = a_{L+N_r}^+, Q^-_L = b_{L+N_r}^+, Q^+_r = a_{L+N_r}^+ \) and \( Q^-_r = b_{L+N_r}^+ \); \( |\text{vac}⟩ \) is the vacuum state; and \( N_l, N_r \) are integer numbers. Since the left and right boundary operators are mutually independent, there are altogether four different VBS states with GOBC. Note that all sites in the spin chain including the left and right boundary sites \(-N_l + 1, L + N_r\) are spin-1’s. Thus this VBS state \( |\text{VBS}⟩ \) is different from that studied in Ref. [7].

We should also note one boundary operator, for example, \( Q^+_L \) changes the boundary state \( a_{L+N_r}^+ |\text{vac}⟩ \) and \( b_{L+N_r}^+ |\text{vac}⟩ \). In fact, the state \( |\text{VBS}⟩ \) is the ground state of the Hamiltonian studied by Affleck et al. [10],

\[
H = \sum_{j=-N_l+1}^{L+N_r-1} \left[ (S_j \cdot S_{j+1}) + \frac{1}{3} (S_j \cdot S_{j+1})^2 \right]. \tag{2}
\]

III. DIVIDING THE CHAIN

For convenience in later calculations, we divide this 1D state into three parts: the left-hand, central, and right-hand parts. The left-hand part is defined as \( |\text{left}, p⟩ \) \( = Q^p_L \prod_{k=-N_l+1}^{0} (a_k^+ b_{k+1}^+ - b_k^+ a_{k+1}^+) |\text{vac}⟩ \). Similarly, the right-hand part is defined as \( |\text{right}, q⟩ \) \( = \prod_{k=L+1}^{L+N_r-1} (a_k^+ b_{k+1}^+ - b_k^+ a_{k+1}^+) Q^p_r |\text{vac}⟩ \). Finally, the central part is written \( |\text{central}⟩ \) \( = \prod_{k=1}^{L-N_l} (a_k^+ b_{k+1}^+ - b_k^+ a_{k+1}^+) |\text{vac}⟩ \).

Note that site 1 appears in both the left and central parts, and acts as two spin-1/2’s; site \( L \) similarly appears in both the central and right parts. Thus the whole VBS state with GOBC now takes the form \(|\text{VBS}; p, q⟩ = |\text{left}, p⟩|\text{central}⟩|\text{right}, q⟩\). We should note that this is not strictly a product state, but that this decomposition is valid for our purposes.

Double-counting is avoided since each bulk spin consists of two spin-1/2’s and the two bosonic operators (spin-1/2’s) in one site constitute a spin-1 state by Fock space representation. For example, terms \( (a_0^+ b_1^+ - b_0^+ a_1^+) |\text{vac}⟩ \) and \( (a_0^+ b_2^+ - b_0^+ a_2^+) |\text{vac}⟩ \) belong to left and central parts, respectively, however, by Fock space representation, the product state will create at site 1 the state \( (a_0^+)^2 |\text{vac}⟩, (b_1^+)^2 |\text{vac}⟩ \) and \( a_0^+ b_2^+ |\text{vac}⟩ \). Thus the three parts are connected to constitute the original state \( |\text{VBS}⟩ \).

Our aim is to now study the von Neumann entropy of the reduced density operator of the contiguous spins from site 1 to \( L \) of the state \(|\text{VBS}; p, q⟩\). For this aim, according to the theory of entanglement, the left- and right part states \(|\text{left}, p⟩\) and \(|\text{right}, q⟩\) can be replaced by two bipartite states, through the Schmidt decomposition.

Without loss of generality, we start from the left part and consider the entanglement of the quantum state \(|\text{left}, p⟩\) between site 1 and the rest; i.e. we consider it a bipartite state with site 1 as one particle and the rest as another particle. According to the Schmidt decomposition, we can first calculate eigenvalues of the reduced density operator of site 1 for state \(|\text{left}, p⟩\).

\[
\text{Denote } |\Psi^−⟩_{\text{left}, p} = (a_0^+ b_1^+ - b_0^+ a_1^+) |\text{vac}⟩, \text{we know } |\Psi^−⟩_{\text{left}, p} = \frac{1}{\sqrt{3}} \sum_{\alpha=1}^{3} |\alpha⟩ |I ∩ σ_α⟩ |\Psi^−⟩_{\text{left}, p}, \text{where } \{σ_α\}_{n=0}^2 = \text{the Pauli group, and we have defined the states } |\alpha⟩ = I ∩ σ_α |\Psi^−⟩. \text{Here } σ_1 = a_0^+ b_1 + a_1 b_0^+, \text{ σ}_2 = -ia_0^+ b_1 + ia_1 b_0^+, \text{ σ}_3 = a_0^+ a_1 - b_0^+ b_1 \text{ and } σ_0 = a_0^+ a_1 + b_0^+ b_1, \text{ the identity. By this result, the state of the left part may be written}
\]

\[
|\text{left}, p⟩ |\text{central}⟩ |\text{right}, q⟩ = \frac{1}{3(N_l-1)/2} \sum_{\alpha_0, ..., α_\text{left}, p} |\alpha⟩ \otimes \cdots \otimes |\alpha_0⟩ \otimes Q^p_L \otimes σ_0 \cdots σ_{N_l+2} |\Psi^−⟩_{\text{left}, p}. \tag{3}
\]

It is now possible to calculate the site 1 reduced density operator. Using the identity \( \sum_{\alpha=1}^{3} (I ∩ σ_α) |\Psi^−⟩ |\Psi^−⟩ (I ∩ σ_α) = I - |\Psi^−⟩⟨\Psi^−| \) (where \( I \) on the l.h.s. and r.h.s. is the identity in \( \mathbb{C}^2 \) and \( \mathbb{C}^2 \otimes \mathbb{C}^2 \), respectively) we find \( \rho_1 = \text{Tr}_L (Q^p_L \otimes I) \frac{1}{4} (1 - f_1) I + f_1 |\Psi^−⟩⟨\Psi^−| (Q^p_L \otimes I) I \), \( f_1 = (1 - 1/N_l)^{-1/3}, \) and the trace is over the first Hilbert space. Now we find that the matrix form of the reduced density operator of site 1 takes a diagonal form \( \rho_1 = \text{diag} (ξ^0_1, ξ^−_1), \) where we have defined \( ξ^±_1 = (3 ± f_1) / 3 \) and \( f_1 = (1 - 1/N_l)^{-1/3} \). For different boundary operators \( Q^p_L \), state \( ρ_1 \) is invariant under a basis transformation. By entanglement theory, we can replace the quantum state of left part by a real bipartite state \(|\phi_1⟩ \equiv \sqrt{ξ^+} a_0^+ b_1^+ - \sqrt{ξ^-} b_0^+ a_1^+⟩ |\text{vac}⟩.\)
We find that the reduced density operator $\rho_l$ converges to the identity exponentially fast with respect to $N_l$, and thus we can simply consider $|\phi_r\rangle$ as a singlet state $|\Psi_{01}\rangle$ when $N_l \to \infty$. Similarly for right part of the state, we have $|\phi_r\rangle \equiv \left(\sqrt{\xi_r^{a_L b_{L+1}^\dagger}} a_{L+1}^\dagger - \sqrt{\xi_r} b_{L+1}^\dagger a_L^\dagger\right) |\text{vac}\rangle$, where the $\xi_r^\pm$ have a similar definition to the $\xi_l^\pm$. Thus the VBS state in Eq. (1) may be rewritten

$$|\text{VBS}\rangle = |\phi_l\rangle \prod_{k=1}^{L-1} (a_k^b b_{k+1}^a - b_k^a a_{k+1}^b) |\phi_r\rangle |\text{vac}\rangle,$$  \hspace{1cm} (5)

where indices $p, q$ are suppressed since they do not change the result. The validity of the transformation from $\Psi^{l}$ to $\Psi^{r}$ in studying the von Neumann entropy of contiguous $L$ spins can also be checked by a method with matrix product state representation introduced in, for example, Ref. [22]. A numerical calculation for small $L$ confirms our result.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig2.png}
\caption{The quantum state of left part is considered as a bipartite state with one particle in site 1 and the rest as another particle. According to the Schmidt decomposition this state is equal to a bipartite state $|\phi_l\rangle$, and each spin is spin-1/2 at site 0 and 1; Finally, the VBS state with GOBC is mapped to a state with $L + 2$ sites with two spin-1/2 boundaries at ends 0 and $L+1$.}
\end{figure}

Expanding this, we find the following form for the density matrix:

$$\hat{\rho}_L = \left( \frac{1-p}{4} (\xi_l^+ \xi_r^-)^2 \begin{array}{cccc}
1+4(\xi_l^+ \xi_r^-)^2 & 0 & -2(\xi_l^+ \xi_r^-)^2 & 0 \\
0 & 1+4(\xi_l^+ \xi_r^-)^2 & -2(\xi_l^+ \xi_r^-)^2 & 0 \\
-2(\xi_l^+ \xi_r^-)^2 & -2(\xi_l^+ \xi_r^-)^2 & 1+4(\xi_l^+ \xi_r^-)^2 & 0 \\
0 & 0 & 0 & 1+4(\xi_l^+ \xi_r^-)^2 
\end{array} \right).$$

When $p$ is small the eigenvalues of the matrix $\hat{\rho}_L$ can be found by a Taylor expansion to be $\lambda_1 = \xi_l^+ \xi_r^- (1-p)$; $\lambda_2 = \xi_l^+ \xi_r^- (1-p)$; $\lambda_3 = \xi_l^+ \xi_r^- (1+p) + O(p^2)$; $\lambda_4 = \xi_l^+ \xi_r^- (1+p) + O(p^2)$. Recall that $|\phi_l\rangle$ is a pure state, so the reduced density operators at sites 0 and 1 are the same under unitary transformation (i.e., $\rho_0 = \rho_1$); similarly for state $|\phi_r\rangle$. By checking the eigenvalues of $\hat{\rho}_L$, we find that $\hat{\rho}_L = \rho_0 \otimes \rho_{L+1} + O(p)$, where the equation is true under a unitary transformation. This transformation has no effect on the von Neumann entropy, and thus we suppress it. The density operator of $\hat{\rho}_L$ converges exponentially fast to the tensor product of two ends; the speed is $p = (-1/3)^L$.

\section{IV. BLOCK ENTROPY}

Finally we calculate explicitly the von Neumann entropy of a block of $L$ spins,

$$S(\hat{\rho}_L) = S(\rho_0) + S(\rho_{L+1}) + O(p).$$  \hspace{1cm} (8)

In the case that $N_l \to \infty$, $N_r \to \infty$ the state takes the form $|\text{VBS}\rangle = \prod_{k=0}^{L} (a_k^b b_{k+1}^a - b_k^a a_{k+1}^b) |\text{vac}\rangle$. The entanglement entropy of this state has been studied previously \cite{3}; it was found that there are no boundary effects. In this paper, one of our main concerns is to show that the VBS state $|\Psi\rangle$ does have a boundary effect. Already we know that if the block of $L$ contiguous spins in Eq. (1) is far from the two boundary sites the boundary effect will decay very rapidly (exponentially). We now present explicitly the entanglement entropy of these $L$ spins. Let us first rewrite the left part state in the form $|\phi_l\rangle = (V_L \otimes I) |\Psi^{\text{r}}\rangle_{01}$, where the matrix form of $V_L$ takes the form $V_l = \text{diag}(\xi_l^+, \xi_l^-)$. Note that $V_l$ is not necessarily unitary. In a similar manner for right part state, $V_r$ can also be defined $V_r = \text{diag}(\xi_r^+, \xi_r^-)$, giving $|\phi_r\rangle = (I \otimes V_r) |\Psi^{\text{r}}\rangle_{L,L+1}$. We can then write the VBS with GOBC in the form:

$$|\text{VBS}\rangle = (V_L \otimes V_r) \sum_{\alpha_L} |\alpha_1\rangle \otimes \cdots \otimes |\alpha_L\rangle \times (\sigma_{\alpha_1} \cdots \sigma_{\alpha_L} \otimes I) |\Psi^{\text{r}}\rangle_{0,L+1},$$

where the summation is from 1 to 3 for indices $\alpha_1, \cdots, \alpha_L$. According to entanglement theory, the von Neumann entropy of the reduced density operator of $L$ spins is the same as the von Neumann entropy of the two ends (sites 0 and $L + 1$). The reduced density operator of these sites takes the form

$$\hat{\rho}_L = (V_L \otimes V_r) \left( \frac{1-p}{4} I + p |\Psi^{\text{r}}\rangle \langle \Psi^{\text{r}}| \right) (V_L \otimes V_r)^\dagger$$

where $p = (-1/3)^L$.
NOTE THAT WHEN p IS COMPARABLE WITH f_l AND f_r, THEN O(p) MAY HAVE CONTRIBUTIONS FOR BOTH f_l AND f_r. CONSIDERING ALL OF THESE POINTS, WE CONCLUDE THAT BOUNDARY EFFECTS DECAY EXPONENTIALLY WHEN THE DISTANCES BETWEEN THE SUBSYSTEM AND THE BOUNDARIES INCREASE. IN THE CASE THAT THERE ARE NO BOUNDARY OPERATORS, THE TRACE IN EQ. (4) IS OVER THE IDENTITY, AND ρ_l REDUCES TO I. HENCE THE BOUNDARY EFFECTS TO THE ENTANGLEMENT ENTROPY NEVER ARISE; THIS IS THE CASE PREVIOUSLY STUDIED [7]. WE REMARK FOR 1D VBS WITH GOBC, THE TERMS CORRESPONDING TO THE TOPOLOGICAL ENTANGLEMENT BETWEEN THE CONSIDERED TWO SPINS. THE CASES VARIES FROM 1 TO 9 FOR R = 1/9, AND Q_r AND Q_r⁺, RESPECTIVELY.

IN ORDER TO QUANTIFY THE TWO-SPIN ENTANGLEMENT IN THIS CASE, WE SHALL USE NEGATIVITY, N [27]. WE FIND THAT THERE IS NO ENTANGLEMENT FOR NON-NEXT-NEIGHBOURING SPINS (REGARDLESS OF BOUNDARY). THE NEAREST-NEIGHBOUR NEGATIVITY FOR A RANGE OF N_l, N_r IS PRESENTED IN TABLE I, WHERE A FACTOR 1/9 IS OMITTED.

CURIOUSLY, WE SEE THAT BOUNDARY OPERATORS DECREASE THE BLOCK VON NEUMANN ENTROPY—SEE EQ. (5)—THEY INCREASE THE NEAREST-NEIGHBOUR NEGATIVITY. ROUGHLY, THIS CAN BE UNDERSTOOD THAT THE ENTANGLEMENT IS MONOGAMOUS [29, 30], I.E., IT CANNOT BE SHARED FREELY BY MANY PARTIES. A SIMPLE EXAMPLE ABOUT THE MONOGAMY OF ENTANGLEMENT IS THAT, SUPPOSE A, B AND C ARE THREE PARTIES, IF A AND B ARE MAXIMALLY ENTANGLED, A AND C WILL NOT BE SEPARABLE. THE RESULT IN THIS PAPER SHOWS THAT THE BOUNDARY OPERATORS HAVE EFFECT ON THE ENTANGLEMENT SHARING IN THIS MANY-BODY SYSTEM.

IN THE TABLE ABOVE, WE SEE THAT FOR FINITE N_l, IT IS ALWAYS THE CASE THAT N_r > 1/9. ASYMMETRIC BOUNDARY OPERATORS MAY ALSO INCREASE THE ENTANGLEMENT. FOR EXAMPLE, N_r = 1.45919/9 FOR N_l = N_r = 1, BUT N_r = 1.50111/9 FOR N_l = 1, N_r = 2. NOW N_r DOES NOT VARY MONOTONICALLY WITH N_l; e.g., when N_r VARIES FROM 1 TO 1 (FOR N_l = 1), N_r OSCILLATES. THIS SEEMINGLY NEW RESULT MAY POTENTIALLY BE USEFUL: NEAREST-NEIGHBOUR ENTANGLEMENT MAY BE CONTROLLED BY TWEAKING BOUNDARIES.

THE DRAWBACK OF THE NEGATIVITY IS THAT THE BLOCK ENTANGLEMENT CANNOT BE DETECTED AND QUANTIFIED. A COMPLEMENTARY QUANTITY DERIVED FROM THE REALIGNMENT SEPARABILITY CRITERION CAN PARTIALLY SOLVE THIS PROBLEM [28].
For a two-site density operator $\rho$, this quantity is defined as $\mathcal{R} = (||R(\rho)|| - 1)/2$, where the matrix $R(\rho)$ is obtained from the density operator $\rho$ by the realignment method, and $|| \cdot ||$ is the trace norm. The larger of the quantities $\mathcal{N}$ and $\mathcal{R}$ gives a lower bound of the concurrence $\mathcal{C}$ for a mixed state in arbitrary dimensional systems; i.e. $\mathcal{C} \geq \max\{\mathcal{N}, \mathcal{R}\}$. 

Using this measure, we still find zero entanglement between detected for non-nearest neighbouring spins regardless of boundary. The entanglement of nearest-neighbouring spins by realignment is presented in Table II and a factor 1/9 is also omitted. We also still find that the boundary operators increase entanglement $\mathcal{R}$, and indeed no entanglement is found for the case without boundary operators: this is due to the limitation of the realignment method. Finally let us remark that for the model studied in this paper, the negativity provides a stronger lower bound for the concurrence. Since the concurrence for a general mixed state in $\mathbb{C}^3 \otimes \mathbb{C}^3$ is difficult to find, the entanglement measures by negativity and realignment are widely accepted.

VII. CONCLUSION

In summary, we studied the boundary effects to the entanglement entropy and the two-site entanglement for the spin-1 VBS state which is the ground state for a gapped model. We showed that the boundary effects are short-ranged, i.e. they decay exponentially in the distance between the subsystem considered and the boundary sites. This is different from the case of XXZ chain which is a gapless model. The two-site entanglement was studied by two entanglement measures, the negativity and the realignment method. For the VBS state, we find the boundary operators decrease the block von Neumann entropy but increase the nearest-neighbour entanglement measured by negativity and realignment.

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