Valence-Bond-Solid state entanglement in a 2-D Cayley tree

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The Valence-Bond-Solid (VBS) states are in general ground states for certain gapped models. We consider the entanglement of VBS states on a two-dimensional Cayley tree. We show that the entropy of the reduced density operator does not depend on the whole size of the Cayley tree. We also show that asymptotically, the entropy is linearly proportional to the number of singlet states cut by the reduced density operator of the VBS state.

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The entanglement of quantum states, and in particular of the ground states, related with spin systems has been attracting a great deal of interest, see for example 123456789101112131415161718. We can quantify the entanglement by the von Neumann entropy of the reduced density operator of the ground states. This quantity for discrete spin chain and lattice models is analogous to the geometric entropy in the continuous field theory 192021. The geometric entropy plays an important role in the quantum field theory and is considered to be related to the Bekenstein-Hawking black hole entropy 22. It has been suggested 1920 that the geometric entropy is proportional to size of the boundary of the block. This problem has been recently studied for discrete case in the real free Klein-Gordon fields 10, and again, the entropy has been found to be related to the surface area of the fields.

The entanglement of a block of contiguous spins has been obtained for various one-dimensional spin chains. The higher-dimensional spin-chain case is in general more complicated, and only recently the entropy of the reduced density operator of ground states for higher-dimensional systems was studied in 1011121314. For discrete 2-D cases, the entropy is found to be linearly proportional to the boundary size of the reduced density operator in the lattice 1011. The fermion case is also studied in 1213. In this Letter, we consider the entropy of a 2-D Valence-Bond Solid (VBS) state on a Cayley tree, which is the ground state of the Affleck-Kennedy-Lieb-Tasaki (AKLT) model 2324. The AKLT model is a gapped model 25 and has been well-studied in condensed matter physics. Certain entanglement properties of the ground state of the AKLT model were already studied 14161718. But the entropy of a block of spins in a 2-D Cayley tree case is not available. There are several reasons that make this quantity of interest to the condensed matter community. First, the entropy quantifies the entanglement between the spins in the reduced density operator with the rest of the ground state. This is important for quantum computation and quantum information, and VBS states for quantum computation are presented in Ref. 26. Secondly, it is interesting to know whether this quantity is related to some macroscopic properties, such as susceptibility as pointed out in Ref. 27. Third, it is generally expected that the entanglement inherent in a system is possibly responsible for the phenomena of quantum phase-transitions 1. Since the AKLT model is a well studied model in condensed matter physics, it is interesting to uncover relationships between the entropy of a block of spins in the ground state and other measurable physical quantities, such as the correlation functions. Finally, the entanglement properties can indicate whether the density matrix renormalization method 28 can be used to efficiently simulate the quantum many-body systems 2930.

The Hamiltonian of the AKLT model is written as 22

\[ H = \sum_{(i,j)} P \bar{S}_i \cdot \bar{S}_j \]  \tag{1}

where \( \bar{S}_i \) is the spin operator on lattice site \( i \), \( P(\bar{S}) \) is the orthogonal projection, and \( (i,j) \) are unordered pairs in the lattice. The ground states of the AKLT model are known as VBS states, which are constructed from the singlet state \( |\Psi^-\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \). For convenience sake, we replace the singlet state by \( |\Psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \). This substitution does not change any properties of the entanglement of the VBS state in this paper.

Let’s consider a \( C_4 \) Cayley tree as in Ref. 23 and as showed in the Figure 1. At each site, three singlet states are connected to it. Each dot represents a spin-\( \frac{1}{2} \). A symmetrization of the three spin-1/2’s creates a spin-3/2 at each site. First, we only consider one lattice site \( A \), and three spin 1/2’s \( (A_1, A_2, A_3) \) are located at this site. The three singlet states are \( |\Psi\rangle_{A_1 A_2} |\Psi\rangle_{A_2 A_3} |\Psi\rangle_{A_3 A_1} \); see Fig 2.

For the VBS state, we need to consider a symmetrization, \( P_A \), at each lattice site \( A \). We realize the symmetrization operator \( P_A \) as follows:

\[ P_A = \frac{1}{4} (|3\uparrow\rangle\langle3\uparrow| + |2\uparrow\downarrow\rangle\langle2\uparrow\downarrow| + |2\uparrow\downarrow\rangle\langle2\downarrow\uparrow| + |3\downarrow\rangle\langle3\downarrow|) \]  \tag{2}

where state \( |i\uparrow,j\downarrow\rangle \) is a symmetrized state with \( i \) spin up, and \( j \) spin down. For example \( |2\uparrow\downarrow\rangle = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \).
The site is maximally entangled with the rest of the sites. So, we know that for the Cayley tree case, each lattice site is maximally entangled with the rest of the sites.

We consider the entanglement across the quantum state \(|\Psi\rangle\). This is a six-partite state, and we show that each lattice site is maximally entangled with the rest of the sites. The notations \(|3\uparrow\rangle = |4\rangle\), \(|2\uparrow, \downarrow\rangle = |3\rangle\), \(|\uparrow, 2 \downarrow\rangle = |2\rangle\), \(|3 \downarrow\rangle = |1\rangle\).

One site reduced density operator: Let's start from lattice site \(A\), three singlet states are connected by \(|\Psi\rangle\), \(|\Psi\rangle\), \(|\Psi\rangle\). The reason follows from the state in (3) that the state \(|\Psi\rangle\) is a six-partite state, and we can find the following

\[
|\Phi\rangle_{A_{123}B_1C_2D_3} = \frac{1}{2}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle + |\downarrow\downarrow\rangle + |\uparrow\uparrow\rangle),
\]

For convenience, we also use the notations \(|3\uparrow\rangle = |4\rangle\), \(|2\uparrow, \downarrow\rangle = |3\rangle\), \(|\uparrow, 2 \downarrow\rangle = |2\rangle\), \(|3 \downarrow\rangle = |1\rangle\).

One site reduced density operator: Let's start from lattice site \(A\), three singlet states are connected by \(|\Psi\rangle\), \(|\Psi\rangle\), \(|\Psi\rangle\). We can verify that even if we just project the state at lattice site \(A\) to the symmetric subspace, then automatically, the rest of the sites \(B_1, C_2, D_3\). We can verify that even if we just project the state at lattice site \(A\) to the symmetric subspace, then automatically, the rest of the sites \(B_1, C_2, D_3\). We can verify that even if we just project the state at lattice site \(A\) to the symmetric subspace, then automatically, the rest of the sites \(B_1, C_2, D_3\).

The reduced density operator of lattice site \(A\) can be found easily: \(\rho_A = \frac{1}{2}I\), which is the identity operator, \(I\), in \(SU(4)\) with a normalization factor so that the trace is 1. For the Cayley tree case presented in Figure 1, the reduced density operator on each lattice site is the same except for the boundary sites. The von Neumann entropy of the reduced density operator is \(S(\rho_A) = 2\).

We know that for the Cayley tree case, each lattice site is maximally entangled with the rest of the sites, and the entanglement is 2 ebits. This result can be directly extended to other types of Cayley tree cases, and we can show that each lattice site is maximally entangled with the rest of the lattice sites.

The entropy of the reduced density operators does not depend on the whole size of the Cayley tree: Let's study the quantum state \(|\Phi\rangle\). This is a six-partite state, and we consider the entanglement across \(B_1 : A_{123}C_2D_3\) cut. It follows directly from the state in (3) that the state across the cut \(B_1 : A_{123}C_2D_3\) cut is maximally entangled. So, we can treat the quantum state \(|\Psi\rangle_{B_1 : A_{123}C_2D_3}\) in (3) as a singlet state as follows,

\[
|\Psi\rangle_{B_1 : A_{123}C_2D_3} = (|\uparrow\Psi\rangle_{B_1,B_1} + |\downarrow\Psi\rangle_{B_1,B_1})/\sqrt{2},
\]

where we denote

\[
|\Psi\rangle_{B_1} = \frac{1}{\sqrt{2}}|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle + |\downarrow\downarrow\rangle + |\uparrow\uparrow\rangle,
\]

One site reduced density operator: Let's start from lattice site \(A\), three singlet states are connected by \(|\Psi\rangle\), \(|\Psi\rangle\), \(|\Psi\rangle\). For a bipartite pure state \(|\Psi_{AB}\rangle\), we know \(S(\rho_A) = S(\rho_B)\), where

This can also be understood as the following: First, we have a singlet state shared by \(B_1, B_2\). To expand the Cayley tree from \(A_1\) to \(A_{123}\) (i.e., one leg is expanded to two legs), we put two additional singlet states shared by \(A_2, C_2\) and \(A_3, C_3\), and perform the symmetrical projection on site \(A_{123}\). The final result is that we just replace the spin up and spin down in \(A_1\) by \(|\uparrow\rangle\) and \(|\downarrow\rangle\). Similarly, we can further expand the Cayley tree from sites \(C_2\), and \(C_3\). If we only consider the bipartite entanglement of the VBS state on a Cayley tree, the bipartite state \(B_1B_2\) is just a singlet state no matter how many legs are represented by \(B_2\).

In this Letter, we will consider the entropy of reduced density operators of the VBS on a Cayley tree. The reduced density operators are one-site, 4-site,..., \(|\rho_{A_{123}}|_{3\times 2^{1}+1-site}|_{N}\rangle\). In Figure 1, the cuts are shown as dashed circles. The entropy of the reduced density operator is the bipartite entanglement across these cuts, i.e., between the spins in the reduced density operator and the rest.

Based on our observations, we present one of our main conclusions in this Letter: The entropy of reduced density operator \(S(\rho_i)\) does not depend on the whole size of the Cayley tree, where \(i = 1, 4, ..., \sum N 3 \times 2^{i}+1-site\) in size. In Figure 1, the cuts are shown as dashed circles. The entropy of the reduced density operator is the bipartite entanglement across these cuts, i.e., between the spins in the reduced density operator and the rest.

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\( \rho_{A(B)} \) is the reduced density operator. To calculate the entropy of the 4-site reduced density operator, we can calculate the entropy of the reduced density operator of six legs; see Figure 3. First we have the state \( |\Psi_{A,B,C,D}\rangle \) which takes the form \( \otimes \) as in Figure 2. Then we can substitute the spin up and spin down in \( B_1, C_2, D_3 \) by \( |\Psi_1\rangle \) and \( |\Psi_\downarrow\rangle \), and now the corresponding Cayley tree reduces to that shown in Figure 3. After tracing over spin-2/3 sites in \( ABCD \), we obtain the reduced density operator as follows:

\[
\bar{\rho}_4 = \frac{2}{3} I_\otimes^3 + \frac{1}{6} \rho_\uparrow_\otimes^3 + \frac{1}{6} \rho_\downarrow_\otimes^3 + X,
\]

where \( I = \frac{1}{2}(\rho_\uparrow + \rho_\downarrow) = \text{diag}(1/3,1/3,1/3) \), \( \rho_\uparrow = \text{diag}(1/2,1/3,1/6) \), \( \rho_\downarrow = \text{diag}(1/6,1/3,1/2) \), the basis chosen here is \( \{|2\uparrow\rangle, |\uparrow,\downarrow\rangle, |2\downarrow\rangle\} \) which are basis vectors of the symmetrical subspace. Moreover, \( \rho_\alpha(\rho_\downarrow) \) is derived from \( |\Psi_\uparrow\rangle(|\Psi_\downarrow\rangle) \) by taking the trace on the spin 2/3 site,

\[
X = \frac{1}{108} [I \otimes (x \otimes x' + x' \otimes x) + (x \otimes x' + x' \otimes x) \otimes I + x \otimes I \otimes x' + x' \otimes I \otimes x],
\]

where \( x = |2\uparrow\rangle, \uparrow, \downarrow, |\uparrow, \downarrow\rangle, (2 \downarrow\rangle \). Since the entropy of the density operator of \( ABCD \) is equal to six legs connected to it, \( S(\rho_4) = S(\bar{\rho}_4) \), the entropy of the 4-site reduced density operator is

\[
S(\rho_4) = \frac{53}{54} + \frac{13}{4} \log 3 - \frac{65}{108} \log 5 \approx 4.735,
\]

where \( \log \) has the base 2. We can find that \( \rho_4 \) is actually like \( I_\otimes^3 \) which has the entropy \( 3 \log 3 \approx 4.755 \). The difference between these two entropies is less than 0.5%.

In fact, the off-diagonal entries \( X \) in \( \rho_4 \) are small, and \( \frac{1}{2} \sum_{\uparrow, \downarrow} \rho_\alpha_\otimes^3 \) is close to \( I_\otimes^3 \). For simplicity, we can use the fidelity to define the distance between \( \rho_\uparrow_\otimes^3 \) and \( I \).

The fidelity is defined as \( F(\rho_A, \rho_B) = \text{Tr} \sqrt{\sqrt{\rho_A} \rho_B \sqrt{\rho_A}} \). The final result shows that \( \rho_4 \approx I_\otimes^3 \), and thus \( S(\rho_4) \approx 6 \log 3 \). Actually, we find \( S(\rho_4) \approx 9.4891 \approx 6 \log 3(1 - \epsilon), \) and \( \epsilon \) is small and is about 0.22%. The fidelity between the term related with \( \rho_\alpha \) in \( \rho_4 \) with identity is 0.994 which is better than the original 0.977 in \( \rho_4 \) case. The Eqs. (9, 10, 11) and Eq. (9) provide us with an algorithm
to find the general reduced density operators of the VBS state on a Cayley tree.

For the general case, we can expand the Cayley tree and obtain the reduced density operator $\rho_i$ by relations (9,10,11). Suppose $i = \sum_{k=0}^{M} 3 \times 2^k + 1$; then the general form will be as follows:

$$
\rho_i = \frac{2}{3} I^{\otimes 3 \times 2^{M-1}} + \frac{1}{6} \sum_{\alpha = \uparrow, \downarrow} (f(\rho_\alpha , I)) + g(x, I) 
\approx I^{\otimes 3 \times 2^{M-1}}. \tag{12}
$$

The last equation follows from the fact that the second term is more like the identity operator as $i$ becomes large, and the third term remains small and can be omitted. We know that $S(\rho_i) \approx 3 \times 2^{M-1} \log 3 , M \geq 1$. The reduced density operator cuts $N = 3 \times 2^M$ singlet states. And we thus estimate that asymptotically the entropy of VBS in a Cayley tree is linearly proportional to the number of singlet states across the boundary.

We should point out that though this is the first order upper bound. We can also compute higher-order upper bounds. But as expected, we get a lower-bound correction for the general form works for all kinds of reduced density operators on the Cayley tree. The only difference is that the substitutions (9,10) will depend on the form of the reduced density operators in the Cayley tree. We expect that our result that asymptotically, the entropy is linearly proportional to the number of singlet states across the boundary, still holds given that the number of cut singlet states is large. We performed the calculations for a density operator with 16 legs (not a circle) extended from $\rho_{10}$, and we found that the Eq. (12) still holds for this case. Some other forms, with fewer legs, have been also checked and our conjecture holds for all these cases as well.

In fact, we actually provide an algorithm to find the reduced density operators of VBS state on a Cayley tree. It will be interesting to apply this algorithm in the simulations of quantum many-body systems.

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