Entanglement in a Valence-Bond Solid State

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We study entanglement in a valence-bond solid state, which describes the ground state of an Affleck-Kennedy-Lieb-Tasaki quantum spin chain, consisting of bulk spin-1's and two spin-1/2's at the ends. We characterize entanglement between various subsystems of the ground state by mostly calculating the entropy of one of the subsystems; when appropriate, we evaluate concurrences as well. We show that the reduced density matrix of a continuous block of bulk spins is independent of the size of the chain and the location of the block relative to the ends. Moreover, we show that the entanglement of the block with the rest of the sites approaches a constant value exponentially fast, as the size of the block increases. We also calculate the entanglement of (i) any two bulk spins with the rest, and (ii) the end spin-1/2's (together and separately) with the rest of the ground state.

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There is considerable current interest in quantifying entanglement in various quantum systems. Entanglement in spin chains, correlated electrons, interacting bosons, and other models has recently been reported [1–13]. Entanglement is a fundamental measure of how much quantum effects we can observe and use, and it is the primary resource in quantum computation and quantum information processing [14,15]. Also, entanglement plays a role in the quantum phase transitions [1,2], and it has been experimentally demonstrated that the entanglement may affect macroscopic properties of solids [3,16].

In this Letter, we will study a spin chain introduced by Affleck, Kennedy, Lieb, and Tasaki (the AKLT model) [17,18]. The ground state of the model is a unique pure state. It is known as the valence-bond solid (VBS), and plays a central role in condensed matter physics. Haldane [19] conjectured that an antiferromagnetic Hamiltonian describing half-odd-integer spins is gapless, but for integer spins it has a gap. The AKLT model describing interaction of spin-1's in the bulk agrees with the conjecture. An implementation of the AKLT model in optical lattices was proposed recently [20], and the use of the AKLT model for *universal quantum computation* was discussed in [21]. The VBS is also closely related to the Laughlin ansatz [22] and to the fractional quantum Hall effect [23].

We investigate the seminal AKLT model from the new perspective of quantum information, and evaluate the entanglement (in terms of entropy) of various subsystems of the VBS. The results and the methodologies adopted herein have several implications from the perspective of both quantum information and condensed matter. For example, while the entanglement in spin chains with periodic boundary conditions has been studied extensively, our results provide entanglement calculations for spin chains with open boundary conditions. Similarly, G. Vidal *et al.* [4] conjectured that for gapped models the entropy of a large block of spins reaches saturation. We confirm this for the AKLT model and find that the entropy of a large block of bulk spins is close to 2. This means that the block can be in four different states, and hence the Hilbert space of states of the large block of bulk spins is four dimensional. Our results also show that the entanglement correlation of the VBS state is *short ranged*, which provides a good understanding of why the density matrix renormalization group method [24] works so efficiently for VBS states; see [25] for recent developments.

The AKLT model consists of a linear chain of N spin-1's in the bulk and two spin-1/2's on the boundary. We shall denote the vector of spin-1 operators by $\vec{S}_k$ and spin-1/2 operators by $\vec{s}_b$, where $b = 0, N+1$. The Hamiltonian is

$$H = \sum_{k=1}^{N-1}\left[\vec{S}_k\vec{S}_{k+1} + \frac{1}{3}(\vec{S}_k\vec{S}_{k+1})^2\right] + \pi_{0,1} + \pi_{N,N+1}. \quad (1)$$

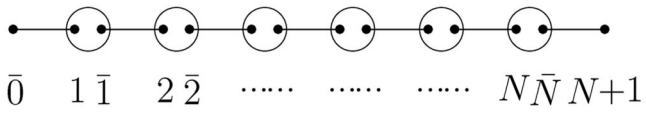
The boundary terms π describe interaction of a spin-1/2 and a spin-1. Each term is a projector on a state with a spin-3/2:

$$\pi_{0,1} = \frac{2}{3}(1 + \vec{s}_0\vec{S}_1), \qquad \pi_{N,N+1} = \frac{2}{3}(1 + \vec{s}_{N+1}\vec{S}_N). \quad (2)$$

The ground state of this model is unique and can be represented as [17,18]

$$|G\rangle = (\otimes_{k=1}^{N} P_{k\bar{k}})|\Psi^-\rangle_{\bar{0}1}|\Psi^-\rangle_{\bar{1}2}\cdots|\Psi^-\rangle_{\bar{N}N+1}. \quad (3)$$

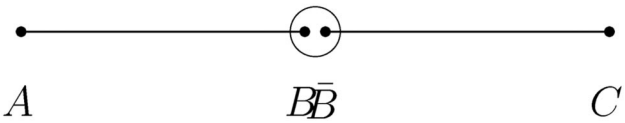
Here P projects a state of two qubits on a symmetric subspace, which describes spin 1. In the formula above $|\Psi^-\rangle = (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$ represents a singlet state, and the subscripts represent the two parties that share the singlet. We have tried to keep our notations as close to those in the Letter of Ref. [9]. We can use the following figure to visualize the ground state:



Black dots represent spin-1/2's, and spin-1's are denoted by circles. To begin with, each bulk site k (where $1 \leq k \leq N$) shares one singlet state $|\Psi^-\rangle$ (represented by a line) with its left and right neighbors. Thus at each bulk site k we start with two spin-1/2's labeled by $(k, \bar{k})$, and then the spin-1's are prepared by projecting the two spin-1/2's (four-dimensional space) on a symmetric three-dimensional subspace of spin 1 (three dimensional). The system has open boundary conditions, and the two ends are numbered as sites $\bar{0}$ (before projection, this site shared a singlet with site #1) and $N+1$.

There is an upper bound on the entropy of a block of L spins. Before projection, the entropy is equal to 2, since the boundary intersects two singlet states. Since the local projections will only decrease the entanglement, we expect that the entropy of a block of L spins to have an upper bound of 2.

In order to calculate the reduced density matrices of various subsystems of the ground state $|G\rangle$ [see Eq. (3)], it is more convenient to express it in a different form based on the singlet chain shown in the preceding figure and the following figure:



Let us first consider a chain of two singlet states, $|\Psi^-\rangle_{AB}$ and $|\Psi^-\rangle_{\bar{B}C}$: A is in site #1, $(B, \bar{B})$ is in site #2, and C is in site #3. The combined state can then be expressed as

$$|\Psi^-\rangle_{AB}|\Psi^-\rangle_{\bar{B}C} = \frac{1}{2}\sum_{\alpha=0}^{3}[(-)^{1+\alpha} I_B \otimes (\sigma_\alpha^*)_{\bar{B}} \otimes I_A \otimes (\sigma_\alpha)_C]|\Psi^-\rangle_{B\bar{B}}|\Psi^-\rangle_{AC}, \quad (4)$$

where both I and σ_0 represent the identity operator, σ_1, σ_2, σ_3 are the Pauli matrices, and the $*$ means complex conjugation. By entanglement swapping similar to teleportation [26], party #2 can perform a Bell state measurement on $(B, \bar{B})$, and then communicate the results of measurements to party #1 or party #3. Then one of them can perform a unitary transformation locally, and finally a maximally entangled state will be shared by them.

Equation (4) can be generalized to a chain of singlet states. First, define quantum states $|\alpha\rangle = (-1)^{1+\alpha} \times (I \otimes \sigma_\alpha^*)|\Psi^-\rangle$. Thus, $|0\rangle$ is the singlet state with the spin-0, while the other three states $|1\rangle, |2\rangle, |3\rangle$ form the symmetric subspace of the spin-1 (within a phase). Repeatedly using the relation (4) and with the help of the property presented later in the proof of our theorem, we obtain

$$|\Psi^-\rangle_{\bar{0}1}|\Psi^-\rangle_{\bar{1}2}\cdots|\Psi^-\rangle_{\bar{N}N+1} = \frac{1}{2^N}\sum_{\alpha_1,\ldots,\alpha_N=0}^{3}|\alpha_1\rangle\cdots|\alpha_N\rangle \times [I_{\bar{0}} \otimes (\sigma_{\alpha_N}\cdots\sigma_{\alpha_1})_{N+1}] \times |\Psi^-\rangle_{\bar{0},N+1}. \quad (5)$$

The quantum states $|\alpha_i\rangle$ are orthonormal states at lattice site $(i, \bar{i})$. Thus, by projecting the quantum state on the symmetric subspace spanned by the states $|1\rangle$, $|2\rangle$, and $|3\rangle$, the ground state of the AKLT model can be rewritten as [9,27]

$$|G\rangle = \frac{1}{3^{N/2}}\sum_{\alpha_1,\cdots,\alpha_N=1}^{3}|\alpha_1\rangle\cdots|\alpha_N\rangle[I_{\bar{0}} \otimes (\sigma_{\alpha_N}\cdots\sigma_{\alpha_1})_{N+1}]|\Psi^-\rangle_{\bar{0},N+1}. \quad (6)$$

It follows directly from Eq. (6) that the reduced density matrix of spin 1 at any bulk site k (recall that $k = 1, \ldots, N$) is

$$\rho_1 \equiv \mathrm{Tr}_{1,\ldots,\{k\},\ldots,N,\bar{0},N+1}|G\rangle\langle G| = \frac{1}{3}\sum_{\alpha_k=1}^{3}|\alpha_k\rangle\langle\alpha_k|, \quad (7)$$

where the trace is taken over all sites (including the two ends), except site number k. We see that all *one-site reduced density operators in the bulk are the same*: the identity or the maximally disordered state in the spin-1 space. Thus, the single-site reduced density matrices are independent of the total size of the spin chain N, and of the distance from the ends (i.e., k or $N-k$). For the more general case, we have the following result.

Theorem: *Consider the reduced density matrix of a continuous block of spins of length L (not including the two boundary 1/2 spins), starting from site k and stretching up to $k+L-1$, where $k \geq 1$ and $k+L-1 \leq N$ (thus, $1 \leq L \leq N$) in the VBS ground state* (6). *Then, all these density operators are the same, and independent of both k (i.e., the location of the block) and of N (the total length of the chain). Thus, the reduced density matrix depends only on L, the length of the block under consideration.*

The proof is based on the following relations: Define $|\Phi^+\rangle = (|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle)/\sqrt{2}$; we know that $|\Phi^+\rangle = (-i) \times (\sigma_2 \otimes I)|\Psi^-\rangle$. For a unitary operator U, we have the property $(U \otimes U^*)|\Phi^+\rangle = |\Phi^+\rangle$. Then $(U_1 \otimes U_2)|\Phi^+\rangle = (U_1 U_2^t \otimes I)|\Phi^+\rangle = (I \otimes U_2 U_1^t)|\Phi^+\rangle$, where U_1, U_2 are two unitary operators (the superindex t denotes the transposition).

By using these relations, we can prove that

$$\mathrm{Tr}_{\bar{0},N+1}(I\otimes U_1 V U_2)|\Psi^-\rangle\times\ \langle\Psi^-|(I\otimes U_1 V' U_2)^\dagger = \mathrm{Tr}_{\bar{0},N+1}(I\otimes V)|\Phi^+\rangle\langle\Phi^+|(I\otimes V')^\dagger. \tag{8}$$

By repeated applications of this relation, and by considering the ground state (6), the reduced density operator of any continuous block of spins of length L is

$$\rho_L = \frac{1}{3^L}\sum_{\alpha,\alpha'}|\alpha_1\rangle\langle\alpha_1'|\cdots|\alpha_L\rangle\langle\alpha_L'|\times\mathrm{Tr}_{\bar{0},N+1}(I\otimes V)|\Phi^+\rangle\langle\Phi^+|(I\otimes V')^\dagger, \tag{9}$$

where $V=\sigma_{\alpha_L}\cdots\sigma_{\alpha_1}$, $V'=\sigma_{\alpha_L'}\cdots\sigma_{\alpha_1'}$. This operator depends only on L. This completes our proof.

Our aim is to calculate the *entanglement* of the VBS state. For a pure bipartite state $|\psi\rangle_{AB}$, the entanglement between spatially separated parties A and B is $S(\rho_A)=S(\rho_B)$, where $\rho_{A(B)}\mathrm{Tr}_{B(A)}|\psi\rangle\langle\psi|$ are the reduced density operators and $S(\rho)=-\mathrm{Tr}\rho\log\rho$ is the von Neumann *entropy*, where we take the logarithms in the base 2. For example, it follows from Eq. (7) that the entropy of the one-site reduced density operator in the bulk is $S(\rho_1(k))=\log 3$. This entropy describes the entanglement between site number k in the bulk (considered as one party) and the rest of the ground state (considered as the other party). The space of the spin-1 is three dimensional, so log3 is the maximum of the entropy. Thus we proved that in the VBS state (6) each individual spin in the bulk is maximally entangled with the rest of the ground state. Later in this Letter, we shall see that this is also true for the boundary spin-1/2's.

Since the reduced density operator of a continuous block of L spins is independent of the total size N of the spin chain, we can consider the case where $L=N$; i.e., we consider a chain of L spin-1's with one spin-1/2 at each end. Now the reduced density operator of two end spin-1/2's takes the following form:

$$\begin{aligned}\rho_{\hat{L}} &= \frac{1}{3^L}\sum_{\alpha_1,\ldots,\alpha_L=1}^{3}(I\otimes\sigma_{\alpha_L}\cdots\sigma_{\alpha_1})|\Psi^-\rangle\langle\Psi^-|\times(I\\ &\quad\otimes\sigma_{\alpha_L}\cdots\sigma_{\alpha 1})^\dagger\\ &= \frac{1}{4}[1-p(L)]\cdot I + p(L)|\Psi^-\rangle\langle\Psi^-|.\end{aligned} \tag{10}$$

Here $p(L)=(-1/3)^L$ and I is the identity in four dimensions. Since the ground state (6) is pure, the entropy of the block of L bulk spin-1's is equal to the entropy of the two ends. So we have

$$\begin{aligned}S_L \equiv S(\rho_L) = S(\rho_{\hat{L}}) &= 2+\frac{3[1-p(L)]}{4}\\ &\times\log[1-p(L)]-\frac{1+3p(L)}{4}\log[1+3p(L)].\end{aligned} \tag{11}$$

As expected, $S_L\le 2$ and approaches 2 exponentially fast in L: $S_L\sim 2-(3/2)p(L)$. This is also clear from (10): the reduced density operator approaches the identity in the four dimensions exponentially fast. Consider the following numbers:

$$\begin{aligned}&S_1=1.58496, \quad S_2=1.97494, \quad S_3=1.99695,\\ &S_4=1.99969, \quad S_5=1.99996, \quad S_6\approx 2.\end{aligned} \tag{12}$$

Note that the correlation function of local spins decays equally fast:

$$\langle\vec{S}_L\vec{S}_1\rangle\sim(-1/3)^L = p(L); \tag{13}$$

see [18,23].

Next we shall study the entropy of *two spin-1's* separated by M sites in the bulk. That is, we calculate the entanglement between two bulk spin-1's and the rest of the spin-1's and the two spin-1/2's. We still can show that the reduced density operator does not depend on the total size of the chain, N, and prove that

$$\rho_2(M) = \frac{1}{9}[1-p(M)]I + p(M)\rho_2, \tag{14}$$

where $p(M)=(-1/3)^M$, ρ_2 is the two-site reduced density operator of nearest neighbors, i.e., the case $M=0$, and the operator I is the identity in nine dimensions. The nearest neighbor two-site reduced density operator can be written explicitly:

$$\begin{aligned}\rho_2 = \frac{1}{9}\Big[&\sum_{\alpha,\beta=1}^{3}|\alpha\rangle\langle\beta|\otimes|\alpha\rangle\langle\beta| + \sum_{\alpha=\beta}(|\alpha\rangle\langle\alpha|\otimes|\beta\rangle\langle\beta|\\ &-|\alpha\rangle\langle\beta|\otimes|\beta\rangle\langle\alpha|)\Big].\end{aligned} \tag{15}$$

So we can calculate the entropy of two spins at distance M:

$$\begin{aligned}S_2(M) = 2\log 3 &-\frac{5}{9}[1-p(M)]\log[1-p(M)]\\ &-\frac{3}{9}[1+p(M)]\log[1+p(M)]\\ &-\frac{1}{9}[1+2p(M)]\log[1+2p(M)].\end{aligned} \tag{16}$$

We see that $S_2(M)$ also approaches the maximum value (since the dimension is 9, the maximum entropy is $2\log 3$) with the exponential rate defined by local correlations (13). Note that $S_2=S_2(0)$ [see Eqs. (11) and (16)]. However, for $M\ge 1$, $S_2(M)$ quickly exceeds S_L. We also can calculate the *concurrence* (another measure of entanglement [28]). We shall use the generalized concurrence in higher dimensions [29]. Two concurrences corresponding to S_L and $S_2(M)$ are equal to $C_L=1-p^2(L)=1-\frac{1}{9^L}$ and $C_2(M)=1-\frac{1}{6}p^2(M)=1-\frac{1}{6\times 9^M}$, respectively.

They look similar because the entanglement of the block also represents the entanglement of two ends with L bulk spins.

Now we turn to the analysis of entanglement of *boundary* spins. We know that the end spin-1/2's are maximally entangled with the rest of the ground state and has an entropy of 1. The density operator of two ends $\rho_{\hat{N}}$ [see Eq. (10)] depends on the total size of the lattice N and is always separable. If the size of the spin chain N increases, $\rho_{\hat{N}}$ approaches quickly the identity matrix in four dimensions. It means that two ends considered as a subsystem are maximally entangled with the bulk spins if N is large.

Next we consider a two-site reduced density operator with *one spin in the bulk* and *another spin at one end*. It is enough to put the end spin at site $\bar{0}$, and the bulk spin at the site $(M+1)$ (the range is $M = 0, \ldots, N-1$). We can calculate the reduced density operator. First, we consider if this state is separable. Since it is the (2×3)-dimensional case, we can use the Peres-Horodecki criterion [30,31]. We find that, when $M = 0$, the state is entangled. For $M \neq 0$, it is a separable state. So, we know that the end spin $\bar{0}$ is entangled only with its nearest neighbor (spin 1). Second, we can study the entropy of this state; it is

$$S[\rho_2(\bar{0}, M+1)] = \log 6 - \frac{2}{3}[1 - p(M)]\log[1 - p(M)] - \frac{1}{3}[1 + 2p(M)]\log[1 + 2p(M)]. \tag{17}$$

Similar to other entropies presented above, it approaches the upper bound log6 with the same exponential speed, defined by local correlations (13). The concurrence corresponding to this entanglement is $C(\bar{0}, M+1) = 1 - \frac{2}{5}p^2(M)$.

In summary, the entanglement properties of the VBS state can be listed as follows: (i) each individual spin is maximally entangled with the rest; (ii) the entanglement of a block of spins of length L with the rest gets to a constant value exponentially fast with L; (iii) the entanglement of any two bulk spins gets maximal exponentially fast in their distance; (iv) each individual boundary spin is maximally entangled with its nearest neighbor and not with the other bulk spins and the other boundary spin; and (v) each individual boundary spin and another individual bulk spin are entangled with the rest, and the entanglement gets maximal exponentially fast with the distance between the boundary spin and its bulk partner.

In the future, it will be interesting to calculate the entropy of a subsystem of the two- and the three-dimensional AKLT model. In fact, we are planning to study the entanglement for the AKLT model on arbitrary graphs using the results of [32]. We believe that it will be useful for universal quantum computation, as in [33].

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