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Entanglement of the valence-bond-solid state on an arbitrary graph

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Abstract

The Affleck–Kennedy–Lieb–Tasaki (AKLT) spin interacting model can be defined on an arbitrary graph. We explain the construction of the AKLT Hamiltonian. Given certain conditions, the ground state is unique and known as the valence-bond-solid (VBS) state. It can be used in measurement-based quantum computation as a resource state instead of the cluster state. We study the VBS ground state on an arbitrary connected graph. The graph is cut into two disconnected parts: the block and the environment. We study the entanglement between these two parts and prove that many eigenvalues of the density matrix of the block are zero. We describe a subspace of eigenvectors of the density matrix corresponding to non-zero eigenvalues. The subspace is the degenerate ground states of some Hamiltonian which we call the block Hamiltonian.

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1. Introduction

The fields of statistical physics, condensed matter physics and quantum information theory share a common interest in the study of interacting quantum many body systems. The concept of entanglement in quantum mechanics has significant importance in all these areas. Much of the current effort is devoted to the description and quantification of the entanglement contained in strongly correlated quantum states. Quantum entanglement is a fundamental measure of how much quantum effects we can observe and use to control one quantum system by another, and it is the primary resource in quantum computation and quantum information processing [6]. Entanglement properties play an important role in condensed matter physics, such as phase transitions and macroscopic properties of solids [43, 44]. Extensive research has been undertaken to investigate quantum entanglement for spin chains, correlated electrons, interacting bosons as well as other models, see [3, 20, 26, 31, 34, 38, 39, 42, 45, 46, 49] for reviews and references. Characteristic functions of quantum entanglement, such as von

Neumann entropy and Rényi entropy, were obtained and discussed through studying reduced density matrices of subsystems [11, 16, 17, 30, 32]. An area law for the von Neumann entropy in harmonic lattice systems has been extensively studied [8, 9, 28].

Much insight in understanding entanglement of quantum systems has been obtained by studying exactly solvable models in statistical mechanics. In 1987, Affleck, Kennedy, Lieb and Tasaki proposed a spin interacting model known as the AKLT model [1, 2]. The model consists of spins on a lattice and the Hamiltonian describes interactions between nearest neighbors. The Hamiltonian density is a linear combination of projectors. The model is similar to the Heisenberg anti-ferromagnet with a gap. The authors (AKLT) of [1, 2] found the exact ground state, which has an exponentially decaying correlation function and a finite energy gap. This model has been attracting enormous research interests since then [10, 13, 33]. It can be defined and solved in higher dimensional and arbitrary lattices [2, 12, 35, 47] and generalizable to the inhomogeneous (non-translational invariant) case (spins at different lattice sites may take different values) and an arbitrary graph [36]. Given certain conditions (as to be described later), the ground state has proven to be unique [4, 36]. It is known as the valence-bond-solid (VBS) state. The Schwinger boson representation of the VBS state (see (17)) relates to the Laughlin ansatz of the fractional quantum Hall effect [4, 26, 29]. The Laughlin wavefunction of the fractional quantum Hall effect is the VBS state on the complete graph [24]. The VBS state illustrates ground state properties of anti-ferromagnetic integer-spin chains with a Haldane gap [23]. In one dimension, the VBS state is related to the matrix product state and deformed VBS models were studied in [37]. The theory of VBS state was generalized to the finitely correlated states and was essentially developed by Fannes, Nachtergaele, Werner and others [14, 15]. In one dimension, the correlation functions were obtained and studied in [15]. The entanglement of formation in the VBS state was estimated in [40]. Brennen and Miyake showed that the VBS state can be used as a resource state in measurement-based quantum computing instead of the cluster state [7]. It was proved in [48] that the VBS state allows universal quantum computation and an implementation of the AKLT Hamiltonian in optical lattices [19] has also been proposed.

We shall consider a part of the system, i.e. a block of spins. It is described by the density matrix of the block, which we call *the density matrix* later for short. The density matrix has been studied extensively in [11, 18, 32, 36, 49]. It contains information of all correlation functions [4, 31, 32, 50]. Furthermore, the entanglement properties of the VBS ground state have been studied by means of the density matrix as in [10, 11, 12, 32, 49]. The von Neumann entropy of the subsystem density matrix is a measure of entanglement of the VBS state. The Rényi entropy is another measure of the entanglement. The entanglement entropy was obtained in [11, 18, 32, 50].

The structure of the density matrix is important. For a one-dimensional AKLT spin chain the density matrix has a lot of zero eigenvalues [50, 51]. The eigenvectors with non-zero eigenvalues are the degenerate ground states of some Hamiltonian, which we shall call the *block* Hamiltonian (see (23)). In the limit of large block, the density matrix is proportional to a projector on the degenerate ground states of the block Hamiltonian. These states are the only eigenstates of the density matrix with non-zero eigenvalues which contribute to the entropy. Also, eigenstates of the density matrix are useful in quantum computing because of quantum measurements. It was conjectured in [50] that eigenvectors of the density matrix with non-zero eigenvalues always form degenerate ground states of some Hamiltonian (the block Hamiltonian), which is generalizable to an arbitrary graph. In this paper we shall give a general proof of this statement.

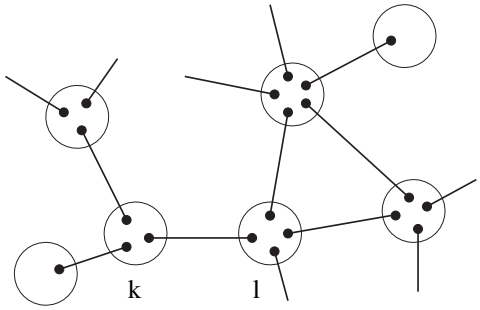

Figure 1. Example of a part of the graph including vertex k with $z_k = 3$ and vertex l with $z_l = 4$. Black dots • represent spin-$\frac{1}{2}$ states, which are enclosed by large circles ○ representing vertices and symmetrization of the product of spin-$\frac{1}{2}$'s at each vertex. Solid lines —— represent edges which anti-symmetrize the pair of connected spin-$\frac{1}{2}$'s.

The paper is divided into five parts:

(i) We define the *basic* AKLT model on an arbitrary connected graph and construct the unique VBS ground state using symmetrization and anti-symmetrization of states. A graphical illustration is included (section 2).

(ii) We introduce the *generalized* (inhomogeneous) AKLT model and give the condition of the uniqueness of the ground state. The VBS ground state is constructed using the Schwinger boson representations. Within this formulation, the relation between the VBS state and the Laughlin states of the fractional quantum Hall effect becomes obvious [4, 24, 26] (section 3).

(iii) In order to study entanglement of the VBS state, we cut the graph into two disconnected parts: the *block* and the *environment*. We define the *block* Hamiltonian, and show that its ground state is degenerate (section 4).

(iv) The density matrix of the block is proved to have a lot of zero eigenvalues. The eigenvectors with non-zero eigenvalues form degenerate ground states of the block Hamiltonian (section 5).

(v) Examples of the density matrix are given explicitly as special cases of the general result. We also formulate some open problems (section 6).

In sections 2 and 3 we follow the paper of Kirillov and Korepin written in 1990, see [36].

2. The basic AKLT model

We start with the definition of the *basic* AKLT model on a connected graph. A *graph* consists of two types of elements, namely *vertices* and *edges*. Every edge *connects* two vertices. As in figure 1, a vertex is drawn as a (large) circle ○ and an edge is drawn as a solid line —— connecting two vertices. For every pair of vertices in the *connected* graph, there is a *walk*[1] from one to the other. Vertices can also be called *sites* and edges sometimes called *links* or *bonds*. In the case of a disconnected graph, the Hamiltonian (1) is a direct sum with respect to

[1] A *walk* is an alternating sequence of vertices and edges, beginning and ending with a vertex, in which each vertex is incident to the two edges that precede and follow it in the sequence, and the vertices that precede and follow an edge are the end vertices of that edge.

connected components and the ground state is a direct product. We shall start with a connected graph. We shall also assume that the graph consists of more than one vertices, otherwise there would be no interaction at all. Let us introduce notations. By $\boldsymbol{S}_l$ we shall denote the spin operator located at vertex l with spin value S_l. In the *basic* model we require that $S_l = \frac{1}{2}z_l$, where z_l is the number of incident edges (connected to vertex l), also known as the valence or coordination number (the number of nearest neighbors of the vertex l). The relation between the spin value and coordination number must be true for any vertex l, including boundaries. This will guarantee uniqueness of the ground state. The Hamiltonian describes interactions between nearest neighbors:

$$H = \sum_{\langle kl \rangle} H(k, l). \tag{1}$$

Here $H(k, l)$ describes the interaction between spins at vertices k and l connected by an edge, and we sum over all edges $\langle kl \rangle$. The Hamiltonian density is $H(k, l)$. To write down an explicit form of $H(k, l)$, we define a projector $\pi_J(k, l)$:

$$\pi_J(k, l) = \prod_{|S_k - S_l| \leqslant j \leqslant S_k + S_l}^{j \neq J} \frac{(\boldsymbol{S}_k + \boldsymbol{S}_l)^2 - j(j+1)}{J(J+1) - j(j+1)}. \tag{2}$$

Operator $\pi_J(k, l)$ projects the edge spin $\boldsymbol{J}_{kl} \equiv \boldsymbol{S}_k + \boldsymbol{S}_l$ on the subspace with fixed total spin value J and $|S_k - S_l| \leqslant J \leqslant S_k + S_l$. Note that we could expand $(\boldsymbol{S}_k + \boldsymbol{S}_l)^2 = 2\boldsymbol{S}_k \cdot \boldsymbol{S}_l + S_k(S_k + 1) + S_l(S_l + 1)$. So that projector $\pi_J(k, l)$ in (2) is a polynomial in the scalar product $(\boldsymbol{S}_k \cdot \boldsymbol{S}_l)$ of degree $2S_{\min}$, where $S_{\min} \equiv \min\{S_k, S_l\}$ is the minimum of the two spin values of the same edge. For example with $S_k = S_l = 1$, we may have a quadratic polynomial:

$$\pi_2(k, l) = \tfrac{1}{6}(\boldsymbol{S}_k \cdot \boldsymbol{S}_l)^2 + \tfrac{1}{2}(\boldsymbol{S}_k \cdot \boldsymbol{S}_l) + \tfrac{1}{3}. \tag{3}$$

In the *basic* model we define the Hamiltonian density $H(k, l)$ as

$$H(k, l) = A(k, l)\pi_{S_k + S_l}(k, l), \qquad H(k, l) \geqslant 0 \tag{4}$$

with $A(k, l)$ an arbitrary positive real coefficient (it may depend on the edge $\langle kl \rangle$). So that the Hamiltonian density for each edge is proportional to the projector on the subspace with the highest possible edge spin value $(S_k + S_l)$. The physical meaning is that interacting spins do not form the highest possible edge spin (this will increase the energy) in the ground state. The Hamiltonian in (1) is a linear combination of projectors with positive coefficients, which shows that H is semi-positive definite.

The Hamiltonian (1) with condition

$$S_l = \tfrac{1}{2}z_l \tag{5}$$

has a unique ground state [1, 2, 4, 36] known as the valence-bond-solid state. It can be constructed as follows. Each vertex l has z_l spin-$\frac{1}{2}$'s. We associate each spin-$\frac{1}{2}$ with an incident edge. In such a way each edge has two spin-$\frac{1}{2}$'s at its ends. We anti-symmetrize the wavefunction of these two spin-$\frac{1}{2}$'s. So that anti-symmetrization is done along each edge. We also symmetrize the product of spin-$\frac{1}{2}$'s at each vertex (each large circle). Let us write down the VBS ground state algebraically. We label the particular dot from vertex l connected with some dot from vertex k by l_k (correspondingly, that dot from vertex k is labeled by k_l). In this way we have specified a unique prescription of labels with dots. Then the anti-symmetrization results in the singlet state

$$|\Phi\rangle_{kl} = \tfrac{1}{\sqrt{2}}\big(|\uparrow\rangle_{l_k}|\downarrow\rangle_{k_l} - |\downarrow\rangle_{l_k}|\uparrow\rangle_{k_l}\big). \tag{6}$$

The direct product of all these $|\Phi\rangle$ singlet states corresponds to all edges in our graph:

$$\prod_{\langle kl\rangle} |\Phi\rangle_{kl}. \tag{7}$$

We still have to complete the symmetrization (circles) at each vertex. We denote the symmetrization operator of z_l dots in vertex l by $\mathbf{P}(l)$, then the symmetrization at each vertex is carried out by taking the product $\prod_l \mathbf{P}(l)$ of all vertices. Finally, the unique VBS ground state can be written as

$$|\mathrm{VBS}\rangle = \prod_l \mathbf{P}(l) \prod_{\langle kl\rangle} |\Phi\rangle_{kl}. \tag{8}$$

Here the first product runs over all vertices and the second over all edges. If the coordination number z_l is a constant over all vertices in the graph except for boundaries, then we would have the same spin value at each bulk vertex. In that case the *basic* model is also referred to as the *homogeneous* model.

3. The generalized AKLT model

In the *generalized* AKLT model, relation (5) is generalized. We associate a positive integer M_{kl} ($M_{kl} \equiv M_{lk}$) to each edge $\langle kl\rangle$ of the graph. We shall call M_{kl} multiplicity numbers. The Hamiltonian describes interactions between nearest neighbors (vertices connected by an edge):

$$H = \sum_{\langle kl\rangle} H(k,l). \tag{9}$$

However, the Hamiltonian density is no longer proportional to a single projector in general. It is a linear combination of projectors

$$H(k,l) = \sum_{J=S_k+S_l-M_{kl}+1}^{S_k+S_l} A_J(k,l)\pi_J(k,l), \qquad H(k,l) \geqslant 0. \tag{10}$$

Projector $\pi_J(k,l)$ is given by (2), and $A_J(k,l)$'s are arbitrary positive coefficients. So that $H(k,l)$ projects the edge spin on the subspace with spin value J greater than $S_k + S_l - M_{kl}$. Physically formation of edge spin higher than $S_k + S_l - M_{kl}$ would increase the energy.

The condition of uniqueness of the ground state was introduced in [36]:

$$2S_l = \sum_k M_{kl}, \qquad \forall\, l. \tag{11}$$

Here S_l is the spin value at vertex l and we sum over all edges incident to vertex l (connected to vertex l). The Hamiltonian (9) has a unique ground state if (11) is valid. The relation $2S_l = z_l$ for the *basic* model is a special case when $M_{kl} = 1$. Condition (11) can be put into an invariant form. Let us define a column vector $\mathbf{S}$, the lth component of which is associated with vertex l of the graph and equal to S_l. The number of components is equal to the number of vertices N. Next, we define another column vector $\mathbf{M}$ with its dimension equal to the number of edges M in the graph. The kth and lth components of this vector are associated with edge $\langle kl\rangle$ and both equal to M_{kl}. The most important geometrical characteristic of the graph is the vertex–edge incidence matrix $\hat{\mathbf{I}}$ (see [27]). This is a rectangular matrix with N rows and M columns. Each row is associated with the vertex and each column is associated with the edge. If the vertex belongs to the edge the corresponding matrix element is equal to one, otherwise zero. Then condition (11) of uniqueness can be re-written as

$$2\mathbf{S} = \hat{\mathbf{I}}\cdot\mathbf{M}. \tag{12}$$

For more details we refer to [36].

Under condition (11) or (12), the unique ground state of Hamiltonian (9) is referred to as the generalized VBS state. It is constructed by introducing the Schwinger boson representation [4, 18, 32, 36, 50, 51]. We define a pair of independent canonical bosonic operators a_l and b_l for each vertex l:

$$\left[a_k, a_l^\dagger\right] = \left[b_k, b_l^\dagger\right] = \delta_{kl} \tag{13}$$

with all other commutators vanishing:

$$[a_k, a_l] = [b_k, b_l] = [a_k, b_l] = \left[a_k, b_l^\dagger\right] = 0, \qquad \forall k, l. \tag{14}$$

Spin operators are represented as

$$S_l^+ = a_l^\dagger b_l, \qquad S_l^- = b_l^\dagger a_l, \qquad S_l^z = \tfrac{1}{2}\left(a_l^\dagger a_l - b_l^\dagger b_l\right). \tag{15}$$

To reproduce the dimension of the spin-S_l Hilbert space at vertex l, a constraint on the total boson occupation number is required:

$$\tfrac{1}{2}\left(a_l^\dagger a_l + b_l^\dagger b_l\right) = S_l. \tag{16}$$

As a result, the VBS ground state in the Schwinger representation is given by

$$|\mathrm{VBS}\rangle = \prod_{\langle kl\rangle} \left(a_k^\dagger b_l^\dagger - b_k^\dagger a_l^\dagger\right)^{M_{kl}} |\mathrm{vac}\rangle. \tag{17}$$

This representation shows that for a full graph (each vertex is connected to every other vertex) the VBS state coincides with the Laughlin wavefunction [4, 24, 26]. In (17) the product runs over all edges and the *vacuum* $|\mathrm{vac}\rangle$ is annihilated by any of the annihilation operators:

$$a_l\,|\mathrm{vac}\rangle = b_l\,|\mathrm{vac}\rangle = 0, \qquad \forall l. \tag{18}$$

Note that $\left[a_k^\dagger, b_l^\dagger\right] = 0, \forall k, l$. To prove that (17) is the ground state we need only to verify for any vertex l and edge $\langle kl\rangle$: (i) the total power of $a_l^\dagger$ and $b_l^\dagger$ is $2S_l$, so that we have spin-S_l at vertex l; (ii) $-\frac{1}{2}\left(\sum_{l'\neq l} M_{l'k} + \sum_{k'\neq k} M_{k'l}\right) \leqslant J_{kl}^z \equiv S_k^z + S_l^z \leqslant \frac{1}{2}\left(\sum_{l'\neq l} M_{l'k} + \sum_{k'\neq k} M_{k'l}\right)$ by a binomial expansion, so that the maximum value of the edge spin J_{kl} is $\frac{1}{2}\left(\sum_{l'\neq l} M_{l'k} + \sum_{k'\neq k} M_{k'l}\right) = S_k + S_l - M_{kl}$ (from $SU(2)$ invariance, see [4]). Therefore, the state $|\mathrm{VBS}\rangle$ defined in (17) has spin-S_l at vertex l and no projection onto the $J_{kl} > S_k + S_l - M_{kl}$ subspace for any edge. The introduction of Schwinger bosons can be used to construct a spin coherent state basis in which spins at each vertex behave as classical unit vectors, see [18, 32, 36, 50, 51].

4. The entanglement between block and environment

The VBS state (see (8) and (17)) has non-trivial entanglement properties. The density matrix of the VBS state is a projector

$$\rho = \frac{|\mathrm{VBS}\rangle\langle\mathrm{VBS}|}{\langle\mathrm{VBS}|\mathrm{VBS}\rangle}. \tag{19}$$

Let us cut the original graph into two subgraphs B and E, that is, we cut through some number of edges such that the resulting graph $B \cup E$ is disconnected (no edge between B and E). We may call one of them, say B, the *block*, and the other one, E, the *environment*. The distinction is arbitrary and the two subsystems are equivalent in measuring entanglement.

Let us focus on the block (subsystem B). It is described by the density matrix ρ_b of the block (obtained by tracing out degrees of freedom of the environment E from the density matrix ρ (19)):

$$\rho_b = \mathrm{Tr}_e[\rho]. \tag{20}$$

In (20) and below we use subscript b for *block* and e for *environment*. The density matrix ρ_b contains all correlation functions in the VBS ground state as matrix entries [4, 31, 32, 50]. The entanglement can be measured by the von Neumann entropy

$$S_{v.N} = -\operatorname{Tr}_b[\rho_b \ln \rho_b] = -\sum_{\lambda \neq 0} \lambda \ln \lambda \tag{21}$$

or the Rényi entropy

$$S_R(\alpha) = \frac{1}{1-\alpha} \ln \left\{ \operatorname{Tr}_b \left[\rho_b^\alpha \right] \right\} = \frac{1}{1-\alpha} \ln \left(\sum_{\lambda \neq 0} \lambda^\alpha \right), \qquad \alpha > 0. \tag{22}$$

Here λ's are (non-zero) eigenvalues of density matrix ρ_b and α is an arbitrary parameter. It was shown by using the Schmidt decomposition [41] that non-zero eigenvalues of the density matrix of subsystem B (block) is equal to those of the density matrix of subsystem E (environment). So the two subsystems are equivalent in measuring entanglement in terms of entanglement entropies, i.e. $S_{v.N}[B] = S_{v.N}[E]$ and $S_R[B] = S_R[E]$. This fact has been used in obtaining entanglement entropies of one-dimensional VBS states as in [11, 32]. We shall show that the spectrum of the density matrix ρ_b contains a lot of zero eigenvalues. In order to understand this and give the subsystem (block) a more complete description, we first introduce the Hamiltonian of the subsystem (called the *block* Hamiltonian).

The *block* Hamiltonian H_b is the sum of Hamiltonian densities $H(k, l)$ with both $k \in B$ and $l \in B$, i.e. nearest neighbor interactions (edge terms) within the block B:

$$H_b = \sum_{\langle kl \rangle \in B} H(k, l), \qquad k \in B, \quad l \in B. \tag{23}$$

Here $H(k, l)$ is given in (4) for the basic model and (10) for the generalized model, for k and l connected by an edge. In (23) no cut edges are present (boundary edges between subgraphs B and E removed). This Hamiltonian has degenerate ground states because uniqueness conditions (5) and (11) are not valid. Let us discuss the degeneracy of ground states of (23). Let us denote by L the number of vertices on the boundary of the block B. The boundary consists of those vertices with one or more cut incident edge, see figure 2. The degeneracy deg of ground states of H_b is given by the Katsura's formula

$$\deg = \prod_{l \in \partial B} \left[\left(\sum_{k \in \partial E} M_{kl} \right) + 1 \right], \qquad \langle kl \rangle \in \{\text{cut edges}\}. \tag{24}$$

Here ∂B denotes vertices on the boundary of the block B and ∂E are vertices on the boundary of the environment E. In (24) we have L terms in the product. Formula (24) is valid for both the basic and the generalized model. For the basic model all $M_{kl} = 1$, including those corresponding to cut edges. Take, for example, a particularly simple case that each vertex on the boundary of the block ∂B was connected to exactly one vertex on the boundary of the environment ∂E. Then the degeneracy $\deg = 2^L$. A general proof of formula (24) is given in the appendix. The subspace spanned by the degenerate ground states is called the *ground space*, with the dimension given by deg in (24). We emphasize at this point that the block B should contain more than one vertices, otherwise the block Hamiltonian vanishes $H_b = 0$ and the whole Hilbert space becomes the *ground space*. We discuss the density matrix for a single vertex block at the end of the following section. It was shown for one-dimensional models in [50, 51] that the spectrum of density matrix ρ_b is closely related to the block Hamiltonian. The density matrix is a projector onto the ground space multiplied by another matrix. We shall prove the statement for an arbitrary graph in the following section.

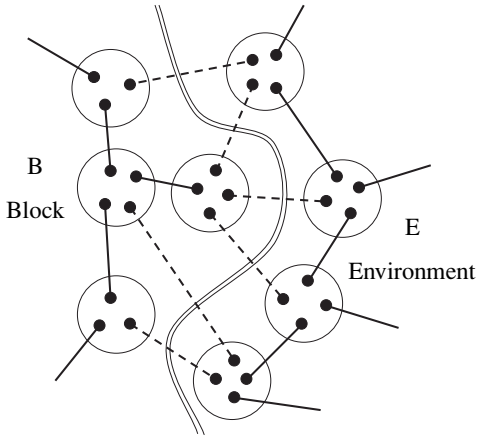

Figure 2. Example of the cutting for the basic model. The curved double line represents the boundary between the two subgraphs. We have the block B on the left and the environment E on the right. Solid lines —— represent edges while dashed lines - - - - represent cut edges. Each dashed line connects two dots. All vertices in the figure belong to the boundary of B or E because of the presence of one or more cut incident edges (dashed lines).

5. The density matrix

Let us denote by N_b the number of vertices in the block B. Then the dimension dim of the Hilbert space of the block B is equal to $\prod_l (2S_l + 1)$ with $l \in B$, which is also the dimension of the density matrix ρ_b. The value is

$$\dim = \prod_{l \in B} [z_l + 1], \tag{25}$$

for the basic model and

$$\dim = \prod_{l \in B} \left[\left(\sum_{k \in (B \cup \partial E)} M_{kl} \right) + 1 \right], \tag{26}$$

for the generalized model. In both expressions (25) and (26) we have N_b factors in the product. Take, for example, a particularly simple basic model in which each vertex is connected with the same number z of vertices, including those corresponding to boundary vertices. Then the dimension $\dim = (z + 1)^{N_b}$. The density matrix ρ_b would have dim number of eigenvalues. However, most of the eigenvalues are vanishing and ρ_b is a projector onto a much smaller subspace multiplied by another matrix. To prove the statement, we define a *support* to be the subspace of the Hilbert space of the block B with non-zero eigenvalues, i.e. it is spanned by eigenstates of ρ_b with non-zero eigenvalues. The dimension of the support is denoted by D. We have the following theorem on the structure of the density matrix ρ_b (assuming that the block have more than one vertices, i.e. $N_b \geqslant 2$, so that H_b is not equal to zero identically):

Theorem 1. *The support of ρ_b (20) is a subspace of the ground space of the block Hamiltonian H_b (23).*

To prove the theorem, we recall that $H = \sum_{\langle kl\rangle \in B} H(k,l)$ and each $H(k,l)$ is a sum of projectors (10). We have $H(k,l) \geqslant 0$. Then the construction of the VBS ground state (8) and (17) guarantees that there is no projection onto the subspace with higher edge spins for *any* edge. Therefore,

$$H(k,l)|\mathrm{VBS}\rangle = 0, \qquad \forall \langle kl\rangle. \tag{27}$$

In particular, this is true for edges inside the block B, i.e. $k \in B$ and $l \in B$. Now, from the definition of ρ_b in (20), we have

$$\begin{aligned} H(k,l)\rho_b &= H(k,l)\,\mathrm{Tr}_e[\rho] \\ &= \frac{H(k,l)\,\mathrm{Tr}_e[|\mathrm{VBS}\rangle\langle\mathrm{VBS}|]}{\langle\mathrm{VBS}|\mathrm{VBS}\rangle} \\ &= \frac{\mathrm{Tr}_e[H(k,l)|\mathrm{VBS}\rangle\langle\mathrm{VBS}|]}{\langle\mathrm{VBS}|\mathrm{VBS}\rangle} = 0, \qquad k \in B, \quad l \in B. \end{aligned} \tag{28}$$

In the last step of (28) we have used (27) and the fact that edge $\langle kl\rangle$ lies completely inside block B so that $H(k,l)$ commutes with tracing in the environment E. Equation (28) is true for any edge in B, so that

$$H_b\rho_b = \sum_{\langle kl\rangle \in B} H(k,l)\rho_b = 0, \qquad k \in B, \quad l \in B. \tag{29}$$

If we diagonalize the density matrix ρ_b

$$\rho_b = \sum_{\lambda\neq 0} \lambda|\lambda\rangle\langle\lambda|, \tag{30}$$

where $|\lambda\rangle$ is the eigenstate corresponding to eigenvalue λ. Then (29) can be re-written as

$$H_b \sum_{\lambda\neq 0} \lambda|\lambda\rangle\langle\lambda| = \sum_{\lambda\neq 0} \lambda H_b|\lambda\rangle\langle\lambda| = 0, \tag{31}$$

Note that $\{|\lambda\rangle\}$ is a linearly independent set. Therefore the solution of (31) means that

$$H_b|\lambda\rangle = 0, \qquad \lambda \neq 0. \tag{32}$$

Expression (32) states that any eigenstate of ρ_b (with non-zero eigenvalue) is a ground state of H_b. As a result, we have proved the *theorem* that the *support* of ρ_b is a subspace of the *ground space* of H_b, so that $D \leqslant \deg$. The density matrix takes the form of a projector multiplied by another matrix and the projector projects on the *ground space*. Also, it is clear from expressions (24)–(26) that $\deg \leqslant \dim$ ($\partial B \subseteq B$ so that $L \leqslant N_b$). Usually, deg is much smaller than dim because the former involves only contributions from boundary vertices of the block while the latter also involves contributions from all bulk vertices. Then as a corollary of the *theorem*, we have $D \leqslant \deg \leqslant \dim$.

If the block B consists of only one vertex with a spin-S, then we conjecture that it is in the maximally entangled state. The *support* has dimension $D = 2S + 1$.

6. Examples of the density matrix and open problems

The density matrix of the block has been studied in [11, 32] and diagonalized directly in [50, 51] for one-dimensional models, which illustrates the *theorem* explicitly. It was shown for different one-dimensional AKLT models that the inequality $D \leqslant \deg$ is always saturated, i.e. $D = \deg$, so that the *support* is exactly equal to the *ground space*. The density matrix is proportional to the projector on the degenerate *ground space* of the block Hamiltonian.

Therefore the projector $\mathbf{P}_D$ on the *support* of ρ_b is equal to the projector $\mathbf{P}_{\text{deg}}$ on the *ground space* of H_b:

$$\mathbf{P}_D = \mathbf{P}_{\text{deg}} \tag{33}$$

If we denote the identity of the Hilbert space of the block by $\mathbf{I}_{\text{dim}}$, then we also have

$$\rho_b(\mathbf{I}_{\text{dim}} - \mathbf{P}_{\text{deg}}) = 0. \tag{34}$$

Using these relations (33) and (34), the density matrix can be put in the following matrix form:

$$\rho_b = \Lambda \cdot \mathbf{P}_{\text{deg}} = \mathbf{P}_{\text{deg}} \cdot \Lambda \tag{35}$$

where Λ is a diagonal matrix with non-zero eigenvalues of ρ_b as entries. It was also proved in [50, 51] that in the large block limit $N_b \to \infty$, all eigenvalues become the same so that

$$\lim_{N_b\to\infty} \Lambda = \frac{1}{D}\mathbf{I}_D, \tag{36}$$

where $\mathbf{I}_D$ is the identity of the *support*. As a consequence, the density matrix approaches the following limit:

$$\lim_{N_b\to\infty} \rho_b \equiv \rho_\infty = \frac{1}{\text{deg}}\mathbf{P}_{\text{deg}} = \frac{1}{D}\mathbf{P}_D, \tag{37}$$

where ρ_∞ behaves as the identity in the *ground space* or *support*.

In below we give explicitly the form of the density matrix for the most general model in one dimension, i.e. the one-dimensional generalized (inhomogeneous) model [51]. Then we formulate some open problems.

For the generalized model in one dimension, we label the left ending site of the block by $l = 1$ with spin value $S_1 = \frac{1}{2}(M_{01} + M_{12})$ and the right ending site by $l = L$ with spin value $S_L = \frac{1}{2}(M_{L-1,L} + M_{L,L+1})$. The block B consists of N_b contiguous bulk vertices and the block Hamiltonian is

$$H_b = \sum_{(l,l+1)\in\text{block}}^{(N_b-1)\text{terms}} \left(\sum_{J=S_l+S_{l+1}-M_{l,l+1}+1}^{S_l+S_{l+1}} A_J(l, l+1)\pi_J(l, l+1) \right) \tag{38}$$

with $\pi_J(l, l+1)$ defined in (2) and $A_J(l, l+1)$ positive coefficients.

As shown in [51], the *ground space* of H_b is $(M_{01}+1)(M_{L,L+1}+1)$-dimensional and can be spanned by $\{|\text{VBS}_{N_b}(J, M)\rangle, J = |J_-|, |J_-|+1, \ldots, J_+, M = -J, -J+1, \ldots, J\}$ (see [51] for an explicit construction of these *degenerate VBS states* of the block). Here $J_- = \frac{1}{2}(M_{01} - M_{L,L+1})$ and $J_+ = \frac{1}{2}(M_{01} + M_{L,L+1})$. These states are eigenstates of ρ_b with non-zero eigenvalues.

In the large block limit, assuming that $M_{01} \to S_-$ and $M_{L,L+1} \to S_+$, we have

$$\lim_{N_b\to\infty} \rho_b \equiv \rho_\infty = \frac{1}{(S_- + 1)(S_+ + 1)}\mathbf{P}_{(S_-+1)(S_++1)}. \tag{39}$$

Here S_- and S_+ are the first and last spins in the block, respectively. The von Neumann entropy is equal to the Rényi entropy

$$S_{v.N} = S_R = \ln[(S_- + 1)(S_+ + 1)] \tag{40}$$

in the limit.

For finite block, $\rho_b|\text{VBS}_{N_b}(J, M)\rangle = \Lambda(J)|\text{VBS}_{N_b}(J, M)\rangle$. The eigenvalues $\Lambda(J)$ are independent of M and given by

$$\Lambda(J) = \frac{1}{(M_{01}+1)(M_{L,L+1}+1)} \left\{ 1 + \sum_{l=1}^{M_<} (2l+1) \left[\prod_{j=1}^{N_b-1} \lambda(l, M_{j,j+1}) \right] \text{poly}(l, J) \right\}, \tag{41}$$

in which $M_< = \min\{M_{j,j+1}, j = 1, \ldots, L-1\}$ being the minimum of the multiplicity numbers, poly(l, J) is a polynomial of J depending on l, and $\lambda(l, M_{j,j+1})$ is given by

$$\lambda(l, M_{ij}) = \frac{(-1)^l M_{ij}!(M_{ij}+1)!}{(M_{ij}-l)!(M_{ij}+l+1)!}. \tag{42}$$

So that matrix $\mathbf{\Lambda}$ consists of these eigenvalues (41) in diagonal form. The density matrix is the projector $\mathbf{P}_{(S_-+1)(S_++1)}$ multiplied by the matrix $\mathbf{\Lambda}$.

Corresponding results for the one-dimensional basic model [11] and homogeneous model [50] can be considered as special cases in which all $M_{j,j+1} = 1$ (all bulk $S_j = 1$, $S_- = S_+ = 1$) for the basic model and all $M_{j,j+1} = S$ ($S_- = S_+ = S$) for the homogeneous model.

One open problem is the calculation of non-zero eigenvalues of the density matrix ρ_b for general and more complicated graphs. One should start with the Cayley tree (also known as the Bethe tree). We expect that an exact explicit expression for the non-zero eigenvalues is possible, because it has no loops. It is also important to calculate non-zero eigenvalues of ρ_b for graphs with loops. In all known examples [11, 50, 51], where the density matrix of a large block has been calculated, all non-zero eigenvalues coincide. So that the density matrix of a large block is proportional to a projector. We conjecture that this will be the case for all connected graphs. In other words, we expect that in the large block limit, each non-zero eigenvalue should approach the same value $\frac{1}{D} = \frac{1}{\deg}$ and the entanglement entropies should be saturated, i.e. $S_{v.N} = S_R = \ln D = \ln(\deg)$.

7. Conclusion

We have studied the entanglement of the AKLT model. We formulate the AKLT model on an arbitrary connected graph. The Hamiltonian (1), (9) is a sum of projectors which describe interactions between nearest neighbors. The condition of uniqueness of the ground state relates the spin value at each vertex with multiplicity numbers associated with edges incident (connected) to the vertex, see (5), (11), (12). The unique ground state is known as the valence-bond-solid state (8), (17). The VBS state can be used instead of the cluster state in measurement-based quantum computation, see [7].

To study the entanglement, the graph is divided into two parts: the *block* and the *environment*. We investigate the density matrix ρ_b of the block and show that it has many zero eigenvalues. We describe the subspace (called the *support*) of eigenvectors of ρ_b with non-zero eigenvalues. We have proved (see *theorem* in section 5) that this subspace is the degenerate *ground space* of some Hamiltonian, we call it the *block* Hamiltonian (23).

The entanglement can be measured by the von Neumann entropy or the Rényi entropy of the density matrix ρ_b. Most eigenvalues of ρ_b vanish and have no contribution to the entanglement entropies. The density matrix takes the form of a projector on the *ground space* multiplied by another matrix (conjectured in [50] for an arbitrary graph).

Non-zero eigenvalues of ρ_b have been calculated for a variety of one-dimensional AKLT models [11, 32, 50, 51]. They are given as illustrations. We find that in these cases the *support* coincides with the *ground space*, so their dimensions are equal $D = \deg$ In the large block limit, all non-zero eigenvalues become the same and the density matrix is proportional to a projector (39). The von Neumann entropy equals the Rényi entropy and both take the saturated value $S_{v.N} = S_R = \ln D = \ln(\deg)$.

For more complicated graphs, non-zero eigenvalues of the density matrix are still unknown. One open problem is to calculate those eigenvalues. One may start with the Cayley tree because there are no loops and we expect to obtain exact explicit expressions of the eigenvalues.

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Appendix. Ground state degeneracy of the block Hamiltonian

We prove Katsura's formula (24) for the degeneracy of ground states of the block Hamiltonian. The block Hamiltonian is defined in (23). We first look at the uniqueness condition (11). For an arbitrary vertex l in the block B, the condition can be written as

$$2S_l = \sum_k M_{kl} = \sum_{k\in B} M_{kl} + \sum_{k\in\partial E} M_{kl}, \qquad l \in B. \tag{A.1}$$

Note that the sum over vertices $k \in \partial E$ is outside the block B. These terms are only present for boundary vertices $l \in \partial B$. Expression (A.1) is valid for *any* vertex in the block (for a bulk vertex the last summation vanishes). Next we define *the block VBS state*

$$|\mathrm{VBS}_{N_b}\rangle = \prod_{\langle kl\rangle\in B} \left(a_k^\dagger b_l^\dagger - b_k^\dagger a_l^\dagger\right)^{M_{kl}} |\mathrm{vac}\rangle, \quad k \in B, \quad l \in B. \tag{A.2}$$

Here edge $\langle kl\rangle$ lies completely inside the block B. Now an *arbitrary* ground state of the block Hamiltonian H_b takes the following form:

$$|\mathrm{G}\rangle = \left[\prod_{l\in\partial B}^{L\text{terms}} f\left(a_l^\dagger, b_l^\dagger\right)\right] |\mathrm{VBS}_{N_b}\rangle, \tag{A.3}$$

where $f\left(a_l^\dagger, b_l^\dagger\right)$ is a polynomial (may depend on the vertex l) in $a_l^\dagger$ and $b_l^\dagger$ and the product runs over all boundary vertices (with the number denoted by L). The degree of this polynomial is equal to $\sum_{k\in\partial E} M_{kl}$. (Each term in the polynomial must have the same total power $\sum_{k\in\partial E} M_{kl}$ of $a_l^\dagger$ and $b_l^\dagger$.) It is straightforward to verify that $|\mathrm{G}\rangle$ in (A.3) is a ground state:

(i) The power of $a_l^\dagger$ and $b_l^\dagger$ in $|\mathrm{VBS}_{N_b}\rangle$ is $\sum_{k\in B} M_{kl}$ (see (A.2)) so that the total power of $a_l^\dagger$ and $b_l^\dagger$ in (A.3) is $\sum_{k\in B} M_{kl} + \sum_{k\in\partial E} M_{kl} = 2S_l$ according to (A.1). Therefore, we have the correct power $2S_l$ of the bosonic operators $a_l^\dagger$ and $b_l^\dagger$ for each vertex l in the block B (constraint (16) is satisfied).

(ii) There is no projection on any edge spin value greater than $S_k + S_l - M_{kl} + 1$ because of the construction of the block VBS state (A.2). (One could use the same reasoning as in section 3.)

Therefore the degeneracy deg of the ground states of H_b is equal to the number of linearly independent states of the form (A.3). Since $a_l^\dagger$'s and $b_l^\dagger$'s are bosonic and commute, the number of linearly independent polynomials $f\left(a_l^\dagger, a_l^\dagger\right)$ for an arbitrary l is equal to its degree plus one, i.e. $\left(\sum_{k\in\partial E} M_{kl}\right) + 1, \forall\, l \in \partial B$. So that the total number of linearly independent polynomials of the form $\prod_{l\in\partial B}^{L\text{terms}} f\left(a_l^\dagger, b_l^\dagger\right)$ is the product of these numbers for each $l \in \partial B$. Finally, the ground state degeneracy of the block Hamiltonian H_b is (Katsura's formula)

$$\mathrm{deg} = \prod_{l\in\partial B} \left[\left(\sum_{k\in\partial E} M_{kl}\right) + 1\right]. \tag{A.4}$$

In the case of the basic model all $M_{kl} = 1$, formula (A.4) has a graphical illustration, see figure 2. We count the number # of all cut edges (dashed lines) incident to one boundary vertex of the block, then add one to the number #. The degeneracy is the product of these (# +1)'s for each boundary vertex.

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