J Stat Phys (2008) 133: 347–377
DOI 10.1007/s10955-008-9617-9

Entanglement and Density Matrix of a Block of Spins in AKLT Model

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Received: 19 April 2008 / Accepted: 13 August 2008 / Published online: 7 September 2008

Abstract We study a 1-dimensional AKLT spin chain, consisting of spins S in the bulk and $S/2$ at both ends. The unique ground state of this AKLT model is described by the Valence-Bond-Solid (VBS) state. We investigate the density matrix of a contiguous block of bulk spins in this ground state. It is shown that the density matrix is a projector onto a subspace of dimension $(S+1)^2$. This subspace is described by non-zero eigenvalues and corresponding eigenvectors of the density matrix. We prove that for large block the von Neumann entropy coincides with Renyi entropy and is equal to $\ln(S+1)^2$.

Keywords AKLT · Density matrix · Entanglement · Valence Bond Solid

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.

NSF Grant DMS-0503712.

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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 [9, 54, 55]. Entanglement properties play an important role in condensed matter physics, such as phase transitions [59, 60] and macroscopic properties of solids [27, 28, 67]. Extensive research has been undertaken to investigate quantum entanglement for spin chains, correlated electrons, interacting bosons as well as other models, see [3, 5, 7, 10–14, 17, 18, 21, 29, 30, 36, 37, 40, 42, 43, 47–51, 53, 57, 58, 61, 63, 64, 66, 67, 69–77] for reviews and references. Characteristic functions of quantum entanglement, such as von Neumann entropy and Renyi entropy, are obtained and discussed through studying reduced density matrices of subsystems [19, 23, 24, 39, 41]. An area law for the von Neumann entropy in harmonic lattice systems has been extensively studied [15, 16, 62].

Much insight in understanding entanglement of quantum systems has been obtained by studying exactly solvable models in statistical mechanics. In this paper we study a celebrated spin chain model introduced by I. Affleck, T. Kennedy, E. H. Lieb and H. Tasaki (AKLT) in 1987 [1, 2]. This model has been attracting enormous research interests since then. It can be defined and solved in higher dimensional and arbitrary lattices [2, 44]. We consider a 1-dimensional AKLT model with spin-S in the bulk and spin-$S/2$ at both ends. The ground state of this model is a unique pure state [6]. It is known as the Valence-Bond-Solid (VBS) state, which plays a central role in condensed matter physics. The VBS state can be defined in higher dimensions [2, 20, 65] and even arbitrary graphs [45, 46]. It is closely related to Laughlin ansatz [38, 52] and fractional quantum Hall effect [6]. It enables us to understand ground state properties of anti-ferromagnetic integer-spin chains where the finite energy gap known as the Haldane gap exists [33, 34]. Universal quantum computation based on VBS states [68] and an implementation of the AKLT Hamiltonian in optical lattices [26] have also been proposed.

The density matrix of a contiguous block of bulk spins as a subsystem (we call it *the density matrix* later for short) has been studied extensively in [19, 25, 41, 45, 46, 69]. It contains information of all correlation functions [6, 40, 41]. Moreover, it has been shown in [19, 41] that the density matrix is independent of the size of the chain and the location of the block relative to the ends. Therefore we can take the length of the block equal to the length of the whole chain. (i.e. we can add two ending spins $S/2$ directly to the block.) Then by using the Schmidt decomposition [56], we can show that the density matrix of the block is equivalent to the density matrix of the two ending spins. By equivalent we mean that all non-zero eigenvalues are the same. Using this method, eigenvalues of the density matrix as well as entanglement entropies were obtained [19, 25, 41] without knowing the eigenvectors explicitly.

However, eigenvectors of the density matrix have their own importance. They can be used to study the structure and symmetries of the density matrix explicitly both for finite block and in large block limit. The construction of eigenvectors also provides us with a possible method to diagonalize the density matrix directly. As to be shown in following sections (see Sects. 2.3, 2.4, 4.3), the eigenvectors also have their own physical meaning as degenerate zero-energy ground states. In the context of the Haldane gap, these degenerate states are known as *edge states* and have been observed in the $S = 1$ spin chain compound [32]. Furthermore, eigenvectors become indispensable in quantum computing algorithms, particularly in discussing quantum measurements.

In this paper, we consider AKLT models with two different boundary conditions. Let's first take spin $S = 1$ for example. The system consists of a linear chain of N spin-1's in the

bulk, and two spin-1/2's on the boundaries. We shall denote by $\mathbf{S}_j$ the vector spin operator at site j ($j = 0, 1, \ldots, N+1$). The Hamiltonian is

$$H_{uniq} = \frac{1}{2}\sum_{j=1}^{N-1}\left(\mathbf{S}_j \cdot \mathbf{S}_{j+1} + \frac{1}{3}\left(\mathbf{S}_j \cdot \mathbf{S}_{j+1}\right)^2 + \frac{2}{3}\right) + \pi_{0,1} + \pi_{N,N+1}. \tag{1}$$

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

$$\pi_{0,1} \equiv \frac{2}{3}\left(1 + \mathbf{S}_0 \cdot \mathbf{S}_1\right), \qquad \pi_{N,N+1} \equiv \frac{2}{3}\left(1 + \mathbf{S}_N \cdot \mathbf{S}_{N+1}\right). \tag{2}$$

The Hamiltonian (1) has a unique ground state (VBS state), thus we shall call it *the unique Hamiltonian*. Alternatively, if we consider spin-1's at every site including the boundaries, then the Hamiltonian takes the form

$$H_{deg} = \frac{1}{2}\sum_{j=1}^{N-1}\left(\mathbf{S}_j \cdot \mathbf{S}_{j+1} + \frac{1}{3}\left(\mathbf{S}_j \cdot \mathbf{S}_{j+1}\right)^2 + \frac{2}{3}\right). \tag{3}$$

The ground states of this Hamiltonian are 4-fold degenerate. We shall call (3) *the degenerate Hamiltonian*.

For generic spin-S, the unique Hamiltonian is

$$H_{uniq} = \sum_{j=1}^{N-1}\sum_{J=S+1}^{2S} C_J P^J_{j,j+1} + \pi_{0,1} + \pi_{N,N+1}, \tag{4}$$

where the projector $P^J_{j,j+1}$ projects the bond spin $\mathbf{J}_{j,j+1} \equiv \mathbf{S}_j + \mathbf{S}_{j+1}$ onto the subspace with total spin J ($J = S+1, \ldots, 2S$). The boundary terms describe interactions between a spin-$S/2$ and a spin-S:

$$\pi_{0,1} \equiv \sum_{J=S/2+1}^{3S/2} D_J P^J_{0,1}, \qquad \pi_{N,N+1} \equiv \sum_{J=S/2+1}^{3S/2} D_J P^J_{N,N+1}. \tag{5}$$

Both coefficients C_J and D_J can take arbitrary positive values. Correspondingly, the degenerate Hamiltonian with spin-S at every site takes the form

$$H_{deg} = \sum_{j=1}^{N-1}\sum_{J=S+1}^{2S} C_J P^J_{j,j+1}. \tag{6}$$

The degeneracy of the ground states is $(S+1)^2$. This will be important in description of eigenvectors of the density matrix (see Sects. 2.4 and 3).

Consider the AKLT spin chain system with the unique Hamiltonian (4) in the VBS ground state. The density matrix $\boldsymbol{\rho}$ of the whole chain is a projector onto the unique VBS ground state (see (10)). If we pick up a block of L contiguous bulk spins as a subsystem and trace out all degrees of freedom outside the block, then we obtain the density matrix $\boldsymbol{\rho}_L$ of the subsystem (see (14)). Because of entanglement with spins outside the block, $\boldsymbol{\rho}_L$ will no longer be a pure state density matrix as $\boldsymbol{\rho}$ is in general. We shall prove that the density matrix $\boldsymbol{\rho}_L$ is a projector onto a $(S+1)^2$-dimensional subspace of the complete Hilbert space

associated with the block (see Sects. 2.4 and 3). The degenerate Hamiltonian (6) becomes essential in description of this subspace. When the degenerate Hamiltonian has its size N equal to that of the block L, it is referred to as *the block Hamiltonian* and denoted by H_b which is defined by (21). It turns out that the block Hamiltonian H_b (i.e. the degenerate Hamiltonian H_{deg} in (6) with $N = L$) defines the density matrix $\boldsymbol{\rho}_L$ completely in the large block limit $L \to \infty$. The zero-energy ground states of the block Hamiltonian H_b span the subspace that the density matrix $\boldsymbol{\rho}_L$ projects onto. So that $\boldsymbol{\rho}_L$ can be represented as the zero-temperature limit of the canonical ensemble density matrix defined by H_b:

$$\boldsymbol{\rho}_L = \lim_{\beta \to +\infty} \frac{e^{-\beta H_b}}{\mathrm{Tr}[e^{-\beta H_b}]}, \quad L \to \infty, \tag{7}$$

where

$$H_b \equiv H_{deg}(\text{with } N = L) = \sum_{j=1}^{L-1} \sum_{J=S+1}^{2S} C_J P^J_{j,j+1}. \tag{8}$$

In the zero-temperature limit, contributions from excited states of H_b all vanish and the right hand side of (7) turns into a projector onto the ground states of the block Hamiltonian.

As main subjects of the paper, we will construct eigenvectors and derive expressions for corresponding eigenvalues of the density matrix. We will show that the density matrix is a projector. The paper is divided into four parts:

1. We calculate the density matrix, prove a theorem on eigenvectors and express eigenvalues in two different forms using the Schwinger representation (Sect. 2).
2. We investigate the structure of the density matrix in the large block limit. As characteristic functions of quantum entanglement, the von Neumann entropy and the Renyi entropy are obtained in the limit (Sect. 3).
3. We study the density matrix using a different representation (a pure algebraic method) for spin $S = 1$ (Sect. 4).
4. An alternative proof of the theorem on eigenvectors is given as we take a different approach (Sect. 5).

2 Density Matrix for Generic Spin-S

2.1 Ground State of the Unique Hamiltonian

We start with the ground state of the unique Hamiltonian (4). It is given in the Schwinger representation by the VBS state [6]

$$|\mathrm{VBS}\rangle \equiv \prod_{j=0}^{N} \left(a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger\right)^S |\mathrm{vac}\rangle, \tag{9}$$

where $a^\dagger$, $b^\dagger$ are bosonic creation operators and $|\mathrm{vac}\rangle$ is destroyed by any of the annihilation operators a, b. These operators satisfy $[a_i, a_j^\dagger] = [b_i, b_j^\dagger] = \delta_{ij}$ with all other commutators vanishing. The spin operators are represented as $S_j^+ = a_j^\dagger b_j$, $S_j^- = b_j^\dagger a_j$, $S_j^z = (a_j^\dagger a_j - b_j^\dagger b_j)/2$. To reproduce the dimension of the spin-S Hilbert space at each site, an additional constraint on the total boson occupation number is required, namely

$(a_j^\dagger a_j + b_j^\dagger b_j)/2 = S$. More details and properties of the VBS state in the Schwinger representation can be found in [6, 8, 45, 46]. The pure state density matrix of the VBS ground state (9) is

$$\boldsymbol{\rho} = \frac{|\mathrm{VBS}\rangle\langle\mathrm{VBS}|}{\langle\mathrm{VBS}|\mathrm{VBS}\rangle}. \tag{10}$$

For normalization $\langle\mathrm{VBS}|\mathrm{VBS}\rangle$ of the VBS state, see Appendix A.

2.2 Density Matrix of a Block of Bulk Spins

We take a block of L contiguous bulk spins as a subsystem. In order to calculate the density matrix of the block, it is convenient to introduce a spin coherent state representation. We introduce spinor coordinates

$$(u, v) \equiv \left(\cos\frac{\theta}{2}e^{i\frac{\phi}{2}}, \sin\frac{\theta}{2}e^{-i\frac{\phi}{2}}\right), \quad 0 \le \theta \le \pi,\ 0 \le \phi \le 2\pi. \tag{11}$$

Then for a point $\hat{\Omega} \equiv (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$ on the unit sphere, the spin-S coherent state is defined as

$$|\hat{\Omega}\rangle \equiv \frac{(ua^\dagger + vb^\dagger)^{2S}}{\sqrt{(2S)!}}|\mathrm{vac}\rangle. \tag{12}$$

Here we have fixed the overall phase (a $U(1)$ gauge degree of freedom) since it has no physical content. Note that (12) is covariant under $SU(2)$ transforms (see Sect. 3). The set of coherent states is complete (but not orthogonal) such that [4, 25]

$$\frac{2S+1}{4\pi}\int d\hat{\Omega}|\hat{\Omega}\rangle\langle\hat{\Omega}| = \sum_{m=-S}^{S}|S, m\rangle\langle S, m| = I_{2S+1}, \tag{13}$$

where $|S, m\rangle$ denote the eigenstate of $\mathbf{S}^2$ and S_z, and I_{2S+1} is the identity of the $(2S+1)$-dimensional Hilbert space for spin-S. The completeness relation (13) can be used in taking trace of an arbitrary operator.

Now we calculate the density matrix of a block of L contiguous bulk spins in the VBS state (9). By definition, this is achieved by taking the pure state density matrix (10) and tracing out all spin degrees of freedom outside the block:

$$\boldsymbol{\rho}_L \equiv \mathrm{Tr}_{0,1,\ldots,k-1,k+L,\ldots,N,N+1}\left[\boldsymbol{\rho}\right], \quad 1 \le k,\ k+L-1 \le N. \tag{14}$$

Here the block of length L starts from site k and ends at site $k+L-1$. $\boldsymbol{\rho}_L$ is no longer a pure state density matrix because of entanglement of the block with the environment (sites outside the block of the spin chain). It was shown in Sect. 2 of [40] that entries of the density matrix are multi-point correlation functions in the ground state. The original proof was for spin $S = 1/2$. This statement is generalized to generic spin-S in Appendix D.

Using the coherent state representation (12) and completeness relation (13), $\boldsymbol{\rho}_L$ can be written as [41]

$$\boldsymbol{\rho}_L = \frac{\int [\prod_{j=0}^{k-1}\prod_{j=k+L}^{N+1} d\hat{\Omega}_j] \prod_{j=0}^{k-2}\prod_{j=k+L}^{N} [\frac{1}{2}(1-\hat{\Omega}_j\cdot\hat{\Omega}_{j+1})]^S B^\dagger |\mathrm{VBS}_L\rangle\langle \mathrm{VBS}_L| B}{[\frac{(2S+1)!}{4\pi}]^L \int [\prod_{j=0}^{N+1} d\hat{\Omega}_j] \prod_{j=0}^{N} [\frac{1}{2}(1-\hat{\Omega}_j\cdot\hat{\Omega}_{j+1})]^S}. \tag{15}$$

Here the boundary operator B and block VBS state $|\mathrm{VBS}_L\rangle$ are defined as

$$B \equiv (u_{k-1}b_k - v_{k-1}a_k)^S (a_{k+L-1}v_{k+L} - b_{k+L-1}u_{k+L})^S, \tag{16}$$

$$|\mathrm{VBS}_L\rangle \equiv \prod_{j=k}^{k+L-2} \left(a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger\right)^S |\mathrm{vac}\rangle, \tag{17}$$

respectively. Note that both B and $|\mathrm{VBS}_L\rangle$ are $SU(2)$ covariant (see Sect. 3). The expression (15) can be simplified. We can perform the integrals over $\hat{\Omega}_j$ ($j = 0, 1, \ldots, k-2, k+L+1, \ldots, N, N+1$) in the numerator and all integrals in the denominator (see Appendix A). After integrating over these variables, the density matrix $\boldsymbol{\rho}_L$ turns out to be independent of both the starting site k and the total length L of the block. This property has been proved in [19] for spin $S = 1$ (using a different representation, namely the maximally entangled states, see Sect. 4) and generalized in [41] for generic spin-S. Therefore, we can choose $k = 1$ and the density matrix takes the form

$$\boldsymbol{\rho}_L = \left[\frac{S+1}{(2S+1)!}\right]^L \frac{(S+1)}{(4\pi)^2} \int d\hat{\Omega}_0\, d\hat{\Omega}_{L+1} B^\dagger |\mathrm{VBS}_L\rangle\langle \mathrm{VBS}_L| B \tag{18}$$

with

$$B^\dagger = \left(u_0^* b_1^\dagger - v_0^* a_1^\dagger\right)^S \left(a_L^\dagger v_{L+1}^* - b_L^\dagger u_{L+1}^*\right)^S, \tag{19}$$

$$|\mathrm{VBS}_L\rangle = \prod_{j=1}^{L-1} \left(a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger\right)^S |\mathrm{vac}\rangle. \tag{20}$$

The last two integral of (18) can be performed, but we keep its present form for later use.

2.3 Ground States of the Block Hamiltonian

In order to describe the eigenvectors of the density matrix (18), we first study the zero-energy ground states of the degenerate Hamiltonian defined in (6). We choose the length of the spin chain equal to that of the block, i.e. $N = L$, then the degenerate Hamiltonian is called the block Hamiltonian and reads

$$H_b \equiv H_{deg}(\text{with } N = L) = \sum_{j=1}^{L-1} \sum_{J=S+1}^{2S} C_J P_{j,j+1}^J. \tag{21}$$

Now we define a set of $S+1$ operators covariant under $SU(2)$

$$A_J^\dagger \equiv \left(ua_1^\dagger + vb_1^\dagger\right)^J \left(a_1^\dagger b_L^\dagger - b_1^\dagger a_L^\dagger\right)^{S-J} \left(ua_L^\dagger + vb_L^\dagger\right)^J, \quad 0 \le J \le S. \tag{22}$$

These operators act on the direct product of Hilbert spaces of spins at site 1 and site L. Then the set of ground states of (21) can be chosen as

$$|\mathrm{G}; J, \hat{\Omega}\rangle \equiv A_J^\dagger |\mathrm{VBS}_L\rangle, \quad J = 0, \ldots, S. \tag{23}$$

Any state $|\mathrm{G}; J, \hat{\Omega}\rangle$ of this set for fixed J and $\hat{\Omega}$ is a zero-energy ground state of (21). To prove this we need only to verify: (i) the total power of $a_1^\dagger$ and $b_1^\dagger$ is $2S$, so that we have spin-S at the first site; (ii) $-S \le J_{1,2}^z \equiv S_1^z + S_2^z \le S$ by a binomial expansion, so that the maximum value of the bond spin $J_{1,2}$ is S (from $SU(2)$ invariance, see [6]). These properties are true for any other site j and bond $(j, j+1)$, respectively. Therefore, the state $|\mathrm{G}; J, \hat{\Omega}\rangle$ defined in (23) has spin-S at each site and no projection onto the $J_{j,j+1} > S$ subspace for any bond.

The set of states $\{|\mathrm{G}; J, \hat{\Omega}\rangle\}$ depend on a discrete parameter J as well as a continuous unit vector $\hat{\Omega}$. States with the same J value are not orthogonal. The rank of a set of states with the same J value is $2J+1$, which can be obtained from the completeness relation (121) (see Appendix B and [35]). Thus the total number of linearly independent states of the set $\{|\mathrm{G}; J, \hat{\Omega}\rangle\}$ is $\sum_{J=0}^{S}(2J+1) = (S+1)^2$, which is exactly the degeneracy of the ground states of (21). So that $\{|\mathrm{G}; J, \hat{\Omega}\rangle\}$ forms a complete set of zero-energy ground states.

We also introduce an orthogonal basis in description of the degenerate zero-energy ground states. It is shown in Appendix B and [35] that $A_J^\dagger$ (22) can be expanded in terms of spin creation operators $\Psi_{JM}^\dagger$ $(M = -J, \ldots, J)$ defined in (119). Operator $\Psi_{JM}^\dagger$ acts on the direct product of two Hilbert spaces of spins at site 1 and site L (120) and can be expressed in terms of bosonic creation operators in the Schwinger representation (115). If we define a set of *degenerate VBS states* $\{|\mathrm{VBS}_L(J, M)\rangle\}$ such that

$$|\mathrm{VBS}_L(J, M)\rangle \equiv \Psi_{JM}^\dagger |\mathrm{VBS}_L\rangle, \quad J = 0, \ldots, S, \ M = -J, \ldots, J, \tag{24}$$

then these $(S+1)^2$ states (24) are not only linearly independent but also mutually orthogonal (Appendix C). Furthermore, any ground state $|\mathrm{G}; J, \hat{\Omega}\rangle$ can be written as a linear superposition over these degenerate VBS states, and *vice versa* (see (122) of Appendix B). The set $\{|\mathrm{VBS}_L(J, M)\rangle\}$ differs from $\{|\mathrm{G}; J, \hat{\Omega}\rangle\}$ by a change of basis, so that it also forms a complete set of zero-energy ground states.

2.4 Eigenvectors of the Density Matrix

Eigenvalues of the density matrix (18) are derived for spin-1 in [19] and for spin-S in [41]. Because the density matrix is independent of both the total length of the spin chain and the starting site of the block, we can add boundary spins directly to the ends of the block. It was shown in [19, 41] by a Schmidt decomposition (see [56]) that non-zero eigenvalues of the density matrix (18) are equal to those of the density matrix of the two boundary spins. All other eigenvalues of the density matrix (18) are zero. This fact reveals the structure of the density matrix as a projector onto a subspace of dimension $(S+1)^2$.

Now we propose a theorem on the eigenvectors of the density matrix given by (18). The explicit construction of eigenvectors allows us to diagonalize the density matrix directly. The set of eigenvectors also spans the subspace that the density matrix projects onto.

Theorem 1 *Eigenvectors of the density matrix* $\boldsymbol{\rho}_L$ (18) *with non-zero eigenvalues are given by the set* $\{|G; J, \hat{\Omega}\rangle\}$ (23), *or, equivalently, by the set* $\{|\mathrm{VBS}_L(J, M)\rangle\}$ (24). *i.e. they are zero-energy ground states of the block Hamiltonian* H_b (21).

We prove the theorem by showing that the density matrix $\boldsymbol{\rho}_L$ (18) can be written as a projector in diagonal form onto the orthogonal degenerate VBS states $\{|\mathrm{VBS}_L(J, M)\rangle\}$ introduced in (24). An alternative proof taking a different approach is given in Sect. 5.

First, it is realized from the definition of spinor coordinates (11) that if we change variables (u, v) to $(iv^*, -iu^*)$, then the unit vector $\hat{\Omega}$ is inverted about the origin to $-\hat{\Omega}$. So that we have [41]

$$(u^* b^\dagger - v^* a^\dagger)^S |\text{vac}\rangle = i^S \sqrt{S!}\, |-\hat{\Omega}\rangle, \tag{25}$$

where $|-\hat{\Omega}\rangle$ means a spin-$S/2$ coherent state for a point opposite to $\hat{\Omega}$ on the unit sphere. Therefore, taking expressions of the boundary operator $B^\dagger$ (19) and the block VBS state $|\text{VBS}_L\rangle$ (20), we have

$$\begin{aligned} &B^\dagger |\text{VBS}_L\rangle \\ &= S! \prod_{j=1}^{L-1} \left(a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger \right)^S |-\hat{\Omega}_0\rangle_1 \otimes |\text{vac}\rangle_2 \otimes \cdots \otimes |\text{vac}\rangle_{L-1} \otimes |-\hat{\Omega}_{L+1}\rangle_L . \end{aligned} \tag{26}$$

Consequently the density matrix $\boldsymbol{\rho}_L$ (18) can be re-written as

$$\begin{aligned} \boldsymbol{\rho}_L = &\left[\frac{S+1}{(2S+1)!} \right]^L \frac{S!S!}{S+1} \prod_{j=1}^{L-1} \left(a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger \right)^S \\ &\times I_{S+1}^{(1)} \otimes |\text{vac}\rangle_2 \langle \text{vac}| \otimes \cdots \otimes |\text{vac}\rangle_{L-1} \langle \text{vac}| \otimes I_{S+1}^{(L)} \prod_{j=1}^{L-1} \left(a_j b_{j+1} - b_j a_{j+1} \right)^S , \end{aligned} \tag{27}$$

where $I_{S+1}^{(1)}$ and $I_{S+1}^{(L)}$ are $(S+1)$-dimensional identities associated with site 1 and site L, respectively. In obtaining (27), we have changed integral variables from $\hat{\Omega}_0$, $\hat{\Omega}_{L+1}$ to $-\hat{\Omega}_0$, $-\hat{\Omega}_{L+1}$ and performed these two integrals using the completeness relation (13). Next we notice that (see Appendix B)

$$\begin{aligned} I_{S+1}^{(1)} \otimes I_{S+1}^{(L)} &= \sum_{J=0}^{S} \sum_{M=-J}^{J} |J, M\rangle_{1,L} \langle J, M| \\ &= \sum_{J=0}^{S} \sum_{M=-J}^{J} \Psi_{JM}^\dagger |\text{vac}\rangle_1 \langle \text{vac}| \otimes |\text{vac}\rangle_L \langle \text{vac}| \Psi_{JM} . \end{aligned} \tag{28}$$

As a result, combining (27) and (28), recalling definitions of $|\text{VBS}_L\rangle$ (20) and $|\text{VBS}_L(J, M)\rangle$ (24), the density matrix $\boldsymbol{\rho}_L$ takes the following final form

$$\begin{aligned} \boldsymbol{\rho}_L &= \left[\frac{S+1}{(2S+1)!} \right]^L \frac{S!S!}{S+1} \sum_{J=0}^{S} \sum_{M=-J}^{J} \Psi_{JM}^\dagger |\text{VBS}_L\rangle \langle \text{VBS}_L| \Psi_{JM} \\ &\equiv \left[\frac{S+1}{(2S+1)!} \right]^L \frac{S!S!}{S+1} \sum_{J=0}^{S} \sum_{M=-J}^{J} |\text{VBS}_L(J, M)\rangle \langle \text{VBS}_L(J, M)| . \end{aligned} \tag{29}$$

The set of degenerate VBS states $\{|\text{VBS}_L(J, M)\rangle\}$ with $J = 0, \ldots, S$ and $M = -J, \ldots, J$ forms an orthogonal basis (see Appendix C). These $(S+1)^2$ states also forms a complete set of zero-energy ground states of the block Hamiltonian (21) (see Sect. 2.3 and Appendix B). So that in expression (29) we have put the density matrix as a projector in diagonal form

over an orthogonal basis. Each degenerate VBS state $|\mathrm{VBS}_L(J,M)\rangle$ is an eigenvector of the density matrix, so as any of the state $|\mathrm{G};J,\hat{\Omega}\rangle$ (because of the degeneracy of corresponding eigenvalues of the density matrix, see Sect. 2.5 and Sect. 2.6). Thus we have proved Theorem 1.

2.5 Eigenvalues of the Density Matrix (Recurrence Formula)

Having constructed eigenvectors, we need to specify the corresponding eigenvalues. An explicit expression of eigenvalues is obtained in Sect. 2.6. In this subsection we express eigenvalues through a conjectured recurrence formula as in [25] and [41]. Let's apply the density matrix $\boldsymbol{\rho}_L$ (18) to the state $|\mathrm{G};J,\hat{\Omega}\rangle$ (23) and get

$$\boldsymbol{\rho}_L|\mathrm{G};J,\hat{\Omega}\rangle=\left[\frac{S+1}{(2S+1)!}\right]^L\frac{S+1}{(4\pi)^2}\int d\hat{\Omega}_0\,d\hat{\Omega}_{L+1}B^\dagger|\mathrm{VBS}_L\rangle\langle\mathrm{VBS}_L|BA_J^\dagger|\mathrm{VBS}_L\rangle. \quad (30)$$

Using the coherent state representation (12) and completeness relation (13), the factor $\langle\mathrm{VBS}_L|BA_J^\dagger|\mathrm{VBS}_L\rangle$ in (30) can be re-written as

$$\begin{aligned}&\langle\mathrm{VBS}_L|BA_J^\dagger|\mathrm{VBS}_L\rangle\\&=\left[\frac{(2S+1)!}{4\pi}\right]^L\int\left(\prod_{j=1}^{L}d\hat{\Omega}_j\right)\prod_{j=1}^{L-1}\left[\frac{1}{2}(1-\hat{\Omega}_j\cdot\hat{\Omega}_{j+1})\right]^S(u_0v_1-v_0u_1)^S\\&\times\left(uu_1^*+vv_1^*\right)^J\left(u_1^*v_L^*-v_1^*u_L^*\right)^{S-J}\left(uu_L^*+vv_L^*\right)^J(u_Lv_{L+1}-v_Lu_{L+1})^S. \quad (31)\end{aligned}$$

The factor $[\frac{1}{2}(1-\hat{\Omega}_j\cdot\hat{\Omega}_{j+1})]^S$ under the integral of (31) can be expanded in terms of Legendre polynomials and further in terms of spherical harmonics as [25, 41]

$$\begin{aligned}\left[\frac{1}{2}(1-\hat{\Omega}_j\cdot\hat{\Omega}_{j+1})\right]^S&=\frac{1}{S+1}\sum_{l=0}^{S}(2l+1)\lambda(l,S)P_l(\hat{\Omega}_j\cdot\hat{\Omega}_{j+1})\\&=\frac{4\pi}{S+1}\sum_{l=0}^{S}\lambda(l,S)\sum_{m=-l}^{l}Y_{lm}(\hat{\Omega}_j)Y_{lm}^*(\hat{\Omega}_{j+1}) \quad (32)\end{aligned}$$

with coefficients $\lambda(l,S)$ given by

$$\lambda(l,S)\equiv\frac{(-1)^lS!(S+1)!}{(S-l)!(S+l+1)!}. \quad (33)$$

Using the expansion (32) and orthogonality of spherical harmonics, the integrals over $\hat{\Omega}_j$ with $j=2,\ldots,L-1$ in (31) can be performed. The result is

$$\begin{aligned}\langle\mathrm{VBS}_L|BA_J^\dagger|\mathrm{VBS}_L\rangle&=\frac{S+1}{(4\pi)^2}\left[\frac{(2S+1)!}{S+1}\right]^L\sum_{l=0}^{S}(2l+1)\lambda^{L-1}(l,S)\\&\times\int d\hat{\Omega}_1\,d\hat{\Omega}_L\,P_l(\hat{\Omega}_1\cdot\hat{\Omega}_L)\,(u_0v_1-v_0u_1)^S\left(uu_1^*+vv_1^*\right)^J\\&\times\left(u_1^*v_L^*-v_1^*u_L^*\right)^{S-J}\left(uu_L^*+vv_L^*\right)^J(u_Lv_{L+1}-v_Lu_{L+1})^S. \quad (34)\end{aligned}$$

We plug the expression (34) into (30). Using transformation properties under $SU(2)$ and binomial expansion (see Sect. 3), the integral over $\hat{\Omega}_0$ yields that

$$\int d\hat{\Omega}_0 \left(u_0^* b_1^\dagger - v_0^* a_1^\dagger\right)^S (u_0 v_1 - v_0 u_1)^S = \frac{4\pi}{S+1} \left(u_1 a_1^\dagger + v_1 b_1^\dagger\right)^S. \tag{35}$$

Similarly we can perform the integral over $\hat{\Omega}_{L+1}$. As a result, the following expression is obtained from (30):

$$\boldsymbol{\rho}_L |\mathrm{G}; J, \hat{\Omega}\rangle = \frac{1}{(4\pi)^2} \sum_{l=0}^{S} (2l+1) \lambda^{L-1}(l, S) K_l^\dagger(\hat{\Omega}) \, |\mathrm{VBS}_L\rangle. \tag{36}$$

The operator $K_l^\dagger(\hat{\Omega})$ involved in (36) is defined as

$$\begin{aligned} K_l^\dagger(\hat{\Omega}) \equiv \int d\hat{\Omega}_1 \, d\hat{\Omega}_L \left(u_1 a_1^\dagger + v_1 b_1^\dagger\right)^S \left(u u_1^* + v v_1^*\right)^J \left(u_1^* v_L^* - v_1^* u_L^*\right)^{S-J} \\ \times \left(u u_L^* + v v_L^*\right)^J \left(u_L a_L^\dagger + v_L b_L^\dagger\right)^S P_l(\hat{\Omega}_1 \cdot \hat{\Omega}_L). \end{aligned} \tag{37}$$

It is expressed as an integral depending on the order l of the Legendre polynomial $P_l(\hat{\Omega}_1 \times \hat{\Omega}_L)$. $K_l^\dagger(\hat{\Omega})$ can be calculated from the lowest few orders (see Sect. 3 for example). It becomes increasingly difficult to perform the integral as order l increases. Based on the eigenvalues of the density matrix obtained in [19, 41], we make a conjecture on the explicit form of the operator $K_l^\dagger(\hat{\Omega})$ for generic order l:

Conjecture 1

$$K_l^\dagger(\hat{\Omega}) = \left(\frac{4\pi}{S+1}\right)^2 I_l \left(\frac{1}{2} J(J+1) - \frac{1}{2} S\left(\frac{1}{2} S + 1\right)\right) A_J^\dagger. \tag{38}$$

Here the polynomial $I_l(x)$ satisfy the recurrence relation

$$I_{l+1}(x) = \frac{2l+1}{(S+l+2)^2} \left(\frac{4x}{l+1} + l\right) I_l(x) - \frac{l}{l+1} \left(\frac{S-l+1}{S+l+2}\right)^2 I_{l-1}(x) \tag{39}$$

with $I_0 = 1$ and $I_1 = \frac{x}{(\frac{S}{2}+1)^2}$.

Note that it is important that $K_l^\dagger(\hat{\Omega}) \propto A_J^\dagger$ defined in (22) and $I_l(x)$ has the same order as the Legendre polynomial $P_l(x)$. The recurrence relation (39) was proposed in [25] and used in [41] to obtain the eigenvalues of the density matrix. (The original definition of $I_l(x)$ differed from our definition in (39) by a factor of $\frac{2l+1}{4\pi}$.) Conjecture 1 (38) is an alternative form of Theorem 1, which also gives eigenvalues through the recurrence relation (39). Indeed, expressions (36), altogether with (38) and (39) yields that

$$\begin{aligned} &\boldsymbol{\rho}_L |\mathrm{G}; J, \hat{\Omega}\rangle \\ &= \frac{1}{(S+1)^2} \sum_{l=0}^{S} (2l+1) \lambda^{L-1}(l, S) I_l \left(\frac{1}{2} J(J+1) - \frac{1}{2} S\left(\frac{1}{2} S + 1\right)\right) |\mathrm{G}; J, \hat{\Omega}\rangle. \end{aligned} \tag{40}$$

Non-zero eigenvalues ($J = 0, 1, \ldots, S$) are seen from (40) as

$$\Lambda(J) \equiv \frac{1}{(S+1)^2} \sum_{l=0}^{S} (2l+1)\lambda^{L-1}(l,S) I_l\left(\frac{1}{2}J(J+1) - \frac{1}{2}S\left(\frac{1}{2}S+1\right)\right). \tag{41}$$

Since all other eigenvalues of the density matrix are vanishing, then we conclude again that the density matrix $\boldsymbol{\rho}_L$ (18) is a projector onto a subspace of dimension $(S+1)^2$. This subspace is spanned by the set of vectors $\{|\mathrm{G}; J, \hat{\Omega}\rangle\}$ (23). (The rank of the set is equal to $(S+1)^2$.) Furthermore, we observe from (41) that non-zero eigenvalues $\Lambda(J)$ depend only on J, not on $\hat{\Omega}$. Therefore, $\{|\mathrm{G}; J, \hat{\Omega}\rangle\}$ with fixed J value spans a degenerate subspace with the same eigenvalue.

2.6 Eigenvalues of the Density Matrix (Normalization of Degenerate VBS States)

Based on the diagonalized form (29), eigenvalues of the density matrix $\boldsymbol{\rho}_L$ can be derived from the normalization of degenerate VBS states. We obtain an explicit expression for eigenvalues in terms of Wigner $3j$-symbols in this subsection.

First, the following property is important: Normalization of the degenerate VBS state $|\mathrm{VBS}_L(J, M)\rangle$ depends only on J and is independent of M. With the introduction of total spin operators of the block $S^{\pm}_{\mathrm{tot}}$, S^{z}_{tot} and $\mathbf{S}^2_{\mathrm{tot}}$ (see Appendix C), we prove the statement as follows:

$$\begin{aligned}
&\langle \mathrm{VBS}_L(J, M \pm 1)|\mathrm{VBS}_L(J, M \pm 1)\rangle \\
&= \frac{1}{(J \mp M)(J \pm M + 1)} \langle \mathrm{VBS}_L(J, M)|S^{\mp}_{\mathrm{tot}} S^{\pm}_{\mathrm{tot}}|\mathrm{VBS}_L(J, M)\rangle \\
&= \frac{1}{(J \mp M)(J \pm M + 1)} \langle \mathrm{VBS}_L(J, M)|(\mathbf{S}^2_{\mathrm{tot}} - (S^{z}_{\mathrm{tot}})^2 \mp S^{z}_{\mathrm{tot}})|\mathrm{VBS}_L(J, M)\rangle \\
&= \langle \mathrm{VBS}_L(J, M)|\mathrm{VBS}_L(J, M)\rangle.
\end{aligned} \tag{42}$$

Here we have used the fact that $|\mathrm{VBS}_L(J, M)\rangle$ is the eigenstate of $\mathbf{S}^2_{\mathrm{tot}}$ and $\mathbf{S}^{z}_{\mathrm{tot}}$ with eigenvalues $J(J+1)$ and M, respectively (see Appendix C).

It is also realized that normalization of $|\mathrm{VBS}_L(J, M)\rangle$ can be calculated from integrating the inner product of $|\mathrm{G}; J, \hat{\Omega}\rangle$ with itself over the unit vector $\hat{\Omega}$ such that

$$\frac{1}{4\pi} \int d\hat{\Omega} \langle \mathrm{G}; J, \hat{\Omega}|\mathrm{G}; J, \hat{\Omega}\rangle = \frac{(S+J+1)!(S-J)!J!J!}{(2J+1)!} \langle \mathrm{VBS}_L(J, M)|\mathrm{VBS}_L(J, M)\rangle. \tag{43}$$

In obtaining this relation (43) we have used expansion (122) and orthogonality (116) in Appendix B.

Let's consider the integral involved in (43). Using coherent state representation (12) and completeness relation (13) as before, we obtain

$$\begin{aligned}
&\frac{1}{4\pi} \int d\hat{\Omega} \langle \mathrm{G}; J, \hat{\Omega}|\mathrm{G}; J, \hat{\Omega}\rangle \\
&= \frac{1}{4\pi} \left[\frac{(2S+1)!}{4\pi}\right]^L \int d\hat{\Omega} \int \left[\prod_{j=1}^{L} d\hat{\Omega}_j\right] \prod_{j=1}^{L-1} \left[\frac{1}{2}(1 - \hat{\Omega}_j \cdot \hat{\Omega}_{j+1})\right]^S
\end{aligned}$$

$$\times \left[\frac{1}{2}(1-\hat{\Omega}_1\cdot\hat{\Omega}_L)\right]^{S-J}\left[\frac{1}{2}(1+\hat{\Omega}_1\cdot\hat{\Omega})\right]^{J}\left[\frac{1}{2}(1+\hat{\Omega}\cdot\hat{\Omega}_L)\right]^{J}. \tag{44}$$

Now we expand $[\frac{1}{2}(1-\hat{\Omega}_i\cdot\hat{\Omega}_j)]^J$ in terms of spherical harmonics as in (32), then integrate over $\hat{\Omega}$ and from $\hat{\Omega}_2$ to $\hat{\Omega}_{L-1}$, the right hand side of (44) is equal to

$$\begin{aligned}&\frac{4\pi((2S+1)!)^L}{(S+1)^{L-1}(S-J+1)(J+1)^2}\\&\times\sum_{l_1=0}^{S}\sum_{l_L=0}^{S-J}\sum_{l=0}^{J}\sum_{m_1=-l_1}^{l_1}\sum_{m_L=-l_L}^{l_L}\sum_{m=-l}^{l}\int d\hat{\Omega}_1\int d\hat{\Omega}_L\lambda^{L-1}(l_1,S)\lambda(l_L,S-J)\\&\times\lambda^2(l,J)Y_{l_1,m_1}(\hat{\Omega}_1)Y_{l_L,m_L}(\hat{\Omega}_1)Y_{l,m}(\hat{\Omega}_1)Y^*_{l_1,m_1}(\hat{\Omega}_L)Y^*_{l_L,m_L}(\hat{\Omega}_L)Y^*_{l,m}(\hat{\Omega}_L).\end{aligned} \tag{45}$$

Here we apply the following useful formula:

$$\begin{aligned}&\int d\hat{\Omega}Y_{l_1,m_1}(\hat{\Omega})Y_{l_L,m_L}(\hat{\Omega})Y_{l,m}(\hat{\Omega})\\&=\sqrt{\frac{(2l_1+1)(2l_L+1)(2l+1)}{4\pi}}\begin{pmatrix}l_1&l_L&l\\0&0&0\end{pmatrix}\begin{pmatrix}l_1&l_L&l\\m_1&m_L&m\end{pmatrix},\end{aligned} \tag{46}$$

where $\begin{pmatrix}l_1&l_L&l\\m_1&m_L&m\end{pmatrix}$ is the Wigner $3j$-symbol. Using formula (46), we carry out the integrals in (45) and obtain

$$\begin{aligned}&\frac{((2S+1)!)^L}{(S+1)^{L-1}(S-J+1)(J+1)^2}\\&\times\sum_{l_1=0}^{S}\sum_{l_L=0}^{S-J}\sum_{l=0}^{J}\sum_{m_1=-l_1}^{l_1}\sum_{m_L=-l_L}^{l_L}\sum_{m=-l}^{l}(2l_1+1)(2l_L+1)(2l+1)\\&\times\lambda^{L-1}(l_1,S)\lambda(l_L,S-J)\lambda^2(l,J)\begin{pmatrix}l_1&l_L&l\\0&0&0\end{pmatrix}^2\begin{pmatrix}l_1&l_L&l\\m_1&m_L&m\end{pmatrix}^2.\end{aligned} \tag{47}$$

The symbols obey the following orthogonality relation:

$$\sum_{m_1,m_L}(2l+1)\begin{pmatrix}l_1&l_L&l\\m_1&m_L&m\end{pmatrix}\begin{pmatrix}l_1&l_L&l'\\m_1&m_L&m'\end{pmatrix}=\delta_{ll'}\delta_{mm'}. \tag{48}$$

Using this orthogonality (48), we can recast expression (47) as

$$\begin{aligned}&\frac{((2S+1)!)^L}{(S+1)^{L-1}(S-J+1)(J+1)^2}\\&\times\sum_{l_1=0}^{S}\sum_{l_L=0}^{S-J}\sum_{l=0}^{J}(2l_1+1)(2l_L+1)(2l+1)\lambda^{L-1}(l_1,S)\\&\times\lambda(l_L,S-J)\lambda^2(l,J)\begin{pmatrix}l_1&l_L&l\\0&0&0\end{pmatrix}^2.\end{aligned} \tag{49}$$

The explicit value of $\left(\begin{smallmatrix} l_1 & l_L & l \\ 0 & 0 & 0 \end{smallmatrix}\right)$ is given by

$$\begin{pmatrix} l_1 & l_L & l \\ 0 & 0 & 0 \end{pmatrix} = (-1)^g \sqrt{\frac{(2g-2l_1)!(2g-2l_L)!(2g-2l)!}{(2g+1)!}} \frac{g!}{(g-l_1)!(g-l_L)!(g-l)!}, \tag{50}$$

if $l_1 + l_L + l = 2g$ ($g \in \mathbf{N}$), otherwise zero. Finally, normalization of degenerate VBS states $|\mathrm{VBS}_L(J, M)\rangle$ is obtained as

$$\begin{aligned} &\langle \mathrm{VBS}_L(J,M)|\mathrm{VBS}_L(J,M)\rangle \\ &= \frac{(2J+1)!((2S+1)!)^L}{(S+1)^{L-1}(S+J+1)!(S-J+1)!(J+1)!(J+1)!} \\ &\quad \times \sum_{l_1=0}^{S} \sum_{l_L=0}^{S-J} \sum_{l=0}^{J} (2l_1+1)(2l_L+1)(2l+1) \\ &\quad \times \lambda^{L-1}(l_1,S)\lambda(l_L,S-J)\lambda^2(l,J) \begin{pmatrix} l_1 & l_L & l \\ 0 & 0 & 0 \end{pmatrix}^2. \end{aligned} \tag{51}$$

Combining results of (29) and (51), we arrive at the following theorem on eigenvalues:

Theorem 2 *Eigenvalues $\Lambda(J)$ $(J = 0, \ldots, S)$ of the density matrix are independent of $\hat{\Omega}$ and/or M in defining eigenvectors (see (23) and (24)). An explicit expression is given by the following triple sum*

$$\begin{aligned} \Lambda(J) &= \left[\frac{S+1}{(2S+1)!}\right]^L \frac{S!S!}{S+1} \langle \mathrm{VBS}_L(J,M)|\mathrm{VBS}_L(J,M)\rangle \\ &= \frac{(2J+1)!S!S!}{(S+J+1)!(S-J+1)!(J+1)!(J+1)!} \\ &\quad \times \sum_{l_1=0}^{S} \sum_{l_L=0}^{S-J} \sum_{l=0}^{J} (2l_1+1)(2l_L+1)(2l+1)\lambda^{L-1}(l_1,S) \\ &\quad \times \lambda(l_L,S-J)\lambda^2(l,J) \begin{pmatrix} l_1 & l_L & l \\ 0 & 0 & 0 \end{pmatrix}^2. \end{aligned} \tag{52}$$

Although not straightforward to verify, this expression (52) should be consistent with eigenvalues given through the recurrence expression (41). We could check the case when $S = 1$ that

$$\begin{aligned} \langle \mathrm{VBS}_L(0,0)|\mathrm{VBS}_L(0,0)\rangle &= \frac{1}{2}(3^L + 3(-1)^L), \\ \langle \mathrm{VBS}_L(1,M)|\mathrm{VBS}_L(1,M)\rangle &= \frac{1}{2}(3^L - (-1)^L), \end{aligned} \tag{53}$$

where we have used the selection rule of the Wigner $3j$-symbol. From (114) we find that $\langle \mathrm{VBS}|\mathrm{VBS}\rangle = 2 \cdot 3^L$, so that we obtain the correct eigenvalues of the density matrix from the above result (52) (see Sect. 4 for comparison).

We shall emphasize at this point that given eigenvalues (52), both von Neumann entropy

$$S_{v.N} = -\mathrm{Tr}\left[\boldsymbol{\rho}_L \ln \boldsymbol{\rho}_L\right] = -\sum_{J=0}^{S}(2J+1)\Lambda(J)\ln\Lambda(J) \tag{54}$$

and Renyi entropy

$$S_R = \frac{1}{1-\alpha}\ln\left\{\mathrm{Tr}\left[\boldsymbol{\rho}_L^{\alpha}\right]\right\} = \frac{1}{1-\alpha}\ln\left\{\sum_{J=0}^{S}(2J+1)\Lambda^{\alpha}(J)\right\} \tag{55}$$

can be expressed directly.

3 Density Matrix in the Large Block Limit

In the limit $L \to \infty$, that is when the size of the block becomes large, we learned from [19, 31, 41] that the von Neumann entropy reaches the saturated value $S_{v.N} = \ln(S+1)^2$. Then the density matrix (denoted by $\boldsymbol{\rho}_\infty$ in the limit) can only take the form (see [56] for a general proof)

$$\boldsymbol{\rho}_\infty = \frac{1}{(S+1)^2} I_{(S+1)^2} \oplus \Phi_\infty, \tag{56}$$

where $I_{(S+1)^2}$ is the identity of dimension $(S+1)^2$ and Φ_∞ is an infinite dimensional matrix with only zero entries. In this section, we give a proof of Conjecture 1 (38) in the limiting case as $L \to \infty$. Then we shall verify the structure of the density matrix (56) explicitly.

We first realize from (33) that as $L \to \infty$, $\lambda^{L-1}(l, S) \to \delta_{l,0}$. Therefore only the first term with $l = 0$ is left in (36). So that we need only to calculate $K_0^{\dagger}(\hat{\Omega})$:

$$\begin{aligned} K_0^{\dagger}(\hat{\Omega}) = \int d\hat{\Omega}_1\, d\hat{\Omega}_L \left(u_1 a_1^{\dagger} + v_1 b_1^{\dagger}\right)^S \left(u u_1^* + v v_1^*\right)^J \\ \times \left(u_1^* v_L^* - v_1^* u_L^*\right)^{S-J} \left(u u_L^* + v v_L^*\right)^J \left(u_L a_L^{\dagger} + v_L b_L^{\dagger}\right)^S. \end{aligned} \tag{57}$$

It is useful to know transformation properties of the integrand in (57) under $SU(2)$. The pair of variables (u, v) defined in (11) and bosonic annihilation operators (a, b) in the Schwinger representation both transform as spinors under $SU(2)$. That is to say, if we take an arbitrary element $\mathbf{D} \in SU(2)$ (2×2 matrix), then (u, v), etc. transform according to

$$\begin{pmatrix} u \\ v \end{pmatrix} \to \mathbf{D} \begin{pmatrix} u \\ v \end{pmatrix}. \tag{58}$$

On the other hand, (u^*, v^*), $(-v, u)$, $(a^{\dagger}, b^{\dagger})$ and $(-b, a)$ transform conjugately to (u, v). That is to say (u^*, v^*), *etc.* transform according to

$$\begin{pmatrix} u^* \\ v^* \end{pmatrix} \to \mathbf{D}^* \begin{pmatrix} u^* \\ v^* \end{pmatrix}. \tag{59}$$

The combinations appeared in $K_0^\dagger(\hat{\Omega})$ (57)

$$u_1 a_1^\dagger + v_1 b_1^\dagger, \quad u u_1^* + v v_1^*, \quad u_1^* v_L^* - v_1^* u_L^*, \quad u u_L^* + v v_L^*, \quad u_L a_L^\dagger + v_L b_L^\dagger \tag{60}$$

as well as $A_J^\dagger$ in (22), boundary operator $B^\dagger$ in (19), etc. all transform covariantly under $SU(2)$, i.e. those expressions keep their form in the new (transformed) coordinates.

These transformation properties (58), (59) can be used to simplify the $K_0^\dagger(\hat{\Omega})$ integral. We first make a $SU(2)$ transform

$$\mathbf{D}_{u_L} = \begin{pmatrix} u_L^* & v_L^* \\ -v_L & u_L \end{pmatrix}, \qquad \mathbf{D}_{u_L} \begin{pmatrix} u_L \\ v_L \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \tag{61}$$

under the part of the integral (57) over $\hat{\Omega}_1$. Then this part of integral becomes

$$\int d\hat{\Omega}_1 \left(u_1 a_1^\dagger + v_1 b_1^\dagger\right)^S \left(u u_1^* + v v_1^*\right)^J \left(-v_1^*\right)^{S-J}. \tag{62}$$

This can be calculated using binomial expansion and the result is

$$\frac{4\pi}{S+1} \left(u a_1^\dagger + v b_1^\dagger\right)^J \left(-b_1^\dagger\right)^{S-J}. \tag{63}$$

Then we make an inverse transform in (63) using $\mathbf{D}_{u_L}^{-1} = \mathbf{D}_{u_L}^\dagger$, consequently (57) is put in a form with a single integral over $\hat{\Omega}_L$ remaining:

$$\begin{aligned} K_0^\dagger(\hat{\Omega}) = {} & \frac{4\pi}{S+1} \left(u a_1^\dagger + v b_1^\dagger\right)^J \\ & \times \int d\hat{\Omega}_L \left(a_1^\dagger v_L^* - b_1^\dagger u_L^*\right)^{S-J} \left(u u_L^* + v v_L^*\right)^J \left(u_L a_L^\dagger + v_L b_L^\dagger\right)^S. \end{aligned} \tag{64}$$

Now we make another $SU(2)$ transform using

$$\mathbf{D}_u = \begin{pmatrix} u^* & v^* \\ -v & u \end{pmatrix}, \qquad \mathbf{D}_u \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \tag{65}$$

then the remaining integral over $\hat{\Omega}_L$ in (64) becomes

$$\int d\hat{\Omega}_L \left(a_1^\dagger v_L^* - b_1^\dagger u_L^*\right)^{S-J} \left(u_L^*\right)^J \left(u_L a_L^\dagger + v_L b_L^\dagger\right)^S. \tag{66}$$

Using again binomial expansion, this integral (66) yields

$$\frac{4\pi}{S+1} \left(a_1^\dagger b_L^\dagger - b_1^\dagger a_L^\dagger\right)^{S-J} \left(a_L^\dagger\right)^J. \tag{67}$$

At last we make an inverse transform in (67) using $\mathbf{D}_u^{-1} = \mathbf{D}_u^\dagger$ and plug the result into (64), the final form is

$$K_0^\dagger(\hat{\Omega}) = \left(\frac{4\pi}{S+1}\right)^2 A_J^\dagger. \tag{68}$$

This expression is consistent with *Conjecture 1* (38), which also proves that $\{|\mathrm{G};J,\hat{\Omega}\rangle\}$ is a set of eigenvectors of the density matrix as $L\to\infty$. Let's denote the density matrix in the limit by $\boldsymbol{\rho}_\infty$. Then (68) leads to the result (see (40))

$$\boldsymbol{\rho}_\infty|\mathrm{G};J,\hat{\Omega}\rangle=\frac{1}{(S+1)^2}|\mathrm{G};J,\hat{\Omega}\rangle. \tag{69}$$

We find from (69) that the limiting eigenvalue $\Lambda_\infty=\frac{1}{(S+1)^2}$ is independent of J. Any vector of the $(S+1)^2$-dimensional subspace spanned by the set $\{|\mathrm{G};J,\hat{\Omega}\rangle\}$ is an eigenvector of $\boldsymbol{\rho}_\infty$ with the same eigenvalue $\frac{1}{(S+1)^2}$. Therefore $\boldsymbol{\rho}_\infty$ acts on this subspace as (proportional to) the identity $I_{(S+1)^2}$. So that we have proved explicitly that the density matrix takes the form (56) in the large block limit. In addition, we also derive from the eigenvalues that the von Neumann entropy $S_{v.N}=-\sum_{J=0}^{S}(2J+1)\Lambda_\infty\ln\Lambda_\infty$ coincides with the Renyi entropy $S_R=\frac{1}{1-\alpha}\ln\{\sum_{J=0}^{S}(2J+1)\Lambda_\infty^\alpha\}$ and is equal to the saturated value $\ln(S+1)^2$.

4 Density Matrix for Spin $S=1$

In the case of spin $S=1$, we could prove Conjecture 1 (38) for finite block by calculating $K_1^\dagger(\hat{\Omega})$ defined in (37) using similar methods as been used in Sect. 3. However, in this special case $S=1$, we have an alternative algebraic proof. We shall use a different representation in which the eigenvectors of the density matrix form an orthogonal basis (maximally entangled states). The formulation is base on [19].

4.1 Ground State of the Unique Hamiltonian

The unique Hamiltonian is given by (1). In order to represent the unique ground state, we first introduce the following notation for convenience [19]:

$$|\alpha\rangle\equiv(-1)^{1+\delta_{\alpha,0}}I\otimes\sigma_\alpha|0\rangle,\quad \alpha=0,1,2,3 \tag{70}$$

where $\sigma_0\equiv I$ (2-dimensional identity), $\sigma_{\alpha=1,2,3}$ are Pauli matrices and $|0\rangle\equiv\frac{-1}{\sqrt{2}}(|\uparrow\downarrow\rangle-|\downarrow\uparrow\rangle)$ is the singlet state (antisymmetric projection) of two spin-1/2's. The four states (70) (maximally entangled states) form an orthonormal basis of the Hilbert space of two spin-1/2 operators.

The spin-1 state at each site is represented by a symmetric projection of two spin-1/2 states given by (70) for $\alpha=1,2,3$. Let's take the jth site for example. The two spin-1/2's are labeled by $(j,\bar{j})$ (from left to right, respectively). Then the spin-1 states are prepared by projecting these two spin-1/2's (4-dimensional space) onto a symmetric 3-dimensional subspace spanned by

$$\begin{aligned}
|1\rangle_{j\bar{j}}&=\frac{1}{\sqrt{2}}(|\uparrow\rangle_j|\uparrow\rangle_{\bar{j}}-|\downarrow\rangle_j|\downarrow\rangle_{\bar{j}}),\\
|2\rangle_{j\bar{j}}&=\frac{-i}{\sqrt{2}}(|\uparrow\rangle_j|\uparrow\rangle_{\bar{j}}+|\downarrow\rangle_j|\downarrow\rangle_{\bar{j}}),\\
|3\rangle_{j\bar{j}}&=\frac{-1}{\sqrt{2}}(|\uparrow\rangle_j|\downarrow\rangle_{\bar{j}}+|\downarrow\rangle_j|\uparrow\rangle_{\bar{j}}).
\end{aligned} \tag{71}$$

Thus the two ending spin-1/2's are labeled as site $\bar{0}$ and $N+1$. The unique ground state in this representation is [1, 2, 19]

$$|\mathrm{G}\rangle = \left(\bigotimes_{j=1}^{N} P_{j\bar{j}}\right)|0\rangle_{\bar{0}1}|0\rangle_{\bar{1}2}\cdots|0\rangle_{\bar{N}N+1}. \tag{72}$$

Here $P_{j\bar{j}}$ projects two spin-1/2 states onto a symmetric subspace, which describes spin-1. Using basis (70), we have

$$P_{j\bar{j}} = \sum_{\alpha=1}^{3} |\alpha\rangle_{j\bar{j}}\langle\alpha|. \tag{73}$$

A crucial step (see [19]) is that the ground state (72) can be expressed in a different form using

$$|0\rangle_{\bar{A}B}|0\rangle_{\bar{B}C} = \frac{-1}{2}\sum_{\alpha=0}^{3} |\alpha\rangle_{B\bar{B}}\left[I_{\bar{A}}\otimes(\sigma_\alpha)_C\right]|0\rangle_{\bar{A}C} \tag{74}$$

for arbitrary labels A, B and C. Repeatedly using relation (74), the product of $|0\rangle$'s in (72) can be rewritten as

$$\begin{aligned} &|0\rangle_{\bar{0}1}|0\rangle_{\bar{1}2}\cdots|0\rangle_{\bar{N}N+1} \\ &= \left(\frac{-1}{2}\right)^{N}\sum_{\alpha_1,\ldots,\alpha_N=0}^{3} |\alpha_1\rangle\cdots|\alpha_N\rangle\left[I_{\bar{0}}\otimes(\sigma_{\alpha_N}\cdots\sigma_{\alpha_1})_{N+1}\right]|0\rangle_{\bar{0}N+1}. \end{aligned} \tag{75}$$

Then by projecting onto symmetric subspace spanned by $|\alpha = 1, 2, 3\rangle$, the ground state (72) takes the form [22, 69]

$$|\mathrm{G}\rangle = \frac{1}{3^{N/2}}\sum_{\alpha_1,\ldots,\alpha_N=1}^{3} |\alpha_1\rangle\cdots|\alpha_N\rangle\left[I_{\bar{0}}\otimes(\sigma_{\alpha_N}\cdots\sigma_{\alpha_1})_{N+1}\right]|0\rangle_{\bar{0}N+1}. \tag{76}$$

Note that this ground state (76) is normalized and we have re-written the overall phase for it has no physical content.

4.2 Density Matrix of a Block of Bulk Spins

Given the ground state in the form (76), we obtain the density matrix of a block of L contiguous spins starting at site k by tracing out spin degrees of freedom outside the block using basis (70):

$$\boldsymbol{\rho}_L \equiv \mathrm{Tr}_{\bar{0},1,\ldots,k-1,k+L,\ldots,N,N+1}\ |\mathrm{G}\rangle\langle\mathrm{G}|. \tag{77}$$

The result is independent of the starting site k and the total length N (see [19]). We choose $k = 1$, $N = L$ so that the density matrix reads [19]

$$\boldsymbol{\rho}_L = \frac{1}{3^L}\sum_{\alpha,\alpha'=1}^{3} |\alpha_1\rangle\langle\alpha'_1|\cdots|\alpha_L\rangle\langle\alpha'_L|\langle 0|I\otimes(\sigma_{\alpha'_1}\cdots\sigma_{\alpha'_L})I\otimes(\sigma_{\alpha_L}\cdots\sigma_{\alpha_1})|0\rangle. \tag{78}$$

4.3 Ground States of the Block Hamiltonian

The degenerate Hamiltonian is given by (3). We choose the length of the spin chain to be equal to that of the block, then the block Hamiltonian $H_b \equiv H_{deg}$ with $N = L$ reads

$$H_b = \frac{1}{2}\sum_{j=1}^{L-1}\left(\mathbf{S}_j \cdot \mathbf{S}_{j+1} + \frac{1}{3}\left(\mathbf{S}_j \cdot \mathbf{S}_{j+1}\right)^2 + \frac{2}{3}\right). \tag{79}$$

Any linear combination of states of the following form

$$|\mathrm{G};\, \chi_1,\, \chi_{\bar{L}}\rangle \equiv \left(\bigotimes_{j=1}^{L} P_{j\bar{j}}\right)|\chi_1\rangle_1|0\rangle_{\bar{1}2}|0\rangle_{\bar{2}3}\cdots|0\rangle_{\overline{L-1}L}|\chi_{\bar{L}}\rangle_{\bar{L}} \tag{80}$$

is a ground state of the block Hamiltonian (79). In (80) we have made notation $|\chi\rangle \equiv |\uparrow \text{ or } \downarrow\rangle$ represents the two spin-1/2 states and $P_{j\bar{j}}$ is defined in (73). Let's make a particular linear combination of these $|\mathrm{G};\, \chi_1,\, \chi_{\bar{L}}\rangle$ states using (70) and write the four ($\alpha = 0, 1, 2, 3$) linearly independent ground states of the block Hamiltonian (79) as follows

$$|\mathrm{G};\, \alpha\rangle \equiv \left(\bigotimes_{j=1}^{L} P_{j\bar{j}}\right)|\alpha\rangle_{\bar{L}1}|0\rangle_{\bar{1}2}|0\rangle_{\bar{2}3}\cdots|0\rangle_{\overline{L-1}L}. \tag{81}$$

Now we go through the same steps as from (72) to (76), the resultant form of the four ground states ($\alpha = 0, 1, 2, 3$) is

$$|\mathrm{G};\, \alpha\rangle = \sum_{\alpha_1,\ldots,\alpha_L=1}^{3} |\alpha_1\rangle\cdots|\alpha_L\rangle\ \langle\alpha_L|\sigma_\alpha \otimes \left(\sigma_{\alpha_{L-1}}\cdots\sigma_{\alpha_1}\right)|0\rangle. \tag{82}$$

Again we have re-written the overall phase for simplicity. These four states are orthogonal, and the normalization is given by

$$\langle \mathrm{G};\, \alpha|\mathrm{G};\, \alpha\rangle = \begin{cases} \dfrac{1}{4}(3^L + 3(-1)^L), & \alpha = 0; \\ \dfrac{1}{4}(3^L - (-1)^L), & \alpha = 1, 2, 3. \end{cases} \tag{83}$$

4.4 Eigenvectors of the Density Matrix

According to Theorem 1, the degenerate ground states (82) are eigenvectors of the density matrix (78). Let's apply $\boldsymbol{\rho}_L$ to $|\mathrm{G};\, \alpha\rangle$ and use orthogonality of the $|\alpha\rangle$ states. Then we obtain

$$\boldsymbol{\rho}_L|\mathrm{G};\, \alpha\rangle = \frac{1}{3^L}\sum_{\alpha_1,\ldots,\alpha_L=1}^{3} |\alpha_1\rangle\cdots|\alpha_L\rangle\ C_{\alpha_1\cdots\alpha_L} \tag{84}$$

with coefficient

$$\begin{aligned} C_{\alpha_1\cdots\alpha_L} = &\sum_{\alpha'_1,\ldots,\alpha'_L=1}^{3} \langle\alpha'_L|\sigma_\alpha \otimes (\sigma_{\alpha'_{L-1}}\cdots\sigma_{\alpha'_1})|0\rangle \\ &\times \langle 0|I \otimes (\sigma_{\alpha'_1}\cdots\sigma_{\alpha'_L})I \otimes (\sigma_{\alpha_L}\cdots\sigma_{\alpha_1})|0\rangle. \end{aligned} \tag{85}$$

It can be shown by induction that

$$\sum_{\alpha'_1,\ldots,\alpha'_{L-1}=1}^{3}(I\otimes\sigma_{\alpha'_{L-1}}\cdots\sigma_{\alpha'_1})|0\rangle\langle 0|(I\otimes\sigma_{\alpha'_1}\cdots\sigma_{\alpha'_{L-1}})=\sum_{\beta=0}^{3}A_\beta|\beta\rangle\langle\beta| \tag{86}$$

with

$$A_\beta=\begin{cases}\dfrac{1}{4}(3^{L-1}+3(-1)^{L-1}), & \beta=0;\\ \dfrac{1}{4}(3^{L-1}-(-1)^{L-1}), & \beta=1,2,3.\end{cases} \tag{87}$$

Therefore the coefficient $C_{\alpha_1\cdots\alpha_L}$ defined in (85) can be simplified as

$$C_{\alpha_1\cdots\alpha_L}=\sum_{\alpha'_L=1,\beta=0}^{3}A_\beta\langle\alpha'_L|\sigma_\alpha\otimes I|\beta\rangle\langle\beta|I\otimes(\sigma_{\alpha'_L}\sigma_{\alpha_L})I\otimes(\sigma_{\alpha_{L-1}}\cdots\sigma_{\alpha_1})|0\rangle. \tag{88}$$

Straightforward calculation using multiplication rules of Pauli matrices shows that (88) can be further simplified as

$$\begin{aligned}C_{\alpha_1\cdots\alpha_L}&=3A_1\delta_{\alpha,0}\langle\alpha_L|I\otimes(\sigma_{\alpha_{L-1}}\cdots\sigma_{\alpha_1})|0\rangle\\&\quad+(A_0+2A_1)(1-\delta_{\alpha,0})\left(\delta_{\alpha\alpha_L}\langle 0|-i\sum_{\beta=1}^{3}\epsilon_{\alpha\alpha_L\beta}\langle\beta|\right)I\otimes(\sigma_{\alpha_{L-1}}\cdots\sigma_{\alpha_1})|0\rangle\end{aligned} \tag{89}$$

where $\epsilon_{\alpha\alpha_L\beta}$ is the totally antisymmetric tensor of three indices with $\epsilon_{123}=1$. By realizing that

$$\delta_{\alpha\alpha_L}\langle 0|-i\sum_{\beta=1}^{3}\epsilon_{\alpha\alpha_L\beta}\langle\beta|=\langle 0|\sigma_{\alpha_L}\sigma_\alpha\otimes I=\langle\alpha_L|\sigma_\alpha\otimes I, \tag{90}$$

we have reached the final form of the coefficient $C_{\alpha_1\cdots\alpha_L}$ such that

$$C_{\alpha_1\cdots\alpha_L}=\left[3A_1\delta_{\alpha,0}+(A_0+2A_1)(1-\delta_{\alpha,0})\right]\langle\alpha_L|\sigma_\alpha\otimes(\sigma_{\alpha_{L-1}}\cdots\sigma_{\alpha_1})|0\rangle. \tag{91}$$

As a result, we plug (91) into (84) and find that

$$\begin{aligned}\boldsymbol{\rho}_L|\mathrm{G};\alpha\rangle&=\frac{3A_1\delta_{\alpha,0}+(A_0+2A_1)(1-\delta_{\alpha,0})}{3^L}\\&\quad\times\sum_{\alpha_1,\ldots,\alpha_L=1}^{3}|\alpha_1\rangle\cdots|\alpha_L\rangle\langle\alpha_L|\sigma_\alpha\otimes(\sigma_{\alpha_{L-1}}\cdots\sigma_{\alpha_1})|0\rangle.\end{aligned} \tag{92}$$

By comparing with (82), we find that (92) is exactly the statement that $|\mathrm{G};\alpha\rangle$ ($\alpha=0,1,2,3$) are eigenvectors of the density matrix $\boldsymbol{\rho}_L$:

$$\boldsymbol{\rho}_L|\mathrm{G};\alpha\rangle=\Lambda_\alpha|\mathrm{G};\alpha\rangle,\quad \alpha=0,1,2,3 \tag{93}$$

with eigenvalues

$$\Lambda_\alpha = \frac{3A_1\delta_{\alpha,0} + (A_0 + 2A_1)(1-\delta_{\alpha,0})}{3^L} = \begin{cases} \frac{1}{4}\left(1 + 3\left(-\frac{1}{3}\right)^L\right), & \alpha = 0; \\ \frac{1}{4}\left(1 - \left(-\frac{1}{3}\right)^L\right), & \alpha = 1, 2, 3. \end{cases} \tag{94}$$

These numbers obtained in (94) are exactly the eigenvalues found in [19, 41] for spin-1, and are consistent with our explicit expression for eigenvalues (52).

We can also prove explicitly that any other eigenvectors of $\boldsymbol{\rho}_L$ orthogonal to the set $\{|\mathrm{G};\alpha\rangle\}$ have zero eigenvalue. Let's note that a complete basis of the Hilbert space $\mathbf{H}_L$ of the block of spins can be chosen as

$$\{|\alpha_1\rangle \cdots |\alpha_L\rangle\}, \quad \alpha = 1, 2, 3. \tag{95}$$

The subspace $\mathbf{H}_\Lambda$ with non-zero eigenvalues is panned by $\{|\mathrm{G};\alpha\rangle\}$, as we have already shown. The Hilbert space can be reduced into a direct sum

$$\mathbf{H}_L = \mathbf{H}_\Lambda \oplus \mathbf{H}_\Phi. \tag{96}$$

We will show that the subspace $\mathbf{H}_\Phi$ orthogonal to $\mathbf{H}_\Lambda$ is a subspace of vanishing eigenvalues. Mathematically, this means that for an arbitrary basis vector $|\beta_1\rangle \cdots |\beta_L\rangle$, we shall have

$$\boldsymbol{\rho}_L(I_L - P_\Lambda)|\beta_1\rangle \cdots |\beta_L\rangle = 0, \tag{97}$$

where I_L is the identity of $\mathbf{H}_L$ and P_Λ is the projector onto $\mathbf{H}_\Lambda$:

$$I_L \equiv \sum_{\alpha_1,\cdots,\alpha_L=1}^{3} |\alpha_1\rangle \cdots |\alpha_L\rangle\langle\alpha_1| \cdots \langle\alpha_L|, \qquad P_\Lambda \equiv \sum_{\alpha=1}^{3} \frac{|\mathrm{G};\alpha\rangle\langle\mathrm{G};\alpha|}{\langle\mathrm{G};\alpha|\mathrm{G};\alpha\rangle}. \tag{98}$$

By taking expressions (78), (98), (93), and realizing that

$$\sum_{\alpha=0}^{3} \frac{3^L \Lambda_\alpha}{\langle\mathrm{G};\alpha|\mathrm{G};\alpha\rangle} |\alpha\rangle\langle\alpha| = \sum_{\alpha=0}^{3} |\alpha\rangle\langle\alpha| = I \otimes I, \tag{99}$$

we find the left hand side of (97) being equal to

$$\begin{aligned} &\boldsymbol{\rho}_L(I_L - P_\Lambda)|\beta_1\rangle \cdots |\beta_L\rangle \\ &= \frac{1}{3^L} \sum_{\alpha_1 \cdots \alpha_L=1}^{3} |\alpha_1\rangle| \cdots |\alpha_L\rangle \ \langle 0|[I \otimes (\sigma_{\beta_1} \cdots \sigma_{\beta_L}), I \otimes (\sigma_{\alpha_L} \cdots \sigma_{\alpha_1})]|0\rangle. \end{aligned} \tag{100}$$

We use multiplication rules of Pauli matrices to write the two terms within the commutator in (100) as

$$\begin{aligned} I \otimes (\sigma_{\beta_1} \cdots \sigma_{\beta_L}) &= e^{i\theta(\beta)} I \otimes \sigma_\beta, \quad \beta = 0, 1, 2, 3; \\ I \otimes (\sigma_{\alpha_L} \cdots \sigma_{\alpha_1}) &= e^{i\theta(\alpha)} I \otimes \sigma_\alpha, \quad \alpha = 0, 1, 2, 3. \end{aligned} \tag{101}$$

Here $e^{i\theta(\beta)}$ and $e^{i\theta(\alpha)}$ are two phase factors. Then the commutator is

$$[I \otimes (\sigma_{\beta_1} \cdots \sigma_{\beta_L}), I \otimes (\sigma_{\alpha_L} \cdots \sigma_{\alpha_1})] = e^{i(\theta(\beta)+\theta(\alpha))} I \otimes [\sigma_\beta, \sigma_\alpha]. \tag{102}$$

There are two possibilities: (i) $\alpha = \beta$ or at least one of the two is equal to zero, then σ_β and σ_α commutes; (ii) $\alpha \neq \beta \neq 0$, then $[\sigma_\beta, \sigma_\alpha] = 2i \sum_{\gamma=1}^{3} \epsilon_{\beta\alpha\gamma}\sigma_\gamma$, but we still have $\langle 0|I \otimes \sigma_\gamma|0\rangle = \langle 0|\gamma\rangle = 0$. Therefore, the factor $\langle 0|[I \otimes (\sigma_{\beta_1} \cdots \sigma_{\beta_L}), I \otimes (\sigma_{\alpha_L} \cdots \sigma_{\alpha_1})]|0\rangle$ in (100) is identically zero. So that we have proved (97). Therefore $\mathbf{H}_\Phi$ is a subspace with only zero eigenvalues.

5 A Different Proof of the Theorem on Eigenvectors

It was shown in Sect. 2.4 that the density matrix takes a diagonal form in the basis of zero-energy ground states of the block Hamiltonian (21). In this section, we show the same result by taking a different approach. This alternative proof of Theorem 1 does not involve coherent state representation.

Let's start with the ground state of the unique Hamiltonian (4) with $N = L$:

$$|\mathrm{VBS}\rangle \equiv \prod_{j=0}^{L} \left(a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger\right)^S |\mathrm{vac}\rangle. \tag{103}$$

In order to calculate the density matrix $\boldsymbol{\rho}_L = \mathrm{Tr}_{0,L+1}[\boldsymbol{\rho}]$, where $\boldsymbol{\rho}$ is defined in (10), we introduce a useful identity:

$${}_{0,L+1}\langle J, M| \left(|s\rangle_{0,1} \otimes |s\rangle_{L,L+1}\right) = \frac{(-1)^{S-J+M}}{(S+1)} |J, -M\rangle_{1,L}, \tag{104}$$

where $|J, M\rangle_{0,L+1}$ is identical to the spin state defined in (120) except for site indices. $|s\rangle_{i,j}$ in (104) is the normalized singlet state with S valence bonds defined as

$$\begin{aligned} |s\rangle_{i,j} &= \frac{1}{S!\sqrt{S+1}} \left(a_i^\dagger b_j^\dagger - b_i^\dagger a_j^\dagger\right)^S |\mathrm{vac}\rangle_i \otimes |\mathrm{vac}\rangle_j \\ &= \frac{(-1)^{\frac{S}{2}}}{\sqrt{S+1}} \sum_{m=-S/2}^{S/2} (-1)^m |S/2, -m\rangle_i \otimes |S/2, m\rangle_j. \end{aligned} \tag{105}$$

Identity (104) is derived using properties of the singlet state (105) and Clebsch-Gordan coefficients as follows:

$$\begin{aligned} &{}_{0,L+1}\langle J, M|s\rangle_{0,1}|s\rangle_{L,L+1} \\ &= \sum_{m_0, m_{L+1}}^{m_0+m_{L+1}=M} (J, M|S/2, m_0; S/2, m_{L+1})_0\langle S/2, m_0|_{L+1}\langle S/2, m_{L+1}| \\ &\quad \times \frac{(-1)^{\frac{S}{2}}}{\sqrt{S+1}} \sum_{m_1=-S/2}^{S/2} (-1)^{m_1} |S/2, -m_1\rangle_0 |S/2, m_1\rangle_1 \\ &\quad \times \frac{(-1)^{\frac{S}{2}}}{\sqrt{S+1}} \sum_{m_L=-S/2}^{S/2} (-1)^{m_L} |S/2, -m_L\rangle_L |S/2, m_L\rangle_{L+1} \\ &= \frac{1}{S+1} \sum_{m_0, m_{L+1}}^{m_0+m_{L+1}=M} (-1)^{m_0+m_{L+1}} (J, M|S/2, m_0; S/2, m_{L+1}) \end{aligned}$$

$$\times |S/2, -m_0\rangle_1 |S/2, -m_{L+1}\rangle_L. \tag{106}$$

Here the Clebsch-Gordan coefficient is defined by

$$(J, M|S/2, m_0; S/2, m_{L+1}) = {}_{i,j}\langle J, M| \left(|S/2, m_0\rangle_i \otimes |S/2, m_{L+1}\rangle_j\right). \tag{107}$$

Then using the symmetry property of Clebsch-Gordan coefficients

$$(J, M|S/2, m_0; S/2, m_{L+1}) = (-1)^{S-J}(J, -M|S/2, -m_0; S/2, -m_{L+1}), \tag{108}$$

and the completeness of the basis $\{|S/2, m_0\rangle_0 \otimes |S/2, m_{L+1}\rangle_{L+1}\}$, we obtain the identity (104).

With the help of identity (104), we calculate the partial inner product of the VBS state with the state $|J, M\rangle_{0,L+1}$, which is involved in taking trace of boundary spins. The VBS state $|\text{VBS}\rangle$ is decomposed into the bulk part and edge parts, then making use of (104), we have

$$\begin{aligned}
&{}_{0,L+1}\langle J, M|\text{VBS}\rangle \\
&= {}_{0,L+1}\langle J, M| \prod_{j=0}^{L} \left(a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger\right)^S |\text{vac}\rangle \\
&= S!(S+1)! \prod_{j=1}^{L-1} \left(a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger\right)^S {}_{0,L+1}\langle J, M|s\rangle_{0,1}|s\rangle_{L,L+1}|\text{vac}\rangle_{2\cdots L-1} \\
&= (S!)^2 \prod_{j=1}^{L-1} \left(a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger\right)^S (-1)^{S-J+M}|J, -M\rangle_{1,L}|\text{vac}\rangle_{2\cdots L-1} \\
&= (-1)^{S-J+M}(S!)^2|\text{VBS}_L(J, -M)\rangle.
\end{aligned} \tag{109}$$

We see that the $(S+1)^2$ degenerate VBS states $|\text{VBS}_L(J, M)\rangle$ defined in (24) appear in the partial inner product (109). As discussed in Sect. 2.3, they form a complete set of zero-energy ground states of the block Hamiltonian (21). These states are nothing but the edge states of the subsystem (block).

Now, it is straightforward to evaluate density matrix as

$$\begin{aligned}
\text{Tr}_{0,L+1}\left[\boldsymbol{\rho}\right] &= \sum_{J,M} \frac{{}_{0,L+1}\langle J, M|\text{VBS}\rangle\langle\text{VBS}|J, M\rangle_{0,L+1}}{\langle\text{VBS}|\text{VBS}\rangle} \\
&= \frac{(S!)^4}{\langle\text{VBS}|\text{VBS}\rangle} \sum_{J,M} |\text{VBS}_L(J, -M)\rangle\langle\text{VBS}_L(J, -M)|.
\end{aligned} \tag{110}$$

This expression is identical to (29) as we change dummy index from M to $-M$. Therefore, in this approach again we arrive at Theorem 1 that the density matrix is proportional to a projector onto a subspace spanned by the $(S+1)^2$ ground states of the block Hamiltonian (21). Normalization $\langle\text{VBS}|\text{VBS}\rangle$ is given in Appendix A. States $|\text{VBS}_L(J, M)\rangle$ are shown to be mutually orthogonal in Appendix C.

6 Conclusion

We have studied the density matrix $\boldsymbol{\rho}_L$ of a block of L contiguous bulk spins in the AKLT model. The unique Hamiltonian for generic spin-S is given by (4), which has a unique ground state described by the VBS state (9) in the Schwinger representation. The density matrix $\boldsymbol{\rho}_L$ (18) of the block is obtained by taking trace (14) of all spin degrees of freedom outside the block. The structure of the density matrix has been investigated both for finite and infinite blocks.

For generic spin-S and finite block, two mathematically rigorous results have been established as Theorem 1 and Theorem 2. In Theorem 1 we constructed eigenvectors of the density matrix with non-zero eigenvalues. These eigenvectors $|\mathrm{G};J,\hat{\Omega}\rangle$ defined in (23), or $|\mathrm{VBS}_L(J,M)\rangle$ defined in (24) equivalently, are proved to be the $(S+1)^2$ zero-energy ground states of the block Hamiltonian (21). The corresponding eigenvalues are obtained in two different forms. Using nonorthogonal basis $\{|\mathrm{G};J,\hat{\Omega}\rangle\}$, the eigenvalues are given through Conjecture 1 (38) and the recurrence relation (39); while using orthogonal basis $\{|\mathrm{VBS}_L(J,M)\rangle\}$, in Theorem 2 an explicit expression (52) for eigenvalues in terms of Wigner $3j$-symbols is derived. Non-zero eigenvalues $\Lambda(J)$ with $J=0,1,\ldots,S$ ((41) and (52)) depend only on J and are independent of $\hat{\Omega}$ and/or M in defining eigenvectors. The density matrix (29) is a projector onto the subspace of dimension $(S+1)^2$ spanned by the set of eigenvectors $\{|\mathrm{G};J,\hat{\Omega}\rangle\}$ and/or $\{|\mathrm{VBS}_L(J,M)\rangle\}$.

In the large block limit $L\to\infty$, Conjecture 1 (38) is proved and all non-zero eigenvalues Λ_∞ become the same (69). The infinite dimensional density matrix $\boldsymbol{\rho}_\infty$ (56) is a projector onto a $(S+1)^2$-dimensional subspace in which it is proportional to the identity. The von Neumann entropy $S_{v.N}$ coincides with the Renyi entropy S_R and is equal to the saturated value $\ln(S+1)^2$. In the limit the Renyi entropy is α independent, which behaves quite differently from the XY model where the Renyi entropy has an essential singularity as a function of α (see [23, 24, 39]).

We have also investigated the structure of the density matrix in a special case when spin $S=1$. Both Theorem 1 and Theorem 2 are proved using a different representation (82) (maximally entangled states) where all four eigenvectors $|\mathrm{G},\alpha\rangle$ are orthogonal. We have also shown (97) explicitly that any vector orthogonal to the subspace spanned by the set $\{|\mathrm{G},\alpha\rangle\}$ has zero eigenvalue.

Based on the main results obtained in this paper, we end our conclusion by making the following conjecture:

Conjecture 2 *The structure of the density matrix as a projector onto a subspace is generalizable to inhomogeneous AKLT spin chains* (*spin values at different lattice sites could be different*) *and lattices of higher dimensions*.[1] *In the large block limit, the density matrix should behave as the identity operator within the subspace. i.e.* (7) *is valid for arbitrary large lattices*.

Acknowledgements The authors would like to thank Professor Heng Fan, Professor Anatol N. Kirillov and Professor Sergey Bravyi for valuable discussions and suggestions. The work is supported by NSF Grant DMS-0503712 and the Japan Society for the Promotion of Science.

[1] It may even be generalizable to certain classes of arbitrary graphs if the limiting sub-graph can be defined properly.

Appendix A: Normalization of the VBS State

The VBS state $|\mathrm{VBS}\rangle$ (also known to be the ground state of the unique Hamiltonian (4)) defined in (9) is not normalized. Using the coherent state formalism (12) and the completeness relation (13), we express the norm square as

$$\langle \mathrm{VBS}|\mathrm{VBS}\rangle = \left[\frac{(S+1)!}{4\pi}\right]^2 \left[\frac{(2S+1)!}{4\pi}\right]^N \int \left(\prod_{j=0}^{N+1} d\hat{\Omega}_j\right) \prod_{j=0}^{N} \left[\frac{1}{2}(1-\hat{\Omega}_j\cdot\hat{\Omega}_{j+1})\right]^S \quad (111)$$

where we have used

$$\langle 0|a^{S+l}b^{S-l}|\hat{\Omega}\rangle = \sqrt{(2S)!}u^{S+l}v^{S-l}. \quad (112)$$

Now we expand $[\frac{1}{2}(1-\hat{\Omega}_j\cdot\hat{\Omega}_{j+1})]^S$ in terms of spherical harmonics as in (32), then integrate from $\hat{\Omega}_0$ to $\hat{\Omega}_{N+1}$. We notice by using the orthogonality of spherical harmonics that each integral contributes a factor of $\frac{4\pi}{S+1}$ except the last one. For example,

$$\begin{aligned}\int d\hat{\Omega}_0 \left[\frac{1}{2}(1-\hat{\Omega}_0\cdot\hat{\Omega}_1)\right]^S &= \frac{4\pi}{S+1}\sum_{l=0}^{S}\lambda(l,S)\sum_{m=-l}^{l}\sqrt{4\pi}Y_{lm}^*(\hat{\Omega}_1)\int d\hat{\Omega}_0 Y_{lm}(\hat{\Omega}_0)Y_{00}^*(\hat{\Omega}_0)\\ &= \frac{4\pi}{S+1}\sqrt{4\pi}Y_{00}^*(\hat{\Omega}_1) = \frac{4\pi}{S+1}. \quad (113)\end{aligned}$$

The last integral over $\hat{\Omega}_{N+1}$ contributes simply a factor of 4π. Consequently, the norm square (111) is equal to

$$\langle \mathrm{VBS}|\mathrm{VBS}\rangle = \left[\frac{(2S+1)!}{S+1}\right]^N S!(S+1)!. \quad (114)$$

Appendix B: Rank of the Set $\{|\mathrm{G};J,\hat{\Omega}\rangle\}$ with Fixed J Value

For notational convenience, we define

$$X_{JM} \equiv \frac{u^{J+M}v^{J-M}}{\sqrt{(J+M)!(J-M)!}}, \qquad \psi_{Sm}^{\dagger} \equiv \frac{(a^{\dagger})^{S+m}(b^{\dagger})^{S-m}}{\sqrt{(S+m)!(S-m)!}}. \quad (115)$$

These two variables transform conjugately with respect to one another under $SU(2)$. X_{JM} has the following orthogonality relation

$$\int d\hat{\Omega} X_{JM}^* X_{JM'} = \frac{4\pi}{(2J+1)!}\delta_{MM'}. \quad (116)$$

$\psi_{Sm}^{\dagger}$ is a spin state creation operator such that

$$\psi_{Sm}^{\dagger}|\mathrm{vac}\rangle = |S,m\rangle. \quad (117)$$

The operator $A_J^\dagger$ defined in (22) can be expanded as (see [35])

$$A_J^\dagger = \sqrt{\frac{(S+J+1)!(S-J)!J!J!}{2J+1}} \times \sum_{M=-J}^{J} X_{JM} \sum_{m_1,m_L}^{m_1+m_L=M} (S/2, m_1; S/2, m_2|J, M)\ \psi^\dagger_{S/2,m_1} \otimes \psi^\dagger_{S/2,m_L}, \quad (118)$$

where $(S/2, m_1; S/2, m_2|J, M)$ are the Clebsch-Gordan coefficients. Note that $\psi^\dagger_{S/2,m_1}$ and $\psi^\dagger_{S/2,m_L}$ are defined in the Hilbert spaces of spins at site 1 and site L, respectively. We realize that the particular form of the sum over m_1 and m_L in (118) can be identified as a single spin state creation operator

$$\Psi^\dagger_{JM} \equiv \sum_{m_1,m_L}^{m_1+m_L=M} (S/2, m_1; S/2, m_2|J, M)\ \psi^\dagger_{S/2,m_1} \otimes \psi^\dagger_{S/2,m_L}. \quad (119)$$

This operator $\Psi^\dagger_{JM}$ acts on the direct product of two Hilbert spaces of spins at site 1 and site L. It has the property that

$$\Psi^\dagger_{JM}|\text{vac}\rangle_1 \otimes |\text{vac}\rangle_L = |J, M\rangle_{1,L}. \quad (120)$$

Now we can derive the completeness relation of the set $\{|\text{G}; J, \hat{\Omega}\rangle\}$ using (116), (118) and (119):

$$\int d\hat{\Omega}|\text{G}; J, \hat{\Omega}\rangle\langle\text{G}; J, \hat{\Omega}| = \frac{4\pi}{(2J+1)!}\frac{(S+J+1)!(S-J)!J!J!}{2J+1} \sum_{M=-J}^{J} \Psi^\dagger_{JM}|\text{VBS}_L\rangle\langle\text{VBS}_L|\Psi_{JM}. \quad (121)$$

The set of states $\{\Psi^\dagger_{JM}|\text{VBS}_L\rangle,\ M = -J, \ldots, J\}$ are linearly independent. So that the rank of $\{|\text{G}; J, \hat{\Omega}\rangle\}$ with fixed J value is $2J+1$. With the introduction of degenerate VBS states $|\text{VBS}_L(J, M)\rangle$ in (24), $|\text{G}; J, \hat{\Omega}\rangle$ can be written as a linear superposition:

$$|\text{G}; J, \hat{\Omega}\rangle = \sqrt{\frac{(S+J+1)!(S-J)!J!J!}{2J+1}} \sum_{M=-J}^{J} X_{JM}|\text{VBS}_L(J, M)\rangle. \quad (122)$$

More details can be found in [35].

Appendix C: Orthogonality of Degenerate VBS States

The set of degenerate VBS states $\{|\text{VBS}_L(J, M)\rangle, J = 0, ..., S, M = -J, ..., J\}$ introduced in (24) are mutually orthogonal. To show this, it is convenient to introduce the total spin operators of the subsystem:

$$S^+_{\text{tot}} = \sum_{j=1}^{L} a_j^\dagger b_j, \qquad S^-_{\text{tot}} = \sum_{j=1}^{L} b_j^\dagger a_j, \qquad S^z_{\text{tot}} = \sum_{j=1}^{L} (a_j^\dagger a_j - b_j^\dagger b_j)/2. \quad (123)$$

First we show that the set of operators $\{S^+_{\rm tot}, S^-_{\rm tot}, S^z_{\rm tot}\}$ commute with the product of valence bonds, i.e.

$$\left[S^{\pm}_{\rm tot}, \prod_{j=1}^{L-1}(a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger)^S\right] = 0, \qquad \left[S^{z}_{\rm tot}, \prod_{j=1}^{L-1}(a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger)^S\right] = 0. \tag{124}$$

These commutation relations (124) can be shown in similar ways. Take the commutator with $S^+_{\rm tot}$ first. We re-write the commutator as

$$\begin{aligned}
&\left[S^+_{\rm tot}, \prod_{j=1}^{L-1}(a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger)^S\right] \\
&= \sum_{j=1}^{L-1}(a_1^\dagger b_2^\dagger - b_1^\dagger a_2^\dagger)^S \cdots [S^+_{\rm tot}, (a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger)^S] \cdots (a_{L-1}^\dagger b_L^\dagger - b_{L-1}^\dagger a_L^\dagger)^S \\
&= \sum_{j=1}^{L-1}(a_1^\dagger b_2^\dagger - b_1^\dagger a_2^\dagger)^S \cdots [S_j^+ + S_{j+1}^+, (a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger)^S] \cdots (a_{L-1}^\dagger b_L^\dagger - b_{L-1}^\dagger a_L^\dagger)^S.
\end{aligned} \tag{125}$$

Then using commutators $[a_i, a_j^\dagger] = \delta_{ij}$ and $[b_i, b_j^\dagger] = \delta_{ij}$, we find that

$$\begin{aligned}
&[S_j^+ + S_{j+1}^+, (a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger)^S] \\
&= [a_j^\dagger b_j + a_{j+1}^\dagger b_{j+1}, (a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger)^S] \\
&= a_j^\dagger [b_j, (a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger)^S] + a_{j+1}^\dagger [b_{j+1}, (a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger)^S] \\
&= a_j^\dagger (-S) a_{j+1}^\dagger (a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger)^{S-1} + a_{j+1}^\dagger S a_j^\dagger (a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger)^{S-1} \\
&= 0.
\end{aligned} \tag{126}$$

Therefore $[S^+_{\rm tot}, \prod_{j=1}^{L-1}(a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger)^S] = 0$. In (126) we have used $[b_j, (a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger)^S] = -S a_{j+1}^\dagger (a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger)^{S-1}$. In a parallel way, we find that the commutator with $S^-_{\rm tot}$ also vanishes. Next we consider the commutator with $S^z_{\rm tot}$:

$$\begin{aligned}
&\left[S^z_{\rm tot}, \prod_{j=1}^{L-1}(a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger)^S\right] \\
&= \sum_{j=1}^{L-1}(a_1^\dagger b_2^\dagger - b_1^\dagger a_2^\dagger)^S \cdots [S_j^z + S_{j+1}^z, (a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger)^S] \cdots (a_{L-1}^\dagger b_L^\dagger - b_{L-1}^\dagger a_L^\dagger)^S.
\end{aligned} \tag{127}$$

In the right hand side of (127), the commutator involved also vanishes because

$$\begin{aligned}
&[S_j^z + S_{j+1}^z, (a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger)^S] \\
&= \frac{1}{2}[a_j^\dagger a_j - b_j^\dagger b_j + a_{j+1}^\dagger a_{j+1} - b_{j+1}^\dagger b_{j+1}, (a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger)^S] \\
&= a_j^\dagger [a_j, (a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger)^S] - b_j^\dagger [b_j, (a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger)^S]
\end{aligned}$$

$$+ a_{j+1}^\dagger [a_{j+1}, (a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger)^S] - b_{j+1}^\dagger [b_{j+1}, (a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger)^S]$$
$$= 0. \tag{128}$$

Substituting (128) into (127), we obtain $[S_{\rm tot}^z, \prod_{j=1}^{L-1}(a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger)^S] = 0$. Now we shall show that the state $|{\rm VBS}_L(J,M)\rangle$ is an eigenstate of $S_{\rm tot}^z$ and the square of the total spin $\mathbf{S}_{\rm tot}^2 = \frac{1}{2}(S_{\rm tot}^+ S_{\rm tot}^- + S_{\rm tot}^- S_{\rm tot}^+) + (S_{\rm tot}^z)^2$ with eigenvalues M and $J(J+1)$, respectively. Using the commutation relations (124), we can show that

$$\begin{aligned} S_{\rm tot}^\pm |{\rm VBS}_L(J,M)\rangle &= \prod_{j=1}^{L-1}(a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger)^S (S_1^\pm + S_L^\pm)|J,M\rangle_{1,L}|{\rm vac}\rangle_{2,\ldots,L-1} \\ S_{\rm tot}^z |{\rm VBS}_L(J,M)\rangle &= \prod_{j=1}^{L-1}(a_j^\dagger b_{j+1}^\dagger - b_j^\dagger a_{j+1}^\dagger)^S (S_1^z + S_L^z)|J,M\rangle_{1,L}|{\rm vac}\rangle_{2,\ldots,L-1}. \end{aligned} \tag{129}$$

Then from the definition of the state $|{\rm VBS}_L(J,M)\rangle$ and the following relations:

$$\begin{aligned} &(S_1^+ + S_L^+)|J,M\rangle_{1,L} = \sqrt{(J\mp M)(J\pm M+1)}|J,M\pm 1\rangle, \\ &(S_1^z + S_L^z)|J,M\rangle_{1,L}\rangle = M|J,M\rangle_{1,L}, \end{aligned} \tag{130}$$

we obtain

$$\begin{aligned} S_{\rm tot}^\pm |{\rm VBS}_L(J,M)\rangle &= \sqrt{(J\mp M)(J\pm M+1)}|{\rm VBS}_L(J,M\pm 1)\rangle, \\ S_{\rm tot}^z |{\rm VBS}_L(J,M)\rangle &= M|{\rm VBS}_L(J,M)\rangle \end{aligned} \tag{131}$$

and hence $\mathbf{S}_{\rm tot}^2|{\rm VBS}_L(J,M)\rangle = J(J+1)|{\rm VBS}_L(J,M)\rangle$. It is now proved that $|{\rm VBS}_L(J,M)\rangle$ is an eigenstate of $S_{\rm tot}^z$ and $\mathbf{S}_{\rm tot}^2$ with eigenvalues M and $J(J+1)$, respectively. Therefore the states with different eigenvalues (J,M) are orthogonal to each other.

Appendix D: Density Matrix and Correlation Functions

The relation between the density matrix and correlation functions was studied in [6, 40, 41]. It was shown in Sect. 2 of [40] that the density matrix contains information of all correlation functions in the ground state. The original proof was for spin $S = 1/2$. In this appendix we shall generalize this result to generic spin-S which is applicable to our AKLT model.

The Hilbert space associated with a spin-S is $(2S+1)$-dimensional. Therefore we could choose a basis of $(2S+1)^2$ linearly independent matrices such that an arbitrary operator defined in the Hilbert space can be written as a superposition over the basis. Let's denote the basis by $\{A_{ab};\ a,b = 1,\ldots,2S+1\}$, in which each matrix A_{ab} is labeled by a pair of indices a and b with totally $(2S+1)^2$ possible combinations. The matrix element is defined as

$$(A_{ab})_{kl} = \delta_{ak}\delta_{bl}, \quad k,l = 1,\ldots,2S+1. \tag{132}$$

In addition to $\{A_{ab}\}$, we introduce an equivalent "conjugate" basis $\{\bar{A}_{ab}\}$ such that

$$(\bar{A}_{ab})_{kl} = \delta_{al}\delta_{bk}, \quad a,b,k,l = 1,\ldots,2S+1. \tag{133}$$

These matrices (132) and (133) are actually matrix representation of operators $\{|S,m\rangle\langle S,m'|; m,m'=-S,\ldots,S\}$. They are normalized such that

$$\mathrm{Tr}(\bar{A}_{ab}A_{cd})=\sum_{k,l}(\bar{A}_{ab})_{kl}(A_{cd})_{lk}=\sum_{k,l}\delta_{al}\delta_{bk}\delta_{cl}\delta_{dk}=\delta_{ac}\delta_{bd}. \tag{134}$$

Here Tr takes trace at one and the same site. Because of the completeness of $\{A_{ab}\}$ at each site, the density matrix of the block can be written as (see (77))

$$\boldsymbol{\rho}_{\mathrm{block}}=\mathrm{Tr}_{\mathrm{outside}}|\mathrm{G}\rangle\langle\mathrm{G}|=\sum_{\{a_jb_j\}}\left(\otimes_{j\in\{\mathrm{block}\}}A_{a_jb_j}\right)\mathrm{coeff}\{a_jb_j\}, \tag{135}$$

where $|\mathrm{G}\rangle$ denotes the unique ground state, $\mathrm{Tr}_{\mathrm{outside}}$ takes traces of sites outside the block and $\mathrm{coeff}\{a_jb_j\}$ denotes the coefficient. Using the normalization property (134), the coefficient $\mathrm{coeff}\{a_jb_j\}$ with label j taking values within the block can be expressed as

$$\begin{aligned}\mathrm{coeff}\{a_jb_j\}&=\sum_{\{c_jd_j\}}\prod_{j\in\mathrm{block}}\mathrm{Tr}(\bar{A}_{a_jb_j}A_{c_jd_j})\mathrm{coeff}\{c_jd_j\}\\&=\mathrm{Tr}_{\mathrm{block}}\left[\left(\otimes_{j\in\mathrm{block}}\bar{A}_{a_jb_j}\right)\boldsymbol{\rho}_{\mathrm{block}}\right]\\&=\mathrm{Tr}_{\mathrm{all}}\left[\left(\otimes_{j\in\mathrm{block}}\bar{A}_{a_jb_j}\right)|\mathrm{G}\rangle\langle\mathrm{G}|\right]\\&=\langle\mathrm{G}|\left(\otimes_{j\in\mathrm{block}}\bar{A}_{a_jb_j}\right)|\mathrm{G}\rangle.\end{aligned} \tag{136}$$

Here $\mathrm{Tr}_{\mathrm{block}}$ takes traces of sites within the block and $\mathrm{Tr}_{\mathrm{all}}$ takes traces of all lattice sites. Combing (135) with (136), we have the final form

$$\boldsymbol{\rho}_{\mathrm{block}}=\sum_{\{a_jb_j\}}\left(\otimes_{j\in\{\mathrm{block}\}}A_{a_jb_j}\right)\langle\mathrm{G}|\left(\otimes_{j\in\mathrm{block}}\bar{A}_{a_jb_j}\right)|\mathrm{G}\rangle. \tag{137}$$

This is the expression of the density matrix with entries related to multi-point correlation functions $\langle\mathrm{G}|\left(\otimes_{j\in\mathrm{block}}\bar{A}_{a_jb_j}\right)|\mathrm{G}\rangle$ in the ground state. All possible combinations $\{a_jb_j\}$ are involved in the summation. Therefore, we have prove for generic spin-S that the density matrix contains information of all correlation functions.

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