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Matrix product representations for all valence bond states

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We introduce a simple representation for irreducible spherical tensor operators of the rotation group of arbitrary integer or half integer rank and use these tensor operators to construct matrix product states corresponding to all the variety of valence bond states proposed in the Affleck–Kennedy–Lieb–Tasaki (AKLT) construction. These include the fully dimerized states of arbitrary spins, with uniform or alternating patterns of spins, which are ground states of Hamiltonians with nearest and next-nearest-neighbor interactions, and the partially dimerized or AKLT/valence bond solid states, which are constructed from them by projection. The latter states are translation-invariant ground states of Hamiltonians with nearest-neighbor interactions.

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I. INTRODUCTION

The problem of introducing exactly solvable models in quantum spin chains has a long history in statistical mechanics and mathematical physics, which encompasses a variety of models and techniques.[1,2] One can mention the XY,[3] the Heisenberg XXX and XXZ,[4] the Affleck–Kennedy–Lieb–Tasaki (AKLT),[5] and the Majumdar–Ghosh models,[6] and the free fermion, the Bethe ansatz, and the matrix product techniques to name only a few of the most important models and techniques which have been developed so far. Finding any exactly solvable model is an important step since it acts as a reference model for developing approximate perturbative solutions for more realistic models. It will also help us to test many of the new ideas about collective behavior of quantum systems, i.e., entanglement properties,[7,8] or the relation of criticality and universality of entanglement.[9,10]

In Ref. 5, Affleck *et al.* suggested a new construction for a variety of spin states, known as valence bond states. The basic element of this construction is a spin-1/2 singlet state, a dimer, $|s\rangle=\frac{1}{\sqrt{2}}(|+,-\rangle-|-,+\rangle)$, which is called a valence bond in Ref. 5. A dimerized state is just a juxtaposition of such dimers on adjacent sites [Fig. 1(a)]. Such a state is clearly seen to be a ground state of a Hamiltonian with three-site interactions (nearest and next-nearest neighbors), the local Hamiltonian of which is the projector to spin-3/2 states, $h=P_{3/2}$. The reason is that due to the presence of a dimer, the sum of spins of three adjacent sites adds up only to spin 1/2. The parent Hamiltonian of this fully dimerized state is known as the Majumdar–Ghosh Hamiltonian and has the form

$$H=\sum_j \sigma_i\cdot\sigma_{i+1}+\frac{1}{2}\sigma_i\cdot\sigma_{i+2}. \tag{1}$$

This Hamiltonian has a twofold ground state degeneracy, the other ground state being simply a one-site translation of dimers to the left or right.

One can also consider fully dimerized states[5] with alternating patterns of spins, where there are alternating number of valence bonds or dimers. An example of this is shown in Fig. 2(a), where the local three-site Hamiltonian should be taken as projector to spin 2, $h=P_2$. Moreover, one can use projection to construct from these fully dimerized states partially dimerized or AKLT/VBS (valence bond solid) states, which are ground states of Hamiltonians with nearest-neighbor interactions. For example, in Fig. 1(b), if one projects each pair of spin-1/2 particles in a bulb of the original chain to the symmetrized triplet, a nondimerized spin-1 state is obtained on a new chain, whose parent Hamiltonian, which annihilates this state, is the sum of spin-2 projectors P_2 on consecutive sites. The reason for this annihilation is that the sum of four initial spins on the original chain (known also as the virtual chain) adds up to at most spin 1, due to the presence of the valence bond, which is a singlet. In this way, a spin-1 quantum chain is obtained, which is the exact ground state of the following Hamiltonian:

$$H=\sum_j S_i\cdot S_{i+1}+\frac{1}{3}(S_i\cdot S_{i+1})^2. \tag{2}$$

Projection can also be used for other types of dimerized state, as shown in Fig. 2(b) to construct states with arbitrary integer or half integer spins. For example, in Fig. 2(b), looking at the number of valence bonds, which are singlets and are not counted in the addition of spins in the virtual sites, one finds that the local Hamiltonians can be chosen as $h_1=\lambda_3P_3$ and $h_2=\lambda_3P_3+\lambda_2P_2$, where P_j is the projector on spin-j states and λ_j's are positive coefficients. To assure translation invariance for the parent Hamiltonian, one then takes $H=\Sigma_j h_{j,j+1}$, where $h=P_3$ is the operator common to both h_1 and h_2. Needless to say, this construction can be

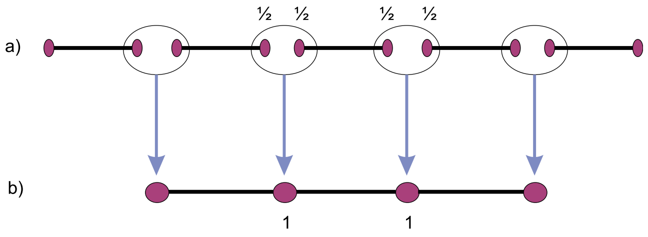

FIG. 1. (Color online) A fully dimerized valence bond state and the AKLT construction of a partially dimerized spin-1 state. The states in each bulb are projected to the symmetrized triplet. The parent Hamiltonian of (a) the upper chain has an interaction range of three lattice sites, while that of (b) the lower chain has a range of two sites.

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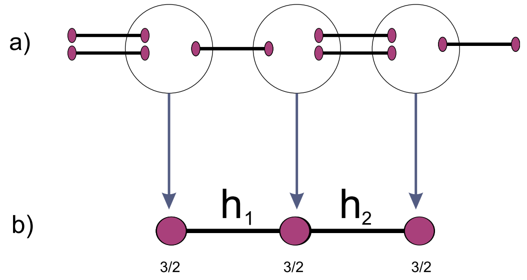

FIG. 2. (Color online) An example of a dimerized state with alternating spin pattern and the AKLT construction of spin-3/2 chain. The interaction ranges are similar to that in Fig. 1.

generalized by taking different alternating numbers of dimers in the virtual chain. This is also the basic idea behind the exactly solvable spin-3/2 spin systems on the honeycomb lattice[11] or, more generally, the basic idea behind projected entangled pair states,[12] which has only recently been discussed in the literature.

In the course of time, the basic idea of AKLT, which in turn was inspired by the work of Majumdar and Ghosh,[6] led to the development of finitely correlated or matrix product representation of states,[13–15] a representation, which when existing, greatly facilitates the calculation of many properties of the ground states of quantum systems.[8,15–26] The matrix product (MP) representation was also found to be closely related to the success of the density matrix renormalization group.[27–29]

When considering spin chains, the basic continuous symmetry is the rotation symmetry captured by the su(2) group, and there has been many different and equivalent implementations of this symmetry in matrix product states.[21,22,25,26,29] While a lot of progress has been made in defining matrix product states having specific symmetries, to our knowledge, the original AKLT variety of states has not been cast into a simple and uniform matrix product form for both integer and noninteger spins. For the integer case, however, such a formulation has been reported in Ref. 30. There is no doubt that such a representation will be of utmost importance for further study of AKLT models and even for similar models on more general geometries such as the Bethe lattice.[31]

To ensure invariance of the matrix product state (MPS) under rotation, it is sufficient that the elementary matrices used in the definition of the MPS constitute a representation of spherical tensor operators of a specific rank. The rank of the tensor depends on the spin of the actual lattice and the dimension of the representation determines the dimension of the auxiliary matrices. Finding a simple and minimal-dimensional representation for such tensors constitutes the basic problem in constructing rotationally invariant MPS, both for spin chain and spin ladders or for two dimensional lattices.

What we will do in this paper is to provide a uniform and simple matrix product representation for all the AKLT or valence bond states and even more general states. The starting point of our analysis is a simple and compact representation of spherical tensor operators of any rank, integer or half integer. These tensors enable us to define MP representations for Majumdar–Ghosh states (which are the ancestors of AKLT states) and their generalization to arbitrary spins, and then we will use them to construct MP representation for partially dimerized states. We then use the projection method to find MP representations for arbitrary spin chains, with nearest-neighbor interaction. The parallel with the AKLT construction is simple: the basic idea is to replace a collection of $2s$ spin-$1/2$ dimers or valence bonds with a single spin-s valence bond and represent the states constructed from these spin-s valence bonds as MPS.

Besides having the benefit of calculability, when we have a MPS representation, the very method of MPS allows us to find a larger family of Hamiltonians than the AKLT method. This larger family with its larger number of couplings will enable us to better adjust or approximate an exactly solvable Hamiltonian with realistic situations. We will see an example of this in this paper.

The structure of this paper is as follows. In Sec. II, we review the matrix product formalism[13–15] in a language which we find convenient[21] for further developments. In particular, we emphasize the symmetry properties of the ground state and the Hamiltonian. In Sec. III, we will introduce a compact formula for spherical tensors of rank s (integer or half integer) and use it to construct dimerized states of arbitrary integer or half-integer spins in Sec. IV. These are the generalization of Majumdar–Ghosh states or fully dimerized states to arbitrary spins. We then go on in Sec. V to define MP representations for other types of dimerized states. In Sec. VI, we find MP representations for AKLT/VBS states. The core of this section is the definition of kinds of tensors, which play the role of auxiliary matrices for the MP representations of these states. Section VII is devoted to some specific examples, where more detailed properties of some of the states and their parent Hamiltonians are derived. We conclude the paper with a discussion.

II. MATRIX PRODUCT STATES

Let us first make a quick review of the matrix product states in a language which we find convenient.[21,22] For more detailed reviews of the subject, the reader can consult a more comprehensive review article such as Ref. 23 or any of the many works where specific examples have been studied.[8,16–22,24–26]

Consider a ring of N sites, where each site describes a d-level state. The Hilbert space C^d of each site is spanned by the basis vectors $|i\rangle$, $i=0,\ldots,d-1$. A state

$$|\Psi\rangle = \sum_{i_1,i_2,\ldots,i_N} \Psi_{i_1 i_2 \cdots i_N} |i_1 i_2 \cdots i_N\rangle \tag{3}$$

is called a matrix product state if there exist D dimensional matrices $A_i \in C^{D\times D}$, $i=0,\ldots,d-1$, such that

$$\Psi_{i_1 i_2 \cdots i_N} = \frac{1}{\sqrt{Z}} \mathrm{tr}(A_{i_1} A_{i_2} \cdots A_{i_N}), \tag{4}$$

where Z is a normalization constant. This constant is given by $Z=\mathrm{tr}(E^N)$, where $E=\sum_{i=0}^{d-1} A_i^* \otimes A_i$. Note that we are here considering homogeneous matrix product states, where the matrices depend on the value of the spin at each site and not on the site itself. More general MPSs can be defined where the matrices also depend on the position of the sites.[23]

The collection of matrices $\{A_i\}$ and $\{\mu U A_i U^{-1}\}$, where μ is an arbitrary complex number, both lead to the same matrix product state; the freedom in scaling with μ is due to its cancellation with Z in the denominator of Eq. (4). This freedom will be useful when we discuss symmetries. There have been discussions on the symmetry of matrix product states in the literature;[13,14,19,21,25,26] here, we use the language or notation used in Ref. 21

A. Symmetries of the ground state

Consider a local continuous symmetry operator R acting on a site as $R|i\rangle = R_{ji}|j\rangle$, where summation convention is being used. R is a d dimensional unitary representation of the symmetry. A global symmetry operator $\mathcal{R} := R^{\otimes N}$ will then change this state to another matrix product state,

$$\Psi_{i_1 i_2 \cdots i_N} \rightarrow \Psi'_{i_1 i_2 \cdots i_N} := \mathrm{tr}(A'_{i_1} A'_{i_2} \cdots A'_{i_N}), \tag{5}$$

where

$$A'_i := R_{ij} A_j. \tag{6}$$

The state $|\Psi\rangle$ is invariant (i.e., a singlet) under this symmetry if there exist an operator $U(R)$ such that

$$R_{ij} A_j = U^{-1}(R) A_i U(R). \tag{7}$$

Repeating this transformation and using the group multiplication of the transformations R puts the constraint

$$U_{R'} U_R = U_{R'R}. \tag{8}$$

Thus, $U(R)$ is a D dimensional representation of the symmetry R. In case that R is a continuous symmetry with generators T_a, Eq. (7) leads to

$$(T_a)_{ij} A_j = [\mathcal{T}_a, A_i], \tag{9}$$

where T_a and $\mathcal{T}_a$ are the d and D dimensional representations of the Lie algebra of the symmetry.

B. Symmetries of the Hamiltonian

Given a matrix product state, the reduced density matrix of k sites is given by

$$\rho_{i_1 \cdots i_k, j_1 \cdots j_k} = \frac{\mathrm{tr}[(A^*_{i_1} \cdots A^*_{i_k} \otimes A_{j_1} \cdots A_{j_k}) E^{N-k}]}{\mathrm{tr}(E^N)}. \tag{10}$$

The null space of this reduced density matrix contains the subspace spanned by the solutions of

$$\sum_{j_1,\ldots,j_k=0}^{d-1} c_{j_1 \cdots j_k} A_{j_1} \cdots A_{j_k} = 0. \tag{11}$$

Let the null space of the reduced density matrix of k adjacent sites, denoted by Δ_k, be spanned by the orthogonal vectors $|e_\alpha\rangle$ $(\alpha = 1, \ldots, s \geq d^k - D^2)$. Then, we can construct the local Hamiltonian acting on k consecutive sites as

$$h := \sum_{\alpha=1}^{s} \lambda_\alpha |e_\alpha\rangle\langle e_\alpha|, \tag{12}$$

where λ_α's are positive constants. These constants together with the parameters of the vectors $|e_\alpha\rangle$ inherited from those of the original matrices A_i determine the total number of coupling constants of the Hamiltonian. If we call the embedding of this local Hamiltonian into sites l to $l+k$ by $h_{l,l+k}$, then the full Hamiltonian on the chain is written as

$$H = \sum_{l=1}^{N} h_{l,l+k}. \tag{13}$$

The state $|\Psi\rangle$ is then a ground state of this Hamiltonian with vanishing energy (see Ref. 21 for a more detailed discussion of the above points).

A Hamiltonian derived as above does not have any particular symmetry. Indeed, the above class includes all types of Hamiltonians, which have the matrix product state as their ground state. A subclass of these Hamiltonians, however, do have the symmetry of the ground state. Consider Eq. (11), multiplying both sides of this equation by $U^{-1}(R)$ from left and $U(R)$ from right and using Eq. (7), we find that if $c_{i\cdots j}$ is a solution of Eq. (11); then, $R_{i,i'} \cdots R_{j,j'} c_{i' \ldots j'}$ is also a solution of the same equation, that is,

$$R_{i,i'} \cdots R_{j,j'} c_{i' \ldots j'} = \lambda(R) c_{i \cdots j}. \tag{14}$$

This means that the null space of the reduced density matrix is an invariant subspace under the action of the symmetry group $R^{\otimes k}$. Thus, the null vectors $|e_\alpha\rangle$ transform into each other under the action of the reducible representation $R^{\otimes k}$. Such vectors can be classified into multiplets such that each multiplet transforms under one irreducible representation of the group R. Let the states transforming under the irreducible representation D^μ of the group be denoted by $|e^\mu_\beta\rangle$. Then, the operators $h^\mu = \sum_\beta |e^\mu_\beta\rangle\langle e^\mu_\beta|$ are scalar under the action of the group, that is,

$$[D^\mu, h^\mu] = 0. \tag{15}$$

Hence, to ensure the symmetry of the local Hamiltonian, we write it as

$$h_{i,i+k} = \sum_\mu \lambda_\mu h^\mu = \sum_{\mu,\beta} \lambda_\mu |e^\mu_\beta\rangle\langle e^\mu_\beta|, \tag{16}$$

where the number of free couplings λ_μ is equal to the number of multiplets, which span the null space Δ_k.

III. REPRESENTATION FOR SPHERICAL TENSORS OF ARBITRARY RANK

We are now equipped with generalities about matrix product states and their symmetry properties. In this section, we specialize the above discussion to the construction of spin-s MPS invariant under rotation in spin space. For such a chain, we take the local Hilbert space to be spanned by the $d = 2s + 1$ states of a spin-s particle, i.e., the states $\{|s,m\rangle, m = -s, \ldots, s\}$. Let us denote the D dimensional matrix assigned to the local configuration m by $A_{s,m}$. Rotational symmetry in the spin space now demands that the matrices $A_{s,m}$ form an irreducible tensor operator of rank s in the space of D dimensional square matrices. In view of Eq. (9), we should find $2s+1$ matrices $A_{s,m}$ such that the following relations are satisfied:

$$[L_z, A_{s,m}] = m A_{s,m},$$

$$[L_+, A_{s,m}] = \sqrt{s(s+1) - m(m+1)} A_{s,m+1},$$

$$[L_-, A_{s,m}] = \sqrt{s(s+1) - m(m-1)} A_{s,m-1}, \tag{17}$$

where L_z, L_+, and L_- are the D dimensional representations (not necessarily irreducible) of the Lie algebra of su(2),

$$[L_z, L_\pm] = \pm L_\pm, \quad [L_+, L_-] = 2L_z. \tag{18}$$

Remark. For simplicity, we will use the notation $|m\rangle$ and A_m instead of $|s,m\rangle$ and $A_{s,m}$, respectively, when the label s is clear from the context.

It is crucial to note that it is not always possible to find tensor operators of a given rank for a given D dimensional representation. For example, while there is a tensor of rank 1, in two dimensions, given by

$$A_1 = -\sqrt{2}\sigma_+, \quad A_0 = \sigma_z, \quad A_{-1} = \sqrt{2}\sigma_-, \tag{19}$$

leading to the spin-1 AKLT model,[5] with parent Hamiltonian (2), there is no rank-1/2 tensor operator in two dimensions. By this, we mean that if we take $D=2$, then there is no nonzero solution for the following system of matrix equations:

$$[L_z, A_\pm] = \pm \frac{1}{2} A_\pm,$$

$$[L_+, A_+] = 0, \quad [L_+, A_-] = A_+,$$

$$[L_-, A_+] = A_-, \quad [L_-, A_-] = 0. \tag{20}$$

Therefore, the first task for the construction of rotationally invariant matrix product states for quantum spin chains or quantum ladders is to have a compact expression for spherical tensors of arbitrary rank.

A possible procedure for obtaining spherical tensors of integer rank is to take two low-rank (possibly identical) tensors and decompose their ordinary or tensor product by the Clebsh–Gordon series to obtain irreducible tensors of higher rank. In fact, if $A_{s,m}$ and $A_{s',m'}$ are two spherical tensors, then one can form the product $A_{s,m}A_{s',m'}$ (if their dimensions are the same) or $A_{s,m} \otimes A_{s',m'}$ (otherwise) and decompose the products by using the Clebsh–Gordon coefficients to obtain spherical tensors of higher rank. For example, take the AKLT tensor of rank 1. Ordinary multiplication of this tensor does not give a tensor of rank 2 since $\sigma_+^2=0$; however, its tensor multiplication gives a tensor of rank 2 of dimension 4, i.e., $A_{2,2}=2\sigma_+ \otimes \sigma_+$, etc. In this way, the product of two rank-1 tensors can be decomposed to give a rank-2, a rank-1, and rank-0 tensor. The obtained tensors can again be multiplied with other tensors and decomposed to obtain tensors of even higher rank. This procedure, however, has several drawbacks: first, the dimensions of the matrices will grow very fast as we increase the rank of tensors; second, it requires multiple use of Clebsh–Gordon coefficients, which make the final expression of the tensors, especially for high-rank tensors, quite cumbersome and not useful. Another useful procedure is to invoke the Wigner–Eckart theorem, which decomposes the matrix elements of any spherical tensor in the angular momentum basis to an angular part, which is the Clebsh–Gordon coefficient, and a reduced part, which essentially defines the tensor. However, this procedure does not always lead to a compact notation for the tensor operators themselves and the multiplication of such tensors requires heavy use of Glebsh–Gordon coefficients. In this paper, we introduce a compact and transparent formula for spherical tensors of rank s, for s integer or half integer, and use it to construct matrix product states for spin chains. For rank-s tensors, the dimensions of the matrices are $2s+2$; thus, the dimension grows linearly with rank.

To construct the spherical rank-s tensor, let us take the orthonormal basis $\{|s,m\rangle, m=-s\cdots s\}$ of the spin-s representation and augment it by the single state $|\tilde{0}\rangle$ of the spin 0 representation,

$$\langle\tilde{0}|\tilde{0}\rangle = 1, \quad \langle\tilde{0}|s,m\rangle = \langle s,m|\tilde{0}\rangle = 0. \tag{21}$$

On this larger space, the following is the reducible $s \oplus 0$ representation of angular momentum algebra:

$$L_z = \sum_{m=-s}^{s} m|s,m\rangle\langle s,m|,$$

$$L_+ = \sum_{m=-s}^{s} \sqrt{s(s+1) - m(m+1)}|s,m+1\rangle\langle s,m|,$$

$$L_- = \sum_{m=-s}^{s} \sqrt{s(s+1) - m(m-1)}|s,m-1\rangle\langle s,m|. \tag{22}$$

Now, it is readily verified that in this $2s+2$ dimensional space, the following matrices form an irreducible rank-s spherical tensor, that is, they satisfy the relations [Eq. (17)]:

$$A_{s,m} := |s,m\rangle\langle\tilde{0}| + (-1)^{s-m}|\tilde{0}\rangle\langle s,-m|, \tag{23}$$

where $-s \le m \le s$.

It is important to note that the rank of these tensors can be integer or half integer. Such operators transform as an irreducible rank-s tensor in the space, which carries the reducible representation $s \oplus 0$.

Note. One can define the tensors more generally as

$$A_{s,m} := a|s,m\rangle\langle\tilde{0}| + b(-1)^m|\tilde{0}\rangle\langle s,-m|,$$

where a and b are arbitrary numbers; however, these tensors are equivalent to the previous ones in the sense that they reduce to them by a suitable unitary transformation. The factor $(-1)^s$ is inserted in the definition to ensure that no complex number enters the expression for half-integer ranks.

While there are many representations for spherical tensors of different ranks, and these have been used in different

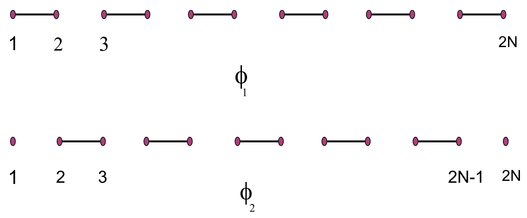

FIG. 3. (Color online) The fully dimerized spin-s states in Eq. (26).

works to construct various examples of invariant MPS,[16–19,21,25,26] we introduced here a unique representation [Eq. (23)]. In the sequel, we show that this representation is very general, in the sense that we can use it to find MP representations for all the variety of AKLT states, including the Majumdar–Ghosh or fully dimerized states of arbitrary spin, the partially dimerized states, and also the various states, which are found from these partially dimerized states by different types of projection. Even more, one can construct other states not listed in the original AKLT papers, these are the symmetry-breaking states.

IV. SPIN-s FULLY DIMERIZED OR MAJUMDAR–GHOSH STATES

Using the definition of A_m, we find

$$A_{m_1}A_{m_2}\cdots A_{m_{2N}} = \prod_{i=1}^{N}(-1)^{s-m_{2i-1}}\delta_{m_{2i-1},-m_{2i}}|\tilde{0}\rangle\langle\tilde{0}| + (-1)^{s-m_{2N}}\prod_{i=1}^{N-1}(-1)^{s-m_{2i}} \times \delta_{m_{2i},-m_{2i+1}}|m_1\rangle\langle -m_{2N}|. \tag{24}$$

Taking the trace, we find

$$\mathrm{Tr}(A_{m_1}\cdots A_{m_{2N}}) = \prod_{i=1}^{N}(-1)^{s-m_{2i-1}}\delta_{m_{2i-1},-m_{2i}} + \prod_{i=1}^{N}(-1)^{s-m_{2i}}\delta_{m_{2i},-m_{2i+1}}. \tag{25}$$

Inserting this into Eqs. (3) and (4), the final simple form of the matrix product ground state is obtained as

$$|\psi\rangle \equiv |\phi_1\rangle + |\phi_2\rangle = |S\rangle_{12}|S\rangle_{34}\cdots|S\rangle_{2N-1,2N} + |S\rangle_{23}|S\rangle_{45}\cdots|S\rangle_{2N,1}, \tag{26}$$

where the singlet states $|S\rangle$ are given by

$$|S\rangle = \frac{1}{\sqrt{2s+1}}\sum_m (-1)^{s+m}|m,-m\rangle. \tag{27}$$

Note that $|S\rangle$ is a singlet state, i.e., $L_z|S\rangle = L_+|S\rangle = L_-|S\rangle = 0$. Thus, $|\phi_1\rangle$ is a juxtaposition of spin-s dimers on sites $(1,2),(3,4),\ldots,(2N-1,2N)$ and $|\phi_2\rangle$ is a one-site translation of $|\phi_1\rangle$, i.e., a collection of spin-s dimers on sites $(2,3),(4,5),\ldots,(2N,1)$ (Fig. 3).

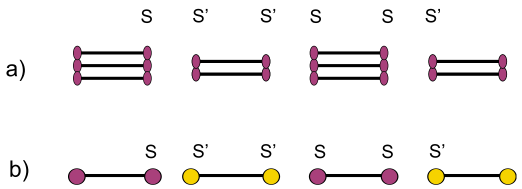

FIG. 4. (Color online) $2s$ valence bonds (spin-1/2 singlets) in the AKLT construction are replaced in our work with a single spin-s valence bond, which is MPS representable by the matrix [Eq. (28)].

V. OTHER TYPES OF DIMERIZED STATES

A general dimerized state is the one which is shown in Fig. 4(a), where each line stands for a spin-1/2 dimer. The numbers of dimers are $2s$ and $2s'$. In our representation, we replace $2s$ spin-1/2 dimers with a single spin-s dimer, as in Fig. 4(b). Such a state has a simple MPS representation in the form

$$|\psi\rangle = \sum \mathrm{tr}(A_{m_1}A_{m_2}B_{m_1'}B_{m_2'}A_{m_3}A_{m_4}B_{m_3'}B_{m_4'}\cdots) \times |m_1 m_2 m_1' m_2' m_3 m_4 m_3' m_4' \cdots\rangle, \tag{28}$$

where the matrices $\{A_m\}$ and $\{B_{m'}\}$ are the embedding of the rank-s and rank-s' tensors [Eq. (23)] into a representation spanned by the vectors $\{|\tilde{0}\rangle, |s,m\rangle, |s',m'\rangle\}$, i.e., the direct sum representation $s \oplus s' \oplus 0$. In fact, it is readily found that with

$$A_{s,m} \equiv A_m = |s,m\rangle\langle\tilde{0}| + (-1)^{s-m}|\tilde{0}\rangle\langle s,-m|,$$

$$A_{s',m'} \equiv B_{m'} = |s',m'\rangle\langle\tilde{0}| + (-1)^{s'-m'}|\tilde{0}\rangle\langle s',-m'|, \tag{29}$$

we have

$$A_{m_1}A_{m_2}B_{m_1'}B_{m_2'} = (-1)^{s-m_1}\delta_{m_1,-m_2}(-1)^{s'-m_1'}\delta_{m_1',-m_2'}|\tilde{0}\rangle\langle\tilde{0}|, \tag{30}$$

which readily yields the following partially dimerized form for the state [Eq. (28)]:

$$|\psi\rangle = |S\rangle_{12}|S'\rangle_{34}|S\rangle_{56}|S'\rangle_{78}\cdots, \tag{31}$$

where $|S\rangle$ and $|S'\rangle$ are, respectively, spin-s and spin-s' singlets defined in Eq. (27).

One can construct even more general states, i.e., the symmetry-breaking states of the form shown in Fig. 5, where the dimers are interspaced by spins which align in a particular direction. Consider the state

$$|\psi\rangle = \mathrm{tr}(A_{m_1}A_{m_2}C_{m_3}A_{m_4}A_{m_5}C_{m_6}\cdots) \times |m_1,m_2,m_3,m_4,m_5,m_6,\cdots\rangle, \tag{32}$$

where A_m is of the form (23) and $C_m = \alpha_m|\tilde{0}\rangle\langle\tilde{0}|$, in which

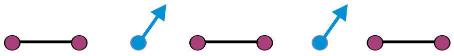

FIG. 5. (Color online) The tensors [Eq. (23)] can also be used to construct symmetry-breaking matrix product states.

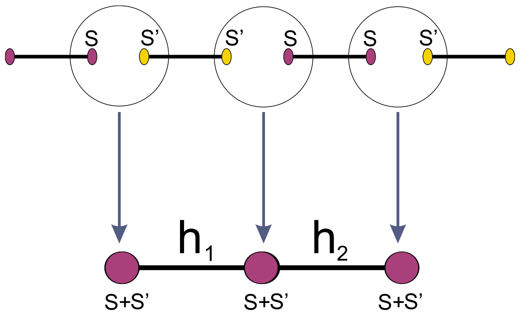

FIG. 6. (Color online) The projection method: From a partially or fully dimerized state, whose parent Hamiltonian has interaction range 3, an AKLT/VBS state is constructed whose parent Hamiltonian has interaction range 2. The form of the Hamiltonian is given in Eqs. (33) and (34).

α_m's $(-s \le m \le s)$ are arbitrary complex numbers. Then, the MPS represents a symmetry-breaking state shown in Fig. 5, where spins 3,6,… are aligned in the state $|\alpha\rangle := \sum_{m=-s}^{s} \alpha_m |s,m\rangle$ and the rest of the sites are dimerized. A suitable projection of these states gives symmetry-breaking nondimerized states.[32]

VI. AFFLECK–KENNEDY–LIEB–TASAKI/VALENCE BOND SOLID STATES

In the AKLT models, one can use the fully dimerized states and project them to states, which are called VBS states. While the parent Hamiltonian of the fully dimerized states has an interaction range of three sites, the VBS states, which are obtained by projection, have parent Hamiltonians with interaction range of two sites. The method is explained in Fig. 6, where we use a single spin-s dimer to replace $2s$ spin-$1/2$ dimers in the original method of AKLT.

The lower state is obtained by projecting the states inside each bulb in the upper chain onto the symmetrized spin sector with total spin $s+s'$. It is now obvious how the parent Hamiltonian of the lower chain, the Hamiltonian which has this state as its ground state, should be constructed. Consider the first bond in Fig. 6, whose local Hamiltonian is denoted by h_1. Due to the $2s'$ singlets, between the two bulbs, here we are only summing over two spin-s states, instead of the apparent two spin-s and two spin-s' states. Hence, all the projectors P_j, with $2s+1 \le j \le 2s+2s'$, annihilate this bond, i.e., the local Hamiltonian h_1 can be constructed as a linear superposition of all the above projectors with positive coefficients. By the same reasoning, the local Hamiltonian h_2 can be a linear superposition of all projectors P_k, with $2s'+1 \le k \le 2s+2s'$. Thus, to construct a translation-invariant Hamiltonian, the parent Hamiltonian of the lower state can be constructed as

$$H = \sum_i h_{i,i+1}, \tag{33}$$

where

$$h = \sum_{j=\max(2s,2s')+1}^{2s+2s'} \lambda_j P_j, \tag{34}$$

where P_j's are the projectors on the spin-j sector of two sites and λ_j are positive coefficients.

Note that the state on the lower chain is no longer dimerized, i.e., spins which are further apart than one lattice spacing are correlated. Needless to say, the projection method although elegant, in principle, is not suitable for the calculation of many properties of the state. Having a matrix product representation for this state turns all calculations into a straightforward and handy procedure. In this section, we show that the irreducible tensors introduced in Sec. III provides a MP representation for these states in a very simple way.

The starting point of our procedure is, however, not to use $2s$ and $2s'$ spin-1/2 dimers, as in Fig. 4(a); rather, we use equivalently one spin-s and one spin-s' singlets, as in Fig. 4(b), for which we have already a MP representation. The spin-s and spin-s' dimers come from rank-s and rank-s' tensors [Eq. (23)]. We multiply and symmetrize these two tensors to obtain a tensor whose highest component is given by

$$V_{s+s',s+s'} = A_{s,s}A_{s',s'} + A_{s',s'}A_{s,s}. \tag{35}$$

From the explicit form of the tensors in Eq. (23), one sees that

$$V_{s+s',s+s'} := |s,s\rangle\langle s',-s'| + |s',s'\rangle\langle s,-s|. \tag{36}$$

Note that this tensor lives in the $2s+2s'+2$ dimensional space spanned by independent vectors $\{|s,m\rangle, |s',m'\rangle, -s \le m \le s, -s' \le m' \le s'\}$.

It is readily verified that

$$[L_z, V_{s+s',s+s'}] = (s+s')V_{s+s',s+s'},$$

$$[L_+, V_{s+s',s+s'}] = 0. \tag{37}$$

Therefore, $V_{s+s',s+s'}$ is indeed the highest-weight component of a spherical tensor of rank $s+s'$. Other components are obtained by successive commutations with L_-. For example, we have

$$\begin{aligned} V_{s+s',s+s'-1} := {} & \sqrt{\frac{s}{s+s'}}(|s,s-1\rangle\langle s',-s'| - |s',s'\rangle\langle s,-s+1|) \\ & + \sqrt{\frac{s'}{s+s'}}(|s',s'-1\rangle\langle s,-s| - |s,s\rangle\langle s',-s' \\ & +1|). \end{aligned} \tag{38}$$

The spherical tensors have the interesting property that they lead to a nonempty null space Δ_2. In fact, it can be verified that these tensors have a peculiar fusion rule (decomposition of the product into irreducible representations), which exactly matches the fusion rule of the original $2s$ and $2s'$ valence bonds in a symmetric way. In the present formalism, this symmetry causes the final local Hamiltonian h to contain projectors common to both h_1 and h_2 (Fig. 6) in the AKLT construction. Using the notation V_s to denote the whole multiplet $V_{s,m}, -s \le m \le s$, the fusion rule of our tensors is

$$V_{s+s'} \otimes V_{s+s'} = \bigoplus_{j=0}^{\max(2s,2s')} c_j V_j. \tag{39}$$

Thus, the multiplets V_j with $\max(2s,2s')+1 \le j \le 2(s+s')$ are absent, i.e., identically vanish, in the decomposition of the left hand side tensors. In the language of matrix product formalism, Sec. II, this means that the null space of the two-site density matrix contains the multiplet of states, which transform as spin-j representations with $\max(2s,2s')+1 \le j \le 2(s+s')$. Therefore, the local Hamiltonian annihilating the dimerized state can be constructed from the projectors to these multiplets, namely,

$$h = \sum_{j=\max(2s,2s')+1}^{2s+2s'} \lambda_j P_j, \tag{40}$$

where P_j's are projectors on spin j and λ_j are positive coefficients. It requires tedious and lengthy calculations, which may not be illuminating to prove Eq. (39), in general. Instead, we will give an idea of the proof by way of examples. First of all, it is readily seen from Eq. (36) that $s, s' \neq 0$,

$$V^2_{s+s',s+s'} = 0,$$

but this is the top state of the multiplet $V_{2s+2s'}$ and hence this multiplet is absent in the right hand side of Eq. (39). In the same way, one can also show from Eqs. (36) and (38) that the top state of the multiplet $V_{2s+2s'-1}$ is zero. This pattern repeats until we arrive at the multiplet $V_{\max(2s,2s')}$. We will give a more detailed and concrete example in Sec. VII.

VII. EXAMPLES

Up until now, we have been able to use our spherical tensors [Eq. (23)] in a uniform manner to construct all the varieties of valence bond states in the AKLT construction. In this section, we will provide a few concrete examples.

A. Properties of fully dimerized or spin-*s* Majumdar–Ghosh states

First, we calculate the normalization of fully dimerized states $|\Psi^{\pm}\rangle$. The basic tool which we use is the following easily verified equation between the singlets, where 1, 2, 3, and 4 are any four different and not necessarily adjacent sites:

$$_{23}\langle S|S\rangle_{12}|S\rangle_{34} = \frac{\epsilon}{2s+1}|S\rangle_{14}, \tag{41}$$

where

$$\epsilon = \begin{cases} 1, & s = \text{integer} \\ -1, & s = \text{half integer}. \end{cases}$$

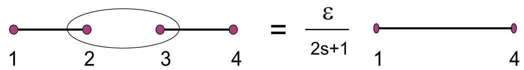

FIG. 7. (Color online) The graphical representation of Eq. (41). A bulb around 2 and 3 means that the state has been multiplied from the left by $_{2,3}\langle S|$, leaving the singlet on the right hand side. Note that labels 1, 2, 3, and 4 denote any four sites.

This relation, which we will use repeatedly in the following, is depicted graphically in Fig. 7. Here, a bulb around two sites (2,3) means that it has been multiplied from the left by a singlet $_{2,3}\langle S|$. Repeatedly using Eq. (41) or graph (7), as in Fig. 8, will give

$$\langle \phi_1|\phi_2\rangle = \frac{\epsilon^N}{(2s+1)^{N-1}}, \tag{42}$$

from which we obtain the normalization

$$\langle \Psi^{\pm}|\Psi^{\pm}\rangle = 2\left[1 \pm \frac{\epsilon^N}{(2s+1)^{N-1}}\right]. \tag{43}$$

In order to find the correlations, we use the following equations:

$$_{12}\langle S|\mathbf{s}_1\cdot\mathbf{s}_2|S\rangle_{12} = -s(s+1) \tag{44}$$

and

$$\begin{aligned} _{23}\langle S|\mathbf{s}_1\cdot\mathbf{s}_2|S\rangle_{12}|S\rangle_{34} &= -s(s+1)\,_{23}\langle S|S\rangle_{12}|S\rangle_{34} \\ &= -\frac{s(s+1)\epsilon^N}{2s+1}|S\rangle_{14}, \end{aligned} \tag{45}$$

which readily gives

$$\langle \phi_1|\mathbf{s}_1\cdot\mathbf{s}_2|\phi_1\rangle = -s(s+1), \quad \langle \phi_2|\mathbf{s}_1\cdot\mathbf{s}_2|\phi_2\rangle = 0. \tag{46}$$

Again, the cross-product term is calculated with the help of graph (8),

$$\langle \phi_1|\mathbf{s}_1\cdot\mathbf{s}_2|\phi_2\rangle = -s(s+1)\langle \phi_1|\phi_2\rangle = -s(s+1)\frac{\epsilon^N}{(2s+1)^{N-1}}. \tag{47}$$

Putting these together, we find the final form of the correlation functions,

$$\frac{\langle \Psi^{\pm}|\mathbf{s}_1\cdot\mathbf{s}_2|\Psi^{\pm}\rangle}{\langle \Psi^{\pm}|\Psi^{\pm}\rangle} = -\frac{s(s+1)}{2}\,\frac{(2s+1)^{N-1} \pm 2\epsilon^N}{(2s+1)^{N-1} \pm \epsilon^N}. \tag{48}$$

To construct the parent Hamiltonian of such states, we use Eq. (11) and find the null space of the reduced density matrices of three consecutive sites Δ_3 (two consecutive sites have no nontrivial null space in this model). From Eq. (23), we have

$$\begin{aligned} A_m A_{m'} A_{m''} = {}& (-1)^{s-m'}\,\delta_{m',-m''}|m\rangle\langle\tilde{0}| + \delta_{m',-m}(-1)^{2s-m-m''}|\tilde{0}\rangle \\ & \times\langle -m''|. \end{aligned} \tag{49}$$

To find the null space Δ_3, we need to solve the matrix equation

$$\sum_{m,m',m''} c_{m,m',m''} A_m A_{m'} A_{m''} = 0, \tag{50}$$

which yields the following conditions:

$$\sum_m (-1)^m C_{m',m,-m} = 0, \quad \forall\, m',$$

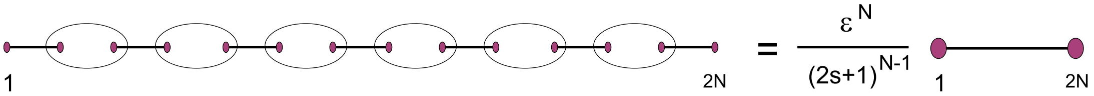

FIG. 8. (Color online) The repeated use of graph (7) for calculating the cross-product terms $\langle\phi_1|\phi_2\rangle$.

$$\sum_m (-1)^m C_{m,-m,m'} = 0, \qquad \forall\, m'. \tag{51}$$

These conditions can be re-expressed in a more useful form, namely, the null space Δ_3 is spanned by vectors of the form

$$|\chi\rangle = \sum_{m,m',m''} c_{m,m',m''}|m,m',m''\rangle, \tag{52}$$

which are perpendicular to the state [Eq. (27)], i.e.,

$${}_{12}\langle S|\chi\rangle = 0, \qquad {}_{23}\langle S|\chi\rangle = 0, \tag{53}$$

where the subscripts indicate the embedding of $\langle S|$ into the local spaces of three consecutive spins. Note that the factor $\sqrt{2s+1}$ has been inserted so that the state $|S\rangle$ is normalized. We will later use these equations to clarify the form of the Hamiltonian, but first let us derive an explicit form for the ground state.

One is tempted to ask if $|\phi_1\rangle$ or $|\phi_2\rangle$ are ground states separately. The answer is positive. To see this, note that the Hamiltonian is written in the form

$$H = \sum_{k=1}^{2N} h_{k,k+1,k+2}, \tag{54}$$

where h is the sum of projectors on the null space Δ_3, i.e.,

$$h = \sum_\alpha \lambda_\alpha |e_\alpha\rangle\langle e_\alpha|, \qquad |e_\alpha\rangle \in \Delta_3. \tag{55}$$

Here, $\{|e_\alpha\rangle\}$ is a basis for Δ_3 and from Eq. (53), we know that $\langle e_\alpha|S\rangle_{12}=\langle e_\alpha|S\rangle_{23}$, $\forall\alpha$. This implies that $H|\phi_1\rangle=H|\phi_2\rangle=0$. Each of the dimerized states $|\phi_1\rangle$ and $|\phi_2\rangle$ breaks the translational symmetry of the Hamiltonian. Finally, let us also derive the parent Hamiltonians for the simplest cases, namely, spin 1/2 which is well known and spin-1 Majumdar–Ghosh states.

1. Parent Hamiltonian for spin-1/2 dimerized state

Using the standard notation $|+\rangle := |\tfrac{1}{2},\tfrac{1}{2}\rangle, |-\rangle := |\tfrac{1}{2},\tfrac{-1}{2}\rangle$, we order the states of auxiliary space as $\{|+\rangle,|\tilde{0}\rangle,|-\rangle\}$. Then from Eq. (23), we have

$$A_+ = |+\rangle\langle\tilde{0}| + |\tilde{0}\rangle\langle - \Bigg| = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix},$$

$$A_- = |-\rangle\langle\tilde{0}| - |\tilde{0}\rangle\Bigg\langle + | = \begin{pmatrix} 0 & 0 & 0 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \tag{56}$$

which transforms as a rank-1/2 tensor with the generators given by

$$L_z = \begin{pmatrix} \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \frac{-1}{2} \end{pmatrix}, \quad L_+ = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad L_- = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}. \tag{57}$$

The singlet states are $|S\rangle = \frac{1}{\sqrt{2}}(|+,-\rangle - |-,+\rangle)$. To find the parent Hamiltonian, we should solve Eq. (51) or, what is the same thing, find states $|\chi\rangle \in C^2\otimes C^2\otimes C^2$ such that ${}_{12}\langle S|\chi\rangle$ $=23\ \langle S|\chi\rangle=0$. It is readily found that there are four such states,

$$|e_1\rangle = |+,+,+\rangle,$$

$$|e_2\rangle = \frac{1}{\sqrt{3}}(|+,+,-\rangle + |+,-,+\rangle + |-,+,+\rangle),$$

$$|e_3\rangle = \frac{1}{\sqrt{3}}(|-,-,+\rangle + |-,+,-\rangle + |+,-,-\rangle),$$

$$|e_4\rangle = |-,-,-\rangle. \tag{58}$$

The vectors $|e_i\rangle$ form the spin-3/2 multiplet, and if they come with the same coefficients in h in Eq. (55), the resulting Hamiltonian will be a scalar. It is known[22,23] that in this case, the parent Hamiltonian will be the Majumdar–Ghosh Hamiltonian, namely,

$$H = \sum_i 2\sigma_i\cdot\sigma_{i+1} + \sigma_i\cdot\sigma_{i+2}.$$

2. Parent Hamiltonian for spin-1 fully dimerized state

Using the abbreviated notation $|1\rangle := |1,1\rangle$, $|0\rangle := |1,0\rangle$, $|\bar{1}\rangle := |1,-1\rangle$, we have as the singlet state in $|S\rangle \in C^3\otimes C^3$,

$$|S\rangle = \frac{1}{\sqrt{3}}(|1,\bar{1}\rangle - |0,0\rangle + |\bar{1},1\rangle). \tag{59}$$

In order to find the null space Δ_3, we note that due to su(2) symmetry [Eq. (14)], the basis vectors of Δ_3 can be grouped into multiplets, which transform irreducibly under su(2). These multiplets come from the decomposition of $1\otimes1\otimes1$ representation, which decomposes as

$$1\otimes1\otimes1 = 3\oplus2\oplus2'\oplus1\oplus1'\oplus1''\oplus0. \tag{60}$$

However, not all the above multiplets belong to Δ_3. In order to determine those which are, we should check the conditions [Eq. (51)]. It is sufficient to check these conditions only for the top state of each multiplet since symmetry guarantees that the other states are present in Δ_3, once the top state is present. With this insight, we readily find that the multiplets with the following top states are present in Δ_3:

$$|e_1\rangle := |t_3\rangle = |1,1,1\rangle,$$

$$|e_2\rangle := |t_2\rangle = |1,1,0\rangle - |0,1,1\rangle,$$

$$|e_3\rangle := |t_{2'}\rangle = |1,1,0\rangle - 2|1,0,1\rangle + |0,1,1\rangle,$$

$$|e_4\rangle := |t_1\rangle = |1,0,0\rangle + |0,0,1\rangle + 3|\bar{1},1,1\rangle + 3|1,1,\bar{1}\rangle - 2|1,\bar{1},1\rangle - 4|0,1,0\rangle,$$

$$|e_5\rangle := |t_0\rangle = |1,\bar{1},0\rangle - |\bar{1},1,0\rangle - |1,0,\bar{1}\rangle + |\bar{1},0,1\rangle + |0,1,\bar{1}\rangle - |0,\bar{1},1\rangle, \tag{61}$$

where $|t_j\rangle$ denotes the top state of the spin-j representation. One can verify that these are actually the top states by checking the equations $L_z|t_j\rangle=j|t_j\rangle$ and $L_+|t_j\rangle=0$ and also that they really belong to Δ_3 by checking ${}_{12}\langle S|e_i\rangle=23\ \langle S|e_i\rangle=0$.

Having five different multiplets in the null space means that the Hamiltonian has five different couplings which can be tuned. Of course, one of the couplings can be set to unity by a choice of energy scale. Let us call the projectors on the representation space j by P_j. Then, the local Hamiltonian h will be

$$h = \lambda_0 P_0 + \lambda_1 P_1 + \lambda_2 P_2 + \lambda_2' P_{2'} + \lambda_3 P_3. \tag{62}$$

Remark. It is important to note that the MPS formalism gives a larger family of parent Hamiltonian than the original AKLT construction. In fact, in the AKLT construction, the presence of projectors P_3, P_2, $P_{2'}$, and P_0 is automatic. However, the presence of the new projector P_1 is the result of the MPS formalism.

The next step, which is not trivial, is to write the projectors in terms of local spin operators. The point is that on the decomposition [Eq. (60)], only some of the representations on the right hand side belong to Δ_3. For those representations which occur with multiplicity 1, we can easily find the expression of the corresponding projectors in terms of local spin operators. Let us denote the sum of spin operators on three sites by $\mathbf{S}$, i.e.,

$$\mathbf{S} := \mathbf{S}_1 + \mathbf{S}_2 + \mathbf{S}_3.$$

The basis states of the representations on the right hand side of Eq. (60) are such that they block diagonalize the generators and hence the operator $\mathbf{S}\cdot\mathbf{S}$. Let us denote the projectors on the totality of spin-j representations by $\mathcal{P}_j$, i.e., $\mathcal{P}_0=P_0$, $\mathcal{P}_1:=P_1+P_{1'}+P_{1''}$, $\mathcal{P}_2=P_2+P_{2'}$, and $\mathcal{P}_3=P_3$. Then, we have the following system of equations $(\mathbf{S}\cdot\mathbf{S})^k=\Sigma_{l=0}^3(l(l+1))^k\mathcal{P}_l$, $k=0,1,2,3$, or more explicitly:

$$I = \mathcal{P}_3 + \mathcal{P}_2 + \mathcal{P}_1 + \mathcal{P}_0,$$

$$\mathbf{S}\cdot\mathbf{S} = 12\mathcal{P}_3 + 6\mathcal{P}_2 + 2\mathcal{P}_1,$$

$$(\mathbf{S}\cdot\mathbf{S})^2 = 144\mathcal{P}_3 + 36\mathcal{P}_2 + 4\mathcal{P}_1,$$

$$(\mathbf{S}\cdot\mathbf{S})^3 = 343\mathcal{P}_3 + 125\mathcal{P}_2 + 27\mathcal{P}_1. \tag{63}$$

Inverting the above equations, we find

$$720\mathcal{P}_3 = 12\mathbf{S}\cdot\mathbf{S} - 8(\mathbf{S}\cdot\mathbf{S})^2 + (\mathbf{S}\cdot\mathbf{S})^3,$$

$$144\mathcal{P}_2 = -24\mathbf{S}\cdot\mathbf{S} + 14(\mathbf{S}\cdot\mathbf{S})^2 - (\mathbf{S}\cdot\mathbf{S})^3,$$

$$80\mathcal{P}_1 = 72\mathbf{S}\cdot\mathbf{S} - 18(\mathbf{S}\cdot\mathbf{S})^2 + (\mathbf{S}\cdot\mathbf{S})^3,$$

$$144\mathcal{P}_0 = 144 - 108\mathbf{S}\cdot\mathbf{S} + 20(\mathbf{S}\cdot\mathbf{S})^2 - (\mathbf{S}\cdot\mathbf{S})^3. \tag{64}$$

A positive linear combination of projectors $\mathcal{P}_3$, $\mathcal{P}_2$, and $\mathcal{P}_0$ gives a three parameter family of Hamiltonians. Projector $\mathcal{P}_1$ should be left out from this combination since only one of the spin-1 representations belongs to the null space Δ_3. In general, those representations which occur with multiplicity one can always be expressed in terms of total spin operator $\mathbf{S}$ on three sites. However, we can construct a more general family of Hamiltonians by calculating explicitly all the projectors in Eq. (62) in terms of the most general set of independent three-body spin operators. A straightforward calculation gives the final form of the Hamiltonian (with the abbreviation $S_{12}:=\mathbf{S}_1\cdot\mathbf{S}_2$),

$$H = \sum_{i=1}^{2N} J_0 + J_1 S_{i,i+1} + J_2 S_{i,i+2} + J_3 S_{i,i+1}^2 + J_4 S_{i,i+2}^2 + J_5\{S_{i,i+1},S_{i+1,i+2}\} + J_6\{S_{i,i+2},\{S_{i,i+1},S_{i+1,i+2}\}\} + J_7(S_{i,i+1}S_{i,i+2}S_{i+1,i+2} + S_{i+1,i+2}S_{i,i+2}S_{i,i+1}),$$

where

$$J_0 = -2\lambda_0 + \frac{3}{5}\lambda_1 + \frac{1}{3}(\lambda_2 + \lambda_{2'}) + \frac{1}{15}\lambda_3,$$

$$J_1 = 2\lambda_0 - \frac{2}{5}\lambda_1 - \frac{1}{3}(\lambda_2 + \lambda_{2'}) + \frac{11}{15}\lambda_3,$$

$$J_2 = -3\lambda_0 + \frac{1}{20}\lambda_1 + \frac{1}{2}(\lambda_2 + \lambda_{2'}) - \frac{3}{10}\lambda_3,$$

$$J_3 = 2\lambda_0 - \frac{13}{20}\lambda_1 - \frac{1}{6}(\lambda_2 - \lambda_{2'}) + \frac{1}{15}\lambda_3,$$

$$J_4 = \lambda_0 + \frac{1}{20}\lambda_1 + \frac{1}{6}(\lambda_2 - \lambda_{2'}) + \frac{1}{30}\lambda_3,$$

$$J_5 = \lambda_0 - \frac{1}{6}(\lambda_2 + \lambda_{2'}) + \frac{1}{6}\lambda_3,$$

$$J_6 = -\lambda_0 + \frac{1}{10}\lambda_1 + \frac{1}{6}\lambda_{2'} - \frac{1}{10}\lambda_3,$$

$$J_7 = \lambda_0 - \frac{1}{40}\lambda_1 - \frac{1}{12}(\lambda_2 + 5\lambda_{2'}) + \frac{7}{30}\lambda_3. \tag{65}$$

This Hamiltonian may seem complicated and not so interesting from the physical point of view. However, we should note that it has effectively four adjustable parameters (since we can take $\lambda_0=1$) and by tuning these parameters, this

Hamiltonian may come close to physically simple and interesting models. For example, if we take the parameters as follows:

$$\lambda_0 := 1, \quad \lambda_1 = 8 + \frac{2}{3}\lambda_2, \quad \lambda_2' = 12 + 2\lambda_2, \quad \lambda_3 = 18 + 4\lambda_2, \tag{66}$$

then the couplings J_3, J_4, J_6, and J_7 all vanish and the Hamiltonian finds the following simple form, modulo additive and positive multiplicative constants:

$$H = \sum_{i=1}^{2N} \mathbf{S}_i \cdot \mathbf{S}_{i+1} + \Delta \mathbf{S}_i \cdot \mathbf{S}_{i+2} + K\{\mathbf{S}_i \cdot \mathbf{S}_{i+1}, \mathbf{S}_{i+1} \cdot \mathbf{S}_{i+2}\}, \tag{67}$$

where $\Delta := \frac{\lambda_2 - 6}{5\lambda_2 + 24}$ and $K = \frac{6 + \lambda_2/2}{5\lambda_2 + 24}$. By taking $\lambda_2 = 6$, we can further set $\Delta = 0$ and $K = \frac{1}{6}$, and hence we can arrive at

$$H = \sum_{i=1}^{2N} \mathbf{S}_i \cdot \mathbf{S}_{i+1} + \frac{1}{6}\{\mathbf{S}_i \cdot \mathbf{S}_{i+1}, \mathbf{S}_{i+1} \cdot \mathbf{S}_{i+2}\}, \tag{68}$$

or by taking λ_2 very large, we can come arbitrarily close to the following Hamiltonian:

$$H = \sum_{i=1}^{2N} \mathbf{S}_i \cdot \mathbf{S}_{i+1} + \frac{1}{5}\mathbf{S}_i \cdot \mathbf{S}_{i+2} + \frac{1}{10}\{\mathbf{S}_i \cdot \mathbf{S}_{i+1}, \mathbf{S}_{i+1} \cdot \mathbf{S}_{i+2}\}. \tag{69}$$

B. Examples of Affleck–Kennedy–Lieb–Tasaki/valence bond solid states

While the MPS representation may not be a necessity when dealing with fully dimerized states, such representation is invaluable when dealing with VBS states.

1. Spin-3/2 valence bond solid state

As our last examples, we consider the MP representation of the spin-3/2 VBS state of the form shown in Fig. 2, which is obtained from a dimerized state with $s=1$ and $s'=1/2$. From Eq. (36), we see that the MP representation of such a chain is given by the following matrices, where we have abbreviated $|1,m\rangle \to |m\rangle$ and $|\frac{1}{2}, \pm\frac{1}{2}\rangle \to |\pm\rangle$:

$$V_{3/2,3/2} = |1\rangle\langle -| + |+\rangle\langle -1|,$$

$$V_{3/2,1/2} = \sqrt{\frac{2}{3}}|0\rangle\langle -| + \sqrt{\frac{1}{3}}|-\rangle\langle -1| - \sqrt{\frac{1}{3}}|1\rangle\langle +| - \sqrt{\frac{2}{3}}|+\rangle\langle 0|,$$

$$V_{3/2,-1/2} = -\sqrt{\frac{2}{3}}|0\rangle\langle +| - \sqrt{\frac{1}{3}}|+\rangle\langle 1| + \sqrt{\frac{1}{3}}|-1\rangle\langle -| + \sqrt{\frac{2}{3}}|-\rangle\langle 0|,$$

$$V_{3/2,-3/2} = -|-1\rangle\langle +| + |-\rangle\langle 1|. \tag{70}$$

Note that we use Eq. (36) to find the highest-weight component of this tensor and the rest of the components are derived by the action of L_-. In a basis with the order $|1,1\rangle, |1,0\rangle, |1,-1\rangle, |+\rangle, |-\rangle$, the five dimensional vectors $V_{3/2,m}$ have the following explicit form:

$$V_{3/2,3/2} = \begin{pmatrix} \cdot & \cdot & \cdot & \cdot & 1 \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix},$$

$$V_{3/2,1/2} = \frac{1}{\sqrt{3}}\begin{pmatrix} \cdot & \cdot & \cdot & -1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \sqrt{2} \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & -\sqrt{2} & \cdot & \cdot & \cdot \\ \cdot & \cdot & 1 & \cdot & \cdot \end{pmatrix}, \tag{71}$$

$$V_{3/2,-1/2} = \frac{1}{\sqrt{3}}\begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & -\sqrt{2} & \cdot \\ \cdot & \cdot & \cdot & \cdot & 1 \\ 1 & \cdot & \cdot & \cdot & \cdot \\ \cdot & -\sqrt{2} & \cdot & \cdot & \cdot \end{pmatrix},$$

$$V_{3/2,-3/2} = \begin{pmatrix} \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & -1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ 1 & \cdot & \cdot & \cdot & \cdot \end{pmatrix}. \tag{72}$$

From Fig. 2 and the discussion following it, we see that the translation-invariant parent Hamiltonian annihilating this state should be constructed from projector P_3 onto spin-3 states. In the matrix product formalism, this means that the null space of the two-site density matrix should contain the multiplet of states, which transform as a spin-3 representation. In view of Eq. (39), this means that in the decomposition of quadratic product of tensors $V_{3/2,m}$, into irreducible representations of su(2), the representation of spin 3 should not appear, i.e., the components of this tensor should identically vanish. This is indeed the case as one can see from Eq. (72) that $V_{3/2,3/2}^2$, which is the component with highest weight of spin-3 representation, vanishes. The other components vanish by symmetry.

Equation (39) generalizes this to arbitrary spins in a nice way, which is exactly what we see in the valence bond picture of Eq. (6). Even more than that, it gives in one shot the Hamiltonian, which is common to both h_1 and h_2 in Fig. 6.

2. Fusion rule of the tensors V_s

As stated above, the properties of valence bonds in the AKLT formalism are nicely captured in the fusion rule of the tensors V_s [Eq. (39)]. Although the complete proof of Eq. (39) is possible, we think that it is not so illuminating. Instead, we try to illustrate the idea by two simple examples. Consider Fig. 6 with $s=3/2$ and $s'=1$. In our picture, the VBS state obtained from projection is a MPS with auxiliary matrices given by $V_{5/2} \coloneqq V_{3/2+1}$. Note that we use V_s to denote the totality of matrices $V_{s,m}$, for all m. We want to show that

$$V_{5/2} \otimes V_{5/2} = V_0 \oplus V_1 \oplus V_2 \oplus V_3, \tag{73}$$

that is, we want to show that in the decomposition of the left hand side, tensors V_4 and V_5 do not appear; hence, local Hamiltonian annihilating the state of the lower chain in Fig. 6 can be constructed from projectors P_4 and P_5. To prove this, we need to only show that the highest-weight components of tensors V_5 and V_4 in the decomposition of the left hand side of Eq. (74) vanish identically. To this end, let us write the explicit form of the components of $V_{5/2}$ obtained from the top component $V_{5/2,5/2}$ by using Eq. (36) and applying the commutation relation $V_{s,m} \propto [L_-, V_{s,m+1}]$. Ignoring the numerical coefficients and signs in front of all states on both sides, which are irrelevant for the following proof, and using the shortened notation $|s,m\rangle \rightarrow |m\rangle$ (i.e., $|1/2\rangle \equiv |3/2,1/2\rangle$, $|-1\rangle \equiv |1,-1\rangle$), we have

$$V_{5/2,5/2} = |3/2\rangle\langle -1| + |1\rangle\langle -3/2|,$$

$$V_{5/2,3/2} = |1/2\rangle\langle -1| + |3/2\rangle\langle 0| + |0\rangle\langle -3/2| + |1\rangle\langle -1/2|.$$

It is now easily seen that $V^2_{5/2,5/2}=0$, implying that the highest weight of V_5 vanishes. Moreover, we see that $V_{5/2,5/2}V_{5/2,3/2}=V_{5/2,3/2}V_{5/2,5/2}=0$, implying the highest weight of V_4 also vanishes. This example corresponds to Fig. 6 with $s=3/2$ and $s'=1$ (or with 3 and 2 valence bonds in the AKLT construction). There is a very interesting point here which we should mention. The point is that a spin-5/2 VBS state can also be constructed in the same way as in Fig. 6 with $s=2$ and $s'=1/2$ or as in the original picture, from partially dimerized states with different numbers, namely, with 4 and 1 valence bonds. Here, we expect that the local Hamiltonian, which is used in the construction of translation-invariant state, be constructed only from projector P_5. This is nicely captured in the fusion rule of our tensors, $W_{5/2} \coloneqq V_{2+1/2}$, which is

$$W_{5/2} \otimes W_{5/2} = W_4 \oplus W_3 \oplus W_2 \oplus W_1 \oplus W_0. \tag{74}$$

In fact, we have (again ignoring numerical coefficients on both sides), and with the same type of shortened notation as in the previous example,

$$W_{5/2,5/2} = |2\rangle\langle -1/2| + |1/2\rangle\langle -2|,$$

$$W_{5/2,3/2} = |1\rangle\langle -1/2| + |2,\rangle\langle 1/2| + |-1/2\rangle\langle -2| + |1/2\rangle\langle -1|.$$

It is now seen that while the top state of W_5 is zero, the top state of W_4, that is, $W_{5/2,5/2}W_{5/2,3/2} - W_{5/2,3/2}W_{5/2,5/2}$, is nonvanishing, proving the fusion rule [Eq. (39)]. This argument can be generalized to the arbitrary spins s and s', although the proof will not be more illuminating than the example given above.

VIII. CONCLUSION

The main emphasis of this paper has been on the rotational symmetry properties of matrix product states. To this end, we have constructed a simple representation of spherical tensors of arbitrary integer or half integer rank. A spherical tensor of rank s is represented in a $2s+2$ dimensional space; hence, the dimension of space increases only linearly with the rank of the tensor. The introduction of these tensors has made possible a unified approach toward fully dimerized and partially dimerized or AKLT/VBS states. In this way, we have been able to find a matrix product representation for all the varieties of valence bond states introduced in the original AKLT paper. Having such a matrix product representation makes the calculation of many properties of such states, specially the nondimerized states, quite easy and straightforward. Moreover, a MPS representation is more powerful since it will give a larger family of Hamiltonians compared with the AKLT construction, since it allows to include more projectors in the local Hamiltonian. This will then lead to more flexibility in approximating realistic interactions with parent Hamiltonians of matrix product states. We have demonstrated this for a spin-1 family of Hamiltonians with nearest and next-nearest-neighbor interactions. Finally, we should remind that the above constructions can be generalized to other symmetry groups such as su(n). At least for a self-conjugate representation of su(n), whose weight diagram is symmetric under reflection, then we can define tensor operators in exactly the same way as in Eq. (23), namely,

$$A_{\mathbf{m}} \coloneqq |\mathbf{m}\rangle\langle\tilde{0}| + |\tilde{0}\rangle\langle -\mathbf{m}|, \tag{75}$$

where $|\mathbf{m}\rangle$ is the $n-1$ dimensional weight vector of that representation. Such a MPS representation may be useful, for example, in recent considerations of AKLT models as in Refs. 33 and 34, where su(2) valence bonds have been replaced with su(n) valence bonds, or in Ref. 34, where trimmer ground states with su(3) symmetry have been studied.

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