Product vacua with boundary states

Sven Bachmann[*] and Bruno Nachtergaele[†]

Department of Mathematics, University of California, Davis, Davis, California 95616, USA
(Received 26 December 2011; revised manuscript received 9 July 2012; published 30 July 2012)

We introduce a family of quantum spin chains with nearest-neighbor interactions that can serve to clarify and refine the classification of gapped quantum phases of such systems. The gapped ground states of these models can be described as a product vacuum with a finite number of particles bound to the edges. The numbers of particles, n_L and n_R, that can bind to the left and right edges of the finite chains serve as indices of the particular phase a model belongs to. All these ground states, which we call product vacua with boundary states (PVBS), can be described as matrix product states (MPS). We present a curve of gapped Hamiltonians connecting the Affleck-Kennedy-Lieb-Tasaki (AKLT) model to its representative PVBS model, which has indices $n_L = n_R = 1$. We also present examples with $n_L = n_R = J$, for any integer $J \geqslant 1$, that are related to a recently introduced class of SO$(2J + 1)$-invariant quantum spin chains.

I. INTRODUCTION

Gapped quantum phases and the transitions between them are a subject of great current interest both for their fundamental importance, as illustrated by the experimental observation of an E_8 symmetry at the critical point of the quantum Ising model,[1] and because of their potential application in quantum information and computation as proposed in Ref. 2. In the latter case the focus is on the topological phases,[3] which cannot be classified using a local order parameter, but depend on global features of the system such as the underlying topology of the model, as, for example, in the quantum Hall effect.[4] These topological orders can be characterized by an equivalent boundary theory.[5]

Several recent works have aimed at classifying the ground state phases of quantum spin chains.[6,7] While true topological order may not occur in one dimension, direct analogs of some essential phenomena are present, including the role of edge states, which is the main topic of this article.

The consensus is that the ground states of two models H_0 and H_1 with short-range interactions are in the same phase if there exists a smooth path of Hamiltonians $H(s)$, $0 \leqslant s \leqslant 1$, $H_0 = H(0), H_1 = H(1)$, such that the gap above the ground state does not close along this path.[8,9] Using the notion of automorphic equivalence, in Ref. 9 we showed how this definition can be made precise so that it can also be applied for infinite systems. In general, proving that the gap does not close is a hard problem but a criterion exists for frustration-free models whose ground states are matrix product states (MPS).[10] Most progress has been made by focusing on such frustration-free models, with or without prescribed symmetries.[7,11]

In this article, we introduce a new family of quantum spin chains with nearest-neighbor interactions with MPS ground states of a special type which we call product vacua with boundary states (PVBS). The bulk phase is a product state (or several product states), but for finite chains there are 2^n ground states that are obtained from the product vacuum by adding up to n distinguishable particles. Of these n particles n_L bind to the left edge of the interval and n_R to the right edge. The equivalence classes of gapped ground states are in one-to-one correspondence with the values of the non-negative integers n_L and n_R. The Hamiltonian preserves the particle number for each type of particle separately. As an example, we identify the classes to which the SO$(2J + 1)$-invariant models of Ref. 12 belong, namely, $n_L = n_R = J$. The Affleck-Kennedy-Lieb-Tasaki (AKLT) model corresponds to $J = 1$. The complete class of PVBS models is more general and will be described elsewhere.

II. PRODUCT VACUA WITH BOUNDARY STATES

We consider a quantum spin chain with spin dimension $d \geqslant n + 1$. There are $n + 1$ states at each site that we interpret as n distinguishable particles and a vacuum. In addition, there may be excited states of positive energy that will play no role in our discussion. For simplicity, we stick to the case $d = n + 1$. We start from a MPS representation of the ground states of the model. The Hamiltonian is constructed as the parent Hamiltonian for the set of MPS ground states and by general arguments we can then conclude that it has a gap and no other ground states.[13]

Let 0 label the empty state and let $1, \ldots, n$ denote the n particle types. The ground states are generated by $n + 1$ square matrices $v_0, v_1, \ldots, v_n$, satisfying the following commutation relations:

$$v_i v_j = e^{i\theta_{ij}} \lambda_i \lambda_j^{-1} v_j v_i, \quad i \neq j, \tag{1}$$

$$v_i^2 = 0, \quad i \neq 0, \tag{2}$$

where $\theta_{ij} \in \mathbb{R}$, $\theta_{ij} = -\theta_{ji}$, and $0 \neq \lambda_i \in \mathbb{R}$, for $0 \leqslant i, j \leqslant n$. By redefining the phases θ_{ij}, we can assume $\lambda_i > 0$ without loss of generality. We will also assume that $\lambda_0 = 1$, which amounts to a choice of normalization for v_0. Although the exact form of the matrices is not essential for our discussion, it is important that such matrices exist. One representation of the commutation relations is most conveniently described in terms of a chain of n spin-$1/2$ particles, yielding matrices of dimension 2^n. Define

$$\sigma^+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad \sigma^- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix},$$

$$w_i = \begin{pmatrix} 1 & 0 \\ 0 & \lambda_i \end{pmatrix}, \quad P_{ij} = \begin{pmatrix} e^{i\theta_{ij}/2} & 0 \\ 0 & 1 \end{pmatrix},$$

for $i,j = 0, \ldots n$. The matrices are given by

$$v_0 = \bigotimes_{i=1}^{n} P_{0i}^2 w_i,$$

$$v_i = \bigotimes_{j=1}^{i-1} P_{ij} w_j \otimes \sigma^+ \otimes \bigotimes_{k=i+1}^{n} P_{ik} w_k, \quad i = 1, \ldots n.$$

Equation (1) follows from $\sigma^+ w_i = \lambda_i w_i \sigma^+$ and $P_{ij} \sigma^+ = e^{i\theta_{ij}/2} \sigma^+ P_{ij}$ as well as $[P_{jk}, w_i] = 0$ for all i,j,k. Finally, (2) is a direct consequence of $(\sigma^+)^2 = 0$.

The MPS generated by this set of matrices for a chain of L spins are given by

$$\psi(B) = \sum_{i_1,\ldots,i_L=0}^{n} \mathrm{Tr}\big(B v_{i_L} \cdots v_{i_1}\big) |i_1, \ldots, i_L\rangle, \qquad (3)$$

where B is an arbitrary $2^n \times 2^n$ matrix. Consider the case $L = 2$. From the commutation relations (1) and (2) it follows that all MPS vectors of the form (3) will be orthogonal to the vectors $\phi_{ij} \in \mathbb{C}^d \otimes \mathbb{C}^d$ given by

$$\phi_i = |0,i\rangle - e^{-i\theta_{i0}} \lambda_i |i,0\rangle, \qquad (4)$$

$$\phi_{ij} = |i,j\rangle - e^{-i\theta_{ji}} \lambda_i^{-1} \lambda_j |j,i\rangle, \qquad (5)$$

$$\phi_{ii} = |i,i\rangle, \qquad (6)$$

for $1 \leqslant i,j \leqslant n$ and $i \neq j$. If $n > 2$, not all combinations of particles can be realized in a ground state of a chain of length 2. Nevertheless, it is sufficient to consider a Hamiltonian with a nearest-neighbor interaction defined by

$$h = \sum_{i=1}^{n} |\hat{\phi}_i\rangle\langle\hat{\phi}_i| + \sum_{1 \leqslant i \leqslant j \leqslant n} |\hat{\phi}_{ij}\rangle\langle\hat{\phi}_{ij}|,$$

where $\hat{\ }$ denotes normalization. The Hamiltonian for a finite chain of spins is then given by

$$H_{[a,b]} = \sum_{x=a}^{b-1} h_{x,x+1}, \qquad (7)$$

where and $h_{x,x+1}$ is a copy of h acting on the pair of spins at the sites x and $x+1$. As a sum of orthogonal projections, $H_{[a,b]}$ is non-negative and it is straightforward to verify that the MPS defined in (3) are eigenvectors with zero energy, hence ground states of the model. It is not hard to show that these are *all* the ground states of $H_{[a,b]}$.[14]

If $b - a + 1 \geqslant n$, for each subset $\{i_1, \ldots, i_m\}$ of $\{1, \ldots, n\}$ there is a ground state $\psi_{[a,b]}^{i_1,\ldots,i_m} = \psi(B^{i_1,\ldots,i_m})$ having exactly one particle of each type $i_1, \ldots, i_m$. The matrices $B^{i_1,\ldots,i_m}$ generating $\psi^{i_1,\ldots,i_m}$ through (3) (up to normalization) can be chosen as

$$B^{i_1,\ldots,i_m} = p^{\otimes(i_1-1)} \otimes \sigma^- \otimes p^{\otimes(i_2-i_1-1)} \otimes \sigma^- \otimes \\ \cdots \otimes \sigma^- \otimes p^{\otimes(n-i_m)},$$

where $p = \sigma^+ \sigma^-$. An interesting example is the ground state containing only particle i,

$$\psi_{[a,b]}^{i} = \sum_{x=a}^{b} (e^{i\theta_{i0}} \lambda_i)^x |0, \ldots, i, \ldots, 0\rangle, \qquad (8)$$

where i is at site x in each term of the sum. We now add the assumption that $\lambda_i \neq 1$, for $1 \leqslant i \leqslant n$. The n_L particles having $\lambda_i < 1$ are bound to the left edge, whereas the $n_R = n - n_L$ particles with $\lambda_i > 1$ are localized near the right edge, as can be seen in (8). The state with $m = 0$ is the product state

$$\Omega = |0, \ldots, 0\rangle.$$

All other ground states differ from Ω only near the edges. Specifically,

$$\lim_{\substack{a \to -\infty \\ b \to +\infty}} \big\langle \hat{\psi}_{[a,b]}^{i_1,\ldots,i_m}, A \hat{\psi}_{[a,b]}^{i_1,\ldots,i_m} \big\rangle = \langle \Omega, A\Omega \rangle$$

for any local observable A. If only one of the edges is taken to infinity, the limiting ground states for the half-infinite chain depend on the particles at the other edge. Concretely, on the chain that extends to infinity on the right but with a left boundary, there remain 2^{n_L} ground states corresponding to the possible combinations of the n_L particles that bind to the left edge. Similarly, there are 2^{n_R} ground states on the left infinite chain with a right boundary.

Using the method of Ref. 10, we can prove that the energy of the first excited state is bounded below by a positive constant, independently of the length of the chain. As at most one particle of each type can bind to the edge, any second particle of that type must be in a scattering state. The dispersion relation of these scattering states can be explicitly calculated by considering the restrictions of the Hamiltonian to any of the n invariant spaces containing exactly one particle. Properly centered and rescaled, these operators reduce to a free hopping Hamiltonian with λ-dependent boundary conditions. A plane wave ansatz yields the dispersion relation

$$\epsilon_i(k) = 1 - \frac{2\lambda_i}{1 + \lambda_i^2} \cos(k + \theta_{i0}).$$

In particular, the gap closes whenever $\lambda_i \to 1$ for some i. Moreover, we conjecture that the *exact* gap in the thermodynamic limit is given by

$$\gamma = \min\left\{ \frac{(1 - \lambda_i)^2}{1 + \lambda_i^2} : 1 \leqslant i \leqslant n \right\}.$$

III. AUTOMORPHIC EQUIVALENCE AND GAPPED GROUND STATE PHASES

Despite their simplicity, the PVBS models introduced in the previous section display the general characteristics of gapped one-dimensional systems with a unique bulk ground state, and we can use them to illustrate the role of edge states in the classification of gapped phases.

In Ref. 15 it is concluded that all gapped, translation invariant, one-dimensional quantum spin systems without symmetry breaking belong to the same phase, and that they are equivalent to a product state. We believe that taking into account edge states, and in particular the behavior of the system on semi-infinite chains, is necessary as it allows for a finer classification closer in spirit to what one would find for models on two- and higher-dimensional manifolds with nontrivial topology.

A. The PVBS classes

It is easily seen that two PVBS models of the type we introduced here belong to the same equivalence class if and only if they have the same values for the non-negative integers n_L and n_R. The reasoning is as follows. Since equivalent phases are related by an automorphism, a unique bulk ground state can only be mapped to another unique bulk state. Similarly, the ground state space dimensions of the half-infinite chains, 2^{n_L} and 2^{n_R}, are also preserved by an automorphism. Hence, if two PVBS models belong to the same phase, they must have equal n_L and n_R. Conversely, if two PVBS models have the same values of n_L and n_R but each with their own sets of parameters $\{\lambda_i(\alpha) \mid 1 \leqslant i \leqslant n_L + n_R\}$ and $\{\theta_{ij}(\alpha) \mid 1 \leqslant i, j \leqslant n_L + n_R\}$, for $\alpha = 0, 1$, an interpolating path along which the gap does not close can be constructed as follows. First, one may apply a strictly local unitary to perform a change of basis in spin space such that both are PVBS expressed in the same spin basis and such that $\lambda_i(\alpha) < 1$ for $1 \leqslant i \leqslant n_L$ and $\lambda_i(\alpha) > 1$ for $n_L + 1 \leqslant i \leqslant n_L + n_R$, for both $\alpha = 0$ and $\alpha = 1$. Let u be the unitary for this change of basis. Then, take a smooth curve of unitaries $u(s)$, $0 \leqslant s \leqslant 1$, with $u(0) = \mathbb{1}$ and $u(1) = u$, and let $U_{[a,b]}(s)$ be the $(b - a + 1)$-fold tensor product of $u(s)$. Now we conjugate the initial $H_{[a,b]}$ with these unitaries to define a smooth path of Hamiltonians with a constant gap. Simultaneously, we can deform the parameters of the two models by linear interpolation:

$$\lambda_i(s) = (1 - s)\lambda_i(0) + s\lambda_i(1),$$

$$\theta_{ij}(s) = (1 - s)\theta_{ij}(0) + s\theta_{ij}(1).$$

This yields a smooth family of vectors $\phi_{ij}(s)$ as in (4)–(6) and thereby a smooth family of nearest-neighbor interactions $h(s)$ and of Hamiltonians. The gap remains open because $\lambda_i(s) \neq 1$ for all $1 \leqslant i \leqslant n$ and $s \in [0, 1]$. By the general result of Ref. 9 this implies the quasilocal automorphic equivalence of the two models. Note that it is essential that in each pair between which we interpolate, the λ_i's are either both <1 or both >1, which is why we had to assume that n_L and n_R are the same for both models. If one uses the same type of interpolation to connect models with different values of n_L and n_R, the gap necessarily closes along the path and there is a quantum phase transition. This is not to say that one could not construct paths along which the gap closes also for the case of constant n_L and n_R and of course this would then not imply a transition between different gapped phases.

The uncountable family of PVBS models which depend on the real parameters $\{\lambda_i\}$ and $\{\theta_{ij}\}$ is completely classified by the pair of integers (n_L, n_R). Given their simplicity, it is natural to choose them as representatives of the much larger phase they belong to.

B. The AKLT model

As a first example, we show that the AKLT model[16] belongs to the same equivalence class as the PVBS models with $n_L = n_R = 1$. The AKLT model is an antiferromagnetic spin-1 chain with a unique, gapped ground state in the thermodynamic limit, and four zero-energy states on a finite chain, which are usually described in terms of a spin-1/2 particle attached to the two

ends of the chain. We found a smooth path of gapped models connecting the AKLT model with a PBVS model with one particle for each boundary. Let us denote the two particle states by $-$ and $+$. For $s \in [0, s_0]$ where $\sin(s_0) = \sqrt{2/3}$, the following four vectors span the ground state space of two neighboring spins of the interpolating models as a function of s:

$$\psi^{00}(s) = \mu(s)\sin(s)[\lambda(s)^2 | -, + \rangle + | +, - \rangle]$$
$$- \cos^2(s)(1 + \lambda(s)^4)|0, 0\rangle,$$
$$\psi^{0-}(s) = -\lambda(s)|0, -\rangle + | -, 0\rangle,$$
$$\psi^{0+}(s) = -\lambda(s)| +, 0\rangle + |0, +\rangle,$$
$$\psi^{-+}(s) = | -, + \rangle - \lambda(s)^2 | +, - \rangle,$$

where $\lambda(s)$ is a smooth function such that $\lambda(s_0) = 1$, $0 < \lambda(s) < 1$, for all $s < s_0$, and $\mu(s) = [1 - \lambda(s)^2 \cos^2(s)]^{1/2}$. The corresponding nearest-neighbor interaction,

$$h(s) = 1 - \sum_{(ij) \in \{(00), (0-), (0+), (-+)\}} |\widehat{\psi^{ij}}(s)\rangle\langle\widehat{\psi^{ij}}(s)|,$$

is the projection onto the orthogonal complement of this four-dimensional space. We then define $H_{[a,b]}(s) = \sum_{x=a}^{b-1} h_{x,x+1}(s)$. It readily follows that $H_{[a,b]}(s_0)$ is the AKLT Hamiltonian and that $H_{[a,b]}(0)$ is the PVBS model with $n_L = n_R = 1$, the coefficients $\lambda_- = \lambda(0)$ and $\lambda_+ = \lambda(0)^{-1}$, and all the phases $\theta_{ij} = \pi$. The path of interactions is smooth as the four ground state vectors are smooth, remain orthogonal to each other and of finite norm for all s, and the spectral gap does not close.[17] Hence, the AKLT model belongs to the same gapped quantum phase as the PVBS model with $n_L = n_R = 1$. In particular, the sets of ground states of these models are automorphically equivalent for the finite, half-infinite, and infinite chains, where they are isomorphic to a pair of qubits, a single qubit, and a unique pure product state, respectively.

The ground states of $H_{[a,b]}(s)$ for $s > 0$ have a minimal matrix product representation with 2×2 matrices $v_i(s)$ defined as follows:

$$v_0 = -\cos(s)\begin{pmatrix} 1 & 0 \\ 0 & -\lambda(s) \end{pmatrix}, \tag{9}$$

$$v_- = \begin{pmatrix} 0 & -\mu(s) \\ 0 & 0 \end{pmatrix}, \quad v_+ = \begin{pmatrix} 0 & 0 \\ \sin(s) & 0 \end{pmatrix}. \tag{10}$$

By contrast, the MPS representation of the ground states of the PVBS model, at $s = 0$, uses 4×4 matrices. In fact, there is no faithful two-dimensional representation of the commutation relations (1) and (2) with $n = 2$. Up to unitary change of basis, the only nilpotent matrix is σ^+, so we can set $v_+ = c_+\sigma^+$ and $v_- = c_- U^*\sigma^+ U$, with $c_\pm \neq 0$ and $U \neq 1$. But their commutation relation implies $\text{Tr}(v_- v_+) = 0$ so that $U = 1$ if $c_\pm \neq 0$. The parent Hamiltonian constructed from the limiting matrices $v_i(0)$ corresponds to a PVBS model with $n_L = 1$ and $n_R = 0$. With a minor modification one can interchange the roles of n_L and n_R, but in either case the limiting matrices lead to a parent Hamiltonian that is *not* in the same phase as the AKLT model; it turns out to be equivalent only in the bulk and on the half-infinite chain tending to ∞ on the right but not on the chain that is infinite on the left. We believe that the finer classification we propose in this paper yields interesting additional information compared to previous

approaches such as Ref. 11. We conclude that it is essential to construct a smooth, gapped family of Hamiltonians, and that it is not sufficient to find a smooth family of MPS matrices only. A similar conclusion was reached in Ref. 18, where "uncle Hamiltonians" were constructed that share the ground state spaces of gapped "parent Hamiltonians" but are gapless in the thermodynamic limit.

C. The $SO(2J + 1)$ models

The SU(2)-symmetric spin-1 AKLT chain has been generalized in a number of different directions: higher SU(2) spins,[19] higher lattice dimensions,[20] SU(N)-invariant models with $N \geqslant 2$,[21] and most recently to a class of spin-J models with an $SO(2J + 1)$-invariant nearest-neighbor interaction.[12] The simplest way to introduce the latter generalization is to note that the kernel of the interaction of the AKLT model, i.e., the ground state space of two neighboring spins is spanned by the antisymmetric vectors, namely, the spin-1 triplet, and the spin singlet state, which is symmetric. As shown in Ref. 14, the antisymmetric subspace of two spins enhanced with one, arbitrary, symmetric state is the ground state space of a frustration-free spin chain with a translation invariant nearest-neighbor interaction. In particular, the spin-J chain, with integral $J \geqslant 1$, with the nearest-neighbor interaction given by the projection onto the orthogonal complement of the span of the antisymmetric vectors and the (symmetric) spin singlet state, is a frustration-free model with a unique gapped MPS ground state of the infinite chain. It is easy to see that this interaction commutes with $SO(2J + 1)$ acting by its fundamental representation on each spin.

In the case of the AKLT model ($J = 1$), the antisymmetry of the ground states is reflected in the fact that the matrices (9) and (10) at $s = s_0$ can be related to the generators of the Clifford algebra $\mathcal{C}_3$:

$$Z_1 = \sqrt{3/2}(v_+ - v_-), \quad Z_2 = -\sqrt{3/2}\mathrm{i}(v_+ + v_-),$$
$$Z_0 = -\sqrt{3}v_0. \tag{11}$$

In fact, the transformation $\{v_-, v_0, v_+\} \to \{Z_0, Z_1, Z_2\}$ corresponds, up to a global rescaling by $\sqrt{3}$, to a change of basis in the local Hilbert space of the spins. Similarly for $J > 1$, the ground states of the $SO(2J + 1)$ model are, up to an overall normalization factor, generated by the matrices $\{Z_\alpha = Z_\alpha^* : 0 \leqslant \alpha \leqslant 2J\}$ of the higher-dimensional Clifford algebra $\mathcal{C}_{2J+1}$ satisfying the anticommutation relations

$$Z_\alpha Z_\beta + Z_\beta Z_\alpha = 2\delta_{\alpha\beta}\mathbb{1}. \tag{12}$$

The symmetry of the ground state is manifest in the invariance of (12) under the transformation $Z'_\beta = \sum_\alpha O_{\beta\alpha} Z_\alpha$ for any orthogonal matrix O. The normalization factor γ can be found by setting $\sum_\alpha \gamma^2 Z_\alpha^2 = 1$, yielding $\gamma = (2J + 1)^{-1/2}$.

A representation of the Clifford algebra $\mathcal{C}_{2J+1}$ can be obtained from a representation of the algebra of canonical anticommutation relations (CARs) with J creation operators

$$a_j^* = \underbrace{(-1)^q \otimes \cdots \otimes (-1)^q}_{j-1} \otimes \sigma^+ \otimes \underbrace{\mathbb{1} \otimes \cdots \otimes \mathbb{1}}_{J-j},$$

where $q = 1 - p = \sigma^- \sigma^+$. Note that $(-1)^q = \sigma^3$. Then, for $1 \leqslant j \leqslant J$,

$$Z_{2j-1} = a_j + a_j^*, \quad Z_{2j} = \mathrm{i}(a_j - a_j^*),$$

and

$$Z_0 = \prod_{j=1}^J (2a_j^* a_j - 1) = \bigotimes_{j=1}^J (-1)^q.$$

The canonical anticommutation relations of the $(a_j^*, a_j)_{j=1}^J$ imply the Clifford relations for the $(Z_\alpha)_{\alpha=0}^{2J}$. This representation is of dimension 2^J.

Now, the matrices

$$V_{2j-1} = \alpha_j a_j, \quad V_{2j} = \beta_j a_j^*, \quad V_0 = \gamma Z_0,$$

are related to the normalized Clifford generators by a change of basis if and only if $|\alpha_j|^2 = |\beta_j|^2 = 2/(2J + 1)$. In that case, the set $\{V_0\} \cup \{V_{2j-1}, V_{2j} : 1 \leqslant j \leqslant J\}$ generate the same matrix product states as the $(Z_\alpha)_{\alpha=0}^{2J}$, namely, the ground states of the $SO(2J + 1)$-invariant model. Note that $\sum_j |\alpha_j|^2 + |\gamma|^2 = 1$, so that it is natural to set

$$\gamma =: \cos(s_0) \quad \text{and} \quad \alpha_j = \frac{1}{\sqrt{J}} \sin(s_0).$$

for all $j = 1, \ldots, J$.

It remains to introduce a deformation of the CAR algebra to relate it to the PVBS algebra with $n_L = n_R = J$. We first note that for any complex number λ,

$$\lambda \cdot \sigma^- \lambda^q = \lambda^q \sigma^-, \quad \sigma^+ \lambda^q = \lambda \cdot \lambda^q \sigma^+, \tag{13}$$

where $\lambda^q = p + \lambda q$. For parameters $\lambda_1, \ldots, \lambda_J$, we introduce the following twisted creation operators

$$a_j^*(\lambda) = (-\lambda_1)^q \otimes \cdots \otimes (-\lambda_{j-1})^q \otimes \sigma^+ \otimes \lambda_{j+1}^q \otimes \cdots \otimes \lambda_J^q,$$

their adjoints, and

$$a_0(\lambda) = (-\lambda_1)^q \otimes \cdots \otimes (-\lambda_J)^q.$$

Clearly, $a_j^*(\lambda)^2 = 0 = a_j(\lambda)^2$. A direct consequence of (13) are the twisted commutation relations

$$a_j^*(\lambda)a_j(\lambda) + \lambda_j^2 a_j(\lambda)a_j^*(\lambda) = a_0(\lambda)^2,$$
$$a_j^*(\lambda)a_k(\lambda) + \lambda_j\lambda_k a_k(\lambda)a_j^*(\lambda) = 0 \quad (j \neq k),$$
$$a_j^*(\lambda)a_0(\lambda) + \lambda_j a_0(\lambda)a_j^*(\lambda) = 0,$$
$$a_j^*(\lambda)a_k^*(\lambda) + \lambda_j\lambda_k^{-1} a_k^*(\lambda)a_j^*(\lambda) = 0,$$

and their adjoint relations. The higher-dimensional analog of the algebraic path (9) and (10) is easily obtained with the following definitions for $s \in [0, s_0]$:

$$V_{2j-1}(s) = \alpha_j(s)a_j(s), \quad V_{2j}(s) = \beta_j(s)a_j^*(s),$$

and $V_0(s) = \gamma(s)a_0(s)$, where $a_j^{\sharp}(s) = a_j^{\sharp}[\lambda(s)]$ for a smooth path of parameter vector $\lambda(s)$ such that $\lambda_j(s) < 1$ for $s < s_0$ and $\lambda_j(s_0) = 1$. Using the commutation relations, the normalization $\sum_\alpha V_\alpha^* V_\alpha = 1$ reads

$$1 = \sum_{j=1}^{J} \left(|\beta_j|^2 - \lambda_j^2|\alpha_j|^2\right)a_j a_j^* + \left[\sum_{j=1}^{J} |\alpha_j|^2 + |\gamma|^2\right]a_0^2,$$

which implies

$$\sum_{j=1}^{J} |\alpha_j|^2 + |\gamma|^2 = 1 \quad \text{and} \quad |\beta_j|^2 = 1 - \lambda_j^2(1 - |\alpha_j|^2).$$

Note that the $SO(2J + 1)$ symmetry is broken as soon as $|\beta_j| \neq |\alpha_j|$. Concretely we choose $\gamma(s) = \cos(s)$ and $\alpha_j(s) = \sin(s)/\sqrt{J}$ for $s \in [0, s_0]$, thereby producing a path that mimics (9) and (10). The commutation relations of the V_α's interpolate between those of the CAR [and therefore of the $SO(2J + 1)$ models] and of the PVBS with parameters

$$\{\lambda_j(0), \lambda_j(0)^{-1} : 1 \leqslant j \leqslant J\}, \tag{14}$$

in particular,

$$V_{2j}(s)V_{2j-1}(s) + \lambda_j(s)^2 V_{2j-1}(s)V_{2j}(s)$$
$$= \frac{\sin(s)\left[1 - \lambda_j^2(1 - \sin^2(s)/J)\right]}{\sqrt{J}\cos^2(s)} V_0^2.$$

This algebraic path of matrices generates a smooth path of matrix product states, from which a smooth family of Hamiltonians with nearest-neighbor interaction can be constructed, for any J. They interpolate between the $SO(2J + 1)$ model and the PVBS model with $n_L = n_R = J$. The properties needed to conclude that the gap remains open along the path can be derived from a suitable generalization of the arguments for the AKLT path, $J = 1$, and will be included in future work.

IV. DISCUSSION

The fact that one of each of the n types of particles can appear in a ground state of the PVBS system, i.e., without raising the energy, should not be interpreted as implying that the particles are massless. Quite to the contrary, there is a mass gap for each of them. It turns out, however, that they can bind to the left or right edge of the chain and the binding energy exactly equals the mass gap so that such states with a particle bound to the edge are degenerate with the vacuum ground state.

As we explained in the previous section, the AKLT model is equivalent to a PVBS model with two types of particles, one that binds to the left edge and one that binds to the right edge. For a finite chain, this yields a four-dimensional ground state space (no particles; one particle on the left boundary; one particle on the right boundary; two particles, one on the left and one on the right). The bulk ground state is unique. It has a finite correlation length in the AKLT model but is a simple product state in the equivalent PVBS model. The unitary transformation relating the two models is quasilocal,[9] meaning that, under conjugation with the unitary,

local observables map to observables that are approximately local, i.e., that up to an arbitrarily small correction depend only on a finite number of spins. Since our goal is to understand the structure of bulk phases and edge states (and, in higher dimensions, also the effects of topology), the quasilocality of this unitary transformation is essential. In finite volume, any unitary will preserve the dimension of the ground state space. The importance of the locality property comes into sharp focus when one takes the thermodynamic limit and considers the resulting ground states on the infinite and half-infinite chains. For example, the nonlocal unitary transformation introduced by Kennedy and Tasaki[22] to reveal the hidden string order[23] transforms the four AKLT ground states into four translation invariant product states, which leads to four distinct bulk ground states in the thermodynamic limit. This example shows that nonlocal unitary transformations do not preserve the structure of the bulk ground state(s) and clearly would not be useful to classify gapped ground state phases.

Similar the bulk ground state of a $SO(2J + 1)$ model for any integer J is equivalent to a unique product state. This however is not sufficient for them to all belong to the same gapped phase as the number of edge states depends on J. The definition of a phase through a quasilocal automorphism yields a finer classification that takes these boundary states into account.

Several generalizations of the PVBS are possible. First, it is straightforward to describe models with more than one vacuum state, e.g., models with a broken discrete symmetry. This could include breaking of the translation symmetry of the lattice to a subgroup, leading to periodic ground states. Second, the construction can easily be generalized to allow more than one particle to occupy the same site. The auxiliary chain of n spin-1/2 particles we have used here has to be replaced by an arbitrary finite spin chain. Third, if all or a subset of the λ parameters are equal, one can describe Hamiltonians with a local continuous symmetry group. Adding symmetry as a constraint considerably enriches the classification problem of the gapped ground state phases and the phase transitions between them.[7,24]

It appears to us that the class of models with PVBS ground states is able to capture the range of behaviors seen in gapped ground states of one-dimensional spin systems with short range interactions. The most interesting phenomena from the physical point of view occur in two dimensions. Some aspects of the classification problem have already been considered in two and higher dimensions. The notion of automorphic equivalence studied in Ref. 9, e.g., applies to arbitrary dimensions. Interesting boundary states in two dimensions have been studied in Ref. 25. Much further work is needed to better understand the landscape of gapped ground state phases in two and three dimensions.

ACKNOWLEDGMENTS

*svenbac@math.ucdavis.edu

†bxn@math.ucdavis.edu

[1] R. Coldea, D. A. Tennant, E. M. Wheeler, E. Wawrzynska, D. Prabhakaran, M. Telling, K. Habicht, P. Smeibidl, and K. Kiefer, Science **327**, 177 (2010).

[2] A. Kitaev, Ann. Phys. **303**, 2 (2003).

[3] X. G. Wen, Phys. Rev. B **40**, 7387 (1989); Int. J. Mod. Phys. B **4**, 239 (1990).

[4] R. B. Laughlin, Phys. Rev. B **23**, 5632 (1981).

[5] B. I. Halperin, Phys. Rev. B **25**, 2185 (1982); J. Fröhlich and U. M. Studer, Rev. Mod. Phys. **65**, 733 (1993); X.-G. Wen, in *Field Theory, Topology and Condensed Matter Physics*, Lecture Notes in Physics Vol. 456, edited by H. Geyer (Springer, Berlin, 1995), pp. 155–176.

[6] F. Verstraete, J. I. Cirac, J. I. Latorre, E. Rico, and M. M. Wolf, Phys. Rev. Lett. **94**, 140601 (2005); B. Yoshida, Ann. Phys. **326**, 15 (2011).

[7] Z.-X. Liu, X. Chen, and X.-G. Wen, Phys. Rev. B **84**, 195145 (2011).

[8] M. B. Hastings and X.-G. Wen, Phys. Rev. B **72**, 045141 (2005); X. Chen, Z.-C. Gu, and X.-G. Wen, *ibid.* **82**, 155138 (2010).

[9] S. Bachmann, S. Michalakis, B. Nachtergaele, and R. Sims, Commun. Math. Phys. **309**, 835 (2012).

[10] B. Nachtergaele, Commun. Math. Phys. **175**, 565 (1996).

[11] N. Schuch, D. Pérez-García, and I. Cirac, Phys. Rev. B **84**, 165139 (2011).

[12] H.-H. Tu, G.-M. Zhang, and T. Xiang, Phys. Rev. B **78**, 094404 (2008).

[13] M. Fannes, B. Nachtergaele, and R. F. Werner, Commun. Math. Phys. **144**, 443 (1992).

[14] M. Fannes, B. Nachtergaele, and R. F. Werner (unpublished).

[15] X. Chen, Z.-C. Gu, and X.-G. Wen, Phys. Rev. B **82**, 155138 (2010).

[16] I. Affleck, T. Kennedy, E. H. Lieb, and H. Tasaki, Commun. Math. Phys. **115**, 477 (1988).

[17] S. Bachmann and B. Nachtergaele (unpublished).

[18] C. Fernández-González, N. Schuch, M. Wolf, J. Cirac, and D. Pérez-García, arXiv:1111.5817v2.

[19] D. P. Arovas, A. Auerbach, and F. D. M. Haldane, Phys. Rev. Lett. **60**, 531 (1988).

[20] T. Kennedy, E. Lieb, and H. Tasaki, J. Stat. Phys. **53**, 383 (1988).

[21] I. Affleck, D. Arovas, J. Marston, and D. Rabson, Nucl. Phys. B **366**, 467 (1991).

[22] T. Kennedy and H. Tasaki, Phys. Rev. B **45**, 304 (1992); Commun. Math. Phys. **147**, 431 (1992).

[23] M. den Nijs and K. Rommelse, Phys. Rev. B **40**, 4709 (1989).

[24] H.-H. Tu, G.-M. Zhang, T. Xiang, Z.-X. Liu, and T.-K. Ng, Phys. Rev. B **80**, 014401 (2009).

[25] X. G. Wen, Phys. Rev. B **43**, 11025 (1991); J. Fröhlich, G. Graf, and J. Walcher, Ann. Henri Poincare **1**, 405 (2000).