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Ground States of VBS Models on Cayley Trees

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We study the thermodynamic limit of the ground states of VBS models on a Cayley tree. We prove uniqueness for coordination numbers $z \leqslant 4$ and the occurrence of Néel order for $z \geqslant 5$. Our main technical tool is a transfer matrix description of VBS states.

KEY WORDS: VBS models; Cayley trees; Néel order.

INTRODUCTION

The main purpose of this paper is to study in detail the thermodynamic limit of the valence-bond-solid models (VBS models) on a Cayley tree as defined in ref. 1. For concreteness let us immediately introduce the Hamiltonians, before going to more technical matters. For any $z \geqslant 2$ we consider the Cayley tree $\mathbb{T}^z$ with coordination number z (for $z = 2$ we recover $\mathbb{Z}$, the one-dimensional lattice). To each site $x \in \mathbb{T}^z$ we assign a quantum spin variable with spin $s = z/2$. Let $\langle x, y \rangle$ denote a pair of nearest neighbors in the tree and $P^{(z)}_{x,y}$ the orthogonal projection onto the subspace in $\mathbb{C}^{z+1} \otimes \mathbb{C}^{z+1}$, located at the sites x and y, which corresponds to maximal total spin, i.e., $z = z/2 + z/2$. The formal Hamiltonian H of our model is then defined as

$$H = \sum_{\langle x, y \rangle} P^{(z)}_{x,y} \tag{0.1}$$

This Hamiltonian is a positive operator (being the sum of positive terms), and it has the peculiar property of possessing a ground state with vanishing

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energy. This is the starting point of the analysis of any VBS model. Using an extension of a technique introduced in ref. 7 for treating one-dimensional VBS models, and also invoking an argument of ref. 2, we can construct an infinite-volume ground state ω of the Hamiltonian (0.1), with the following property: for any finite volume $\Lambda \in \mathbb{T}^z$ and any finite-volume ground state η_Λ of the local Hamiltonian $H_\Lambda = \sum_{\langle x, y \rangle \subset \Lambda} P^{(z)}_{x,y}$, there exists a constant $C > 0$ such that

$$\eta_\Lambda(A^*A) \leqslant C\omega(A^*A)$$

for any observable A in the volume Λ. In other terms: the local restriction ω_Λ of ω is a convex combination in which all ground states of the volume Λ appear.

We are now ready to formulate the problem we want to analyze in this paper: Determine all states ω_0 of the infinite tree which are weak limits of the following type:

$$\omega_0(A) = \operatorname*{w-lim}_{n \to \infty} \omega_{b_{\Lambda_n}}(A)$$

where the Λ_n are a sequence of increasing finite volumes in the tree (eventually covering all of it) and the b_{Λ_n} represent a specification of the state of the spins at the border of Λ_n, i.e., a boundary condition.

The results of ref. 1 concerning this question are the following: taking only homogeneous product boundary conditions (i.e., fixing all the spins of the boundary in one and the same direction), one obtains a unique limit in the cases $z = 2$ and $z = 3$ and nonuniqueness for $z \geqslant 5$. Numerical evidence for uniqueness in the case $z = 4$ was found.

Here we extend these results in the following way: we consider arbitrary nonhomogeneous boundary conditions of tensor product type and prove uniqueness in the cases $z \leqslant 4$. Furthermore, in the case of homogeneous product boundary conditions and $z \geqslant 5$, we find all possible limits.

The paper is organized as follows:

Section 1. We introduce a construction of states for quantum spin systems on an infinite Cayley tree. The construction contains the valence-bond-solid (VBS) states, which are exact ground states of the class of models under consideration. The construction we use is a generalization of the so-called finitely correlated states which were analyzed in ref. 7. The term "finitely correlated" refers to a fundamental property of such states: the space of functionals obtained by conditioning on the "left" half of the system is finite dimensional. As we do not intend here to study such a class of states on a tree in its full generality, we will still use the name VBS state. We will study in particular how these states depend on boundary conditions and obtain a transfer matrix technique which appears to be more effective than the VBS formalism as used in ref. 1, especially to determine questions like symmetry breaking in the thermodynamic limit.

Section 2. Here we make the ideas of Section 1 concrete by introducing the "master" ground state for the VBS models (0.1), i.e., we construct the ground state ω which is a mixture of all possible ground states. It is this state that we are going to decompose using boundary conditions of a specific type.

Section 3. In this section we prove uniqueness in the cases $z \leqslant 4$.

Section 4. This section is devoted to the analysis of the case $z \geqslant 5$.

Section 5. To obtain the explicit expressions for the states in the thermodynamic limit from the results of Sections 3 and 4, an additional equation has to be solved. The solution is needed, e.g., for computing the exact value of the Néel order parameter in cases of nonuniqueness. It is then also straightforward to obtain the spin–spin correlation function of the model.

Appendix. In the Appendix useful formulas which arise in the representation theory of $SU(2)$ are collected.

1. CONSTRUCTION OF VBS STATES ON CAYLEY TREES

Let $z \geqslant 2$ be an integer and consider the Cayley tree $\mathbb{T}^z$ with coordination number z ($\mathbb{T}^z$ is the unique homogeneous graph with coordination number z and no loops; see Fig. 1). By cutting one bond, one divides the tree into two disconnected parts, the branches (sometimes called rooted trees), which are isomorphic with one another. Sometimes one removes a site and thus obtains z equivalent branches. We will mostly work with only one of the parts and call it $\mathbb{T}^z_+$. We call the site of $\mathbb{T}^z_+$ which belonged to the broken bond the origin (or the root) of the tree.

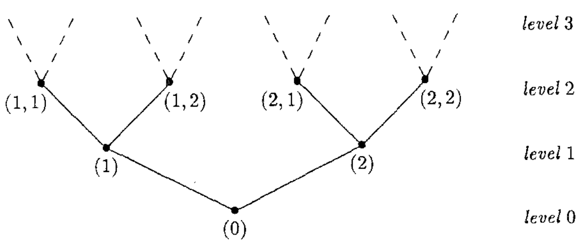

Fig. 1. The first three levels of the branch $\mathbb{T}^z_+$ with $z = 3$.

Useful coordinates on the positive branch $\mathbb{T}^z_+$ are given by

$$\mathbb{T}^z_+ = \{(i_1,..., i_n) \mid n \in \mathbb{N}, i_k \in \{1,..., z-1\} \text{ for } 1 \leqslant k \leqslant n\} \cup \{(0)\}$$

(0) constitutes level 0 of the tree and the sites $(i_1,..., i_n)$ form level n, containing $(z-1)^n$ sites. If $x \in \mathbb{T}^z_+$, $x = (i_1,..., i_n)$, we define $N(x) = n$ to be the *level* of x.

$\mathbb{T}^z_+$ acts as a semigroup of translations on itself (non-Abelian for $z \geqslant 3$): define the translations $\tau_{(i_1,..., i_n)}$ by

$$\tau_{(i_1,..., i_n)}(j_1,..., j_m) = (i_1,..., i_n) \vee (j_1,..., j_m) \equiv (i_1,..., i_n, j_1,..., j_m)$$

and of course

$$(i_1,..., i_n) \vee (0) = (0) \vee (i_1,..., i_n) = (i_1,..., i_n)$$

such that $\tau_{(0)} = \text{id}$.

The "rotations" of $\mathbb{T}^z_+$ are generated by the following set of actions of the symmetric group of $\{1,..., z-1\}$, $\mathscr{S}_{z-1}$: for $\sigma \in \mathscr{S}_{z-1}$ define

$$\pi^{(\sigma)}_{(0)}(0) = (0)$$

$$\pi^{(\sigma)}_{(0)}(i_1,..., i_m) = (\sigma(i_1), i_2,..., i_m)$$

for all $m \geqslant 1$. For $n \geqslant 1$ and any element $(j_1,..., j_n)$ of the tree we define a rotation $\pi^{(\sigma)}_{(j_1,..., j_n)}$ at the point $(j_1,..., j_n)$ by: for every point y of the form $\tau_{(j_1,..., j_n)}(x)$

$$\pi^{(\sigma)}_{(j_1,..., j_n)}(y) = \tau_{(j_1,..., j_n)}(\pi^{(\sigma)}_{(0)}(x)) \tag{1.1}$$

and all other points of $\mathbb{T}^z_+$ are left invariant by $\pi^{(\sigma)}_{(j_1,..., j_n)}$. It is then obvious that

$$\pi^{(\sigma)}_{(j_1,..., j_n)} \circ \tau_{(j_1,..., j_n)} = \tau_{(j_1,..., j_n)} \circ \pi^{(\sigma)}_{(0)}$$

For all $x \in \mathbb{T}^z_+$, and $n \in \mathbb{N}$, we define a finite volume $(x, n) \subset \mathbb{T}^z$ as follows:

$$(x, n) = \tau_x(0, n) = \{\tau_x(y) \mid y \in (0, n)\} \tag{1.2}$$

where

$$(0, n) = \{y \in \mathbb{T}^z_+ \mid N(y) \leqslant n\}$$

with $N(y)$ the level to which y belongs. We call a finite volume of the type (x, n) a *triangle* in the tree. This local structure is extended to the whole tree by taking as the origin an arbitrary site $x \in \mathbb{T}^z$.

In any site $x \in \mathbb{T}^z$ we now consider a copy $\mathscr{A}_x$ of a finite-dimensional C^*-algebra $\mathscr{A}$ with unit. $\mathscr{A}_{(x,n)}$ is then defined by

$$\mathscr{A}_{(x,n)} = \bigotimes_{y \in (x,n)} \mathscr{A}_y$$

and the full algebra $\mathscr{A}_{\mathbb{T}^z}$ of the tree is obtained in the usual way by an inductive limit[10]

$$\mathscr{A}_{\mathbb{T}^z} = \overline{\bigcup_{x \in \mathbb{T}^z, n \in \mathbb{N}} \mathscr{A}_{(x,n)}}$$

In this paper we will only be concerned with the case where the one-site algebra is the algebra $\mathscr{M}_d$ of complex $d \times d$ matrices.

We will first give an explicit formula for a local VBS state ω on a finite volume of the type $(0, n)$. We consider therefore a linear map $\mathbb{E}$,

$$\mathbb{E}: \quad \mathscr{A} \otimes (\otimes \mathscr{B})^{(z-1)} \to \mathscr{B}$$

where $\mathscr{B}$ is some auxiliary finite-dimensional C^*-algebra with unit element. The map $\mathbb{E}$ will play a role similar to that of the transition matrix in the context of classical Markov processes. Clearly, it must possess specific positivity properties. The natural notion of positivity here is that of complete positivity.[10] This positivity is preserved under tensoring and composition. As we will restrict our attention to matrix algebras, all completely positive maps $\mathbb{P}$ from a matrix algebra $\mathscr{M}_{d_1}$ into $\mathscr{M}_{d_2}$ are of the type

$$\mathbb{P}(X) = \sum_{i=1}^{k} V_i^* X V_i$$

where the V_i are linear maps from $\mathbb{C}_{d_2}$ into $\mathbb{C}_{d_1}$. Besides this positivity requirement, we will also impose that $\mathbb{P}$ be unity preserving; in terms of the V_i this means that $\sum_i V_i^* V_i = \mathbb{1}_{d_2}$. In fact, we will only need to consider the case where $\mathbb{P}$ is defined by a single V. Clearly, $\mathbb{P}$ will then be unity preserving iff V is an isometry.

Define for all $n \in \mathbb{N}$, the nth-level algebras $\mathscr{A}^{(n)}$ and $\mathscr{B}^{(n)}$ by

$$\mathscr{A}^{(n)} = \bigotimes_{x, N(x) = n} \mathscr{A}_x, \qquad \mathscr{B}^{(n)} = \bigotimes_{x, N(x) = n} \mathscr{B}_x$$

For all $X \in \mathscr{A}$ we define

$$\mathbb{E}_X: \quad \mathscr{B}^{\otimes (z-1)} \to \mathscr{B}: \quad Y \mapsto \mathbb{E}_X(Y) = \mathbb{E}(X \otimes Y)$$

and furthermore we put $\mathbb{E}_X^{(0)} \equiv \mathbb{E}_X$ and for all $n \geqslant 1$ and $X = \bigotimes_{x, N(x)=n} X_x \in \mathscr{A}^{(n)}$ and Y of the form $Y = \bigotimes_{y, N(y)=n} Y_y$, $Y_y \in \mathscr{B}^{\otimes (z-1)}$, we have

$$\mathbb{E}_X^{(n)}: \quad \mathscr{B}^{(n+1)} \to \mathscr{B}^{(n)}: \quad Y \mapsto \mathbb{E}_X^{(n)}(Y) = \left(\bigotimes_{x, N(x)=n} \mathbb{E}_{X_x}^{(0)} \right) (Y)$$

We then extend this map linearly to general $X \in \mathscr{A}^{(n)}$ and $Y \in \mathscr{B}^{(n+1)}$. We also define

$$\hat{\mathbb{E}}^{(n)} = \mathbb{E}_{\mathbb{1}}^{(n)} \tag{1.3}$$

where $\mathbb{1}$ is the unit element of $\mathscr{A}^{(n)}$.

With *boundary conditions* for the volume $(0, n)$ we mean a positive functional $\rho_{(0,n)}$ of $\mathscr{B}$ and a positive element $b_{(0,n)} \in \mathscr{B}^{(n+1)}$. For any such boundary condition we define a state of $\mathscr{A}_{(0,n)}$ by the linear extension of the following formula: for all $X_k \in \mathscr{A}^{(k)}$, $0 \leqslant k \leqslant n$,

$$\omega_{(0,n)}(X_0 \otimes X_1 \otimes \cdots \otimes X_n) = \rho_{(0,n)}(\mathbb{E}_{X_0}^{(0)} \circ \mathbb{E}_{X_1}^{(1)} \circ \cdots \circ \mathbb{E}_{X_n}^{(n)}(b_{(0,n)})) \tag{1.4}$$

The complete positivity of $\mathbb{E}$ guarantees the positivity of the functional: as the set of completely positive maps is closed under taking tensor products and composition of maps, all the maps $\hat{\mathbb{E}}^{(0)} \circ \cdots \circ \hat{\mathbb{E}}^{(n)}$ are completely positive; together with the positivity of the boundary conditions, this implies the positivity of the functional ω. If the boundary conditions are chosen such that $\omega(\mathbb{1}) = 1$, we have defined a state of $\mathscr{A}_{(0,n)}$. A state ω on the volume (x, n) can then be obtained by applying a suitable translation and using boundary conditions $(\rho_{(x,n)}, b_{(x,n)})$.

It is obvious that two sets of "boundary conditions"

$$(\rho_{(x,n)}, b_{(x,n)}) \qquad \text{and} \qquad (\rho'_{(x,n)}, b'_{(x,n)})$$

normalized such that both define a state of $\mathscr{A}_{(x,n)}$, and related by a positive constant λ as follows

$$\rho'_{(x,n)} = \lambda \rho_{(x,n)}, \qquad b'_{(x,n)} = \lambda^{-1} b_{(x,n)}$$

define the same state. So we do not have to distinguish between them.

To obtain states ω of the infinite-volume tree, one needs sets of boundary conditions $\{(\rho_{(x,n)}, b_{(x,n)}) \mid x \in \mathbb{T}^z, n \in \mathbb{N}_0\}$ which satisfy the compatibility conditions

$$\text{if} \quad (x, n) \subset (y, m), \qquad \text{then} \quad \omega_{(y,m)} \restriction_{\mathscr{A}_{(x,n)}} = \omega_{(x,n)} \tag{1.5}$$

Indeed, if (1.5) is satisfied, then there exists a unique state ω on $\mathscr{A}_{\mathbb{T}^z}$ such that for all x and n, $\omega_{(x,n)} = \omega \restriction_{\mathscr{A}_{(x,n)}}$. In general, compatibility conditions impose strong constraints on the construction of correlation functions. It is, however, a particular merit of the VBS construction, as presented in (1.4), that one is always able to find boundary conditions that guarantee compatibility. In the sequel we will only consider boundary conditions that are simple tensor products, i.e., each $b_{(x,n)}$ is a simple tensor product of elements of $\mathscr{B}$. This kind of boundary condition is exactly equivalent to fixing the state of the spins (of the system itself) at the boundary of the volume. Moreover, we will take the boundary conditions local in the following sense:

$$\rho_{(x,n)} = \rho_{(x,m)} \equiv \rho_x \qquad \text{for all} \quad n, m \geqslant 0 \tag{1.6}$$

$$\begin{aligned} b_{(x,n)} &= b_{(x \vee (1), n-1)} \otimes \cdots \otimes b_{(x \vee (z-1), n-1)} \\ &= \bigotimes_{y, N(y)=n} b_{(x \vee y, 0)} \equiv \bigotimes_{y, N(y)=n} c_{x \vee y} \end{aligned} \tag{1.7}$$

This means that the boundary conditions can be attached to the sites of the tree. Therefore we call such boundary conditions $\{(\rho_x, c_x) \mid x \in \mathbb{T}^z\}$ *local* boundary conditions. In this situation we have the following theorem, which provides us with sufficient conditions for compatibility.

Theorem 1.1. For all $x \in \mathbb{T}^z$, let $\rho_{(x,n)}$ be a state of $\mathscr{B}$ and c_x a positive element of $\mathscr{B}$. Consider the local boundary condition $\{(\rho_x, c_x) \mid x \in \mathbb{T}^z\}$ as described in (1.6)–(1.7); then formula (1.4) defines the local restrictions of a unique state ω on the tree, i.e., $\omega \mid_{\mathscr{A}_{(x,n)}} = \omega_{(x,n)}$, if the following three conditions are satisfied:

(i) $\rho_x(c_x) = 1$ for all $x \in \mathbb{T}^z$.

(ii) $\hat{\mathbb{E}}^{(n)}(b_{(x,n)}) = b_{(x,n-1)} \Leftrightarrow c_x = \hat{\mathbb{E}}(c_{x \vee (1)} \otimes \cdots \otimes c_{x \vee (z-1)})$.

(iii) For all $Y \in \mathscr{B}$, and $k = 1,..., z-1$,

$$\rho_x(\hat{\mathbb{E}}(c_{x \vee (1)} \otimes \cdots \otimes c_{x \vee (k-1)} \otimes Y \otimes c_{x \vee (k+1)} \otimes \cdots c_{x \vee (z-1)})) = \rho_{x \vee (k)}(Y)$$

Proof. Let (x, n) and (y, m) be two triangles in $\mathbb{T}^z$ such that $(y, m) \subset (x, n)$. We have to show that

$$\omega_{(x,n)} \mid_{\mathscr{A}_{(y,m)}} = \omega_{(y,m)}$$

It is easy to see that it is sufficient to consider the following two situations:

1. $x = y$, $n = m + 1$.
2. $n = m + 1$, $y = x \vee (k)$, for some $1 \leqslant k \leqslant z - 1$.

In the case 1 one applies (ii). In the case 2 one applies (iii). Then (i) guarantees the normalization of the state. ∎

2. THE MODEL AND MAIN RESULTS

On the Cayley tree $\mathbb{T}^z$ with coordination number $z \geqslant 2$, we consider a spin-s model with $s = z/2$. So $\mathscr{A} = \mathscr{M}_{z+1}$. The $(z+1)$-dimensional irreducible representation of $SU(2)$ on $\mathbb{C}^{z+1}$ is denoted by $D_{z/2}$. Its generators are denoted by S^x, S^y, S^z. For any two half-integers $s_1, s_2 \in \frac{1}{2}\mathbb{N}$ the representation $D_{s_1} \otimes D_{s_2}$ decomposes according to the Clebsch–Gordan series:

$$D_{s_1} \otimes D_{s_2} \cong D_{|s_1 - s_2|} \oplus D_{|s_1 - s_2| + 1} \cdots \oplus D_{s_1 + s_2}$$

We denote by $P^{(z)}$ the orthogonal projection onto the spin-z subspace of $\mathbb{C}^{z+1} \otimes \mathbb{C}^{z+1}$. The bonds of the tree are the nearest neighbor pairs of the form $\{x, x \vee (k)\}$, $1 \leqslant k \leqslant z-1$, and we write $P^{(z)}_{x, x \vee (k)}$ for the spin-z projection located at the bond $\{x, x \vee (k)\}$.

The following $SU(2)$-invariant Hamiltonian with nearest neighbor interaction was first introduced in ref. 1. It is of exactly the same type as in the one-dimensional VBS models and therefore much of the analysis is similar to that developed in ref. 7. For all $x \in \mathbb{T}^z$, $n \geqslant 1$,

$$H_{(x,n)} = \sum_{y \in (x, n-1)} \sum_{k=1}^{z-1} P^{(z)}_{y, y \vee (k)} \tag{2.1}$$

where (x, n) is the triangle defined in (1.2).

Using formula (1.4), we now define a set of positive functionals of the local algebras $\mathscr{A}_{(x,n)}$. Take $\mathscr{B} = \mathscr{M}_2$ and $b_{(x,n)}$ an arbitrary positive element of $\mathscr{B}^{(n+1)}$, and ρ_x a positive functional of $\mathscr{B}$. As in the construction of the ground states of the one-dimensional VBS models in ref. 6, we define $\mathbb{E}$ with the aid of an isometry. It follows from the Clebsch–Gordan series that there exists an up to a phase unique isometry $V: \mathbb{C}^2 \to \mathbb{C}^{z+1} \otimes (\otimes \mathbb{C}^2)^{(z-1)}$ satisfying

$$D_{z/2}(g) \otimes (\otimes D_{1/2}(g))^{z-1}\, V = V D_{1/2}(g) \qquad \text{for all} \quad g \in SU(2)$$

and

$$V^* V = \mathbb{1} \in \mathscr{M}_2$$

Then one defines for all $X \in \mathscr{M}_{z+1}$ and $Y \in (\otimes \mathscr{M}_2)^{z-1}$

$$\mathbb{E}(X \otimes Y) = V^* X \otimes Y V \tag{2.2}$$

With these ingredients we can describe the finite-volume ground states of the Hamiltonians (2.1).

Theorem 2.1. (i) All the local states $\omega_{(x,n)}$, constructed with the completely positive map $\mathbb{E}$ (2.2) and arbitrary boundary conditions, are ground states of (2.1); indeed, for all $y \in (x, n-1)$ and all $k = 1,..., z-1$, we have that

$$\omega_{(x,n)}(P^{(z)}_{y, y \vee (k)}) = 0$$

(ii) All ground states of $H_{(x,n)}$ defined in (2.1) are contained in the face generated by the set of all states $\omega_{(x,n)}$ constructed with the completely positive map $\mathbb{E}$ and arbitrary boundary conditions.

Proof. This is a mere application of Theorem 2.1 of ref. 2. ∎

The interesting thing now is to determine the infinite-volume ground states of the models. For this to make sense, one has to define first what exactly the infinite-volume model is and also what is meant by ground state. There are at least the following four possibilities:

(i) A ground state is a state of $\mathscr{A}_{\mathbb{T}^z}$ such that for all $x \in \mathbb{T}^z$ and all $k = 1,..., z-1$, $\omega(P^{(z)}_{x, x \vee (k)}) = 0$.

(ii) A ground state is a weak limit of the form

$$\omega(X) = \lim_{\Lambda \uparrow \mathbb{T}^z} \omega_\Lambda(X)$$

where for the finite volumes Λ (forming an net increasing to $\mathbb{T}^z$), ω_Λ is a ground state of the corresponding finite-volume Hamiltonian, and X is any local observable.

(iii) A ground state is weak limit as in (ii), but where the states ω_Λ are now states of the local algebra $\mathscr{A}_\Lambda$ with minimal energy for Hamiltonians of the form

$$H_\Lambda = \sum_{\text{bonds in } \Lambda} P^{(z)}_{\text{bond}} + Y_{\delta\Lambda}$$

where $Y_{\delta\Lambda}$ is a self-adjoint element in the algebra of the boundary sites of Λ.

(iv) A ground state is a state of the infinite-volume algebra which satisfies for any local observable X the inequality

$$\lim_{(x,n) \uparrow \mathbb{T}^z} \omega(X^*[H_{(x,n)}, X]) \geqslant 0$$

where the $H_{(x,n)}$ are defined in (2.1).

The Cayley tree is a pathological lattice in the sense that it is not at all clear that even the energy density is the same for all ground states in the sense of (iii) or (iv). This is due to the fact that for any finite volume the number of boundary sites is larger than the number of interior sites (see, e.g., the discussions in refs. 3, 5, and 9). This is a good reason to prefer (i) or (ii) as a definition of ground state. In fact, one can show that for the models under consideration the definitions (i) and (ii) are equivalent.

As mentioned earlier, we will restrict the class of boundary conditions in the following sense: we will consider *local* boundary conditions of the tensor product type [see Eqs. (1.6) and (1.7)]. Such local boundary conditions are of the form

$$b_{(x,n)} = \bigotimes_{y, N(y) = n} c_{x \vee y} \tag{2.3}$$

where for all $x, y \in \mathbb{T}^z$, $0 \neq c_{x \vee y}$ is a positive 2×2 matrix. If the c_x depend only on the level $N(x)$ of x, we will call the boundary conditions *homogeneous*. It should be remarked that the notion of homogeneity is defined in terms of the levels and that the notion of level itself depends on the orientation of the branch in the tree and the choice of the root. It can be seen that homogeneous boundary conditions of periodicity two, i.e., only depending on the parity of the level, are consistent with any choice of the root and branch orientation. The conditions of Theorem 1.1 now are as follows:

$$\text{(i)} \quad \rho_x(c_x) = 1 \qquad \text{for all} \quad x \in \mathbb{T}^z \tag{2.4}$$

$$\text{(ii)} \quad c_x = \hat{\mathbb{E}}(c_{x \vee (1)} \otimes \cdots \otimes c_{x \vee (z-1)}) \tag{2.5}$$

(iii) For $1 \leqslant k \leqslant z-1$, for all $y \in \mathscr{B}$,

$$\rho_x(\hat{\mathbb{E}}(c_{x \vee (1)} \otimes \cdots \otimes c_{x \vee (k-1)} \otimes Y \otimes c_{x \vee (k+1)} \otimes \cdots c_{x \vee (z-1)})) = \rho_{x \vee (k)}(Y) \tag{2.6}$$

At this point we remark that in the usual setup of the VBS construction (see, e.g., ref. 1), where one works with a set of vectors $\Omega_{\alpha,\beta}$, the most general boundary conditions one naturally considers are exactly the ones we have introduced here.

Next we show that for the models under consideration there is at least one solution of (2.4)–(2.6).

Proposition 2.2. Define $c_x = \mathbb{1} \in \mathscr{M}_2$ and $\rho_x(Y) = \frac{1}{2}\operatorname{Tr} Y$, $Y \in \mathscr{M}_2$. Then Eqs. (2.4)–(2.6) are satisfied, and therefore they define an infinite-volume ground state of (2.1) in the above sense.

Proof. $\mathbb{E}$ is defined with an isometry V, so it is unity preserving and (2.5) is automatically satisfied. (2.4) is also obvious. To check (2.6), we use the intertwining property of V:

$$
\begin{aligned}
&\operatorname{Tr} \hat{\mathbb{E}}(\mathbb{1} \otimes \cdots \otimes Y \otimes \cdots \otimes \mathbb{1}) \\
&\quad = \operatorname{Tr} \hat{\mathbb{E}}(Y \otimes \mathbb{1} \otimes \cdots \otimes \mathbb{1}) \\
&\quad = \int_{SU(2)} dg \operatorname{Tr} D^*_{1/2}(g)\, V^*(Y \otimes \mathbb{1} \cdots \otimes \mathbb{1})\, V D_{1/2}(g) \\
&\quad = \operatorname{Tr} V^* \int_{SU(2)} dg\, D^*_{1/2}(g)\, Y D_{1/2}(g) \otimes \mathbb{1} \cdots \otimes \mathbb{1} V \\
&\quad = \operatorname{Tr} \hat{\mathbb{E}}(\mathbb{1})\, \tfrac{1}{2} \operatorname{Tr} Y \\
&\quad = \operatorname{Tr} Y \quad \blacksquare
\end{aligned}
$$

It is also straightforward to see that the thermodynamic limits of local states obtained with boundary conditions of the tensor product type are infinite-volume ground states whose local restrictions are all VBS states determined by boundary conditions satisfying (2.4)–(2.6).

The next section is devoted to the proof of the uniqueness of the solution for the c_x of (2.5) in the case $z \leqslant 4$. In Section 5 we will then also show that there is a unique solution for the ρ_x such that (2.4) and (2.6) are satisfied. Section 4 is devoted to the study of (2.5) in the case $z \geqslant 5$ and homogeneous boundary conditions, i.e., the c_x appearing in (2.3) depend only on the level of x. Together, Sections 3–5 give the complete proof of the following result.

Theorem 2.3. (i) $z \leqslant 4 \Rightarrow$ *uniqueness of infinite-volume ground state*: Let ω be the infinite-volume ground state of the Hamiltonian (2.1) defined in Proposition 2.2. For any set of boundary conditions of the product type (2.3) $\{b_{x,n} \mid x \in \mathbb{T}^z, n \in \mathbb{N}\}$ let $\omega_{x,n}$ be the state on the volume (x, n) defined in (1.4) using the $\mathbb{E}$ defined in (2.2). Then,

$$\lim_{(x,n) \uparrow \mathbb{T}^z} \omega_{(x,n)} = \omega$$

(ii) $z \geqslant 5 \Rightarrow$ *occurrence of Néel order*: For $z \geqslant 5$ there are two types of ground states of the Hamiltonian (2.1) obtained with homogeneous boundary conditions of product type:

(a) A translation- and $SU(2)$-invariant ground state with free boundary conditions, i.e., for $x \in \mathbb{T}^z$, $c_x = \mathbb{1}$ and $\rho_x =$ the normalized trace in (2.4)–(2.6).

(b) All other ground states with homogeneous boundary conditions of product type have a nonvanishing Néel order parameter as defined in the introduction of Section 4. They break both the translation and $SU(2)$ invariance and can be explicitly constructed using the homogeneous solutions of the compatibility conditions (2.4)–(2.6). These solutions are given in Sections 4 and 5.

The translation-invariant solution (a) is unstable in the sense that any other homogeneous product boundary condition will produce one of the Néel ordered ground states described in (b).

3. THE CASE $z \leqslant 4$, PROOF OF UNIQUENESS

In fact in this section we are only going to study the solutions of (2.5): we will show that in the case $z \leqslant 4$ there is only one solution [up to a trivial constant to be determined by (2.4)], namely $c_x = \mathbb{1}$ for all $x \in \mathbb{T}^z$. Strictly speaking, to prove the uniqueness of the solution of (2.4)–(2.6), this result has to be complemented with the uniqueness of the solution of (2.6) for any given set $\{c_x\}$ and this we will do in Section 5 (for all z).

So the problem of this section is to prove that for $z = 2, 3, 4$ the only set $\{c_x \geqslant 0 \mid x \in \mathbb{T}^z\}$ satisfying

$$c_x = \hat{\mathbb{E}}(c_{x \vee (1)} \otimes \cdots \otimes c_{x \vee (z-1)})$$

consists of multiples of $\mathbb{1}$. Let us start by giving the explicit form of the maps $\hat{\mathbb{E}}$, defined in the previous section, in a more convenient representation.

$\hat{\mathbb{E}}$: $(\mathcal{M}_2)^{\otimes z-1} \to \mathcal{M}_2$ and as a basis for $\mathcal{M}_2$ we choose $\{\mathbb{1}, \sigma_x, \sigma_y, \sigma_z\}$, where the σ_α are the usual Pauli matrices. We denote the three Pauli matrices put together in a vector by $\boldsymbol{\sigma}$ ($\sigma_\alpha = 2S^\alpha$). $\hat{\mathbb{E}}$ is linear and invariant under arbitrary permutations of the $z-1$ factors of its argument [see (A2) of the Appendix] and therefore the maps $\hat{\mathbb{E}}$ are completely determined by the following relations:

For $z = 2$,

$$\hat{\mathbb{E}}(\mathbb{1}) = \mathbb{1}$$
$$\hat{\mathbb{E}}(\sigma_\alpha) = -\tfrac{1}{3}\sigma_\alpha$$

For $z = 3$,

$$\hat{\mathbb{E}}(\mathbb{1} \otimes \mathbb{1}) = \mathbb{1}$$
$$\hat{\mathbb{E}}(\sigma_\alpha \otimes \mathbb{1}) = -\tfrac{1}{3}\sigma_\alpha$$
$$\hat{\mathbb{E}}(\sigma_\alpha \otimes \sigma_\beta) = \tfrac{1}{3}\delta_{\alpha,\beta}\mathbb{1}$$

For $z=4$,

$$\hat{\mathbb{E}}(\mathbb{1}\otimes\mathbb{1}\otimes\mathbb{1})=\mathbb{1}$$
$$\hat{\mathbb{E}}(\sigma_\alpha\otimes\mathbb{1}\otimes\mathbb{1})=-\tfrac{1}{3}\sigma_\alpha$$
$$\hat{\mathbb{E}}(\sigma_\alpha\otimes\sigma_\beta\otimes\mathbb{1})=\tfrac{1}{3}\delta_{\alpha,\beta}\mathbb{1}$$
$$\hat{\mathbb{E}}(\sigma_\alpha\otimes\sigma_\alpha\otimes\sigma_\alpha)=-\tfrac{1}{5}\sigma_\alpha$$
$$\hat{\mathbb{E}}(\sigma_\alpha\otimes\sigma_\beta\otimes\sigma_\beta)=-\tfrac{1}{15}\sigma_\alpha,\qquad \alpha\neq\beta$$
$$\hat{\mathbb{E}}(\sigma_x\otimes\sigma_y\otimes\sigma_z)=0$$

These relations can be obtained using the information on $SU(2)$-intertwiners collected in the Appendix.

The $c_x\in\mathcal{M}_2$ are supposed to be positive and $\neq 0$ (otherwise the state cannot be normalized). It is therefore sufficient to prove the following theorem:

Theorem 3.1. For $z=2$, 3, 4 and the $\hat{\mathbb{E}}^{(n)}$ defined as in (1.3), and *any* sequence (b_n), $b_n=\bigotimes_{x,N(x)=n}c_x$, with the $c_x\in\mathcal{M}_2$ positive and nonzero, we have

$$\lim_{n\to\infty} 2\frac{\hat{\mathbb{E}}^{(1)}\circ\cdots\circ\hat{\mathbb{E}}^{(n)}(b_n)}{\mathrm{Tr}\{\hat{\mathbb{E}}^{(1)}\circ\cdots\circ\hat{\mathbb{E}}^{(n)}(b_n)\}}=\mathbb{1}\in\mathcal{M}_2$$

Proof. As the c_x are positive and nonzero, we can normalize them such that $\mathrm{Tr}\,c_x=2$. The positive $c\in\mathcal{M}_2$ such that $\mathrm{Tr}\,c=2$ can be conveniently parametrized in terms of the Pauli matrices: $c=\mathbb{1}+\mathbf{x}\cdot\boldsymbol{\sigma}$ where $\mathbf{x}\in\mathbf{B}_3=\{\mathbf{y}\in\mathbb{R}^3 \mid \|\mathbf{y}\|\leqslant 1\}$. The map $\hat{\mathbb{E}}$ can then be studied in terms of a map $\mathbb{F}$: $(\mathbf{B}_3)^{\times(z-1)}\to\mathbf{B}_3$ defined by

$$\mathbb{1}+\mathbb{F}(\mathbf{x}_1,\ldots,\mathbf{x}_{z-1})\cdot\boldsymbol{\sigma}=2\frac{\hat{\mathbb{E}}(c_1\otimes\cdots\otimes c_{z-1})}{\mathrm{Tr}\{\hat{\mathbb{E}}(c_1,\ldots,c_{z-1})\}}$$

where $c_i=\mathbb{1}+\mathbf{x}_i\cdot\boldsymbol{\sigma}$. In terms of these $\mathbb{F}$ we have to prove that for an arbitrary choice of vectors $\mathbf{x}_{i_1,\ldots,i_n}\in\mathbf{B}_3$, $n=1$, 2, 3,..., and $1\leqslant i_j\leqslant z-1$, we have

$$\lim_{n\to\infty}\mathbb{F}\circ\mathbb{F}^{(2)}\circ\cdots\circ\mathbb{F}^{(n)}((\mathbf{x}_{i_1,\ldots,i_n}))=0\in\mathbb{R}^3 \tag{3.1}$$

where the $\mathbb{F}^{(n)}$ are defined in analogy with the $\hat{\mathbb{E}}^{(n)}$ in (1.3). Note that $\mathbb{F}$ inherits from $\hat{\mathbb{E}}$ the permutation symmetry

$$\mathbb{F}(\mathbf{x}_1,\ldots,\mathbf{x}_{z-1})=\mathbb{F}(\mathbf{x}_{\pi(1)},\ldots,\mathbf{x}_{\pi(z-1)}) \tag{3.2}$$

We now prove (3.1) for the cases $z=2$, 3, and 4 separately. In each case our strategy is to show that, provided $\|\mathbf{x}_1\|,..., \|\mathbf{x}_{z-1}\| \leqslant r$, we have a bound $\|\mathbb{F}(\mathbf{x}_1,..., \mathbf{x}_{z-1})\| \leqslant \beta^{(z)}(r)$, from which one gets

$$\|\mathbb{F} \circ \mathbb{F}^{(2)} \circ \cdots \mathbb{F}^{(n)}((\mathbf{x}_{i_1,..., i_n}))\| \leqslant (\circ\beta^{(z)})^n (\max\{\|\mathbf{x}_{i_1,..., i_n}\|\})$$

We then show that the iterates $(\circ\beta^{(z)})^n (r)$ converge to zero.

$z=2$

This is the case of the one-dimensional lattice; the result is well-known from refs. 1 and 6. For completeness we formulate it here in terms of $\mathbb{F}$. In this case $\mathbb{F}$ is given by $\mathbb{F}(\mathbf{x}) = -(1/3)\mathbf{x}$. Hence we have $\beta^{(2)}(r) = r/3$, and the iteration converges exponentially fast.

$z=3$

From the formulas for $\hat{\mathbb{E}}$ we easily compute $\mathbb{F}$:

$$\mathbb{F}(\mathbf{x}_1, \mathbf{x}_2) = -\frac{\mathbf{x}_1 + \mathbf{x}_2}{3 + \mathbf{x}_1 \cdot \mathbf{x}_2}$$

and hence

$$\|\mathbb{F}(\mathbf{x}_1, \mathbf{x}_2)\|^2 = \frac{\|\mathbf{x}_1\|^2 + \|\mathbf{x}_2\|^2 + 2\mathbf{x}_1 \cdot \mathbf{x}_2}{9 + 6\mathbf{x}_1 \cdot \mathbf{x}_2 + (\mathbf{x}_1 \cdot \mathbf{x}_2)^2}$$

In order to maximize this over $\mathbf{x}_1$, $\mathbf{x}_2$ with norm less than r, first fix $\mathbf{x}_2$ and the scalar product $\mathbf{x}_1 \cdot \mathbf{x}_2$. The latter constraint leaves $\mathbf{x}_1$ free to change within a plane. It is clear from the above expression that $\|\mathbb{F}(\mathbf{x}_1, \mathbf{x}_2)\|^2$ becomes maximal if we choose $\|\mathbf{x}_1\| = r$, and similarly $\|\mathbf{x}_2\| = r$. Hence, with $\gamma = r^{-2}\mathbf{x}_1 \cdot \mathbf{x}_2$ we have

$$\|\mathbb{F}(\mathbf{x}_1, \mathbf{x}_2)\|^2 = \frac{2r^2(1+\gamma)}{(3+r^2\gamma)^2} \leqslant \frac{4r^2}{(3+r^2)^2}$$

Hence

$$\beta^{(3)}(r) = \frac{2r}{3+r^2} \leqslant \frac{2}{3} r$$

and convergence is exponentially fast.

$z=4$

We follow the same lines as in the previous case, the only difference being that now the various estimates become more delicate.

Using the formulas for $\hat{\mathbb{E}}$, it is easy to verify that $\mathbb{F}$ is now given by

$$\mathbb{F}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3) = -\frac{(5+\mathbf{x}_2\cdot\mathbf{x}_3)\,\mathbf{x}_1 + (5+\mathbf{x}_1\cdot\mathbf{x}_3)\,\mathbf{x}_2 + (5+\mathbf{x}_1\cdot\mathbf{x}_2)\,\mathbf{x}_3}{5(3+\mathbf{x}_1\cdot\mathbf{x}_2+\mathbf{x}_1\cdot\mathbf{x}_3+\mathbf{x}_2\cdot\mathbf{x}_3)}$$

Again we can assume that $\|\mathbf{x}_1\| \geqslant \|\mathbf{x}_2\| \geqslant \|\mathbf{x}_3\|$. Furthermore, we adopt the notation $s_1 = \mathbf{x}_2\cdot\mathbf{x}_3$, $s_2 = \mathbf{x}_1\cdot\mathbf{x}_3$, $s_3 = \mathbf{x}_1\cdot\mathbf{x}_2$.

We compute

$$\|\mathbb{F}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3)\|^2 = \frac{(5+s_1)^2\,\|\mathbf{x}_1\|^2 + 2(5+s_1)(5+s_2)\,s_3 + \text{cycl. perm.}}{25(3+s_1+s_2+s_3)^2} \tag{3.3}$$

Notice that again we can restrict ourselves to vectors of equal length. To see this, we use the fact that we can always find two vectors $\mathbf{y}_2$ and $\mathbf{y}_3$ such that $r = \|\mathbf{x}_1\| = \|\mathbf{y}_2\| = \|\mathbf{y}_3\|$ and $s_1 = \mathbf{y}_2\cdot\mathbf{y}_3$, $s_2 = \mathbf{x}_1\cdot\mathbf{y}_3$, and $s_3 = \mathbf{x}_1\cdot\mathbf{y}_2$ and we observe that

$$\|\mathbb{F}(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3)\|^2 \leqslant \|\mathbb{F}(\mathbf{x}_1, \mathbf{y}_2, \mathbf{y}_3)\|^2$$

Next we compare this situation of three vectors of equal length with the case $\mathbf{x}_1 = \mathbf{x}_2 = \mathbf{x}_3$; we will show

$$\|\mathbb{F}(\mathbf{x}_1, \mathbf{y}_2, \mathbf{y}_3)\| \leqslant \|\mathbb{F}(\mathbf{x}_1, \mathbf{x}_1, \mathbf{x}_1)\| \tag{3.4}$$

from which one gets

$$\beta^{(4)}(r) = r\,\frac{5+r^2}{5+5r^2}$$

The iterates of this function still converge to $r=0$, albeit at a much slower rate: there is a constant $C>0$ such that

$$(\circ\beta^{(4)})^n\,(r) \leqslant \frac{C}{n^{1/2}}$$

Let us finally prove (3.4). Define $\varepsilon_1, \varepsilon_2, \varepsilon_3 \geqslant 0$ by

$$\varepsilon_3 = 1 - \frac{\mathbf{x}_1\cdot\mathbf{x}_2}{r^2} \text{ and cycl. perm.}$$

and put $\zeta = \varepsilon_1 + \varepsilon_2 + \varepsilon_3$, $\xi = \varepsilon_1^2 + \varepsilon_2^2 + \varepsilon_3^2$, $\eta = \varepsilon_1\varepsilon_2\varepsilon_3$. The numerator of (3.3) is then given by

$$\begin{aligned} P = {} & r^2(225 - 50\zeta) + r^4(90 - 50\zeta + 10\zeta^2 - 10\xi) \\ & + r^6(9 - 8\zeta - 2\xi - 6\eta + 3\xi^2) \end{aligned}$$

and the denominator by

$$Q = 25[9 + 6r^2(3 - \zeta) + r^4(3 - \zeta)^2]$$

Proving (3.4) then amounts to showing that

$$\frac{25P}{r^2Q} \leqslant \frac{25 + 10r^2 + r^4}{1 + 2r^2 + r^4}$$

or equivalently we have to show that

$$\begin{aligned} g(r^2) \equiv {} & 25\zeta + (5\xi - 5\zeta^2)\, r^2 + (3\eta - 26\zeta + 11\xi + \zeta^2)\, r^4 \\ & + (7\xi + 6\eta - 3\zeta^2)\, r^6 + (\xi + 3\eta + \zeta - \zeta^2)\, r^8 \\ \geqslant {} & 0 \end{aligned}$$

Note that coefficients of η and ξ are positive. So, using $\eta \geqslant 0$ and $3\xi \geqslant \zeta^2$, we have

$$\begin{aligned} \frac{3g(r^2)}{\zeta(1 - r^2)} & \geqslant 75 + 75r^2 - 3r^4 - 3r^6 - 2r^2\zeta(5 - 2r^2 - r^4) \\ & \equiv h(r^2, \zeta) \end{aligned}$$

As $r^2 \leqslant 1$, the coefficient of ζ in $h(r^2, \zeta)$ is negative; furthermore, as $0 \leqslant \zeta \leqslant 6$, it suffices to observe that

$$h(r^2, 6) = 75 + 15r^2 + 21r^4 + 9r^6 \geqslant 0$$

to conclude the proof. ∎

4. NONUNIQUENESS IN THE CASE $z \geqslant 5$

In this section we will restrict ourselves to homogeneous boundary conditions. When more than one homogeneous solution of (2.5) is found, one can immediately see that there is also an infinite number of nonhomogeneous solutions. This fact was already pointed out in ref. 1. Working with the subset of homogeneous boundary conditions is reasonable because of the π-symmetry of the Hamiltonians $H_{(x,n)}$, i.e.,

$$\pi_x^{(\sigma)}(H_{(x,n)}) = H_{(x,n)}$$

with the $\pi_x^{(\sigma)}$ defined in (1.1). Also, the completely positive map $\mathbb{E}$ is permutation invariant in the sense that

$$\mathbb{E}(X \otimes \pi_0^{(\sigma)}(Y)) = \mathbb{E}(X \otimes Y)$$

and the $\mathbb{E}^{(n)}$ satisfy certain covariance relations under "rotations." It is therefore natural to look at weak limits of ground states which are determined by homogeneous boundary conditions. By this we mean that the boundary spins belonging to the same level in the tree are put into the same state. So we still allow for dependence of the boundary condition on the level. This is important because we are especially interested in the question of whether there are solutions which exhibit Néel order: i.e., whether there are states $\omega_{g,\pm}$, $g \in SU(2)$, which satisfy

$$\omega_{g,\pm}(D_{z/2}(g)^* S_x^z D_{z/2}(g)) = \pm n_0(-1)^{d(0,x)}$$

for all $x \in \mathbb{T}^z$. Remark that on a Cayley tree

$$(-1)^{d(x,y)} = (-1)^{N(x)-N(y)}$$

$d(x, y)$ being defined as the number of steps in the shortest path over bonds connecting x and y; $N(x)$ is the level to which x belongs, that is, $N(x) = d(x, 0)$.

So, our problem is to determine all the solutions $\{c_x\}$ of (2.5) such that the c_x depend only on $N(x)$. In other words, we are looking for sequences (c_n), $c_n \in \mathcal{M}_2$, positive and nonzero, such that

$$\hat{\mathbb{E}}((\otimes c_{n+1})^{z-1}) = c_n \qquad \text{for all} \quad n \geq 0 \tag{4.1}$$

This analysis will be done for arbitrary $z \geq 2$ and we will see that nonuniqueness occurs iff $z \geq 5$. The fact that there is always at least one solution was demonstrated in Proposition 2.2.

Proposition 4.1. If $(c_n)_{n=0}^{\infty}$, $c_n \geq 0$, satisfies

$$c_{n-1} = \hat{\mathbb{E}}((\otimes c_n)^{z-1})$$

then there exists a $g \in SU(2)$ and a sequence (μ_n) of strictly positive numbers such that

$$c_n = \mu_n D_{1/2}(g)^* \begin{pmatrix} 1 + (-1)^{n+1}(\alpha_n - 1) & 0 \\ 0 & 1 - (-1)^{n+1}(\alpha_n - 1) \end{pmatrix} D_{1/2}(g) \tag{4.2}$$

where the $\alpha_n \in [0, 2]$ satisfy

$$t^{(z)}(\alpha_n) = 2 - \alpha_{n+1}$$

with $t^{(z)}$: $[0, 2] \to [0, 2]$ defined by

$$t^{(z)}(x) = \frac{2}{z+1} \frac{\sum_{k=0}^{z-1} (z-k)\, x^k (2-x)^{z-k-1}}{\sum_{k=0}^{z-1} x^k (2-x)^{z-k-1}} \tag{4.3}$$

Proof. Define a (nonlinear) operator $T^{(z)}$ by

$$T^{(z)}: \quad \mathscr{M}_2 \to \mathscr{M}_2: \quad c \mapsto T^{(z)}(c) = f^{(z)}(c)\, \hat{\mathbb{E}}((\otimes c)^{z-1})$$

where $f^{(z)}$ is a scalar function which will be specified later. Any positive $c \in \mathscr{M}_2$ can be diagonalized with a unitary of the type $D_{1/2}(g)$, $g \in SU(2)$, and by the intertwining property of V we have

$$T^{(z)}\left(D_{1/2}(g)^* \begin{pmatrix} \alpha & 0 \\ 0 & \beta \end{pmatrix} D_{1/2}(g)\right) = D_{1/2}(g)^*\, T^{(z)}\left(\begin{pmatrix} \alpha & 0 \\ 0 & \beta \end{pmatrix}\right) D_{1/2}(g)$$

Using the formulas for the Clebsch–Gordan coefficients given in the Appendix, it is easy to verify that

$$\hat{\mathbb{E}}\left(\left(\otimes \begin{pmatrix} \alpha & 0 \\ 0 & \beta \end{pmatrix}\right)^{z-1}\right) = \begin{pmatrix} g_+^{(z)}(\alpha, \beta) & 0 \\ 0 & g_-^{(z)}(\alpha, \beta) \end{pmatrix}$$

with $g_+^{(z)}(\alpha, \beta) = g_-^{(z)}(\beta, \alpha)$ and

$$\begin{aligned} g_+^{(z)}(\alpha, \beta) &= \sum_M \sum_{m_1, \ldots, m_{z-1}} \\ &\quad \times |\langle 1/2; 1/2 \mid z/2, 1/2, \ldots, 1/2; M, m_1, \ldots, m_{z-1} \rangle|^2 \\ &\quad \times \alpha^{\{\sum_{i=1}^{z-1} (m_i + 1/2)\}} \beta^{\{z-1-\sum_{i=1}^{z-1} (m_i + 1/2)\}} \\ &= \sum_{k=0}^{z-1} \frac{2}{(z+1)!} \binom{z-1}{k} \alpha^k \beta^{z-1-k} (z-k)!\, k! \\ &= \frac{2}{z(z+1)} \sum_{k=0}^{z-1} (z-k)\, \alpha^k \beta^{z-1-k} \end{aligned}$$

and also

$$g_-^{(z)}(\alpha, \beta) = \frac{2}{z(z+1)} \sum_{k=0}^{z-1} (k+1)\, \alpha^k \beta^{z-1-k}$$

It is now convenient to choose the scalar function $f^{(z)}$ in the definition of $T^{(z)}$ as follows:

$$\begin{aligned} f^{(z)}(\alpha, \beta) &= 2\{g_+^{(z)}(\alpha, \beta) + g_-^{(z)}(\alpha, \beta)\}^{-1} \\ &= \left\{\frac{1}{z} \sum_{k=0}^{z-1} \alpha^k \beta^{z-1-k}\right\}^{-1} \end{aligned}$$

The operator $T^{(z)}$ is now completely described by

$$T^{(z)}\left(\begin{pmatrix}\alpha & 0\\ 0 & 2-\alpha\end{pmatrix}\right)=\begin{pmatrix}t^{(z)}(\alpha) & 0\\ 0 & 2-t^{(z)}(\alpha)\end{pmatrix}$$

where

$$t^{(z)}(\alpha)=f^{(z)}(\alpha, 2-\alpha)\, g_{+}^{(z)}(\alpha, 2-\alpha)$$

It is then clear that $t^{(z)}$: $[0, 2]\to[0, 2]$ and that it has the following symmetry:

$$t^{(z)}(2-\alpha)=2-t^{(z)}(\alpha)$$

Using this symmetry property, one can write the c_n as stated in the theorem. ∎

It is now obvious that we have to study the asymptotics of the dynamical system on $[0, 2]$ given in (4.2)–(4.3) or equivalently the asymptotics of $(\circ t^{(z)})^n$. We first study the function $t^{(z)}$ in detail (Fig. 2).

Proposition 4.2. Let z be an integer $\geqslant 2$ and define for all $x\in[0, 2]$

$$t^{(z)}(x)=\frac{2}{z+1}\,\frac{\sum_{k=0}^{z-1}(z-k)\,x^k(2-x)^{z-1-k}}{\sum_{k=0}^{z-1}x^k(2-x)^{z-1-k}}$$

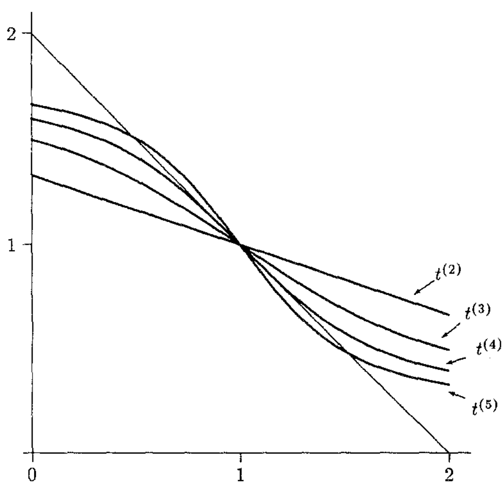

Fig. 2. Graph of the functions $t^{(z)}$ for $z=2, 3, 4, 5$.

Then $t^{(z)}$: $[0, 2] \to [0, 2]$ has the following properties:

(a) $t^{(z)}$ is monotonically decreasing.

(b) $t^{(z)}$ is concave on $[0, 1]$.

(c) $t^{(z)}$ is convex on $[1, 2]$.

(d) $t^{(z)}$ is analytic.

(e) $t^{(z)}(2-x) = 2 - t^{(z)}(x)$ for all $x \in [0, 2]$.

(f) $t^{(z)}(0) = 2z/(z+1)$, $t^{(z)}(2) = 2/(z+1)$.

(g) $t^{(z)}(1) = 1$.

(h) $t^{(z)\prime}(0) = t^{(z)\prime}(2) = -2/(z+1)$.

(i) $t^{(z)\prime}(1) = -(z-1)/3$.

(j) We have

$$\lim_{z \to \infty} t^{(z)}(x) = \begin{cases} 1 & \text{if} \quad x = 1 \\ 2 & \text{if} \quad 0 \leqslant x < 1 \\ 0 & \text{if} \quad 1 < x \leqslant 2 \end{cases}$$

and for all $x \in [0, 2]$ this limit converges monotonically.

Proof. Only the properties (a), (b), and (c) really require a proof.

(a) Monotonicity. We start by making the following substitution: $r = (2-x)/x \in [0, +\infty]$. One then has

$$\frac{z+1}{2} t^{(z)}(x) = g(r) \equiv \frac{zr^{z+1} - (z+1) r^z + 1}{(r-1)(r^z - 1)} \tag{4.4}$$

As

$$\frac{dr}{dx} = -\frac{2}{x^2} \leqslant 0$$

it is sufficient to prove that

$$\frac{dg}{dr} \equiv g' \geqslant 0$$

to obtain the monotonicity of $t^{(z)}$. One first checks that

$$\begin{aligned} &(r-1)^2 (r^z - 1)^2 g'(r) \\ &\quad = \{(r^{z-1} + r^{z-2} + \cdots + 1)^2 - z^2 r^{z-1}\}(r-1)^2 \end{aligned} \tag{4.5}$$

The proof will be finished if we show that for all $z \geqslant 2$, $r \geqslant 0$,

$$(r^{z-1} + r^{z-2} + \cdots + 1)^2 \geqslant z^2 r^{z-1} \tag{4.6}$$

This we do by induction on z.

For $z = 2$, (4.6) follows by the concavity of the square root function. Suppose that we have the inequality for z. In order to obtain it for $z+1$, it is sufficient to show that

$$r^z \geqslant (z+1)\, r^{z/2} - z r^{(z-1)/2}$$

which is equivalent to

$$\frac{z}{y} + y^z \geqslant z + 1$$

for all $y \geqslant 0$. The latter can be seen by observing that the function $y \mapsto y^z + z/y$ is convex for $y > 0$ with a unique minimum at $y = 1$.

(b, c) Concavity–convexity. Starting from (4.4) and (4.5), we verify that

$$-2g(r)' \frac{dr}{dx} = \{(r-1)^{-2} - z^2 r^{z-1}(r^z - 1)^{-2}\}(r+1)^2$$

Then we calculate the second derivative:

$$\frac{z+2}{2} \frac{d^2 t^{(z)}}{dx^2} = (z+2) \frac{d}{dr}\left(g'(r) \frac{dr}{dx}\right) \frac{dr}{dx} = -\frac{z+2}{x^2} \frac{r+1}{(r^z - 1)^3} h(r)$$

with $h(r)$ defined by

$$\begin{aligned} h(r) &= 4(1 + r + \cdots + r^{z-1})^3 \\ &\quad - z^2 r^{z-2}\{(z-1)\, r^{z+1} + (z+1)\, r^z + (z+1) r + z - 1\} \end{aligned}$$

We show that for all $z \geqslant 2$ and all $r \geqslant 0$, $h(r) \geqslant 0$. We develop a similar but slightly different argument for z even and z odd. Therefore, for $n = 1, 2, \ldots$, define

$$h_{1,n}(r) = \frac{1}{2r^{3n}} h(r) \qquad \text{for} \quad z = 2n+1$$

$$h_{2,n}(r) = \frac{1}{4r^{3n-1/2}} h(r) \qquad \text{for} \quad z = 2n$$

With these definitions we have

$$h_{1,n}(r) = 2(r^{-n} + r^{-n+1} + \cdots + r^n)^3 - (2n+1)^2 \{nr^{n+1} + (n+1)\, r^n + (n+1)\, r^{-n} + nr^{-n-1}\}$$

$$h_{2,n}(r) = (r^{-n+1/2} + r^{-n+3/2} + \cdots + r^{n-1/2})^3 - n^2\{(2n-1)\, r^{n+1/2} + (2n+1)\, r^{n-1/2} + (2n+1)\, r^{-n+1/2} + (2n-1)\, r^{-n-1/2}\}$$

We have to show that these two functions are positive.

1. We first treat $h_{1,n}$. For any $k \geqslant 0$ define a variable x_k by

$$x_0 = 1$$

$$x_k = r^k + r^{-k} \qquad \text{for} \quad k \geqslant 1$$

All the x_k are considered as functions of x_1. Because of the symmetry $h_{1,n}(r) = h_{1,n}(r^{-1})$, it is sufficient to consider $r \geqslant 1$ and this makes $r \leftrightarrow x_1$ and $x_1 \leftrightarrow x_k$, $k \geqslant 1$, good substitutions. Now $h_{1,n}$ can be written as a function of $n+2$ variables:

$$h_{1,n} = 2(x_0 + x_1 + \cdots + x_n)^3 - (2n+1)^2\, [nx_{n+1} + (n+1)\, x_n]$$

As $h_{1,n}(1) = 0$, it is sufficient to prove

$$\frac{d}{dx_1} h_{1,n} \geqslant 0 \qquad \text{for all} \quad x_1 \geqslant 0$$

First check that $x_k \geqslant 2$ for $k \geqslant 1$ and that

$$\frac{dx_k}{dx_1} = \begin{cases} k(x_{k-1} + x_{k-3} + \cdots + x_0) & \text{for } \; k \text{ odd} \\ k(x_{k-1} + x_{k-3} + \cdots + x_1) & \text{for } \; k > 0 \text{ and even} \\ 0 & \text{for } \; k = 0 \end{cases}$$

All this permits us to obtain the estimate

$$\begin{aligned} \frac{d}{dx_1} h_{1,n}(x_1) &= 6(x_0 + x_1 + \cdots + x_n)^2 \left(\frac{dx_1}{dx_1} + \cdots + \frac{dx_n}{dx_1}\right) \\ &\quad - n(n+1)(2n+1)(x_0 + x_1 + \cdots + x_n) \\ &\geqslant (x_0 + \cdots + x_n)(2n+1)\left\{6 \sum_{k=1}^{n} k^2 - n(n+1)(2n+1)\right\} \\ &\geqslant 0 \end{aligned}$$

2. To prove $h_{2,n} \geqslant 0$, we use similar reasoning. We need an additional set of variables

$$y_k = r^{k-1/2} + r^{-k+1/2} \qquad \text{for} \quad k = 1, 2, 3,...$$

Again $h_{2,n}(r) = h_{2,n}(r^{-1})$, $h_{2,n}(1) = 0$, and for all $r \geqslant 1$

$$\begin{aligned} \frac{d}{dy_1} h_{2,n}(y_1) &= 3(y_1 + \cdots + y_n)^2 \sum_{k=0}^{n-1} (n^2 - k^2)\, x_k \\ &\quad - n^2 \left\{ (2n-1) \frac{dy_{n+1}}{dy_1} + (2n+1) \frac{dy_n}{dy_1} \right\} \\ &= 3(y_1 + \cdots + y_n)^2 \sum_{k=0}^{n-1} (n^2 - k^2)\, x_k \\ &\quad - n^2(2n+1)(2n-1)\, y_1(y_1 + \cdots + y_n) \\ &\geqslant y_1(y_1 + \cdots + y_n) \left\{ 6n \left[\sum_{k=0}^{n-1} (n^2 - k^2) - \frac{n^2}{2} \right] \right. \\ &\quad \left. - n^2(2n+1)(2n-1) \right\} \\ &\geqslant 0 \end{aligned}$$

where we have used the relations

$$\frac{dy_k}{dy_1} = (2k-1)(x_0 + \cdots + x_{k-1}) \qquad \text{for} \quad k = 1, 2,...$$

$$\frac{dy_1}{dy_1} + \cdots + \frac{dy_n}{dy_1} = \sum_{k=0}^{n-1} (n^2 - k^2)\, x_k$$

and the inequalities

$$x_k \geqslant 2 \qquad \text{for} \quad k \geqslant 1$$

$$x_0 = 1$$

$$y_k \geqslant y_{k-1} \geqslant \cdots \geqslant y_1 \geqslant 0$$

This concludes the proof of the convexity property of $t^{(z)}$. ∎

As a consequence of the properties (a)–(j), we have a quite precise idea of the graph of $t^{(z)}$: see Fig. 2.

Proposition 4.3. The solutions $\alpha \in [0, 2]$ of

$$t^{(z)}(\alpha) = 2 - \alpha \tag{4.7}$$

are the following:

(i) If $2 \leqslant z \leqslant 4$, then $\alpha = 1$ is the unique solution of (4.7).

(ii) If $z \geqslant 5$, there are exactly three solutions: α_0, 1, and $1 - \alpha_0$, where $0 < \alpha_0 < 1$. Furthermore, α_0 is monotonically decreasing to 0 for z tending to infinity.

Proof. The proof is a straightforward application of the properties of the function $t^{(z)}$ which are proved in Proposition 4.2. ▮

In the next proposition we collect our results concerning the asymptotics of $(\circ t^{(z)})^n$. For the case $z \leqslant 4$ the stated properties are actually implied by the results of Section 3.

Proposition 4.4. Define the asymptotic invariant set of the dynamics $(\circ t^{(z)})^n$ as follows:

$$C_z = \bigcap_{n \geqslant 0} (\circ t^{(z)})^n ([0, 2])$$

Then

$$\begin{aligned} C_z &= \{\alpha_0 \in [0, 2] \mid t^{(z)}(\alpha_0) = 2 - \alpha_0\} \\ &= \{\alpha_0, 1, 2 - \alpha_0\} \end{aligned}$$

where α_0 satisfies (4.7). In particular, $C_2 = C_3 = C_4 = \{1\}$ and for $z \geqslant 5$, C_z contains exactly three points. Furthermore, $(\circ t^{(z)})^n$ converges uniformly to a stationary point or a limit cycle of period 2, i.e.,

$$\lim_{n \to \infty} \sup_{\alpha \in [0,2]} \inf_{\alpha_0 \in C_z} |t^{(z)}(\alpha) - \alpha_0| = 0$$

The limit cycle of period two occurs when $z \geqslant 5$ and corresponds to ..., α_0, $2 - \alpha_0$, α_0,... .

Proof. Define $\Delta = \alpha - 1$ and for all $z \geqslant 2$, $\Delta' = t^{(z)}(1 + \Delta) - 1$; it is then easy to derive the following formulas:

$$\text{for } z = 2 \qquad \Delta' = -\frac{1}{3} \Delta$$

$$\text{for } z = 3 \qquad \Delta' = -\Delta \frac{2}{3 + \Delta^2}$$

$$\text{for } z = 4 \qquad \Delta' = -\Delta \frac{\Delta^2 + 5}{5\Delta^2 + 5}$$

Using this information, one immediately obtains for $z=2, 3$ that there exists a $\gamma>0$ such that for all $n\geqslant 0$

$$(\circ t^{(z)})^n([0, 2])\subset[1-e^{-n\gamma}, 1+e^{-n\gamma}]$$

the results then follows and $C=\{1\}$.

For $z=4$, also $C=\{1\}$, and one has that

$$|1-(\circ t^{(4)})^n(\alpha)|\leqslant|1-(\circ t^{(4)})^n(0)|$$

As

$$\lim_{n\to\infty}(\circ t^{(4)})^n(0)=1$$

the uniform convergence follows and $C=\{1\}$.

For $z\geqslant 5$, it is easy to see from the properties of $t^{(z)}$, proved in Proposition 4.2, that there is uniform exponential convergence to a limit cycle of period 2, for all initial conditions $\neq 1$. This cycle is determined by the unique solution $\alpha_0\in(0, 1)$ of $t^{(z)}(\alpha_0)=2-\alpha_0$. So $C_z=\{\alpha_0, 1, 2-\alpha_0\}$. ∎

To summarize, we can conclude that the solutions of (4.1) are given as follows:

(i) If $2\leqslant z\leqslant 4$, there is, up to a normalization factor, a unique solution: $c_n=\mathbb{1}$ for all n.

(ii) If $z\geqslant 5$, there are two types of solutions: (a) the translation- and $SU(2)$-invariant solution $c_n=\mathbb{1}$; and (b) solutions that break the translation and $SU(2)$ invariance. They are determined by formula (4.2) with α_n equal to one of the nontrivial solutions of Eq. (4.7).

A more detailed analysis of the behavior of the functions $t^{(z)}$ easily shows that in the case (ii) only the symmetry-breaking solutions are stable.

5. COMPLETING THE PROOF OF THEOREM 2.3

In Sections 3 and 4 we have found various homogeneous solutions of (2.5). Remember that homogeneous means that c_x depends only on $N(x)$. In the case of uniqueness, $z\leqslant 4$, the solution for the $\{c_x\}$ is homogeneous. In the case $z\geqslant 5$, we found nonuniqueness within the class of homogeneous $\{c_x\}$. Given such a homogeneous $\{c_x\}$, we now want to solve Eq. (2.6) for the ρ_x:

$$\rho_x(\hat{\mathbb{E}}(c_{N(x)+1}\otimes\cdots c_{N(x)+1}\otimes \underset{k\text{th place}}{Y}\otimes c_{N(x)+1}\otimes\cdots c_{N(x)+1}))=\rho_{x\vee(k)}(Y)\quad(5.1)$$

From the permutation invariance of $\hat{\mathbb{E}}$ and the homogeneity of the boundary conditions, it is easy to see that (5.1) implies that $\rho_{x \vee (k)}$ is independent of k. Therefore, the ρ_x only depend on the level $N(x)$ of x:

$$\rho_x = \rho_{N(x)}$$

In Sections 3 and 4 we obtained the solutions c_n of (2.5). The constants μ_n can be calculated using the renormalizing function $f^{(z)}$ which appears in the proof of Proposition 4.1:

$$\begin{aligned}
\mu_n &= \prod_{m=1}^{n} f^{(z)}(\alpha_m)^{-1} \\
&= \prod_{m=1, m \text{ odd}}^{n} f^{(z)}(2-\alpha_0)^{-1} \prod_{m=1, m \text{ even}}^{n} f^{(z)}(\alpha_0)^{-1} \\
&= \begin{cases} \left(\dfrac{1}{2z} \dfrac{1-\alpha_0}{(2-\alpha_0)^z - \alpha_0^z} \right)^n & \text{if} \quad \alpha_0 \neq 1 \\ 1 & \text{if} \quad \alpha_0 = 1 \end{cases}
\end{aligned}$$

With the same choice of α_0 the c_n are then given by

$$c_n = \mu_n D_{1/2}(g)^* \begin{pmatrix} 1+(-1)^{n+1}(\alpha_0 - 1) & 0 \\ 0 & 1-(-1)^{n+1}(\alpha_0 - 1) \end{pmatrix} D_{1/2}(g) \tag{5.2}$$

We now solve Eq. (2.6) to obtain the ρ_n.

Proposition 5.1. The ρ_n which satisfy (2.6) are given by

$$\rho_n = \nu_n \delta_{\varepsilon(n)}$$

where $\varepsilon(n) = 0$ for n even and $\varepsilon(n) = 1$ for n odd. δ_0 and δ_1 are the density matrices determined by

$$\delta_0 = D_{1/2}(g) \begin{pmatrix} r(\alpha_0) & 0 \\ 0 & 1 - r(\alpha_0) \end{pmatrix} D_{1/2}(g)^*$$

$$\delta_1 = D_{1/2}(g) \begin{pmatrix} 1 - r(\alpha_0) & 0 \\ 0 & r(\alpha_0) \end{pmatrix} D_{1/2}(g)^*$$

$r(\alpha_0) \in [0, 1]$ is uniquely determined by imposing that for all $Y \in \mathcal{M}_2$,

$$\delta_\varepsilon(\hat{\mathbb{E}}(Y \otimes (\otimes c_{1-\varepsilon})^{z-2})) = \lambda \delta_{1-\varepsilon}(Y)$$

where c_0 and c_1 are given in Proposition 4.1 (forgetting about the μ_n):

$$c_0 = \begin{pmatrix} 2-\alpha_0 & 0 \\ 0 & \alpha_0 \end{pmatrix}$$

$$c_1 = \begin{pmatrix} \alpha_0 & 0 \\ 0 & 2-\alpha_0 \end{pmatrix}$$

and $\alpha_0 \in [0, 2]$ is determined in (4.7); $g \in SU(2)$ and α_0 are the same as those which appear in (5.2). We also have

$$\lambda = \frac{1}{z} \sum_{k=0}^{z-1} \alpha_0^k (2-\alpha_0)^{z-1-k} = \mu_1^{-1}$$

and the normalizing constants v_n are

$$v_n = \{\mu_n \delta_0(c_0)\}^{-1}$$

Proof. The dependence of the solutions on the group element $g \in SU(2)$ is easily determined; so we can suppose that g is the neutral element and we are left with the following set of equations to solve:

$$\delta_0(\hat{\mathbb{E}}(b \otimes (\otimes c_1)^{z-2}) = \lambda_1 \delta_1(b) \tag{5.3}$$

$$\delta_1(\hat{\mathbb{E}}(b \otimes (\otimes c_0)^{z-2}) = \lambda_0 \delta_0(b) \tag{5.4}$$

in the sense that we have to find δ_0 and δ_1 satisfying (5.3) and (5.4) for all $b \in \mathcal{M}_2$ and with $\lambda_0 > 0$ and $\lambda_1 > 0$. The c_0 and c_1 are given in Proposition 4.1 (up to normalization).

Now, (5.3)–(5.4) is a linear equation for (δ_0, δ_1), and it is not difficult to derive that it has a unique positive solution. In fact (5.3)–(5.4) can be solved explicitly. Consider for

$$\sigma = \begin{pmatrix} \alpha & 0 \\ 0 & \beta \end{pmatrix}$$

the linear operator

$$L_\sigma\colon\ \mathcal{M}_2 \to \mathcal{M}_2\colon\ \ b \mapsto \hat{\mathbb{E}}(b \otimes (\otimes \sigma)^{z-2})$$

Define also the automorphism

$$\tau\colon\ \mathcal{M}_2 \to \mathcal{M}_2\colon\ \ b \mapsto \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} b \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Then (5.3)–(5.4) can be written as

$$\delta_0(L_{c_1}(b)) = \lambda_1 \delta_1(b)$$
$$\delta_1(L_{\tau(c_1)}(\tau(b)) = \lambda_0 \delta_0(b)$$

Observe that

$$L_{\tau(c_1)}(\tau(b)) = \tau(L_{c_1}(b))$$

Therefore, we can rewrite the equations as

$$\delta_0(L_{c_1}(b)) = \lambda_1 \delta_1(b)$$
$$\delta_1 \circ \tau(L_{c_1}(b)) = \lambda_0(\delta_0 \circ \tau)(b)$$

The unique solution (δ_0, δ_1) will therefore satisfy $\delta_0 = \delta_1 \circ \tau$, $\delta_1 = \delta_0 \circ \tau$, and

$$\delta_1((\tau \circ L_{c_1})(b)) = \lambda_0 \delta_1(b)$$

The diagonalization of $(\tau \circ L_\sigma)^*$: $\mathscr{M}_2^* \to \mathscr{M}_2^*$ is given as follows:

1. One negative eigenvalue, doubly degenerate:

$$\lambda_-(\alpha, \beta) = -\frac{2}{(z-1)\, z(z+1)} \sum_{k=0}^{z-2} (z-1-k)(k+1)\, \alpha^k \beta^{z-2-k}$$

with eigenvectors

$$\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

2. A positive eigenvalue

$$\tilde{\lambda} = \tfrac{1}{2}(\delta(\alpha, \beta) + \delta(\beta, \alpha)) - \tfrac{1}{2}\{[\delta(\alpha, \beta) - \delta(\beta, \alpha)]^2 + 4\lambda_-(\alpha, \beta)^2\}^{1/2}$$

where

$$\delta(\alpha, \beta) = \frac{2}{(z-1)\, z(z+1)} \sum_{k=0}^{z-2} (k+1)(k+2)\, \alpha^k \beta^{z-2-k}$$

with a nonpositive (diagonal) eigenvector.

3. A positive eigenvalue

$$\lambda_0 = \frac{1}{z} \sum_{k=0}^{z-1} \alpha^k \beta^{z-1-k}$$

with a positive eigenvector of the form

$$\delta_1 = \begin{pmatrix} r(\alpha, \beta) & 0 \\ 0 & 1 - r(\alpha, \beta) \end{pmatrix}$$

where $r(\alpha, \beta)$ is such that for all $\alpha \in (0, 1)$, $1/2 < r(\alpha, 2-\alpha) < 1$. Of course, $r(\alpha, \beta)$ can be calculated explicitly if necessary.

Furthermore, one has that

$$\lambda_0 > \tilde{\lambda} \qquad \text{and} \qquad \lambda_0 > |\lambda_-|$$

This immediately shows that the positive solution δ_1 is unique if $\alpha_0 \in (0, 1)$ and by symmetry also when $\alpha_0 \in (1, 2)$. The case $\alpha_0 = 1$ is straightforward to check. ∎

Theorem 5.2. Within the class of boundary conditions we studied, in the thermodynamic limit, the model (2.1) (i) does not exhibit Néel order in the ground state if $z = 2$, 3, 4, and (ii) has Néel ordered ground states whenever $z \geqslant 5$.

Proof. The only fact that still remains to be checked is that the Néel order parameter does not vanish when $z \geqslant 5$. In order to compute this parameter, we have to insert the information that is contained in Section 4 and in Proposition 5.1 into the definition (1.4) of the state. Doing so, we find

$$n_0 = \rho_0(\mathbb{E}(S^z \otimes c_0^{\otimes(z-1)})$$

Taking $\alpha_0 \in (0, 1)$, there is a constant $0 < r < 1/2$ such that

$$\rho_0 = \begin{pmatrix} r & 0 \\ 0 & 1-r \end{pmatrix}$$

and it is also straightforward to determine

$$\mathbb{E}(S^z \otimes (c_0)^{\otimes(z-1)}) = \begin{pmatrix} s_+ & 0 \\ 0 & s_- \end{pmatrix}$$

with $|s_+| < |s_-|$. This implies $|n_0| > 0$. ∎

Remark 5.3. For all $z \geqslant 2$ the symmetric ground state is obtained by taking $\rho_x = \frac{1}{2}\mathrm{Tr}$ and $b_{(x,n)} = \mathbb{1}$ for all $x \in \mathbb{T}^z$ and all $n \in \mathbb{N}$. The two-point correlation function is then given by

$$\omega(S_0^\alpha S_x^\beta) = \frac{(z+2)^2}{12}\,\delta_{\alpha,\beta}\left(-\frac{1}{3}\right)^{N(x)}$$

In fact, one observes this kind of exponential clustering for arbitrary local observables.

Proof. According to formula (1.4), we have to compute

$$\tfrac{1}{2}\mathrm{Tr}\ \mathbb{E}(S^{\alpha}\otimes \mathbb{L}^{N(\alpha)-1}(\mathbb{E}(S^{\beta}\otimes \mathbb{1}_2^{\otimes(z-1)}))\otimes \mathbb{1}_2^{\otimes(z-2)})$$

with, for all $Y\in \mathcal{M}_2$,

$$\mathbb{L}(Y)=\hat{\mathbb{E}}(Y\otimes \mathbb{1}_2^{\otimes(z-2)})$$

Using formula (A9) of the Appendix, we have

$$\mathbb{E}(S^{\beta}\otimes \mathbb{1}_2^{\otimes(z-1)})=\frac{z+2}{3}J^{\beta} \tag{5.5}$$

where the J^{β} are the generators of the two-dimensional irreducible representation of $SU(2)$. Using (A10), we have

$$\mathbb{L}(J^{\beta})=-\tfrac{1}{3}J^{\beta} \tag{5.6}$$

and furthermore

$$\mathbb{E}(S^{\alpha}\otimes J^{\beta}\otimes \mathbb{1}_2^{\otimes z-2})=-\delta_{\alpha,\beta}\frac{z+2}{12}\mathbb{1}_2 \tag{5.7}$$

Combining (5.5)–(5.7), we get the desired result. ∎

Conjecture 5.4. In the cases $z=3$ and $z=4$ the VBS state constructed above is a pure state of the algebra $\mathcal{A}_{\mathbb{T}^z}$ with nonvanishing entropy density (calculated with the local structure of the tree that we adopted in Section 1).

APPENDIX

For convenience we list here some useful "generalized" Clebsch–Gordan coefficients. The j's are half-integers, the corresponding m's and M range from $-j$ to j in integer steps, and $k\geqslant 1$ is an integer, indicating the number of factors D_j that are considered. D_j is the $(2j+1)$-dimensional irreducible unitary representation of $SU(2)$. The formulas are taken or derived from ref. 8. We have

$$\langle kj;M\mid j,\ldots,j;m_1,\ldots,m_k\rangle$$
$$=\delta_{M,m_1+\cdots+m_k}\left\{\binom{2j}{j-m_1}\cdots\binom{2j}{j-m_k}\Big/\binom{2kj}{kj-M}\right\}^{1/2}$$

For $j=1/2$ this becomes

$$\langle k/2; M \mid 1/2,\ldots, 1/2; m_1,\ldots, m_k\rangle$$
$$= \delta_{M, m_1+\cdots+m_k}\left[\frac{(k/2+m_1+\cdots+m_k)!\,(k/2-m_1-\cdots-m_k)!}{k!}\right]^{1/2}$$

For clarity: these are the coefficients in the k-fold tensor product basis of the representation space of $(\otimes D_j)^k$ of the $2kj+1$ vectors supporting the component D_{kj} in the irreducible decomposition of $(\otimes D_j)^k$.

Let $V_{k,j}$ be the intertwining isometry between $D_{(k+1)j}\otimes(\otimes D_j)^k$ and D_j (which is unique up to a phase), i.e.,

$$D_{(k+1)j}(g)\otimes(\otimes D_j)^k(g)\, V_{k,j} = V_{k,j} D_j(g) \tag{A1}$$

for all $g\in SU(2)$. The invariance under permutations of the m_i, $i=1,\ldots, k$, is immediately visible. This entails, with $Q_{k,j}$ the orthogonal projection onto the permutation symmetric subspace of $(\otimes \mathbb{C}^{2j+1})^k$, the relation

$$(\mathbb{1}_{2kj+1}\otimes Q_{k,j})\, V_{k,j} = V_{k,j} \tag{A2}$$

We also need, for $j_1 \geqslant j_2$,

$$\langle j_1-j_2; M \mid j_1, j_2; m_1, m_2\rangle$$
$$= \delta_{M, m_1+m_2}(-1)^{j_2+m_2}\left\{\frac{[2(j_1-j_2)+1]!\,(2j_2)!}{(2j_1+1)!}\right\}^{1/2}$$
$$\times\left\{\frac{(j_1+m_1)!\,(j_1-m_1)!}{(j_2+m_2)!\,(j_2-m_2)!\,(j_1-j_2+M)!\,(j_1-j_2-M)!}\right\}^{1/2}$$

In particular, for $j_1-j_2=1/2$,

$$\langle 1/2; M \mid j, j-1/2; m_1, m_2\rangle$$
$$= \delta_{M, m_1+m_2}(-1)^{j-1/2+m_2}\left[\frac{1}{(2j+1)j}\right]^{1/2}$$
$$\times\left\{\frac{(j+m_1)!\,(j-m_1)!}{(j-1/2+m_2)!\,(j-1/2-m_2)!\,(1/2+M)!\,(1/2-M)!}\right\}^{1/2}$$

With this information one readily computes the CG coefficients which determine $V_{z-1,1/2}$, used in the proof of Proposition 4.1:

$$\langle 1/2; m \mid z/2, 1/2,\ldots, 1/2; M, m_1,\ldots, m_{z-1}\rangle$$
$$= \sum_{\mu_1,\mu_2} \langle 1/2; m \mid z/2, (z-1)/2; \mu_1, \mu_2\rangle$$
$$\times \langle z/2, (z-1)/2; \mu_1, \mu_2 \mid z/2, 1/2,\ldots, 1/2; M, m_1,\ldots, m_{z-1}\rangle$$

$$= \langle 1/2; m \mid z/2, (z-1)/2; M, m_1 + \cdots + m_{z-1} \rangle$$
$$\times \langle (z-1)/2; m_1 + \cdots + m_{z-1} \mid 1/2,..., 1/2; M, m_1,..., m_{z-1} \rangle$$
$$= \delta_{m, M+m_1+\cdots+m_{z-1}} (-1)^{(z-1)/2+m_1+\cdots+m_{z-1}} [2/(z+1)!]^{1/2}$$
$$\times [(z/2+m-m_1-\cdots-m_{z-1})!\,(z/2-m+m_1+\cdots+m_{z-1})!]^{1/2}$$

We now derive some relations that are useful in the calculation of correlation functions of VBS states on $\mathbb{T}^z$.

By taking derivatives of (A1), we obtain the intertwining property of the isometry $V_{k,j}$ expressed in terms of the generators of the representations. Denote by $\{S^\alpha \mid \alpha = x, y, z\}$ the generators of D_s, and by $\{J^\alpha \mid \alpha = x, y, z\}$ the generators of D_j; then, with $s = (k+1)j$, for $\alpha = x, y, z$,

$$(S^\alpha \otimes (\otimes \mathbb{1}_{2j+1})^k + \mathbb{1}_{2s+1} \otimes J^\alpha \otimes (\otimes \mathbb{1}_{2j+1})^{k-1}$$
$$+ \cdots \mathbb{1}_{2s+1} \otimes (\otimes \mathbb{1}_{2j+1})^{k-1} \otimes J^\alpha)\, V_{k,j} = V_{k,j} J^\alpha$$

Up to trivial phases, by the uniqueness of the subrepresentations, $V_{k,j}$ can be written as

$$V_{k,j} = W_{k,j} U_{s,\,kj,\,j}$$

where for $|s'-r| \leqslant l \leqslant s'+r$, $r, s' \in \frac{1}{2}\mathbb{N}$, and $l, s'+r \in \mathbb{N}$, $U_{s',r,l}$ is the intertwining isometry satisfying

$$(D_{s'} \otimes D_r)\, U_{s',r,l} = U_{s',r,l} D_l$$

and for $j \in \frac{1}{2}\mathbb{N}$, $k \in \mathbb{N}_0$, $W_{k,j}$ is the intertwining isometry satisfying

$$(\otimes D_j)^k\, W_{k,j} = W_{k,j} D_{kj}$$

Denote the generators of the representation D_{kj} by $\{K^\alpha\}$; then

$$\{J^\alpha \otimes (\otimes \mathbb{1}_{2j+1})^{k-1} + \cdots \mathbb{1}_{2j+1} \otimes J^\alpha (\otimes \mathbb{1}_{2j+1})^{k-2}$$
$$+ \cdots (\otimes \mathbb{1}_{2j+1})^{k-1} \otimes J^\alpha\}\, W_{k,j} = W_{k,j} K^\alpha$$

and by the permutation symmetry of the k factors

$$J^\alpha \otimes (\otimes \mathbb{1}_{2j+1})^{k-1}\, W_{k,j} = \frac{1}{k}\, W_{k,j} K^\alpha \tag{A3}$$

For the $U_{s,r,l}$, denoting by L^α the generators of D_l, and by R^α the generators of D_r,

$$(S^\alpha \otimes \mathbb{1}_{2r+1} + \mathbb{1}_{2s+1} \otimes R^\alpha)\, U_{s,r,l} = U_{s,r,l} L^\alpha \tag{A4}$$

We want to show that there exists a $\lambda \in \mathbb{R}$ such that, for $\alpha = x, y, z$,

$$U^*_{s,r,l}(S^\alpha \otimes \mathbb{1}_{2r+1})\, U_{s,r,l} = \lambda L^\alpha \tag{A5}$$

$$U^*_{s,r,l}(\mathbb{1}_{2s+1} \otimes R^\alpha)\, U_{s,r,l} = (1-\lambda)\, L^\alpha \tag{A6}$$

The S^α, R^α, and L^α form irreducible representations of the Lie-algebra $su(2)$, and satisfy

$$\begin{aligned}
[U^*_{s,r,l}(S^\alpha \otimes \mathbb{1}_{2r+1})\, U_{s,r,l}, L^\beta] &= U^*_{s,r,l}([S^\alpha, S^\beta] \otimes \mathbb{1}_{2r+1})\, U_{s,r,l} \\
&= \sum_\gamma i\varepsilon_{\alpha,\beta,\gamma} U^*_{s,r,l}(S^\gamma \otimes \mathbb{1}_{2r+1})\, U_{s,r,l} \\
[U^*_{s,r,l}(\mathbb{1}_{2s+1} \otimes R^\alpha)\, U_{s,r,l}, L^\beta] &= U^*_{s,r,l}(\mathbb{1}_{2s+1} \otimes [R^\alpha, R^\beta])\, U_{s,r,l} \\
&= \sum_\gamma i\varepsilon_{\alpha,\beta,\gamma} U^*_{s,r,l}(\mathbb{1}_{2s+1} \otimes R^\gamma)\, U_{s,r,l}
\end{aligned}$$

Together with (A4), this proves (A5) and (A6). Next we calculate the value of λ. Note that $\mathbf{S}^2 = s(s+1)\mathbb{1}$, $\mathbf{R}^2 = r(r+1)\mathbb{1}$, and $\mathbf{L}^2 = l(l+1)\mathbb{1}$, where $\mathbf{S}^2 = \sum_\alpha (S^\alpha)^2$, etc. Also define $\mathbf{S} \dot{\otimes} \mathbf{R} = \sum_\alpha S^\alpha \otimes R^\alpha$. Then, using the intertwining property twice, we find

$$\mathbf{S} \dot{\otimes} \mathbf{R} U_{s,r,l} = \tfrac{1}{2}\{l(l+1) - s(s+1) - r(r+1)\}\, U_{s,r,l} \tag{A7}$$

From (A5), using again the intertwining property, we obtain

$$U^*_{s,r,l} \mathbf{S} \dot{\otimes} \mathbf{R} U_{s,r,l} = \{\lambda l(l+1) - s(s+1)\}\, \mathbb{1}_{2l+1} \tag{A8}$$

One can now find λ from (A7) and (A8):

$$\lambda = \frac{1}{2} + \frac{1}{2}\frac{s(s+1) - r(r+1)}{l(l+1)}$$

If $s = z/2$, $r = (z-1)/2$, and $l = 1/2$, with $z \geqslant 2$, this becomes

$$\lambda = \frac{z+2}{3}$$

Using this result together with (A3), one can check that, with $k = z - 1$, $j = 1/2$, and $V = V_{z-1,1/2}$,

$$\begin{aligned}
&V^* S^\alpha \otimes (\otimes \mathbb{1}_2)^{z-1}\, V \\
&\quad = U^*_{z/2,(z-1)/2,1/2} W^*_{z-1,1/2}(S^\alpha \otimes (\otimes \mathbb{1}_2)^{z-1})\, W_{z-1,1/2} U_{z/2,(z-1)/2,1/2} \\
&\quad = U^*_{z/2,(z-1)/2,1/2}(S^\alpha \otimes \mathbb{1}_z)\, U_{z/2,(z-1)/2,1/2} \\
&\quad = \frac{z+2}{3} J^\alpha
\end{aligned} \tag{A9}$$

Analogously,

$$\begin{aligned} V^* \mathbb{1}_{z+1} \otimes J^\alpha \otimes (\otimes \mathbb{1}_2)^{z-2} V &= \frac{1}{z-1} U^*_{z/2,(z-1)/2,1/2} (\mathbb{1}_{z+1} \otimes K^\alpha)\, U_{z/2,(z-1)/2,1/2} \\ &= \frac{1}{z-1} (1-\lambda) J^\alpha \\ &= -\frac{1}{3} J^\alpha \end{aligned} \tag{A10}$$

Using the $SU(2)$ symmetry, one easily checks that

$$V^* S^\alpha \otimes J^\beta \otimes (\otimes \mathbb{1}_2)^{z-2} V = 0 \qquad \text{if} \quad \alpha \neq \beta \tag{A11}$$

From (A7) and (A3) one gets

$$V^* \mathbf{S} \dot{\otimes} \mathbf{J} \otimes (\otimes \mathbb{1}_2)^{z-2} V = -\frac{z+2}{4} \mathbb{1}_2$$

and combining this with (A11), we find

$$V^* S^\alpha \otimes J^\beta \otimes (\otimes \mathbb{1}_2)^{z-2} V = -\delta_{\alpha,\beta} \frac{z+2}{12} \mathbb{1}_2$$

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