

PRODUCT VACUA AND BOUNDARY STATE MODELS IN d -DIMENSIONS

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ABSTRACT. We introduce and analyze a class of quantum spin models defined on d -dimensional lattices $\Lambda \subseteq \mathbb{Z}^d$, which we call *Product Vacua with Boundary States* (PVBS). We characterize their ground state spaces on arbitrary finite volumes and study the thermodynamic limit. Using the martingale method, we prove that the models have a gapped excitation spectrum on \mathbb{Z}^d except for critical values of the parameters. For special values of the parameters we show that the excitation spectrum is gapless. We demonstrate the sensitivity of the spectrum to the existence and orientation of boundaries. This sensitivity can be explained by the presence or absence of edge excitations. In particular, we study a PVBS models on a slanted half-plane and show that it has gapless edge states but a gapped excitation spectrum in the bulk.

1. INTRODUCTION

Gapped ground state phases of quantum lattice systems are receiving much renewed attention lately because they may support topological order, a feature of interest as a potential path to realizing robust quantum memory [18]. Particular effort has been devoted to classifying gapped ground state phases [1, 3, 7, 8, 11, 13, 14, 17, 24].

In this work we generalize the class of models introduced in [2], called *Product Vacua with Boundary States* (PVBS), to higher dimensions and provide a proof for a subclass of these models that they have a non-vanishing gap above the ground state. These models are quantum spin systems with nearest neighbor interactions defined on \mathbb{Z}^d . The bulk ground state is a simple product state (the vacuum) but there is also an interesting structure of edge states. These models are defined in Section 2.

PVBS models have in common with many other examples of multidimensional models with known or expected gapped ground states that they are frustration-free and that they can be considered as particularly simple representatives of a ‘gapped ground state phase’. The PVBS models have a product ground state, which we shall refer to as the vacuum. The excited states can be thought as interacting particle states. Depending on the parameters and the shape of the domain or the boundary condition, there may be an additional ground state carrying one particle. This particle is bound to the edge of the domain. As was shown in [2] in one dimension, the number of such boundary states is an invariant of gapped phases in the sense of [8]. Toy models of this type are sometimes referred to in the literature as Renormalization Group Fixed Points (RGFP). Well-known examples are the Toric Code model [18] and the models with Product of Entangled Pairs (PEPS) ground states studied in [9, 23, 25, 27]. In contrast to most of the previously studied models for which a non-vanishing spectral gap is proved, the interaction terms of the PVBS models are not mutually commuting and the excitations have a physical, in particular non-flat, dispersion relation.

The focus of the present paper is to prove the non-vanishing spectral gap and study the nature of the edge states. Section 3 carries out a detailed discussion of the finite volume ground state spaces and of their limits to various infinite volumes. In particular, we show that the ground state degeneracy depends on the geometry of the infinite volume and on the presence of edges or corners. Obtaining rigorous lower bounds for the spectral gap of multidimensional models with non-commuting interaction terms has proved to be notoriously difficult. In this work we prove such lower bounds for PVBS models with one species of particles in d -dimensions on infinite volumes that

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are obtained as limits of rectangular boxes. We use the martingale method from [21] to accomplish this in Section 4. In Section 5 we show that PVBS models defined on specific infinite volumes, such as the half-infinite plane with a 45 degree boundary, that have the exact same interactions as the PVBS models that we prove are gapped in Section 4, can have a gapless excitation spectrum, meaning the GNS Hamiltonian has gapless spectrum. It is then also clear that, in both finite and infinite volumes, the size of the gap above the ground state(s) depends on the shape of the domain and, specifically, on the orientations of its edges.

It is important that the ground state and spectral gap for the PVBS models are stable under small perturbations of the interactions. The essential ingredient in proving stability for frustration-free models in [20] is the so-called ‘Local Topological Quantum Order’ condition, which we prove holds for the ground states of the PVBS models in Section 6. We conclude the paper by clarifying the fundamental difference between two possible ways of closing the gap in PVBS models. The first, the vanishing of the gap at a critical value of the coupling (here $\lambda = 1$) is a bulk phenomenon. The second involves the geometry of the boundary of the system and the gap closes due to edge excitations. As we explain, in the second case the ‘bulk gap’ stays open.

2. GENERAL SETUP AND RESULTS

2.1. The d -Dimensional PVBS Model. The class of quantum spin chains introduced in [2], called Product Vacua with Boundary States (PVBS), has an $(n + 1)$ - dimensional state space at each site for which $n \geq 1$ denotes the number of particle species in the model, labeled $i = 1, \dots, n$. At most one particle may occupy a given site at any time. If a particle of species i occupies site x , the state at site x is denoted by $|i\rangle$, and if no particle occupies the site, then the state is denoted by $|0\rangle$. The Hamiltonian for a chain of L spins is given by

$$H_{[1,L]} = \sum_{x=1}^{L-1} h_{x,x+1},$$

where $h_{x,x+1}$ acts non-trivially on the states of the nearest neighbor pair at sites x and $x + 1$ by a copy of the interaction term h . The interaction h contains both hopping terms for the particles and a repulsive interaction between two particles of the same species occupying neighboring sites. Specifically, h is of the form

$$(2.1) \quad h = \sum_{i=1}^n |\hat{\phi}_i\rangle\langle\hat{\phi}_i| + \sum_{1 \leq i < j \leq n} |\hat{\phi}_{ij}\rangle\langle\hat{\phi}_{ij}|,$$

where the vectors $\phi_{ij} \in \mathbb{C}^{n+1} \otimes \mathbb{C}^{n+1}$ are given by

$$\phi_i = |0, i\rangle - \lambda_i |i, 0\rangle, \quad \phi_{ij} = \lambda_i |i, j\rangle - \lambda_j |j, i\rangle, \quad \phi_{ii} = |i, i\rangle$$

for $i = 1, \dots, n$ and $i \neq j = 1, \dots, n$. The parameters satisfy $\lambda_i \geq 0$, for $0 \leq i \leq n$, and we put $\lambda_0 = 1$ for later convenience. The notation $\hat{\phi}$ denotes the normalized vector $\|\phi\|^{-1}\phi$. Although the two groups of terms in (2.1) are of the same form, we separated them to emphasize their individual roles. The first sum describes the hopping of each particle species, while the second contains the pair interactions.

We are interested in defining higher-dimensional PVBS models. To do this we consider finite connected subsets $\Lambda \subseteq \mathbb{Z}^d$ as oriented graphs with edges of the form $(\mathbf{x}, \mathbf{x} + e_k)$, where e_k , $1 \leq k \leq d$, are the canonical basis vectors of \mathbb{Z}^d . For each oriented edge $(\mathbf{x}, \mathbf{x} + e_k)$ of a graph Λ , we then consider an interaction term of the same form as that of the one-dimensional model defined in (2.1):

$$(2.2) \quad H_\Lambda = \sum_{\mathbf{x} \in \Lambda} \sum_{\substack{k=1, \dots, d \\ \mathbf{x} + e_k \in \Lambda}} h_{\mathbf{x}, \mathbf{x} + e_k}^{(k)}$$

Here, for each direction $k = 1, \dots, d$, we may choose different values for the parameter, say $\lambda_{(i,k)}$, appearing in the PVBS interaction (2.1).

As in the one-dimensional case, the ground states space of H_Λ is equal to its kernel and can be explicitly constructed. If Λ is connected, has at least n vertices, and $\lambda_{(i,k)} \in (0, \infty)$ for all $i = 1, \dots, n$ and $k = 1, \dots, d$, then the dimension of the ground state space is 2^n . Under these assumptions, the ground state space has a basis $\{\psi_M^\Lambda\}$ labeled by the subsets $M \subset \{1, \dots, n\}$. For $M = \emptyset$, we have

$$\psi_\emptyset^\Lambda = \bigotimes_{x \in \Lambda} |0\rangle.$$

For $M = \{i_1, \dots, i_m\}$, the corresponding ground state vector is given by

$$(2.3) \quad \psi_M^\Lambda = \sum_{\substack{\mathbf{y}_1, \dots, \mathbf{y}_m \in \Lambda \\ \mathbf{y}_j \neq \mathbf{y}_i \text{ if } i \neq j}} \prod_{j=1}^m \prod_{k=1}^d \lambda_{(i_j, k)}^{y_{jk}} \xi(M, \mathbf{y}_1, \dots, \mathbf{y}_m)$$

$$\mathbf{y}_j = (y_{j1}, \dots, y_{jd}),$$

where $\mathbf{y}_1, \dots, \mathbf{y}_m \in \Lambda$, all \mathbf{y}_j distinct, $\xi(M, \mathbf{y}_1, \dots, \mathbf{y}_m)$ denotes the unit vector with a particle of type i_j in position \mathbf{y}_j . It is straightforward to check that $h_{\mathbf{x}, \mathbf{x}+e_k}^{(k)} \psi_M^\Lambda = 0$, for all pairs $\{\mathbf{x}, \mathbf{x}+e_k\} \subset \Lambda$. Therefore, the vectors (2.3) are 2^n mutually orthogonal zero-energy ground states of (2.2). More details on the ground state space for the one-species case are given in Section 3.

The scope of this paper will be to describe various properties of the d -dimensional PVBS model with a single species of particle. For the single species model, the local Hilbert space at each site \mathbf{x} is then \mathbb{C}^2 and we can simplify the notation and the definition of the Hamiltonian as follows. We abbreviate $\lambda_{(1,k)}$ by λ_k , and write the Hamiltonian on any finite $\Lambda \subseteq \mathbb{Z}^d$ as

$$(2.4) \quad H_\Lambda = \sum_{k=1}^d \sum_{\mathbf{x}, \mathbf{x}+e_k \in \Lambda} h_{\mathbf{x}, \mathbf{x}+e_k}^{(k)}$$

where $h_{\mathbf{x}, \mathbf{x}+e_k}^{(k)}$ acts non-trivially on the states associated with the sites $\mathbf{x}, \mathbf{x} + e_k$ and is defined by

$$(2.5) \quad h_{\mathbf{x}, \mathbf{x}+e_k}^{(k)} = |1, 1\rangle\langle 1, 1| + |\hat{\phi}_k\rangle\langle \hat{\phi}_k|,$$

$$(2.6) \quad \hat{\phi}_k = \frac{1}{\sqrt{1 + \lambda_k^2}} (|0, 1\rangle - \lambda_k |1, 0\rangle).$$

The Hamiltonian H_Λ preserves particle number, a fact that will be useful throughout the paper.

We define the following orthonormal basis for the Hilbert space of the one-species model, \mathcal{H}_Λ . Let $X \subseteq \Lambda$ where Λ is finite. We define $\xi_X^\Lambda \in \mathcal{H}_\Lambda$ to be the product state vector with exactly $|X|$ particles occupying the sites $\mathbf{x} \in X$, namely

$$(2.7) \quad \xi_X^\Lambda = \bigotimes_{\mathbf{x} \in \Lambda} |\xi_X^\Lambda(\mathbf{x})\rangle \text{ with } \xi_X^\Lambda(\mathbf{x}) = \begin{cases} 1 & \mathbf{x} \in X \\ 0 & \mathbf{x} \in \Lambda \setminus X \end{cases}$$

We refer to the basis $\{\xi_X^\Lambda : X \subseteq \Lambda\}$ as the canonical orthonormal basis \mathcal{B}_Λ of \mathcal{H}_Λ . Note that contrary to the one-dimensional PVBS models discussed above, there is only one particle species here and the label X refers to their positions.

In the case of a single-species PVBS model defined on a finite connected graph $\Lambda \subseteq \mathbb{Z}^d$ with $\lambda_k \in (0, \infty)$ for $k = 1, \dots, d$, the ground state space is two-dimensional. The normalized ground

state space vectors are given by

$$(2.8) \quad \psi_0^\Lambda = \xi_\emptyset^\Lambda = \bigotimes_{\mathbf{x} \in \Lambda} |0\rangle, \quad \psi_1^\Lambda = \frac{1}{\sqrt{C_\Lambda}} \sum_{\mathbf{x} \in \Lambda} \lambda^{\mathbf{x}} \xi_{\{\mathbf{x}\}}^\Lambda$$

where

$$(2.9) \quad C(\Lambda) = \sum_{\mathbf{x} \in \Lambda} \lambda^{2\mathbf{x}},$$

with, for any $\mathbf{x} = (x_1, x_2, \dots, x_d) \in \mathbb{Z}^d$, $\lambda^{\mathbf{x}} = \prod_{k=1}^d \lambda_k^{x_k}$. Note that the subscript 0, 1 refers here to whether or not the ground state has a particle.

We briefly comment on the assumption $\lambda_k > 0$. First, if some but not all of the $\lambda_k = 0$, then there exist finite connected $\Lambda \subseteq \mathbb{Z}^d$ on which the model has other ground states in addition to the ones given by (2.7). These additional ground states correspond to ‘stuck particles’ and do not appear to be of particular interest to us. Second, the model with complex parameters $\lambda_k \in \mathbb{C}$ is unitarily equivalent to the model with each parameter replaced by its absolute value. Therefore, we can restrict our attention to the case of $\lambda_k > 0$, for all $k = 1, \dots, d$.

2.2. Other Representations. The model with one species of particles we study here is equivalent to an XY model with a particular choice of magnetic field. In fact, our analysis applies to the following family of models of XXZ type as long as the additional parameter $\Delta > -1$. With the same notations as in (2.5), the generalization is defined by

$$(2.10) \quad H_\Lambda(\Delta) = \sum_{k=1}^d \sum_{\mathbf{x}, \mathbf{x}+e_k} h_{\mathbf{x}, \mathbf{x}+e_k}^{(k)}(\Delta)$$

$$(2.11) \quad \begin{aligned} h_{\mathbf{x}, \mathbf{x}+e_k}^{(k)}(\Delta) &= (1 + \Delta)|1, 1\rangle\langle 1, 1| + |\hat{\phi}_k\rangle\langle \hat{\phi}_k|, \\ &= -\frac{\lambda_k}{1 + \lambda_k^2} (S^+ \otimes S^- + S^- \otimes S^+) + \Delta S^3 \otimes S^3 \\ &\quad + \left(\frac{\lambda_k^2}{1 + \lambda_k^2} + \frac{\Delta}{2} \right) S^3 \otimes \mathbb{1} + \left(\frac{1}{1 + \lambda_k^2} + \frac{\Delta}{2} \right) \mathbb{1} \otimes S^3 \\ &\quad + \frac{1}{2} \left(1 + \frac{\Delta}{2} \right) \mathbb{1} \otimes \mathbb{1}. \end{aligned}$$

The PVBS models are recovered by setting $\Delta = 0$, yielding a representation of the PVBS interaction in terms of the spin operators with the convention that $S^3|1\rangle = (1/2)|1\rangle$ and $S^3|0\rangle = -(1/2)|0\rangle$.

Alternatively, the model can be written in terms of creation and annihilation operators for hard-core bosons on the lattice, which is why the particle language is natural. We let

$$a_{\mathbf{x}}^* = S_{\mathbf{x}}^+, \quad a_{\mathbf{x}} = S_{\mathbf{x}}^-, \quad n_{\mathbf{x}} = a_{\mathbf{x}}^* a_{\mathbf{x}} = S_{\mathbf{x}}^3 + 1/2,$$

for any $\mathbf{x} \in \Lambda$. With these operators,

$$(2.12) \quad h_{\mathbf{x}, \mathbf{x}+e_k}^{(k)} = \frac{1}{2} + \frac{1}{1 + \lambda_k^2} [\lambda_k^2 n_{\mathbf{x}} - \lambda_k (a_{\mathbf{x}}^* a_{\mathbf{y}} + a_{\mathbf{y}}^* a_{\mathbf{x}}) + n_{\mathbf{y}}]$$

$$(2.13) \quad = \frac{1}{2} + \frac{1}{1 + \lambda_k^2} (\lambda_k a_{\mathbf{x}} - a_{\mathbf{y}})^* (\lambda_k a_{\mathbf{x}} - a_{\mathbf{y}}).$$

Despite the appealing appearance of this expression, the interaction is not quadratic in bosonic creation and annihilation operators due to the hard-core constraint, namely $a^*|1\rangle = 0$. Hence, it cannot be diagonalised by a Bogoliubov transformation.

2.3. Results. We extend some of the results for the one-dimensional PVBS models, in particular the lower and upper bounds for the spectral gap above the ground states, to the d -dimensional models. We also describe some new phenomena related to gapless edge states that only occur for $d > 1$.

We first prove that the ground state space is, in fact, two-dimensional and spanned by the orthonormal states given in equation (2.8). We then discuss the thermodynamic limit taken over different sequences of finite volumes. The nature of the ground states on infinite systems and the spectrum of low-lying excitations depends on the choice of the infinite volume, in particular on the presence and the nature of boundaries. Our main results are the following.

Proposition 2.1 (Ground States on Finite Volumes). *For the one-species PVBS model defined on a finite, connected subset $\Lambda \subseteq \mathbb{Z}^d$ as given in (2.4), and (2.5) with $\lambda_k \in (0, \infty)$ for all $k = 1, \dots, d$, the ground state space \mathcal{G}_Λ is given by the kernel of H_Λ , is two dimensional, and spanned by*

$$(2.14) \quad \psi_0^\Lambda = \bigotimes_{\mathbf{x} \in \Lambda} |0\rangle, \quad \psi_1^\Lambda = \frac{1}{\sqrt{C(\Lambda)}} \sum_{\mathbf{x} \in \Lambda} \lambda^{\mathbf{x}} \zeta_{\{\mathbf{x}\}}^\Lambda$$

where $C(\Lambda)$ is the normalization constant defined in (2.9).

We are interested in the ground states defined for the system on infinite subsets $\Gamma \subseteq \mathbb{Z}^d$, that can be obtained as weak limits of the finite volume ground states associated with the vectors ψ_0^Λ and ψ_1^Λ of (2.14). Such limits are taken over increasing sequences of finite subsets $\Lambda_n \rightarrow \Gamma$. Regardless of the infinite volume Γ to which the sequence Λ_n increases, the sequence of functionals $\omega_0^{\Lambda_n}(\cdot) = \langle \psi_0^{\Lambda_n}, \cdot \psi_0^{\Lambda_n} \rangle$ will converge to the product state $\omega_0^\Gamma(\cdot)$ such that with respect to its the GNS representation $(\pi_0^\Gamma, \mathcal{H}_0^\Gamma, \Omega_0^\Gamma)$, it is given by the vector state

$$(2.15) \quad \omega_0^\Gamma(\cdot) = \left\langle \Omega_0^\Gamma, \pi_{\omega_0^\Gamma}(\cdot) \Omega_0^\Gamma \right\rangle.$$

Depending on Γ and the value of the parameters λ_k , one of two possible scenarios is realized for the thermodynamic limit of the one-particle ground state $\omega_1^{\Lambda_n}(\cdot) = \langle \psi_1^{\Lambda_n}, \cdot \psi_1^{\Lambda_n} \rangle$. Either, it also converges to the product vacuum, in which case ω_0^Γ is the unique limiting zero-energy ground state, or it converges to a one-particle ground state which is realized by a unit vector Ω_1^Γ also in the GNS space of the product vacuum ω_0^Γ . The state Ω_1^Γ is orthogonal to Ω_0^Γ and represents the particle in a bound state. We will refer to the first possibility as *Scenario I* and the second as *Scenario II*. An example of Scenario I is given by $\Gamma = \mathbb{Z}^d$ in which case the product vacuum is the unique ground state in the thermodynamic limit. An explicit expression of $\Omega_1^\Gamma \in \mathcal{H}_0^\Gamma$ in Scenario II is given by

$$(2.16) \quad \Omega_1^\Gamma = \frac{1}{\sqrt{C(\Gamma)}} \sum_{\mathbf{x} \in \Gamma} \lambda^{\mathbf{x}} \pi_{\omega_0^\Gamma}(\sigma_{\mathbf{x}}^1) \Omega_0^\Gamma$$

where $C(\Gamma) = \sum_{\mathbf{x} \in \Gamma} \lambda^{2\mathbf{x}}$ and $\sigma_{\mathbf{x}}^1$ is the first Pauli matrix.

From the expression for ψ_1^Λ , it is clear that the probability amplitude for the particle in the one-particle ground state is concentrated on the sites \mathbf{x} in Λ where $\lambda^{\mathbf{x}}$ is maximized. If Λ is a rectangular box and all $\lambda_k \neq 1$, then the particle will concentrate in a corner. It is then easy to see that an example of Scenario II is realized if all $\lambda_k \in (0, 1)$, and the thermodynamic limit is taken over an increasing sequence of hypercubes of the form $\Lambda_n = [0, n]^d$. The thermodynamic limit of the one-particle ground states then shows a particle in a bound state concentrated at the origin of $\Gamma = [0, \infty)^d \subset \mathbb{Z}^d$. Which scenario, I or II, that occurs for a given infinite volume Γ and set of model parameters is summarized by the following proposition.

Proposition 2.2. *Let Γ be an arbitrary infinite lattice and let $(\Lambda_n)_{n \in \mathbb{N}}$ be a sequence of increasing and absorbing finite sets converging to Γ . Then, in the weak- $*$ topology,*

- i. (*Scenario I*): *If $\lim_{n \rightarrow \infty} C(\Lambda_n) = +\infty$, then $\omega_1^{\Lambda_n} \rightarrow \omega_0^\Gamma$,*

ii. (*Scenario II*): If $\lim_{n \rightarrow \infty} C(\Lambda_n) < +\infty$, then $\Omega_1^\Gamma \in \mathcal{H}_0^\Gamma$, $\langle \Omega_1^\Gamma, \Omega_0^\Gamma \rangle = 0$ and $\omega_1^{\Lambda_n} \rightarrow \omega_1^\Gamma$ where

$$\omega_1^\Gamma(\cdot) = \langle \Omega_1^\Gamma, \pi_0^\Gamma(\cdot) \Omega_1^\Gamma \rangle.$$

The *excitation spectrum* of the model defined on an infinite volume $\Gamma \subset \mathbb{Z}^d$ with respect to a ground state ω is defined as the spectrum of the GNS Hamiltonian, H_ω , i.e., the densely defined self-adjoint operator on the GNS Hilbert space \mathcal{H}_ω , that generates the dynamics of the infinite system and is such that $H_\omega \Omega_\omega = 0$. We say that there is a *spectral gap* above the ground state ω if there exists a $\delta > 0$ such that

$$\text{spec}(H_\omega) \cap (0, \delta) = \emptyset.$$

In this situation the *spectral gap*, γ , is defined by

$$(2.17) \quad \gamma_\omega = \sup\{\delta > 0 : \text{spec}(H_\omega) \cap (0, \delta) = \emptyset\}.$$

If such $\delta > 0$ does not exist we put $\gamma = 0$ and say that the ground state has gapless excitations.

We will show that any infinite volume obtained as a limit of increasing rectangular boxes will have a nonzero gap in the associated excitation spectrum given that $\lambda_k \neq 1$ for all $k = 1, \dots, d$. Specifically, this indicates that both $\Gamma = [0, \infty)^d$ and $\Gamma = \mathbb{Z}^d$ will have gapped excitation spectrum given that no $\lambda_k = 1$. Hence, a gapped excitation spectrum can arise for models belonging to both scenarios I and II. We believe the excitation spectrum is gapped for any model categorized by Scenario II. However, we present other cases of Scenario I that have a gapless excitation spectrum above the ground state even if $\lambda_k \neq 1$, for all $k = 1, \dots, d$. For example, the thermodynamic limit of diamond shaped $\Lambda_n \subset \mathbb{Z}^2$ with $\lambda_1 = \lambda_2 \in (0, 1]$ discussed in Section 5, has gapless excitations above the unique ground state.

In the following proposition, which we prove in sections 4 and 5, the key tools to studying the spectral gap are the upper and lower bounds for the system on rectangular boxes of the form $\Gamma_{\mathbf{N}} = [0, N_1] \times \dots \times [0, N_d] \subset \mathbb{Z}^d$, $N_1, \dots, N_d \geq 1$. Let $\gamma(\Gamma)$ denote the spectral gap of the system defined on Γ , namely the spectral gap of the Hamiltonian (2.4) for finite systems and that of the GNS Hamiltonian H_0^Γ of the corresponding vacuum state ω_0^Γ in the case of an infinite system. Let B_d be the d -dimensional unit hypercube in \mathbb{Z}^d .

Theorem 2.3 (Bounds for the Spectral Gap).

For the PVBS model with local Hamiltonians defined in (2.4), and $\lambda_k \in (0, \infty)$, $k = 1, \dots, d$, we have the following bounds on the spectral gap:

(i) For any finite rectangular solid $\Gamma = \Gamma_{\mathbf{N}}$, or any infinite $\Gamma \subset \mathbb{Z}^d$ that can be obtained as the limit of a sequence of increasing rectangular solids (i.e., translations of finite volumes $\Gamma_{\mathbf{N}}$), we have the following lower bound:

$$(2.18) \quad \gamma(\Gamma) \geq \frac{\gamma(B_d)}{2^d} \prod_{k=1}^d (1 - \epsilon(\lambda_k) \sqrt{2})^2$$

where

$$(2.19) \quad \epsilon(\lambda_k) = \begin{cases} \frac{\lambda_k}{\sqrt{1+\lambda_k^2}} & \lambda_k < 1 \\ \frac{1}{\sqrt{1+\lambda_k^2}} & \lambda_k > 1 \end{cases}$$

(ii) For the model on \mathbb{Z}^d , the gap of the GNS Hamiltonian satisfies the upper bound

$$(2.20) \quad \gamma(\mathbb{Z}^d) \leq \sum_{k:\lambda_k \neq 1} \frac{(1 - \lambda_k)^2}{1 + \lambda_k^2}.$$

In particular, it is gapless if $\lambda_k = 1$ for all k .

Note that there is a discrepancy between the upper and lower bounds of the theorem, namely the lower bound is equal to zero as soon as *one* of the model parameters is equal to 1, while the upper bound vanishes only if *all* of them equal 1. This is due to the fact that the lower bound is a finite volume calculation while the upper bound is a true infinite volume statement. While in finite volume, there is a zero-energy state in the one-particle subspace, this is no longer true in the GNS Hilbert space of the model on \mathbb{Z}^d . Observe that the restriction of the Hamiltonian for finite or infinite rectangular solids to the one-particle sector is separable in the sense that it is a sum of terms each of which acts on one of the particle's coordinates only. Hence, it is possible in finite volume to construct a vector in the one-particle space which is a ground state of the terms corresponding to all but one coordinate directions, but such a vector does not exist in the GNS space for the model on \mathbb{Z}^d , and any variational state in the one-particle sector there will have an energy which is at least the sum of all one-dimensional gaps. This suggests that the GNS Hamiltonian on \mathbb{Z}^d is gapless only if all model parameters are equal to one.

The upper bounds in this proposition are proved in the usual way by constructing suitable variational states. For the lower bounds we use the martingale method of [21]. The constant $\gamma(B_d)$ is positive by definition. For example, when $d = 2$,

$$\gamma(B_2) = 2 - \sqrt{1 + \frac{4\lambda_1\lambda_2}{(1 + \lambda_1^2)(1 + \lambda_2^2)}}.$$

We comment on the extension of our results to the XXZ formulation given in (2.10)-(2.11). The ground state space for this extension is the same as the ground state space for the one species, d -dimensional PVBS model as long as $\Delta > -1$. As the martingale method is a calculation on the ground state space of a model, it follows that the spectral gap claim from Theorem 2.3(i) also holds for this more general case with the slight modification that the constant $\gamma(B_d)$ is the spectral gap of the generalized Hamiltonian $H_{B_d}(\Delta)$.

We also show that the presence of edge states can cause the spectrum in the thermodynamic limit to be gapless. In Section 5 we consider the PVBS models on $D_\infty = \{(x, y) : y \geq -x\} \subseteq \mathbb{Z}^2$ with $\lambda_1 = \lambda_2 \in (0, 1)$ for which Scenario I is realized, and we prove that the excitation spectrum of the GNS Hamiltonian is gapless. Under the latter condition, a particle can 'bind' to one of the 45 degree boundaries while remaining delocalized on the boundary. This gives rise to a gapless band of edge states.

Specifically, we consider a sequence $\phi_L \in \mathcal{H}_0^{D_\infty}$ of one-particle states in the GNS Hilbert space for which the particle is confined to a finite diamond $D_L \subset \Gamma$, see Figure 1 in Section 5. We show that the energy $E_L = \|\phi_L\|^{-1} \langle \phi_L, H_0^{D_\infty} \phi_L \rangle$ is of the order L^{-2} , showing that the excitation spectrum of the GNS Hamiltonian is gapless in this case.

Proposition 2.4. *Let $d = 2$, and $\lambda_1 = \lambda = \lambda_2$ where $\lambda \in (0, 1)$. Then the GNS Hamiltonian of the one-species PVBS model is gapless on $D_\infty = \{(x, y) : y \geq -x\}$.*

Due to the symmetry of the model, the spectrum remains unchanged if $\lambda_k \rightarrow \lambda_k^{-1}$ and $x_k \rightarrow -x_k$. Therefore, similar statements about the ground states and the excitation spectrum can also be made for the model defined on suitable lattices with coupling constants in $(1, \infty)$.

3. GROUND STATE SPACE

Since we consider the one species class of models, the Hilbert space at any site $\mathbf{x} \in \mathbb{Z}^d$ is a copy of \mathbb{C}^2 . Let Λ be any finite connected subset of \mathbb{Z}^d . For $0 \leq N \leq |\Lambda|$, let

$$\mathcal{H}_\Lambda^N := \text{span} \{ \psi_X^\Lambda : |X| = N \},$$

which we refer to as the N -particle subspace. Clearly, $\mathcal{H}_\Lambda = \bigoplus_{0 \leq N \leq |\Lambda|} \mathcal{H}_\Lambda^N$. The interactions defined in (2.5) are such that $H_\Lambda \mathcal{H}_\Lambda^N \subset \mathcal{H}_\Lambda^N$. Thus, the Hamiltonian preserves particle number.

By the definition of the Hamiltonian, $H_\Lambda \xi_\emptyset^\Lambda = 0$. Since the Hamiltonian H_Λ is a sum of positive semi-definite operators, $H_\Lambda \geq 0$, the ground state space \mathcal{G}_Λ is given by its non-empty kernel

$$\ker(H_\Lambda) = \bigcap_{\substack{k=1, \dots, d \\ \mathbf{x}, \mathbf{x}+e_k \in \Lambda}} \ker(h_{\mathbf{x}, \mathbf{x}+e_k}^{(k)}).$$

In other words,

$$(3.1) \quad \psi \in \mathcal{G}_\Lambda \text{ iff } h_{\mathbf{x}, \mathbf{x}+e_k}^{(k)} \psi = 0 \text{ for all } \mathbf{x}, k \text{ such that } \{\mathbf{x}, \mathbf{x}+e_k\} \subset \Lambda.$$

Proof of Proposition 2.1. Since the Hamiltonian preserves particle number we can just look for solutions of (3.1) in each N -particle subspaces \mathcal{H}_Λ^N separately.

(i) $N = 0$. $\mathcal{H}_\Lambda^0 = \{\mathbb{C}\xi_\emptyset^\Lambda\}$ is one-dimensional and we have already seen that $\psi_0^\Lambda = \xi_\emptyset^\Lambda$ is a ground state.

(ii) $N = 1$. Any $\psi \in \mathcal{H}_\Lambda^1$ has an orthogonal expansion of the form

$$\psi = \sum_{\mathbf{x} \in \Lambda} a_{\mathbf{x}} \xi_{\{\mathbf{x}\}}^\Lambda$$

and for this case, the equations given in (3.1) are equivalent to the following equations for the coefficients $a_{\mathbf{x}}$:

$$(3.2) \quad a_{\mathbf{x}+e_k} = \lambda_k a_{\mathbf{x}}, \text{ for all } \mathbf{x}, k \text{ such that } \{\mathbf{x}, \mathbf{x}+e_k\} \subset \Lambda.$$

The equations

$$(3.3) \quad a_{\mathbf{x}} = \lambda^{\mathbf{x}} \quad \text{where} \quad \lambda^{\mathbf{x}} = \prod_{k=1}^d \lambda_k^{x_k},$$

are a non-zero solution to (3.2). We argue that this is the only linearly independent solution in \mathcal{H}_Λ^1 . Since Λ is connected, for any two distinct $\mathbf{x}, \mathbf{y} \in \Lambda$, there is a path $\mathbf{x} = \mathbf{x}_0 \rightarrow \mathbf{x}_1 \rightarrow \dots \rightarrow \mathbf{x}_n = \mathbf{y}$ contained in Λ such that for all $i = 0, \dots, n-1$, $\mathbf{x}_{i+1} = \mathbf{x}_i + p_i e_{k_i}$ where $p_i \in \{\pm 1\}$ and $k_i \in \{1, \dots, d\}$. This implies that $\mathbf{y} - \mathbf{x} = (n_1, n_2, \dots, n_d)$ where $n_k = \sum_{i, k_i=k} p_i$ and applying (3.2) shows

$$a_{\mathbf{y}} = \lambda^{\mathbf{y}-\mathbf{x}} a_{\mathbf{x}}.$$

Hence, the solution of (3.2) is unique up to a multiplicative constant.

(iii) $N \geq 2$. Any $\psi \in \mathcal{H}_\Lambda^N$ has an expansion of the form

$$\psi = \sum_{X \subset \Lambda, |X|=N} a_X \xi_X^\Lambda.$$

Due to the first term in the general interaction defined in (2.5), the equations (3.1) imply that $a_X = 0$ whenever X contains a nearest neighbor pair. In particular, for a connected Λ with at least two sites, it follows that there are no non-zero solutions with $N = |\Lambda|$. Consider any X a subset of Λ such that it contains no nearest neighbor pairs and $|X| = N < |\Lambda|$. Fix $\mathbf{x} \in X$ and let $\mathbf{x}' \in \Lambda \setminus X$ be a nearest neighbor of \mathbf{x} , i.e., $\mathbf{x}' = \mathbf{x} + p e_k$, for some $p \in \{-1, +1\}$ and $k \in \{1, \dots, d\}$. Let \tilde{X} denote the set obtained from X by replacing \mathbf{x} with \mathbf{x}' . The equations (3.1) then imply

$$(3.4) \quad a_{\tilde{X}} = \lambda_k^p a_X.$$

Since $|X| \geq 2$ and Λ is connected, for any pair of distinct sites $\mathbf{x}, \mathbf{y} \in X$ there is a path $\mathbf{x} = \mathbf{x}_0 \rightarrow \mathbf{x}_1 \rightarrow \dots \rightarrow \mathbf{x}_n = \mathbf{y}$ contained in Λ such that for all $i = 0, \dots, n-1$, $\mathbf{x}_{i+1} = \mathbf{x}_i + p_i e_{k_i}$ with $p_i \in \{\pm 1\}$ and $k_i \in \{1, \dots, d\}$. For any $\mathbf{x} \in X$, pick a $\mathbf{y} \in X$ such that there is connecting path in Λ of shortest length among all paths in Λ connecting \mathbf{x} to a site of $X \setminus \{\mathbf{x}\}$. For such \mathbf{y} , the shortest

connecting path contained in Λ satisfies $\{\mathbf{x}_1, \dots, \mathbf{x}_{n-1}\} \subset \Lambda \setminus X$. By moving \mathbf{y} along this path to the position \mathbf{x}_1 , which is nearest neighbor to \mathbf{x} and applying (3.4) at each step, we conclude

$$a_X = \lambda^{\mathbf{y}-\mathbf{x}} \lambda_{k_1}^{-p_1} a_{X'}$$

with X' a set containing the nearest neighbor pair $\{\mathbf{x}, \mathbf{x}_1\}$. As argued above, $a_{X'} = 0$ and since $\lambda_k \neq 0$ for all k we conclude that $a_X = 0$. Hence, there are no ground states with $N \geq 2$. \square

In Proposition 2.1 we have assumed that $\lambda_k > 0$ for all $k = 1, \dots, d$, and we will continue to make that assumption throughout the rest of the paper. Note that if some of the λ_k vanish, there may be additional solutions of the equations (3.2). This happens, e.g., when there are sites for which the only outgoing edges are in the coordinate directions k and the associated $\lambda_k = 0$.

We now turn to the proof of Proposition 2.2:

Proof. Let $A \in \mathcal{A}_{\text{loc}}$, and $X = \text{supp}(A)$. Then,

$$(3.5) \quad \omega_1^{\Lambda_n}(A) = \frac{1}{C(\Lambda_n)} \left[\sum_{\mathbf{x}, \mathbf{y} \in X} \lambda^{\mathbf{x}+\mathbf{y}} \left\langle \xi_{\{\mathbf{x}\}}^{\Lambda_n}, A \xi_{\{\mathbf{x}\}}^{\Lambda_n} \right\rangle + \sum_{\mathbf{x} \in \Lambda_n \setminus X} \lambda^{2\mathbf{x}} \left\langle \xi_{\emptyset}^{\Lambda_n}, A \xi_{\emptyset}^{\Lambda_n} \right\rangle \right].$$

Since X is a finite set, both scalar products above do not depend on n . The first sum is a finite constant, independent on n , while the second is equal to $C(\Lambda_n \setminus X) \omega_0^\Gamma(A)$. As $n \rightarrow \infty$, the first term tends to zero if and only if $C(\Lambda_n) \rightarrow \infty$. Furthermore, and again since X is finite, $C(\Lambda_n \setminus X)$ and $C(\Lambda_n)$ are either both convergent or both divergent. In the latter case

$$\lim_{n \rightarrow \infty} \frac{C(\Lambda_n \setminus X)}{C(\Lambda_n)} = 1.$$

Hence, if $C(\Lambda_n) \rightarrow \infty$, then $\omega_1^{\Lambda_n}(A) \rightarrow \omega_0^\Gamma(A)$.

On the other hand, if $C(\Gamma) := \lim_{n \rightarrow \infty} C(\Lambda_n) < +\infty$, then $\omega_1^{\Lambda_n}(A)$ converges, but $\lim_{n \rightarrow \infty} \omega_1^{\Lambda_n}(A) \neq \omega_0^\Gamma(A)$. Let Ω_1^Γ be the formal expression (2.16). Since

$$\left\| \sum_{\mathbf{x} \in \Gamma} \lambda^{\mathbf{x}} \pi_{\omega_0^\Gamma}(\sigma_{\mathbf{x}}^1) \Omega_0^\Gamma \right\| \leq \sum_{\mathbf{x} \in \Gamma} \lambda^{2\mathbf{x}} < \infty,$$

as $(\sigma_{\mathbf{x}}^1)^* \sigma_{\mathbf{x}}^1 = 1$, we see that Ω_1^Γ is a well-defined vector and $\Omega_1^\Gamma \in \mathcal{H}_{\omega_0^\Gamma}$. Moreover,

$$\langle \Omega_0^\Gamma, \Omega_1^\Gamma \rangle_{\mathcal{H}_{\omega_0^\Gamma}} = \sum_{\mathbf{x} \in \Gamma} \lambda^{\mathbf{x}} \omega_0^\Gamma(\sigma_{\mathbf{x}}^1) = \sum_{\mathbf{x} \in \Gamma} \lambda^{\mathbf{x}} \langle 0, \sigma_{\mathbf{x}}^1 0 \rangle_{\mathcal{H}_{\mathbf{x}}} = 0.$$

It remains to prove that $\omega_1^{\Lambda_n}$ converges to the vector state given by Ω_1^Γ . Since $\xi_{\{\mathbf{x}\}}^{\Lambda_n} = \sigma_{\mathbf{x}}^1 \xi_{\emptyset}^{\Lambda_n}$, we have that

$$\omega_1^{\Lambda_n}(A) = \frac{1}{C(\Lambda_n)} \sum_{\mathbf{x}, \mathbf{y} \in X} \lambda^{\mathbf{x}+\mathbf{y}} \langle \xi_{\emptyset}^{\Lambda_n}, \sigma_{\mathbf{x}}^1 A \sigma_{\mathbf{y}}^1 \xi_{\emptyset}^{\Lambda_n} \rangle + \frac{C(\Lambda_n \setminus X)}{C(\Lambda_n)} \langle \xi_{\emptyset}^{\Lambda_n}, A \xi_{\emptyset}^{\Lambda_n} \rangle.$$

So if $C(\Lambda_n)$ converges, then

$$\begin{aligned} \lim_{n \rightarrow \infty} \omega_1^{\Lambda_n}(A) &= \frac{1}{C(\Gamma)} \sum_{\mathbf{x}, \mathbf{y} \in X} \lambda^{\mathbf{x}+\mathbf{y}} \omega_0^\Gamma(\sigma_{\mathbf{x}}^1 A \sigma_{\mathbf{y}}^1) + \frac{C(\Gamma \setminus X)}{C(\Gamma)} \omega_0^\Gamma(A) \\ &= \frac{1}{C(\Gamma)} \sum_{\mathbf{x}, \mathbf{y} \in \Gamma} \lambda^{\mathbf{x}+\mathbf{y}} \left\langle \pi_{\omega_0^\Gamma}(\sigma_{\mathbf{x}}^1) \Omega_0^\Gamma, \pi_{\omega_0^\Gamma}(A) \pi_{\omega_0^\Gamma}(\sigma_{\mathbf{y}}^1) \Omega_0^\Gamma \right\rangle \\ &= \omega_1^\Gamma(A), \end{aligned}$$

which concludes the proof for Scenario II. \square

We note that the first term in (3.5) corresponds to the projection $\sum_{\mathbf{x} \in X} |\xi_{\{\mathbf{x}\}}^{\Lambda_n}\rangle \langle \xi_{\{\mathbf{x}\}}^{\Lambda_n}|$, and produces the probability of finding the particle within X . Hence the theorem could be restated as follows: $\omega_1^{\Lambda_n}$ converges to the vacuum state if and only if the probability to find the particle within any fixed finite volume tends to 0 as $\Lambda_n \rightarrow \Gamma$.

To conclude this section we show that in Scenario II, any infinite volume ground state obtained as a weak-* limit of finite volume ground states is realized as a vector in the GNS Hilbert space that is a linear combination of the two vectors Ω_0^Γ and Ω_1^Γ . Let ω be the weak-* limit of a sequence of finite volume ground state functionals $\omega_{a_n, b_n}^{\Lambda_n}(\cdot) = \langle \psi_n, \cdot \psi_n \rangle$ which are generated by normalized vectors $\psi_n = a_n \psi_0^{\Lambda_n} + b_n \psi_1^{\Lambda_n} \in \mathcal{G}_{\Lambda_n}$. We call such ω zero-energy ground states. Since $\{a_n\}$ and $\{b_n\}$ are bounded sequences in \mathbb{C} , there exists some subsequence n_i such that $a_{n_i} \rightarrow a$, and $b_{n_i} \rightarrow b$ for some $a, b \in \mathbb{C}$. Now,

$$\omega(A) = \lim_{i \rightarrow \infty} \omega_{a_{n_i}, b_{n_i}}^{\Lambda_{n_i}}(A) = |a|^2 \omega_0^\Gamma(A) + |b|^2 \omega_1^\Gamma(A) + \lim_{i \rightarrow \infty} \left[\overline{a_{n_i}} b_{n_i} \langle \psi_0^{\Lambda_{n_i}}, A \psi_1^{\Lambda_{n_i}} \rangle + c.c. \right].$$

But by the argument above,

$$\lim_{i \rightarrow \infty} \langle \psi_0^{\Lambda_{n_i}}, A \psi_1^{\Lambda_{n_i}} \rangle = \sum_{\mathbf{x} \in \Gamma} \lambda^{\mathbf{x}} \omega_0^\Gamma(A \sigma_{\mathbf{x}}^1) = \langle \Omega_0^\Gamma, \pi_{\omega_0^\Gamma}(A) \Omega_1^\Gamma \rangle,$$

so that, altogether,

$$\omega(A) = \langle \Omega_\omega^\Gamma, \pi_{\omega_\omega^\Gamma}(A) \Omega_\omega^\Gamma \rangle,$$

where $\Omega_\omega^\Gamma := a \Omega_0^\Gamma + b \Omega_1^\Gamma$.

This result proves, in particular, that if Ω_1^Γ converges as a vector in the GNS space of ω_0^Γ , the associated vector state is a second pure ground state, which we denote by ω_1^Γ . The GNS representation of ω_0^Γ can also serve as the GNS representation of ω_1^Γ . The GNS Hamiltonian, which we denote by H_0^Γ , has a kernel given by $\text{span}\{\Omega_0^\Gamma, \Omega_1^\Gamma\}$. To see this one relies on the frustration free property of the Hamiltonian. It follows that H_0^Γ is the sum of positive local terms, each of which only act non-trivially on a nearest neighbor pair. It then follows from similar calculations done in the finite volume case that the ground state space of H_0^Γ can be at most two-dimensional, and is two-dimensional if and only if Ω_1^Γ converges.

4. LOWER BOUNDS FOR THE SPECTRAL GAP

4.1. The Martingale Method. To prove the existence of a spectral gap in the thermodynamic limit, we appeal to the following theorem.

Theorem 4.1. *Let H_ω be the GNS Hamiltonian of a zero-energy ground state ω for the model defined on an subset $\Gamma \subseteq \mathbb{Z}^d$, and let $\gamma(\Gamma)$ be the spectral gap of H_ω as defined in (2.17). Then*

$$\gamma(\Gamma) \geq \liminf_{N \geq 1} \lambda_1(N)$$

where $\lambda_1(N)$ is the smallest nonzero eigenvalue of the frustration-free Hamiltonians H_{Λ_N} , and Λ_N is an increasing and absorbing sequence of finite volumes $\Lambda_N \rightarrow \Gamma$.

The martingale method provides a means for estimating the lower bound for the spectral gap of the Hamiltonian H_{Λ_N} , for suitable finite volumes Λ_N . To apply Theorem 4.1 to obtain a lower bound for the infinite volume spectral gap $\gamma(\Gamma)$, we need to find a sequence of absorbing finite volumes Λ_N for which the martingale method yields a uniform lower bound for the finite volume spectral gaps. For a fixed finite volume Λ_N , the martingale method requires a finite sequence of volumes Λ_n that increase to Λ_N , for which one can verify the following three conditions.

Conditions for the Martingale Method.

The following conditions must hold for a suitable value of $l > 0$.

(1) There exists a constant d_l for which the local Hamiltonians satisfy

$$0 \leq \sum_{n=l}^N H_{\Lambda_n \setminus \Lambda_{n-l}} \leq d_l H_{\Lambda_N}.$$

(2) The local Hamiltonians H_{Λ_n} have a non-trivial kernel $\mathcal{G}_{\Lambda_n} \subseteq \mathcal{H}_{\Lambda_n}$ and a nonvanishing spectral gap $\gamma_l > 0$ such that:

$$H_{\Lambda_n \setminus \Lambda_{n-l}} \geq \gamma_l (\mathbb{I} - G_{\Lambda_n \setminus \Lambda_{n-l}})$$

for all $n \geq n_l$. We denote by G_{Λ_n} the orthogonal projection onto \mathcal{G}_{Λ_n} . For $\Lambda_n \subseteq \Lambda_N$, G_{Λ_n} projects onto $\mathcal{G}_{\Lambda_n} \otimes \mathcal{H}_{\Lambda_N \setminus \Lambda_n}$.

(3) There exists a constant $\epsilon_l < \frac{1}{\sqrt{l}}$ and some n_l such that for all $n_l \leq n \leq N-1$,

$$\|G_{\Lambda_{n+1} \setminus \Lambda_{n+1-l}} E_n\| \leq \epsilon_l$$

where $E_n = G_{\Lambda_n} - G_{\Lambda_{n+1}}$.

Theorem 4.2 (The Martingale Method). *Assume that conditions (1)-(3) are satisfied for the same integer l . Then for any $\psi \in \mathcal{H}_{\Lambda_N}$ such that $G_{\Lambda_N} \psi = 0$, one has*

$$(4.1) \quad \langle \psi, H_{\Lambda_N} \psi \rangle \geq \frac{\gamma_l}{d_l} (1 - \epsilon_l \sqrt{l})^2 \|\psi\|^2.$$

A proof of Theorem 4.2 can be found in [21].

4.2. The Spectral Gap for PVBS Models on Rectangular Boxes. By virtue of Theorem 4.1, the proof of the lower bound in Theorem 2.3(i) will follow from appropriate lower bounds for the spectral gap for the model on rectangular boxes, which is the focus of this section. Recall that in the statement of the theorem we assume $\lambda_k \in (0, \infty)$. We additionally assume that $\lambda_k \neq 1$ for all k as the lower bound in Theorem 2.3 is trivial if any value $\lambda_k = 1$.

Let $\mathbf{N} = (N_1, \dots, N_d)$ with $N_k \geq 1$ for all k . By the translation invariance of the PVBS models, proving the lower bound (2.18) on any rectangular volume of the form

$$\Gamma_{\mathbf{N}} = \prod_{k=1}^d [0, N_k] \subset \mathbb{Z}^d$$

is sufficient to prove the lower bound for any d -dimensional rectangular solid. The remainder of this section will be dedicated to proving the lower bound on the spectral gap for a PBVS model defined on a general lattice of the form $\Gamma_{\mathbf{N}}$.

Proof of Theorem 2.3 (i). Define

$$\Gamma_{\mathbf{N}}^{(k)} = \prod_{i=1}^{d-k} [0, N_i] \times \prod_{i=d-k+1}^d [0, 1].$$

and note that $\Gamma_{\mathbf{N}} = \Gamma_{\mathbf{N}}^{(0)}$. Using the martingale method we prove for $\epsilon(\lambda_k)$ defined as in (2.19) that

$$(4.2) \quad \gamma(\Gamma_{\mathbf{N}}) \geq \frac{\gamma(\Gamma_{\mathbf{N}}^{(1)})}{2} (1 - \epsilon(\lambda_d) \sqrt{2})^2.$$

By relabeling the axes and permuting the model parameters accordingly, the result (4.2) actually proves

$$(4.3) \quad \gamma(\Gamma_{\mathbf{N}}^{(k)}) \geq \frac{\gamma(\Gamma_{\mathbf{N}}^{(k+1)})}{2} (1 - \epsilon(\lambda_{d-k}) \sqrt{2})^2$$

for $0 \leq k \leq d-1$. Additionally, since $\Gamma_{\mathbf{N}}^{(d)} = B_d$, the unit hypercube, we will obtain the desired uniform lower bound by recursively applying (4.3):

$$(4.4) \quad \gamma(\Gamma_{\mathbf{N}}) \geq \frac{\gamma(B_d)}{2^d} \prod_{k=1}^d (1 - \epsilon(\lambda_k)\sqrt{2})^2.$$

Let $N_d > 1$, since if $N_d = 1$ the bound given in (4.2) is trivial since $\Gamma_{\mathbf{N}} = \Gamma_{\mathbf{N}}^{(1)}$ and $\frac{1}{2}(1 - \epsilon(\lambda_d)\sqrt{2})^2 < 1$. As the sequence of finite volumes increasing to $\Gamma_{\mathbf{N}}$ we choose

$$\Lambda_n = \prod_{i=1}^{d-1} [0, N_i] \times [0, n]$$

for $1 \leq n \leq N_d$. Note that $\Lambda_{N_d} = \Gamma_{\mathbf{N}}$. We will use $l = 2$ to satisfy the conditions of the martingale method. For this value of l , conditions (1) and (2) are easily verified since the PVBS Hamiltonians have range-one interactions, are translation invariant and are frustration-free. Specifically, we find

$$d_l = 2, \quad \text{and} \quad \gamma_l = \gamma(\Gamma_{\mathbf{N}}^{(1)}).$$

It remains to prove condition (3). For our choice of l this is equivalent to showing there exists an $\epsilon < \frac{1}{\sqrt{2}}$ such that

$$(4.5) \quad \sup_{\psi \in \mathcal{G}_{\Lambda_n} \cap \mathcal{G}_{\Lambda_{n+1}}^\perp} \frac{\|G_{\Lambda_{n+1} \setminus \Lambda_{n-1}} \psi\|^2}{\|\psi\|^2} < \epsilon^2.$$

Let $\lambda = (\lambda_1, \dots, \lambda_d)$ be the collection of PVBS model parameters, and $\mathbf{x} = (x_1, x_2, \dots, x_d) \in \mathbb{Z}^d$. In the discussion that follows, the definition of the following set and constants will be useful:

$$(4.6) \quad T_{\mathbf{N}} = \prod_{k=1}^{d-1} [0, N_k] \subseteq \mathbb{Z}^{d-1}$$

$$C(T_{\mathbf{N}}) = \prod_{k=1}^{d-1} c(\lambda_k, N_k), \quad \text{where} \quad c(\lambda_k, m) = \sum_{i=0}^m \lambda_k^{2i}.$$

Furthermore, for $\mathbf{x} \in T_{\mathbf{N}}$, we define $(\mathbf{x}, x_d) \in \mathbb{Z}^d$ to be the d -tuple obtained from appending x_d to \mathbf{x} .

Recall the expressions for the ground states ψ_0^Λ and ψ_1^Λ given in (2.14). Since the ground state space on any connected lattice consists of states with at most one particle, it is sufficient to only consider vectors $\psi \in \mathcal{G}_{\Lambda_n} \cap \mathcal{G}_{\Lambda_{n+1}}^\perp$ in equation (4.5) that have at most one particle on $\Lambda_{n+1} \setminus \Lambda_n$, as vectors with more than one particle will be annihilated by $G_{\Lambda_{n+1} \setminus \Lambda_{n-1}}$. The following is the general form for the vector ψ of interest.

$$(4.7) \quad \psi = b_0 \psi_1^{\Lambda_n} \otimes \psi_0^{\Lambda_{n+1} \setminus \Lambda_n} + \sum_{\mathbf{x} \in T_{\mathbf{N}}} \left[a_{\mathbf{x}} \psi_0^{\Lambda_n} \otimes \xi_{\{(\mathbf{x}, n+1)\}}^{\Lambda_{n+1} \setminus \Lambda_n} + b_{\mathbf{x}} \psi_1^{\Lambda_n} \otimes \xi_{\{(\mathbf{x}, n+1)\}}^{\Lambda_{n+1} \setminus \Lambda_n} \right]$$

where

$$(4.8) \quad b_0 = -\frac{1}{\sqrt{C(T_{\mathbf{N}})c(\lambda_d, n)}} \sum_{\mathbf{x} \in T_{\mathbf{N}}} \lambda^{(\mathbf{x}, n+1)} a_{\mathbf{x}}.$$

Recall that $G_{\Lambda_{n+1} \setminus \Lambda_{n-1}}$ is of the form

$$G_{\Lambda_{n+1} \setminus \Lambda_{n-1}} = |\psi_0^{\Lambda_{n+1} \setminus \Lambda_{n-1}}\rangle \langle \psi_0^{\Lambda_{n+1} \setminus \Lambda_{n-1}}| + |\psi_1^{\Lambda_{n+1} \setminus \Lambda_{n-1}}\rangle \langle \psi_1^{\Lambda_{n+1} \setminus \Lambda_{n-1}}|$$

with

$$\psi_1^{\Lambda_{n+1} \setminus \Lambda_{n-1}} = \frac{1}{\sqrt{(1 + \lambda_d^2)C(T_{\mathbf{N}})}} \sum_{\mathbf{x} \in T_{\mathbf{N}}} \left[\lambda^{(\mathbf{x}, 0)} \xi_{\{(\mathbf{x}, n)\}}^{\Lambda_{n+1} \setminus \Lambda_{n-1}} + \lambda^{(\mathbf{x}, 1)} \xi_{\{(\mathbf{x}, n+1)\}}^{\Lambda_{n+1} \setminus \Lambda_{n-1}} \right].$$

Applying $G_{\Lambda_{n+1} \setminus \Lambda_{n-1}}$ to ψ yields

$$\begin{aligned} G_{\Lambda_{n+1} \setminus \Lambda_{n-1}} \psi &= \left(\frac{b_0 \lambda_d^n}{\sqrt{c(\lambda_d, n)(1 + \lambda_d^2)}} + \sum_{\mathbf{x} \in T_{\mathbf{N}}} \frac{a_{\mathbf{x}} \lambda^{(\mathbf{x}, 1)}}{\sqrt{(1 + \lambda_d^2)C(T_{\mathbf{N}})}} \right) \psi_0^{\Lambda_{n-1}} \otimes \psi_1^{\Lambda_{n+1} \setminus \Lambda_{n-1}} \\ &\quad + \left(\sum_{\mathbf{x} \in T_{\mathbf{N}}} \frac{b_{\mathbf{x}} \lambda^{(\mathbf{x}, 1)} \sqrt{c(\lambda_d, n-1)}}{\sqrt{c(\lambda_d, n)(1 + \lambda_d^2)C(T_{\mathbf{N}})}} \right) \psi_1^{\Lambda_{n-1}} \otimes \psi_1^{\Lambda_{n+1} \setminus \Lambda_{n-1}} \\ &\quad + \frac{b_0 \sqrt{c(\lambda_d, n-1)}}{\sqrt{c(\lambda_d, n)}} \psi_1^{\Lambda_{n-1}} \otimes \psi_0^{\Lambda_{n+1} \setminus \Lambda_{n-1}}. \end{aligned}$$

Replacing b_0 by the expression given in (4.8) and applying the Cauchy-Schwarz inequality, we find that $\|G_{\Lambda_{n+1} \setminus \Lambda_{n-1}} \psi\|^2$ is bounded above by

$$\begin{aligned} \|G_{\Lambda_{n+1} \setminus \Lambda_{n-1}} \psi\|^2 &\leq \frac{\lambda_d^2 c(\lambda_d, n-1)}{(1 + \lambda_d^2) c(\lambda_d, n)} \left(\sum_{\mathbf{x} \in T_{\mathbf{N}}} (|a_{\mathbf{x}}|^2 + |b_{\mathbf{x}}|^2) + \frac{1}{c(\lambda_d, n) C(T_{\mathbf{N}})} \left| \sum_{\mathbf{x} \in T_{\mathbf{N}}} \lambda^{(\mathbf{x}, n+1)} a_{\mathbf{x}} \right|^2 \right) \\ &= \frac{\lambda_d^2 c(\lambda_d, n-1)}{(1 + \lambda_d^2) c(\lambda_d, n)} \|\psi\|^2. \end{aligned}$$

Hence,

$$\sup_{\psi \in \mathcal{G}_{\Lambda_n} \cap \mathcal{G}_{\Lambda_{n+1}}^\perp} \frac{\|G_{\Lambda_{n+1} \setminus \Lambda_{n-1}} \psi\|^2}{\|\psi\|^2} \leq \frac{\lambda_d^2 c(\lambda_d, n-1)}{(1 + \lambda_d^2) c(\lambda_d, n)}.$$

We must consider the cases $\lambda_d < 1$ and $\lambda_d > 1$ separately. When $\lambda_d < 1$ we see that as $n \rightarrow \infty$

$$\frac{c(\lambda_d, n-1)}{c(\lambda_d, n)} \rightarrow 1.$$

So for all n ,

$$\frac{\lambda_d^2 c(\lambda_d, n-1)}{(1 + \lambda_d^2) c(\lambda_d, n)} \leq \frac{\lambda_d^2}{1 + \lambda_d^2}.$$

In this case, since $0 < \lambda_d < 1$, $\frac{\lambda_d^2}{1 + \lambda_d^2} < \frac{1}{2}$. In the case that $\lambda_d > 1$, taking the limit $n \rightarrow \infty$ produces

$$\frac{c(\lambda_d, n-1)}{c(\lambda_d, n)} \rightarrow \frac{1}{\lambda_d^2}.$$

Therefore, when $\lambda_d > 1$ we have that for all n

$$\frac{\lambda_d^2 c(\lambda_d, n-1)}{(1 + \lambda_d^2) c(\lambda_d, n)} \leq \frac{1}{1 + \lambda_d^2}.$$

Since $\lambda_d > 1$ it follows that $\frac{1}{1 + \lambda_d^2} < \frac{1}{2}$. Therefore, for all values of λ_d ,

$$\sup_{\psi \in \mathcal{G}_{\Lambda_n} \cap \mathcal{G}_{\Lambda_{n+1}}^\perp} \frac{\|G_{\Lambda_{n+1} \setminus \Lambda_{n-1}} \psi\|^2}{\|\psi\|^2} \leq \epsilon(\lambda_d)^2 < \frac{1}{2}$$

where $\epsilon(\lambda_d)$ is as defined in (2.19). Thus, the third condition of the martingale method is satisfied, and by Theorem 4.2

$$\gamma(\Gamma_{\mathbf{N}}) \geq \frac{\gamma(\Gamma_{\mathbf{N}}^{(1)})}{2} (1 - \epsilon(\lambda_d) \sqrt{2})^2,$$

as desired. Then, appealing to equations (4.3) and (4.4), and Theorem 4.1 we obtain all of the desired lower bounds of Theorem 2.3(i). \square

5. UPPER BOUNDS AND CLOSURES OF THE SPECTRAL GAP

In this section we prove the upper bound for $\gamma(\mathbb{Z}^d)$ given in Theorem 2.3 as well as discuss two ways in which the spectral gap can close. Specifically, we show that the PVBS models are gappless if all $\lambda_k = 1$, and we prove Proposition 2.4 which shows through an example that the existence of spectral gap in the thermodynamic limit is dependent on the boundary of the infinite lattice. We use the variational principle in the GNS Hilbert space to prove both claims.

5.1. The Bulk Phase Transition. We first prove part (ii) of the theorem. By Proposition 2.2, the ground state of the PVBS model is unique for all value of the parameters $\lambda_1, \dots, \lambda_d$. Let $(\pi_0^{\mathbb{Z}^d}, \mathcal{H}_0^{\mathbb{Z}^d}, \Omega_0^{\mathbb{Z}^d})$ be its GNS representation. For any finite volume Λ , and any $\mathbf{z} = (z_1, \dots, z_d)$, with $z_i \in \mathbb{C}$, let $\tilde{\varphi}_\Lambda(\mathbf{z}) \in \mathcal{H}_0^{\mathbb{Z}^d}$ be the vector given by

$$\tilde{\varphi}_\Lambda(\mathbf{z}) = \pi_0^{\mathbb{Z}^d}(A_\Lambda(\mathbf{z}))\Omega_0^{\mathbb{Z}^d}$$

where the local observable $A_\Lambda(\mathbf{z}) \in \mathcal{A}_\Lambda$ is given by

$$A_\Lambda(\mathbf{z}) = \sum_{\mathbf{x} \in \Lambda} \mathbf{z}^{\mathbf{x}} \sigma_{\mathbf{x}}^1.$$

We first note that

$$\langle \tilde{\varphi}_\Lambda(\mathbf{z}), \Omega_0^{\mathbb{Z}^d} \rangle = \sum_{\mathbf{x} \in \Lambda} \mathbf{z}^{\mathbf{x}} \langle \Omega_0^{\mathbb{Z}^d}, \pi_0^{\mathbb{Z}^d}(\sigma_{\mathbf{x}}^1) \Omega_0^{\mathbb{Z}^d} \rangle = \sum_{\mathbf{x} \in \Lambda} \mathbf{z}^{\mathbf{x}} \langle 0, \sigma_{\mathbf{x}}^1 0 \rangle = 0$$

so that $\tilde{\varphi}_\Lambda(\mathbf{z})$ is a good variational vector for any $\mathbf{z} \in \mathbb{C}^d$. Furthermore,

$$\|\tilde{\varphi}_\Lambda(\mathbf{z})\|^2 = \|A_\Lambda(\mathbf{z})\psi_0^\Lambda\|^2 = \sum_{\mathbf{x} \in \Lambda} |\mathbf{z}|^{2\mathbf{x}}$$

and we shall denote $\varphi_\Lambda(\mathbf{z}) := A_\Lambda(\mathbf{z})\psi_0^\Lambda = \sum_{\mathbf{x} \in \Lambda} \mathbf{z}^{\mathbf{x}} \xi_{\{\mathbf{x}\}}^\Lambda$. Finally,

$$\langle \tilde{\varphi}_\Lambda(\mathbf{z}), H_0^{\mathbb{Z}^d} \tilde{\varphi}_\Lambda(\mathbf{z}) \rangle = \omega_0^{\mathbb{Z}^d}(A_\Lambda(\mathbf{z})^* \delta(A_\Lambda(\mathbf{z}))) = \omega_0^{\mathbb{Z}^d}(A_\Lambda(\mathbf{z})^* [H_{\Lambda(1)}, A_\Lambda(\mathbf{z})]) = \langle \varphi_\Lambda(\mathbf{z}), H_{\Lambda(1)} \varphi_\Lambda(\mathbf{z}) \rangle$$

where we denoted $\Lambda^{(1)} := \{x \in \mathbb{Z}^d : d(x, \Lambda) \leq 1\}$ and used that $H_{\Lambda(1)}\psi_0^{\Lambda(1)} = 0$.

For any $\mathbf{x} \in \Lambda$ and $1 \leq k \leq d$ such that $\mathbf{x}, \mathbf{x} + e_k \in \Lambda$ (i.e. the bulk terms) we compute

$$h_{\mathbf{x}, \mathbf{x} + e_k}^{(k)} \varphi_\Lambda(\mathbf{z}) = \frac{\mathbf{z}^{\mathbf{x}}(z_k - \lambda_k)}{1 + \lambda_k^2} \left(\xi_{\{\mathbf{x} + e_k\}}^\Lambda - \lambda_k \xi_{\{\mathbf{x}\}}^\Lambda \right)$$

so that

$$\langle \varphi_\Lambda(\mathbf{z}), H_\Lambda \varphi_\Lambda(\mathbf{z}) \rangle = \sum_{\mathbf{x} \in \Lambda} |\mathbf{z}|^{2\mathbf{x}} \sum_{k=1}^d \frac{(z_k - \lambda_k)(\bar{z}_k - \lambda_k)}{1 + \lambda_k^2}.$$

For the boundary terms, we have for any $1 \leq k \leq d$,

$$\langle \varphi_\Lambda(\mathbf{z}), h_{\mathbf{x}, \mathbf{x} + e_k}^{(k)} \varphi_\Lambda(\mathbf{z}) \rangle = \begin{cases} \frac{\lambda_k^2}{1 + \lambda_k^2} |\mathbf{z}|^{2\mathbf{x}} & \text{if } \mathbf{x} \in \Lambda, \mathbf{x} + e_k \notin \Lambda \\ \frac{|z_k|^2}{1 + \lambda_k^2} |\mathbf{z}|^{2\mathbf{x}} & \text{if } \mathbf{x} \notin \Lambda, \mathbf{x} + e_k \in \Lambda \end{cases}$$

We now choose for convenience the finite set to be

$$\Lambda = \bar{\Gamma}_\mathbf{N} = \prod_{k=1}^d [-N_k, N_k] \subset \mathbb{Z}^d.$$

with $|\bar{\Gamma}_\mathbf{N}| = \prod_{k=1}^d (2N_k + 1)$. The sum of all boundary terms reads

$$\sum_{k=1}^d \frac{1}{1 + \lambda_k^2} \left(\lambda_k^2 |z_k|^{2N_k} + |z_k|^{-2(N_k-1)} \right) \prod_{i \neq k} \sum_{\alpha = -N_i}^{N_i} |z_i|^{2\alpha}.$$

Let us consider the special case $z_k = 1$ for all k . Then $\|\tilde{\varphi}_\Lambda(\mathbf{z})\|^2 = |\bar{\Gamma}_\mathbf{N}|$ and the boundary contributions read

$$|\bar{\Gamma}_\mathbf{N}| \sum_{k=1}^d \frac{1}{2N_k + 1}.$$

Both of these expressions are independent of λ . Furthermore, the bulk terms are bounded by

$$|\bar{\Gamma}_\mathbf{N}| \sum_{k:\lambda_k \neq 1} \frac{(1 - \lambda_k)^2}{1 + \lambda_k^2},$$

so that

$$\frac{\langle \tilde{\varphi}_{\bar{\Gamma}_\mathbf{N}}(1), H_0^{\mathbb{Z}^d} \tilde{\varphi}_{\bar{\Gamma}_\mathbf{N}}(1) \rangle}{\|\tilde{\varphi}_{\bar{\Gamma}_\mathbf{N}}(1)\|^2} \leq \sum_{k:\lambda_k \neq 1} \frac{(1 - \lambda_k)^2}{1 + \lambda_k^2} + \sum_{k=1}^d \frac{1}{2N_k + 1}.$$

which yields the estimate

$$\gamma(\mathbb{Z}^d) \leq \liminf_{\mathbf{N} \rightarrow \infty} \frac{\langle \tilde{\varphi}_{\bar{\Gamma}_\mathbf{N}}(1), H_0^{\mathbb{Z}^d} \tilde{\varphi}_{\bar{\Gamma}_\mathbf{N}}(1) \rangle}{\|\tilde{\varphi}_{\bar{\Gamma}_\mathbf{N}}(1)\|^2} \leq \sum_{k:\lambda_k \neq 1} \frac{(1 - \lambda_k)^2}{1 + \lambda_k^2}$$

In particular, the model is gapless if $\lambda_k = 1$ for all $1 \leq k \leq d$.

5.2. Low-lying Edge States. In this section we explore how the thermodynamic behavior depends on the boundary of the infinite lattice. We previously showed that the existence of a unique GNS ground state vector is closely tied with the geometry, and more specifically the boundary, of the infinite volume one considers. It is then natural to ask whether the geometry will effect other properties in the thermodynamic limit.

As an example, we discuss the case of the diagonal-edged infinite volume $D_\infty \subset \mathbb{Z}^2$ defined by $(x, y) \in D_\infty$ if and only if $y \geq -x$ and prove that, unlike an infinite lattice obtained as the limit of finite rectangles, the PVBS model with one species of particle is in fact gapless when $\lambda_1 = \lambda = \lambda_2$ with $\lambda < 1$. The closure of the gap in this case is due to the existence of boundary states in which a single particle is delocalized across the boundary.

Proof of Proposition 2.4. We construct a sequence of variational vectors in the GNS Hilbert space for which the energy decays polynomially. The vectors we choose belong to the one particle sector with the particles bound to the finite volume D_L defined by:

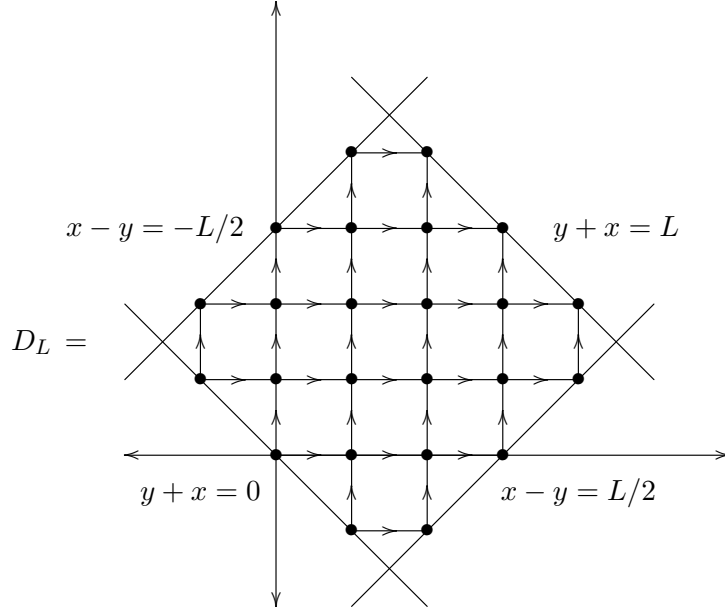
$$(5.1) \quad D_L = \{(x, y) : 0 \leq x + y \leq L, |x - y| \leq L/2\}.$$

For convenience, we choose $L = 2k$ where k is an odd integer. An example of the sector D_L to which to particles are bound is given in Figure 1. We partition D_L into the following subsets:

$$\begin{aligned} D_L^{\text{int}} &= \{(x, y) : 0 < x + y < L, |x - y| < L/2\} \\ D_L^{\text{edge}} &= \{(x, y) : x + y = 0\} \\ D_L^{\text{opp}} &= \{(x, y) : x + y = L\} \\ D_L^{\text{uside}} &= \{(x, y) : x - y = -L/2\} \\ D_L^{\text{lside}} &= \{(x, y) : x - y = L/2\} \end{aligned}$$

We consider the GNS Hamiltonian $H_0^{D_\infty}$ associated with the infinite volume ground state given in (2.15), where $\Omega_0^{D_\infty} = \bigotimes_{(x,y) \in D_\infty} |0\rangle$. The variational vectors $\tilde{\varphi}_L \in \mathcal{H}_0^{D_\infty}$ are defined by

$$(5.2) \quad \tilde{\varphi}_L = \pi_0^{D_\infty}(A_L)\Omega_0^{D_\infty}$$

FIGURE 1. The sector D_L for $L = 6$.

where $A_L \in \mathcal{A}_{D_L}$ is the local observable

$$A_L = \sum_{\mathbf{x}=(x,y) \in D_L} \lambda^{x+y} \sin(k(x-y)) \sigma_{\mathbf{x}}^1$$

with $k = \frac{2\pi}{L}$. Again, $\|\tilde{\varphi}_L\| = \|A_L \psi_0^{D_L^\partial}\|$ and

$$\langle \tilde{\varphi}_L, H_0^{D_\infty} \tilde{\varphi}_L \rangle = \langle A_L \psi_0^{D_L^\partial}, H_{D_L^\partial} A_L \psi_0^{D_L^\partial} \rangle$$

where

$$D_L^\partial = \{(x, y) : 0 \leq x + y \leq L + 1, |x - y| \leq L/2 + 1\}.$$

and we used that $H_{D_L^\partial} \psi_0^{D_L^\partial} = 0$. Notice that $(x, y) \in D_L^{\text{edge}}$ if and only if $(x + \frac{L}{2}, y + \frac{L}{2}) \in D_L^{\text{opp}}$, and so

$$(5.3) \quad \sum_{(x,y) \in D_L^{\text{opp}}} \sin^2 k(x-y) = \sum_{(x,y) \in D_L^{\text{edge}}} \sin^2 k(x-y).$$

Using (5.3) and our choice of k ,

$$(5.4) \quad \langle A_L \psi_0^{D_L^\partial}, H_{D_L^\partial} A_L \psi_0^{D_L^\partial} \rangle = 2(1 - \cos(k)) \left[\sum_{(x,y) \in D_L^{\text{int}}} \lambda^{2(x+y)} \sin^2 k(x-y) + \frac{\lambda^2 + \lambda^{2L}}{1 + \lambda^2} \sum_{(x,y) \in D_L^{\text{opp}}} \sin^2 k(x-y) \right] \\ + \frac{2\lambda^{2L+2}}{1 + \lambda^2} \sum_{(x,y) \in D_L^{\text{opp}}} \sin^2 k(x-y)$$

and

$$\|A_L \psi_0^{D_L^\partial}\|^2 = \sum_{(x,y) \in D_L^{\text{int}}} \lambda^{2(x+y)} \sin^2 k(x-y) + (1 + \lambda^{2L}) \sum_{(x,y) \in D_L^{\text{opp}}} \sin^2 k(x-y).$$

All in all, it follows that the spectral gap is bounded above by

$$\gamma(D_\infty) \leq \frac{\langle \tilde{\varphi}_L, H_0^{D_\infty} \tilde{\varphi}_L \rangle}{\|\tilde{\varphi}_L\|^2} \leq 2(1 - \cos(2\pi/L)) + \frac{2\lambda^{2L+2}}{1 + \lambda^2},$$

where we used that $\sum_{(x,y) \in D_L^{\text{opp}}} \sin^2 k(x-y) \leq \|\tilde{\varphi}_L\|^2$. Since $\lambda < 1$, the second term decays exponential in L as $L \rightarrow \infty$, while the first one is of order L^{-2} . \square

Analogously, we expect that this type of gap closure to occur for any d -dimensional infinite volume with slant boundary when the outward pointing normal is given by the vector $\vec{n} = (\log \lambda_1, \dots, \log \lambda_d)$.

6. DISCUSSION

6.1. Stability. *Stability* refers to the continuous behavior of certain spectral properties of quantum spin Hamiltonians under small local perturbations. Although the case of perturbations around classical Hamiltonians was considered in great detail long ago [4, 10, 12, 15, 16, 19], results for perturbations of frustration-free quantum models with interesting ground states have only been achieved rather recently [5, 6, 9, 20, 26, 28]. The most basic stability results establish two properties; for models with a unique ground state in the infinite volume limit and for sufficiently small perturbations, one proves first of all that the spectral gap above the ground state energy does not close, and secondly, that the unique ground state depends continuously on the perturbation. In [20], such stability results are obtained for models with a unique frustration-free ground state under two additional conditions. First, the perturbation is of the form $\sum_{X \subset \Lambda} \Psi(X)$ where, roughly speaking, $\|\Psi(X)\|$ decays faster than any polynomial as a function of the diameter of X . Second, the possibly many finite volume ground states satisfy what is referred to as the *local topological order* condition in [20]. For any hypercube Λ_L of length L , consider sets $X \subset \Lambda_L$ such that $X^{(l)} \subset \Lambda_L$, where $X^{(l)} = \{x \in \Gamma : d(x, X) \leq l\}$. In the case of a multi-dimensional finite volume ground state space, the ground states are called topologically ordered if there exists a positive function f decaying faster than any polynomial such that for any $A \in \mathcal{A}(X)$,

$$(6.1) \quad \|G_{X^{(l)}} A G_{X^{(l)}} - c_l(A) G_{X^{(l)}}\| \leq \|A\| f(l)$$

where

$$c_l(A) = \text{Tr}(G_{X^{(l)}})^{-1} \text{Tr}(G_{X^{(l)}} A).$$

We now prove that the models considered here satisfy (6.1). The spaces $G_{X^{(l)}}$ are two-dimensional and spanned by $\psi_0^{X^{(l)}}$ and $\psi_1^{X^{(l)}}$. We shall use the bound

$$\|G_{X^{(l)}} A G_{X^{(l)}} - c_l(A) G_{X^{(l)}}\| \leq 2 \sup_{i,j \in \{0,1\}} \left| \langle \psi_i^{X^{(l)}}, A \psi_j^{X^{(l)}} \rangle - c_l(A) \delta_{ij} \right|.$$

Since A is supported in X , we have that

$$\langle \psi_1^{X^{(l)}}, A \psi_1^{X^{(l)}} \rangle = \frac{C(X)}{C(X^{(l)})} \langle \psi_1^X, A \psi_1^X \rangle + \frac{C(X^{(l)} \setminus X)}{C(X^{(l)})} \langle \psi_0^{X^{(l)} \setminus X}, A \psi_0^{X^{(l)} \setminus X} \rangle,$$

and the last scalar product can be replaced by $\langle \psi_0^X, A \psi_0^X \rangle$. With this, both cases $i = j = 0$ and $i = j = 1$ are bounded above by

$$\frac{1}{2} \left| \langle \psi_1^{X^{(l)}}, A \psi_1^{X^{(l)}} \rangle - \langle \psi_0^{X^{(l)}}, A \psi_0^{X^{(l)}} \rangle \right| \leq \frac{\|A\|}{2} \left[\left| \frac{C(X)}{C(X^{(l)})} \right| + \left| 1 - \frac{C(X^{(l)} \setminus X)}{C(X^{(l)})} \right| \right] = \|A\| \left| \frac{C(X)}{C(X^{(l)})} \right|$$

where we used that $C(X^{(l)}) - C(X^{(l)} \setminus X) = C(X)$ by the definition (2.9) of $C(\cdot)$. The off-diagonal case can be computed similarly,

$$\left| \langle \psi_0^{X^{(l)}}, A \psi_1^{X^{(l)}} \rangle \right| = \left| \left(\frac{C(X)}{C(X^{(l)})} \right)^{1/2} \langle \psi_0^X, A \psi_1^X \rangle \right| \leq \|A\| \left| \frac{C(X)}{C(X^{(l)})} \right|^{1/2}.$$

Hence, (6.1) holds with $f(l) = 2\sqrt{C(X)/C(X^{(l)})}$, which decays exponentially in l .

The models considered here have open boundary conditions, while the theorem of [20] assumes periodic boundary conditions. We believe, however, that stability holds in the present more general setting, given the frustration-free and topological quantum order conditions. This means that there is an open neighborhood of local interactions around the models presented in this work which have a spectral gap above the ground state energy, on \mathbb{Z}^d .

6.2. Edge versus Bulk Gapless Excitations. To conclude, we would like to underline the physical difference between the gapless spectrum that arises in the case of $\lambda_k = 1$ for all k , and the gapless spectrum we found in Section 5 for a class of models on the slanted half-infinite plane D_∞ . As explained above, the limit $\lambda \rightarrow 1$ corresponds to a quantum phase transition in the sense that the bulk dispersion relation becomes gapless. In the case of the slanted edge the low-lying excited states are localized along the edge and nothing special happens in the bulk. In particular, excited states localized away from the edge show a gapped energy spectrum, and the dynamics of observables whose support is at a distance d from the edge is unaffected by the gapless excitations up to times t that are of the same order of magnitude as d/v , where the constant v is the Lieb-Robinson velocity of the model.

To make these statements more precise, consider the PVBS model on $D_\infty \subset \mathbb{Z}^2$, the half-space with a 45 degree edges as discussed in Section 5, and let $\omega_0^{D_\infty}$ be the unique vacuum state of this system with $(\pi_0^{D_\infty}, \mathcal{H}_0^{D_\infty}, \Omega_0^{D_\infty})$ its GNS representation. Let $D_\infty^{\text{edge}} \subset D_\infty$ denote the sites at the 45 degree boundary of D_∞ .

Let

$$\mathcal{H}_0^{\text{bulk}} := \text{span}\{\pi(A)\Omega_0^{D_\infty} : d(\text{supp}(A), D_\infty^{\text{edge}}) \geq 1\} \subset \mathcal{H}_0^{D_\infty},$$

and P_0^{bulk} the orthogonal projection onto $\mathcal{H}_0^{\text{bulk}}$. Finally, let $H_0^{D_\infty}$ be the GNS Hamiltonian associated with $\omega_0^{D_\infty}$. Although the GNS Hamiltonian $H_0^{D_\infty}$ for the model on D_∞ does not have a gap above the ground state, the self-adjoint operator $P_0 H_0^{D_\infty} P_0$ regarded as an operator on $\mathcal{H}_0^{D_\infty}$ does have a spectral gap above its ground state at least as large as the gap of the model defined on \mathbb{Z}^2 .

Proposition 6.1. *With the notations above, let*

$$H_0^{\text{bulk}} := P_0^{\text{bulk}} H_0^{D_\infty} P_0^{\text{bulk}} : \mathcal{H}_0^{\text{bulk}} \rightarrow \mathcal{H}_0^{\text{bulk}}.$$

Then, $\inf \text{Spec}(H_0^{\text{bulk}}) = 0$ is an eigenvalue and if $\lambda \neq 1$, there is a spectral gap $\gamma \geq \gamma(\mathbb{Z}^2)$.

Proof. First, we observe that $P_0^{\text{bulk}} \Omega_0^{D_\infty} = \Omega_0^{D_\infty}$ so that

$$H_0^{\text{bulk}} \Omega_0^{D_\infty} = P_0^{\text{bulk}} H_0^{D_\infty} \Omega_0^{D_\infty} = 0$$

which shows that $\Omega_0^{D_\infty}$ belongs to the kernel of the positive operator H_0^{bulk} .

We consider $A \in \mathcal{A}_X$, with $d(X, D_\infty^{\text{edge}}) \geq 1$, and observe that the generator of the dynamics on D_∞ , namely δ_{D_∞} , satisfies

$$(6.2) \quad \delta_{D_\infty}(A) = \lim_{\Lambda \uparrow D_\infty} [H_\Lambda, A] = \lim_{\Lambda \uparrow \mathbb{Z}^2} [H_\Lambda, A] = \delta_{\mathbb{Z}^2}(A).$$

Hence,

$$\begin{aligned} \langle \pi_0^{D_\infty}(A)\Omega_0^{D_\infty}, H_0^{\text{bulk}} \pi_0^{D_\infty}(A)\Omega_0^{D_\infty} \rangle &= \langle \pi_0^{D_\infty}(A)\Omega_0^{D_\infty}, H_0^{D_\infty} \pi_0^{D_\infty}(A)\Omega_0^{D_\infty} \rangle = \omega_0^{D_\infty}(A^* \delta_{D_\infty}(A)) \\ &= \omega_0^{\mathbb{Z}^2}(A^* \delta_{\mathbb{Z}^2}(A)), \end{aligned}$$

where in the last equality we first use (6.2) and then the fact that both ground states are the same product state on local observables. Now let A be such that $\pi_0^{D_\infty}(A)\Omega_0^{D_\infty} \perp \Omega_0^{D_\infty}$, or equivalently $0 = \omega_0^{D_\infty}(A) = \omega_0^{\mathbb{Z}^2}(A)$. Since the model on \mathbb{Z}^2 has a gap $\gamma(\mathbb{Z}^2) > 0$, this implies

$$(6.3) \quad \langle \pi_0^{D_\infty}(A)\Omega_0^{D_\infty}, H_0^{\text{bulk}} \pi_0^{D_\infty}(A)\Omega_0^{D_\infty} \rangle \geq \gamma(\mathbb{Z}^2) \omega_0^{D_\infty}(A^* A) = \gamma(\mathbb{Z}^2) \|\pi_0^{D_\infty}(A)\Omega_0^{D_\infty}\|^2.$$

The inequality (6.3) shows that H_0^{bulk} has a spectral gap above 0 at least equal to $\gamma(\mathbb{Z}^2)$, which we have shown to be strictly positive. \square

Finally, we show that the dynamics of observables supported away from the edge is unaffected by the gapless edge modes. In particular, multi-time correlation functions for such observables behave as if the system was gapped for times that are not too large. To this end, recall that a nearest-neighbor interaction defined on a regular lattice – such as the present PVBS models – satisfies a Lieb-Robinson bound, with velocity v . In particular, the difference of the dynamics generated by two finite-volume Hamiltonians H_{Λ_1} and H_{Λ_2} , where $\Lambda_2 \subset \Lambda_1$, can be estimated by

$$\left\| \tau_t^{\Lambda_1}(A) - \tau_t^{\Lambda_2}(A) \right\| \leq C \|A\| |X| e^{-a[d(X, \Lambda_1 \setminus \Lambda_2) - v|t|]},$$

where $A \in \mathcal{A}_X$, $X \subset \Lambda_2$, and with suitable constants $a, C > 0$ (see [22, equation (2.28)]). Let $\Lambda_{1,n} \rightarrow \mathbb{Z}^2$ and $\Lambda_{2,n} \rightarrow D_\infty$ be increasing sequences such that $\Lambda_{2,n} \subset \Lambda_{1,n}$ for all $n \in \mathbb{N}$. For n large enough, $d(X, \Lambda_{1,n} \setminus \Lambda_{2,n}) = d(X, D_\infty^{\text{edge}})$, and in particular

$$\left\| \tau_t^{D_\infty}(A) - \tau_t^{\mathbb{Z}^2}(A) \right\| \leq C \|A\| |X| e^{-a[d(X, D_\infty^{\text{edge}}) - v|t|]}.$$

Hence, for times $t \ll d(X, D_\infty^{\text{edge}})/v$, the half-plane dynamics of A are well-approximated by the dynamics in the bulk generated by the gapped Hamiltonian.

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