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A Two-Dimensional Isotropic Quantum Antiferromagnet with Unique Disordered Ground State

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We continue the study of valence-bond solid antiferromagnetic quantum Hamiltonians. These Hamiltonians are invariant under rotations in spin space. We prove that a particular two-dimensional model from this class (the spin-3/2 model on the hexagonal lattice) has a unique ground state in the infinite-volume limit and hence no Néel order. Moreover, all truncated correlation functions decay exponentially in this ground state. We also characterize all the finite-volume ground states of these models (in every dimension), and prove that the two-point correlation function of the spin-2 square lattice model with periodic boundary conditions has exponential decay.

KEY WORDS: Quantum antiferromagnet; Néel order.

1. INTRODUCTION

The properties of the ground states of quantum antiferromagnets are usually difficult to determine. Even in those rare cases in which the ground states can be explicitly found, the properties of the explicit solution can require further efforts. The usual Heisenberg antiferromagnet in three dimensions was shown by Dyson *et al.*[6] to have Néel order in the ground state and at low temperature when the spin is at least 1. Fernando Perez and Jordão Neves[8] extended this result to the two-dimensional model in the ground state for spin 3/2 or more. This latter result actually holds for spin 1 or more, as was pointed out in ref. 2. The possibility of an isotropic [i.e., $SU(2)$ invariant], two-dimensional quantum antiferromagnet which does not Néel order in the ground state is of great interest. In the present paper we provide a rigorous example of such a model.

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The results of this paper were conjectured in ref. 2. The Hamiltonian for the valence-bond solid (VBS) models studied here and in ref. 2 is

$$H = \sum_{(i,j)} P^{2S}_{(i,j)}$$

where the sum is over all nearest neighbor bonds in the lattice, and $P^{2S}_{(i,j)}$ is the projection onto the states whose restriction to sites i and j has total spin $2S$. The spin S at each site is taken to be half of the coordination number of the lattice. The operator $P^{2S}_{(i,j)}$, like the usual Heisenberg $\boldsymbol{S}_i \cdot \boldsymbol{S}_j$ operator, is antiferromagnetic and isotropic. In fact, $P^{2S}_{(i,j)}$ can be written as a polynomial in $\boldsymbol{S}_i \cdot \boldsymbol{S}_j$. Ground states for these models—the VBS states—were explicitly described in refs. 1 and 2. The VBS states were first constructed by Affleck.[1] One of the new results of the present paper is a proof that they are the *only* ground states. Even though we know the ground states of these models explicitly, the properties of these ground states have only been determined for a few of the models.

The simplest of the VBS models in ref. 2 is a one-dimensional spin-1 model with the above Hamiltonian. For this model we were able to show that there is a unique infinite-volume ground state, that the truncated correlation functions all decay exponentially in this ground state, and that there is a gap between the ground-state energy and the rest of the spectrum. This is the only example known so far for which Haldane's conjecture about spin chains has been rigorously proven (see ref. 15 for a discussion and partial resolution of this conjecture).

For the spin-3/2 VBS model on the hexagonal lattice it was shown in ref. 2 that the two-point function decays exponentially, but only for the case of periodic boundary conditions. In the present paper we prove that in the infinite-volume limit this model has a unique ground state and the truncated correlation functions all have exponential decay. Of course, the uniqueness of the infinite-volume ground state implies the absence of Néel order.

We also prove in the present paper that the two-point function for the spin-2 model on the square lattice has exponential decay when periodic boundary conditions are used. The exponential decay of the two-point function for other choices of the boundary conditions and the uniqueness of the infinite-volume ground state for this square lattice model are open questions.

The results of the present paper were all made possible by the representation for the VBS ground states found by Arovas *et al.*[3] Their representation and the unique factorization theorem for polynomials are used in Section 2 to characterize explicitly all the ground states of a general

class of VBS models in a finite volume. Their representation also leads to a simple random walk representation for the correlation functions. For the case of periodic boundary conditions all the terms in this random walk representation are nonnegative. This fact is exploited in Section 3 to prove exponential decay of the two-point function for the hexagonal and square lattice VBS models. For boundary conditions other than the periodic one the terms in the random walk representation have mixed signs. We handle this situation in Section 4 by using the machinery of polymer expansions. For the hexagonal lattice model we can prove this expansion converges and from this deduce the uniqueness of the infinite-volume ground state. Proving that the expansion converges requires numerous tedious estimates concerning the number of polymers of various types. This counting, which is done with the help of a computer, is explained in the appendix.

Before closing this section, we recall two conjectures about the VBS models which were made in ref. 2 and are still unproven.

1. There is an energy gap above the ground state for the two-dimensional hexagonal and square lattice models considered here. This conjecture is based on the fact that correlations decay exponentially. In ref. 2 the existence of the energy gap was proved for the one-dimensional spin-1 model. An elegant argument of Knabe[10] reduces the problem of proving the gap to a calculation involving only finite systems. For the one-dimensional chain Knabe has suceeded in carrying out the required calculation with the help of a computer, but for the higher dimensional models the required calculation is beyond the capacity of the computer.

2. For sufficiently high dimensions, the VBS model on a hypercubic lattice has Néel order in the ground state. Some support for this conjecture is the fact that the Cayley tree model with large coordination number has Néel order, but it does not when the coordination number is small.[2]

2. EXPLICIT CHARACTERIZATION OF FINITE-VOLUME GROUND STATES

The VBS states are described here and shown to be the only ground states of the VBS Hamiltonian.

A *lattice* consists of a finite set of sites and a finite set of bonds. The former is denoted by Λ and the latter by $\mathbf{B}$. The symbol $|\Lambda|$ denotes the number of sites in Λ. We assume that the number of sites connected to a given site (i.e., the coordination number) is at most z and at least one. The *boundary* $\partial\Lambda$ is the set of sites which have coordination number strictly smaller than z.

We define a quantum spin system on the lattice by associating an $S = z/2$ quantum spin with each site. As in ref. 2, we consider the following isotropic antiferromagnetic Hamiltonian:

$$H = \sum_{(i,j) \in \mathbf{B}} P^{2S}_{(i,j)} \tag{2.1}$$

Here $P^{2S}_{(i,j)}$ is the orthogonal projection onto the states whose restriction to sites i and j has total spin $2S = z$ (i.e., the maximum possible value).

A beautiful representation of the VBS states was given by Arovas *et al.*[3] We review their representation by first reviewing the Weyl[14] representation of the Lie algebra of $SU(2)$. Consider the space of polynomials in the two variables u and v with coefficients in $\mathbf{C}$ such that for each monomial in the polynomial the power of u plus the power of v equals $2S$. These polynomials form a vector space over $\mathbf{C}$. The action of the spin operators on this $(2S+1)$-dimensional vector space is given by the linear operators

$$\begin{aligned} S^+ &\leftrightarrow u\, \partial/\partial v \\ S^- &\leftrightarrow v\, \partial/\partial u \\ S^z &\leftrightarrow \tfrac{1}{2}(u\, \partial/\partial u - v\, \partial/\partial v) \end{aligned} \tag{2.2}$$

The eigenstates of S^z are the polynomials $u^j v^{2S-j}$, $j = 0, 1, \ldots, 2S$. We define an inner product on this space of polynomials by requiring that the vectors $u^j v^{2S-j}[\binom{2S}{j}(2S+1)]^{1/2}$ be an orthonormal basis. It is a straightforward computation to check that (2.2) and this inner product yield the $(2S+1)$-dimensional irreducible unitary representation of $SU(2)$.

We can explicitly realize this inner product as follows. Let

$$u = e^{i\phi/2} \cos(\theta/2), \qquad v = e^{-i\phi/2} \sin(\theta/2) \tag{2.3}$$

where θ and ϕ are the usual angles for the sphere, so $0 \leqslant \theta < \pi$, $0 \leqslant \phi < 2\pi$. The inner product of two polynomials Ψ and Φ is then given by

$$(\Psi, \Phi) = \int d\Omega\, \overline{\Psi(u, v)}\, \Phi(u, v) \tag{2.4}$$

where $d\Omega = (4\pi)^{-1} \sin\theta\, d\theta\, d\phi$ is the usual normalized, invariant measure on the sphere. It is a straightforward calculation to check that this formula does indeed yield the desired inner product.

An important rule for computing expectation values was derived in ref. 3. Consider one spin (with S fixed), let Ψ and Φ be two vectors (i.e., polynomials in u, v), and let A be any operator that conserves S (i.e., the

degree of Ψ and Φ, which is $2S$). This means that A can be written as the differential operator

$$A = \sum_{k,l,j} a_{klj} (\partial/\partial u)^k (\partial/\partial v)^l u^{k+j} v^{l-j} \tag{2.5}$$

The assertion is that there are constants

$$C_{kl} = (2S+2)(2S+3)\cdots(2S+k+l+1), \qquad \text{with} \quad C_{00} = 1 \tag{2.6}$$

which are independent of Ψ *and* Φ, such that

$$(\Psi, A\Phi) = \sum_{k,l,j} C_{kl} a_{klj} (u^k v^l \Psi, u^{k+j} v^{l-j} \Phi) \tag{2.7}$$

[Note that $u^k v^l \Psi$ and $u^{k+j} v^{l-j} \Phi$ have degree $2S+k+l$, but the inner products in (2.7) are still well defined by formula (2.4).] This formula (2.7) can be checked by expanding Ψ and Φ in a monomial basis.

The significance of (2.7) is this. Corresponding to every A there is a polynomial P in $u, v, \bar{u}, \bar{v}$ [and hence a function $A(\mathbf{\Omega})$ of θ, ϕ by (2.3)] such that

$$(\Psi, A\Phi) = \int d\mathbf{\Omega}\, \overline{\Psi(u, v)}\, \Phi(u, v)\, A(\mathbf{\Omega}) \tag{2.8}$$

holds, regardless of Ψ and Φ. This formula (2.8) will be important for us in computing expectation values. The formula obviously extends to operators acting on the tensor product of several spin spaces.

To describe states on the lattice Λ, we associate variables u_i, v_i with each site i in Λ. We let $\mathscr{H}_i$ denote the polynomials in u_i and v_i such that for each monomial in the polynomial the power of u_i plus the power of v_i equals $2S$. The *state space* $\mathscr{H}$ for Λ is given by $\bigotimes_i \mathscr{H}_i$, i.e., it consists of all polynomials which are jointly homogeneous of degree $2S$ in each pair u_i, v_i for each $i \in \Lambda$.

The main result of this section is the following theorem, which explicitly characterizes the ground states of H in (2.1). Since H is clearly positive semidefinite, this theorem also proves that the ground-state energy of H is zero.

Theorem 2.1 (Characterization of Ground States). Let $\Psi \in \mathscr{H}$ be such that $H\Psi = 0$. Then there exists a unique polynomial Φ in the variables u_i and v_i with $i \in \partial\Lambda$ such that

$$\Psi = \Phi \prod_{(i,j) \in \mathbf{B}} (u_i v_j - u_j v_i) \tag{2.9}$$

Conversely, any state Ψ of the form (2.9) satisfies $H\Psi = 0$.

Remarks. 1. We refer to states of the form (2.9) as VBS states, since these states contain a valence bond (i.e., a singlet pair) for each bond in the lattice. The polynomial representation (2.9) of the VBS states was introduced by Arovas *et al.*[3] The new features of our Theorem 2.1 are the assertions that all the ground states of H are given in (2.9) and that Φ is unique.

2. There is another way to think of these VBS states. Following refs. 1 and 2, we think of each spin S as the symmetrization of the product of $2S$ spin-1/2's. We first consider an extended (or unphysical) Hilbert space which has $2S$ spin-1/2's at each site of Λ. The projection operator $\mathscr{P} = \otimes_i \mathscr{P}_i$, where $\mathscr{P}_i$ is the symmetrization operator for the $2S$ spin-1/2's of the site i, projects this unphysical Hilbert space onto the physical Hilbert space for spin S at each site. The VBS states can now be written as follows:

$$\Psi = \mathscr{P}\left\{\left(\bigotimes_{(i,j)\in \mathbf{B}} V_{ij}\right) \otimes \Psi_{\partial\Lambda}\right\} \tag{2.10}$$

Here the valence bond V_{ij} denotes the singlet state which can be formed using a spin 1/2 at site i and a spin 1/2 at site j. The representation (2.10) follows in a straightforward, but tedious way from Theorem 2.1. Since we shall have no need of (2.10) here, we shall not bother to prove the equivalence. Note that, unlike the situation for Φ in Theorem 2.1, the state $\Psi_{\partial\Lambda}$ in (2.10) is not unique in general. Following ref. 2, we can represent these VBS states diagrammatically as shown in Fig. 1.

3. Theorem 2.1 was conjectured in ref. 2 and proven for the one-dimensional spin-1 case. The proof we give here not only covers the general case, but is also considerably simpler than the proof in ref. 2. Our proof,

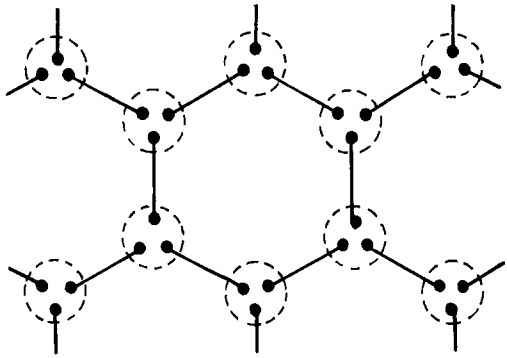

Fig. 1. The VBS state on the hexagonal lattice. Each dot represents a spin 1/2. The solid lines indicate singlet pairs, and the dotted circles indicate the symmetrization of three spin 1/2's to form a spin 3/2.

however, does not apply to the Majumdar–Ghosh model[11,12] and its generalizations.[2,10] Chayes *et al.*[5] have recently proved the corresponding theorem for some of these models.

4. The reader should note that Theorem 2.1 does not require Λ to be bipartite. There can be "frustration." For example, if there are three spins with $S=1$ arranged in a triangle, the ground state is unique and has zero energy.

We now turn to the proof of Theorem 2.1. For a bond (i, j) we define two subspaces of $\mathscr{H}_i \otimes \mathscr{H}_j$ as follows [in the following we use the abbreviations $(u, v)=(u_i, v_i)$ and $(u', v')=(u_j, v_j)$]:

$$\mathscr{S}_1 = \{(uv' - vu')\, \Phi(u, v, u', v')\}$$

$$\mathscr{S}_2 = \{\Psi(u, v, u', v') | P^{2S}_{(i,j)} \Psi = 0\}$$

Here Φ is an arbitrary polynomial such that the product $(uv'-vu')\Phi$ is in $\mathscr{H}_i \otimes \mathscr{H}_j$. This means that Φ has degree $2S-1$ in (u, v) and $2S-1$ in (u', v'). The $P^{2S}_{(i,j)}$ is the orthogonal projection onto the subspace where the total spin of the two sites is $2S$, and $\mathscr{S}_2$ is just the ground states of the one-bond Hamiltonian. Then we have the following elementary lemma.

Lemma 2.2. $\mathscr{S}_1 = \mathscr{S}_2$.

Proof. We first prove the inclusion $\mathscr{S}_1 \subset \mathscr{S}_2$, i.e., if $\Psi \in \mathscr{S}_1$, then $P^{2S}_{(i,j)} \Psi = 0$. Let $T^\alpha = S^\alpha_i + S^\alpha_j$ $(\alpha = x, y, z)$ be the total spin operators. Each S^α_i is given by (2.2) as a differential operator. We easily find that $T^\alpha(uv' - vu') = 0$ for all α and, since T^α is a derivation and $\Psi = (uv' - vu')\Phi$, we have that $T^\alpha \Psi = (uv' - vu')\, T^\alpha \Phi$. Repeating this and adding, we have $T^2 \Psi = (uv' - vu')\, T^2 \Phi$. Now Φ is a polynomial and can be written as a sum $\sum \Phi_j$, where $T^2 \Phi_j = j(j+1)\Phi_j$. Then $T^2(uv' - vu')\Phi_j = j(j+1)(uv' - vu')\Phi_j$ and hence $(uv' - vu')\Phi_j$ is an eigenstate of T^2. But $\Phi_{2S} = 0$ since Φ has degree $2S-1$ in i and in j. Therefore $T^2 \Psi$ has no component in the $T^2 = 2S(2S+1)$ subspace, which means that $\Psi \in \mathscr{S}_2$.

To prove the identity $\mathscr{S}_1 = \mathscr{S}_2$, we simply calculate the dimensions of the spaces. Clearly we have $\dim \mathscr{S}_2 = (2S+1)^2 - (4S+1) = (2S)^2$. Note that in the definition of $\mathscr{S}_1$ we can take $(2S)^2$ linearly independent Φ, namely $u^{2S-l-1} v^l (u')^{2S-m-1} (v')^m$ with $0 \leqslant l,\ m \leqslant 2S-1$. After multiplication by $(uv' - vu')$, this gives us $(2S)^2$ linearly independent vectors in $\mathscr{S}_1$. This is so because if $(uv' - vu')P$ is identically zero, then P is identically zero. Thus we have $\dim \mathscr{S}_1 = (2S)^2 = \dim \mathscr{S}_2$, which proves the lemma. ∎

Lemma 2.3. If $\Psi \in \mathscr{H} = \bigotimes_k \mathscr{H}_k$ satisfies $P^{2S}_{(i,j)} \Psi = 0$ for some particular (i, j), then it factorizes as $\Psi = (u_i v_j - v_i u_j)\Phi$. Conversely, if Ψ can be written as $\Psi = (u_i v_j - v_i u_j)\Phi$, then it satisfies $P^{2S}_{(i,j)} \Psi = 0$.

Proof. The space of all Ψ satisfying $P^{2S}_{(i,j)}\Psi = 0$ is $\mathscr{S}_2 \otimes (\bigotimes_{k\neq i,j} \mathscr{H}_k)$ and that of all Ψ which can be written as $\Psi = (u_i v_j - v_i u_j)\Phi$ is $\mathscr{S}_1 \otimes (\bigotimes_{k\neq i,j} \mathscr{H}_k)$. Thus, the lemma follows from the identity $\mathscr{S}_1 = \mathscr{S}_2$. ∎

Proof of Theorem 2.1. Let $\Psi \in \mathscr{H}$ be a state which satisfies $H\Psi = 0$. Then, from (the first part of) Lemma 2.3 we see that Ψ contains the factor $(u_i v_j - v_i u_j)$ for each bond (i, j). The polynomial ring over $\mathbf{C}$ in the variables u_i, v_i for $i \in \Lambda$ is a unique factorization domain (ref. 7, Section 3.2). This means that if Ψ contains the irreducible polynomials A and B as factors (i.e., $\Psi = A\alpha$ and $\Psi = B\beta$), then Ψ contains AB as a factor, i.e., $\Psi = AB\gamma$ for some *unique* γ. Applying this remark to the irreducible polynomials $u_i v_j - v_i u_j$ for each bond, we have that Ψ has the form of (2.9) and that Φ is unique. The second part of the theorem follows immediately from the second part of Lemma 2.3. ∎

3. ABSENCE OF NÉEL ORDER IN THE HEXAGONAL AND SQUARE LATTICE VBS MODELS

Two basic results for the VBS states on the hexagonal and square lattice will be proved here. The proofs are based on a simple random walk expansion derived from the representation of Arovas *et al.*[3] For the hexagonal lattice, much stronger results will be proved in the next section.

In ref. 2 it was shown for the hexagonal lattice (with periodic boundary conditions) that the two-point function decays exponentially. The first theorem of this section extends this result to the square lattice.

In the following theorem we consider a finite hexagonal or square lattice Λ wrapped on a torus so that there are no boundary spins. We assume that Λ is bipartite, i.e., there is no "frustration." The importance of this condition is explained after Eq. (3.8). In this case the ground state Ψ is unique (Theorem 2.1) and one can define the expectation value of an operator A by

$$\langle A \rangle = (\Psi, A\Psi)/(\Psi, \Psi)$$

Theorem 3.1 (Bounds on the Two-Point Function). Let Λ be a finite, bipartite, two-dimensional hexagonal or square lattice with periodic boundary conditions. The two-point function of the VBS state on Λ satisfies the bounds

$$0 \leqslant (-1)^{|i-j|} \langle \boldsymbol{S}_i \cdot \boldsymbol{S}_j \rangle \leqslant C \exp(-|i-j|/\xi) \tag{3.1}$$

where C and ξ are positive constants which are independent of the lattice size, and $|i-j|$ is the minimum number of bonds needed to connect i and j (i.e., the graph-theoretic distance).

The theorem is also valid for a general bipartite lattice without boundary and with coordination number $z=3$ or 4. The constants C and ξ depend on the lattice structure. For the hexagonal (or any bipartite lattice with $z=3$), we can choose $\xi=2.5$. For the two-dimensional square lattice, we have to choose $\xi=160$, though we suspect that the true correlation length is much smaller in this case.

The existence of exponential decay strongly suggests, but does not prove, the absence of Néel order in the state. This may be tested directly by considering the VBS state with boundary conditions which favor Néel order. Consider the hexagonal or square lattice Λ with boundary $\partial\Lambda$. Since Λ is bipartite, we can decompose Λ into a disjoint union $\Lambda=\Lambda_+\cup\Lambda_-$ with the property that for any $(i,j)\in\mathbf{B}$ either $i\in\Lambda_+$, $j\in\Lambda_-$ or $j\in\Lambda_+$, $i\in\Lambda_-$. Then the VBS state with Néel boundary conditions is defined as

$$\Psi_{\text{Néel}}=\prod_{(i,j)\in\mathbf{B}}(u_iv_j-v_iu_j)\prod_{k\in\Lambda_+\cap\partial\Lambda}u_k^{z-z(k)}\prod_{l\in\Lambda_-\cap\partial\Lambda}v_l^{z-z(l)} \tag{3.2}$$

where $z(k)$ $(<z)$ denotes the coordination number of the boundary site k. We define the corresponding expectation value as

$$\langle A\rangle_{\text{Néel}}=(\Psi_{\text{Néel}},A\Psi_{\text{Néel}})/(\Psi_{\text{Néel}},\Psi_{\text{Néel}})$$

Intuitively, one would expect the Néel boundary conditions to favor Néel order more than any other choice of boundary conditions, i.e., choice of Φ in (2.9). The representation of ref. 3 can be used to prove the following theorem, which could not be proved by the methods in ref. 2.

Theorem 3.2 (Bounds on the Néel Order). Let Λ be a finite two-dimensional hexagonal or square lattice with boundary $\partial\Lambda$. The Néel order parameter of the VBS state on Λ with Néel boundary conditions satisfies the bounds

$$0\leqslant(-1)^i\langle S_i^z\rangle_{\text{Néel}}\leqslant C'\,|\partial\Lambda|\exp[-\text{dist}(i,\partial\Lambda)/\xi] \tag{3.3}$$

where C' and ξ are positive constants which are independent of the lattice size. $|\partial\Lambda|$ is the number of sites in the boundary, $\text{dist}(i,\partial\Lambda)$ is the minimum of $|i-j|$ for $j\in\partial\Lambda$, and $(-1)^i=1$ if $i\in\Lambda_+$ and -1 if $i\in\Lambda_-$. Therefore, when the lattice size tends to infinity and $i\in\Lambda$ is fixed, $\langle S_i^z\rangle_{\text{Néel}}$ goes to zero.

Again we can prove Theorem 3.2 for a more general class of lattices. Since we expect the Néel order parameter to assume its maximum value for Néel boundary conditions, the above theorem strongly indicates the absence of Néel order for any boundary conditions. However, our simple

proof in this section only works in the "hardest" case of Néel boundary conditions. For the particular case of the hexagonal lattice, however, we will be able to treat *arbitrary* boundary conditions in the next section. *Rigorous treatment of the square lattice with arbitrary boundary conditions is still an open problem.*

We begin the proofs of Theorems 3.1 and 3.2 by developing a random walk expansion for the norm of the VBS state and expectations in that state. From Eqs. (2.4) and (2.9), we get the following formula[3] for the norm of the VBS state Ψ:

$$(\Psi, \Psi) = \int d\mathbf{\Omega} \prod_{(i,j)\in \mathbf{B}} |u_i v_j - v_i u_j|^2 |\Phi|^2 = \int d\mathbf{\Omega} \prod_{(i,j)\in \mathbf{B}} \left[\frac{1-\mathbf{\Omega}_i \cdot \mathbf{\Omega}_j}{2}\right] f(\Omega) \tag{3.4}$$

where $d\mathbf{\Omega} = \prod_{i\in\Lambda} d\mathbf{\Omega}_i$. The second equality follows from the identity

$$|u_i v_j - v_i u_j|^2 = \tfrac{1}{2}(1 - \mathbf{\Omega}_i \cdot \mathbf{\Omega}_j)$$

and $f(\mathbf{\Omega})$ is simply equal to $|\Phi|^2$. We can carry out a similar construction for the quantity $(\Psi, A\Psi)$, where A is an arbitrary operator, to get the following formula:

$$(\Psi, A\Psi) = \int d\mathbf{\Omega}\, A(\mathbf{\Omega}) \prod_{(i,j)\in \mathbf{B}} \left[\frac{1-\mathbf{\Omega}_i \cdot \mathbf{\Omega}_j}{2}\right] f(\mathbf{\Omega}) \tag{3.5}$$

Here $A(\mathbf{\Omega})$ is a function of $\{\mathbf{\Omega}_i : i \in \text{support of } A\}$ given by (2.8). When A is $\boldsymbol{S}_i$ or $\boldsymbol{S}_i \cdot \boldsymbol{S}_j$, $A(\mathbf{\Omega})$ is simply $(S+1)\mathbf{\Omega}_i$ or $(S+1)^2 \mathbf{\Omega}_i \cdot \mathbf{\Omega}_j$.

Combining (3.4) and (3.5), we finally get the Arovas–Auerbach–Haldane representation[3] for expectation values in the VBS states

$$\langle A \rangle = \frac{(\Psi, A\Psi)}{(\Psi, \Psi)} = \frac{\int d\mathbf{\Omega}\, A(\mathbf{\Omega}) \prod_{(i,j)\in \mathbf{B}} (1 - \mathbf{\Omega}_i \cdot \mathbf{\Omega}_j) f(\mathbf{\Omega})}{\int d\mathbf{\Omega} \prod_{(i,j)\in \mathbf{B}} (1 - \mathbf{\Omega}_i \cdot \mathbf{\Omega}_j) f(\mathbf{\Omega})} \tag{3.6}$$

It is worth noting that the right side of (3.6) can be regarded as the expectation value of a *classical* Heisenberg model with the unusual (but non-negative) Boltzmann weight[3] $(1 - \mathbf{\Omega}_i \cdot \mathbf{\Omega}_j)$. The classical nature of the representation will allow us to use some of the standard techniques for classical spin systems.

Let us first treat the case with periodic boundary conditions, so that $\partial\Lambda = \varnothing =$ *empty set*. We denote the denominator and the numerator in (3.6) by Z and $Z(A)$, respectively. We expand the product in Z as follows:

$$Z = \sum_{\Gamma \subset \mathbf{B}} \int d\mathbf{\Omega} \prod_{(i,j)\in\Gamma} (-\mathbf{\Omega}_i \cdot \mathbf{\Omega}_j)$$

Here the sum runs over all subsets Γ of $\mathbf{B}$. Since the measure is invariant under the local change of variable $\mathbf{\Omega}_i \to -\mathbf{\Omega}_i$, we see that the integrand in the final equation must contain even numbers of $\mathbf{\Omega}_i$ for each i in order to contribute to Z. In geometric language, the relevant Γ must satisfy $\partial\Gamma = \varnothing$, where the boundary ∂B of any $B \subset \mathbf{B}$ is defined as the set of sites i which belong to an odd number of bonds in B. By decomposing Γ into connected components as $\Gamma = \gamma_1 \cup \cdots \cup \gamma_n$, we get the *polymer representation*

$$Z = \sum_{\substack{\{\gamma_1,\ldots,\gamma_n\} \\ \gamma_i \cap \gamma_j = \varnothing}} W(\gamma_1) \cdots W(\gamma_n) \tag{3.7}$$

where the statistical weight of a polymer is defined as follows:

$$W(\gamma) = \int d\mathbf{\Omega} \prod_{(i,j)\in\gamma} (-\mathbf{\Omega}_i \cdot \mathbf{\Omega}_j) = \int d\mathbf{\Omega} \prod_{(i,j)\in\gamma} \mathbf{\Omega}_i \cdot \mathbf{\Omega}_j \tag{3.8}$$

The final identity is true because the number of bonds contained in γ is alway even (if is here that the fact that Λ is bipartite is used). Each loop γ_i is by definition a connected subset of $\mathbf{B}$ satisfying $\partial\gamma_i = \varnothing$. By the statement $\gamma_i \cap \gamma_j = \varnothing$ we mean that γ_i and γ_j have no common *sites*. The summation in (3.7) runs over the integers $n = 0, 1, \ldots$, and all possible $\{\gamma_1, \ldots, \gamma_n\}$.

By repeating exactly the same procedure, we will get a similar polymer representation for the quantity $Z(A)$. When $A = \boldsymbol{S}_i \cdot \boldsymbol{S}_j$ we get the following:

$$\begin{aligned}
&(S+1)^{-2}(-1)^{|i-j|} Z(\boldsymbol{S}_i \cdot \boldsymbol{S}_j) \\
&\quad = (-1)^{|i-j|} \int d\mathbf{\Omega}\, (\mathbf{\Omega}_i \cdot \mathbf{\Omega}_j) \prod_{(k,l)\in\mathbf{B}} (1 - \mathbf{\Omega}_k \cdot \mathbf{\Omega}_l) \\
&\quad = \sum_{\substack{\gamma_0 \\ \partial\gamma_0 = \{i,j\}}} \sum_{\substack{\{\gamma_1,\ldots,\gamma_n\} \\ \gamma_m \cap \gamma_p = \varnothing \\ (m,p=0,1,\ldots,n)}} W_{ij}(\gamma_0)\, W(\gamma_1) \cdots W(\gamma_n)
\end{aligned} \tag{3.9}$$

Here γ_0 is a connected set of bonds whose boundary is $\{i, j\}$, and the corresponding statistical weight is

$$W_{ij}(\gamma_0) = \int d\mathbf{\Omega}\, (\mathbf{\Omega}_i \cdot \mathbf{\Omega}_j) \prod_{(k,l)\in\gamma_0} \mathbf{\Omega}_k \cdot \mathbf{\Omega}_l \tag{3.10}$$

We have used the fact that $(-1)^{|i-j|} = (-1)^{|\gamma_0|}$ for any γ_0 with $\partial\gamma_0 = \{i, j\}$, where $|\gamma_0|$ is the number of bonds in γ_0.

The following elementary lemma is useful in our proof.

Lemma 3.3. Let $\mathbf{\Omega}_1, \ldots, \mathbf{\Omega}_{2n}$ be unit vectors in $\mathbf{R}^3$. Then we have the following identity:

$$\int_{S^2} d\mathbf{\Omega} \prod_{i=1}^{2n} \mathbf{\Omega} \cdot \mathbf{\Omega}_i = \frac{1}{2n+1} \sum_{j=2}^{2n} \mathbf{\Omega}_1 \cdot \mathbf{\Omega}_j \int_{S^2} d\mathbf{\Omega} \prod_{\substack{i=2 \\ i\neq j}}^{2n} \mathbf{\Omega} \cdot \mathbf{\Omega}_i \tag{3.11}$$

Proof. By Wick's theorem,

$$\int d^3\mathbf{x}\, e^{-|\mathbf{x}|^2/2} \prod_{i=1}^{2n} \mathbf{x}\cdot\boldsymbol{\Omega}_i = \sum_{j=2}^{2n} \boldsymbol{\Omega}_1\cdot\boldsymbol{\Omega}_j \int d^3\mathbf{x}\, e^{-|\mathbf{x}|^2/2} \prod_{\substack{i=2\\ i\neq j}}^{2n} \mathbf{x}\cdot\boldsymbol{\Omega}_i \quad (3.12)$$

where $\mathbf{x}$ is integrated over $\mathbf{R}^3$. Letting $\mathbf{x} = r\boldsymbol{\Omega}$ with $0 \leqslant r < \infty$ and $\boldsymbol{\Omega}$ a unit vector, we have $d^3\mathbf{x} = 4\pi r^2\, dr\, d\boldsymbol{\Omega}$. We also have that

$$\int_0^\infty r^{2n} e^{-r^2/2}\, dr = (2\pi)^{1/2}\cdot 1\cdot 3\cdot 5\cdots(2n-1)$$

Substituting this in (3.2) gives (3.11). ∎

Let us consider only the hexagonal lattice for the moment. Note that any loop in the hexagonal lattice has no self-intersections, since the coordination number of the lattice is three. By using (3.11) with $n=1$ repeatedly, we can evaluate the statistical weights $W(\gamma)$, $W_{ij}(\gamma_0)$ as follows:

$$\left.\begin{aligned} W(\gamma) &= 3^{-|\gamma|+1} \\ W_{ij}(\gamma_0) &= 3^{-|\gamma_0|+g(\gamma_0)} \end{aligned}\right\} \quad \text{hexagonal lattice} \quad (3.13)$$

Here $g(\gamma_0) = 0, 1, 2$ is the number of loops in γ_0, and $|\gamma|$ denotes the number of bonds in γ. γ_0 can contain at most two loops, since it can intersect itself only at sites i and j.

Since $W(\gamma)$, $W_{ij}(\gamma_0)$ are nonnegative, we can bound $Z(\boldsymbol{S}_i\cdot\boldsymbol{S}_j)$ as

$$\begin{aligned} 0 &\leqslant (S+1)^{-2}(-1)^{|i-j|}\, Z(\mathbf{S}_i\cdot\boldsymbol{S}_j) \\ &\leqslant \sum_{\substack{\gamma_0\\ \partial\gamma_0=\{i,j\}}} \sum_{\substack{\{\gamma_1,\ldots,\gamma_n\}\\ \gamma_m\cap\gamma_p=\varnothing\\ (m,p=1,2,\ldots,n)}} W_{ij}(\gamma_0)\, W(\gamma_1)\cdots W(\gamma_n) \\ &= Z \sum_{\substack{\gamma_0\\ \partial\gamma_0=\{i,j\}}} W_{ij}(\gamma_0) = Z \sum_{\substack{\gamma_0\\ \partial\gamma_0=\{i,j\}}} 3^{-|\gamma_0|+g(\gamma_0)} \end{aligned} \quad (3.14)$$

where we simply omitted the constraint $\gamma_0\cap\gamma_m = \varnothing$ in the middle expression in (3.14). Note that any connected set γ_0 such that $\partial\gamma_0 = \{i, j\}$ can be associated with a (not necessarily unique) self-avoiding walk $w = \{i_0, i_1, \ldots, i_l\}$, where $i_0 = i$, $i_l = j$, $(i_k, i_{k+1}) \in \mathbf{B}$, and $(i_k, i_{k+1}) \neq (i_m, i_{m+1})$ if $k \neq m$. Therefore from (3.14) we get

$$0 \leqslant (-1)^{|i-j|}\langle \boldsymbol{S}_i\cdot\boldsymbol{S}_j\rangle \leqslant (S+1)^2 \sum_{\substack{\gamma_0\\ \partial\gamma_0=\{i,j\}}} 3^{-|\gamma_0|+2} \leqslant \left(\frac{5}{2}\right)^2 \sum_{w: i\to j} 3^{-|w|+2}$$

where the sum runs over all the (bond) self-avoiding walks (in the sense that no bond is traversed more than once) connecting i and j, and $|w|$ is the number of bonds in w. Since the hexagonal lattice has coordination number three, the total number of (bond) self-avoiding walks with $|w| = l$ is bounded by $3 \cdot 2^{l-1}$. Thus we can bound the above sum as

$$\sum_{w: i \to j} 3^{-|w|+2} \leqslant \sum_{l=|i-j|}^{\infty} 3 \cdot 2^{l-1} \cdot 3^{-l+2} = \frac{81}{2} \left(\frac{2}{3}\right)^{|i-j|}$$

This proves Theorem 3.1 for the hexagonal lattice.

The extension of the above proof to the square lattice requires a more careful treatment of the statistical weight. We will construct upper bounds for $W_{ij}(\gamma_0)$ in an inductive manner as follows. For an arbitrary integer $n = 0, 1, 2, \ldots$ and connected γ_0 such that $\partial\gamma_0 = \{i, j\}$, we define

$$X_{ij}^{(n)}(\gamma_0) = \sum_{\substack{w: i \to j \\ w \subset \gamma_0, |w| \leqslant n}} 3^{-|w|} W(\gamma_0 \backslash w) + \sum_{\substack{k \in \gamma_0 \\ k \neq j}} \sum_{\substack{w: i \to k \\ w \subset \gamma_0, |w| = n}} 3^{-|w|} W_{kj}(\gamma_0 \backslash w) \tag{3.15}$$

where w always denotes a (bond) self-avoiding walk. The weights $W(\gamma_0 \backslash w)$ and $W_{kj}(\gamma_0 \backslash w)$ are defined as in (3.8) and (3.10), respectively. The symbol $\gamma_0 \backslash w$ means γ_0 with the bonds in w deleted, and the condition $k \in \gamma_0$ means that $k \in \Lambda$ and that γ_0 contains a bond with k as one of its endpoints.

Lemma 3.4. For any γ_0, i, j, the quantity $X_{ij}^{(n)}(\gamma_0)$ is nondecreasing in n.

Proof. Consider a site k and a walk w that contributes to the second term in (3.15). Because the boundary of $\gamma_0 \backslash w$ is $\{k, j\}$ and the square lattice has coordination number four, one of the following is true: (i) There is a unique k' such that the bond $(k, k') \in \gamma_0 \backslash w$. (ii) There are three sites k_p $(p = 1, 2, 3)$ such that $(k, k_p) \in \gamma_0 \backslash w$. Suppose that (i) is the case. We use (3.11) with $n = 1$ by setting $\mathbf{\Omega} = \mathbf{\Omega}_k$ to get

$$W_{kj}(\gamma_0 \backslash w) = \tfrac{1}{3} W_{k'j}(\gamma_0 \backslash w') \tag{3.16}$$

where $w' = w \cup (k, k')$. When (ii) is the case, we use (3.11) with $n = 2$ in the form

$$\int d\mathbf{\Omega}_k \, (\mathbf{\Omega}_k \cdot \mathbf{\Omega}_j) \prod_{p=1,2,3} \mathbf{\Omega}_k \cdot \mathbf{\Omega}_{k_p}$$

$$= \frac{1}{5} \left\{ (\mathbf{\Omega}_{k_1} \cdot \mathbf{\Omega}_j) \int d\mathbf{\Omega}_k \, (\mathbf{\Omega}_k \cdot \mathbf{\Omega}_{k_2})(\mathbf{\Omega}_k \cdot \mathbf{\Omega}_{k_3}) + (\text{two permutations}) \right\}$$

to get

$$W_{kj}(\gamma_0 \backslash w) = \frac{1}{5} \sum_{p=1,2,3} W_{k_p j}(\gamma_0 \backslash w_p) \leqslant \frac{1}{3} \sum_{p=1,2,3} W_{k_p j}(\gamma_0 \backslash w_p) \tag{3.17}$$

where $w_p = w \cup \{k, k_p\}$.

In both cases k' or k_p may equal j. If this happens, the new walk w' or w_p goes from i to j and we make use of the equality $W_{jj}(\gamma_0 \backslash w) = W(\gamma_0 \backslash w)$. If this does not happen, the new walk w' or w_p has length $n+1$ and goes from i to some site $k' \in \gamma_0$. Using (3.16) and (3.17), we thus obtain the following bound:

$$\sum_{\substack{k \in \gamma_0 \\ k \neq j}} \sum_{\substack{w : i \to k \\ w \subset \gamma_0,\, |w| = n}} 3^{-|w|} W_{kj}(\gamma_0 \backslash w)$$

$$\leqslant \sum_{\substack{w' : i \to j \\ w' \subset \gamma_0,\, |w'| = n+1}} 3^{-|w'|} W(\gamma_0 \backslash w')$$

$$+ \sum_{\substack{k' \in \gamma_0 \\ k' \neq j}} \sum_{\substack{w' : i \to k' \\ w' \subset \gamma_0,\, |w'| = n+1}} 3^{-|w'|} W_{k'j}(\gamma_0 \backslash w')$$

Substituting the above bound in (3.15), the desired inequality $X_{ij}^{(n)}(\gamma_0) \leqslant X_{ij}^{(n+1)}(\gamma_0)$ follows. ∎

From Lemma 3.4 we see that

$$W_{ij}(\gamma_0) = X_{ij}^{(0)}(\gamma_0) \leqslant X_{ij}^{(n)}(\gamma_0) = \sum_{\substack{w : i \to j \\ w \subset \gamma_0}} 3^{-|w|} W(\gamma_0 \backslash w)$$

where $n \geqslant |\gamma_0|$. Substituting the above bound in (3.9), we find

$$(S+1)^{-2}(-1)^{|i-j|} Z(\boldsymbol{S}_i \cdot \boldsymbol{S}_j)$$

$$\leqslant \sum_{\substack{\gamma_0 \\ \partial\gamma_0 = \{i,j\}}} \sum_{\substack{w : i \to j \\ w \subset \gamma_0}} 3^{-|w|} \sum_{\substack{\{\gamma_1, \ldots, \gamma_n\} \\ \gamma_m \cap \gamma_p = \varnothing \\ (m,p = 0,1,\ldots,n)}} W(\gamma_0 \backslash w)\, W(\gamma_1) \cdots W(\gamma_n)$$

We now switch the order of the summations over γ_0 and w. Fix a w and consider the sums over γ_0 and $\gamma_1, \ldots, \gamma_n$. The constraints are that $\gamma_0 \supset \omega$, $\gamma_1, \ldots, \gamma_n$ are pairwise disjoint, and each of $\gamma_1, \ldots, \gamma_n$ is disjoint from γ_0. We obtain an upper bound on the sum if we replace the last constraint by the constraint that each of $\gamma_1, \ldots, \gamma_n$ is disjoint from $\gamma_0 \backslash w$. This sum over $\gamma_0, \gamma_1, \ldots, \gamma_n$ then equals Z. Thus,

$$(-1)^{|i-j|} Z(\boldsymbol{S}_i \cdot \boldsymbol{S}_j) \leqslant Z(S+1)^2 \sum_{w : i \to j} 3^{-|w|}$$

Now we have the following simple upper bound for the correlation function:

$$(-1)^{|i-j|}\langle \boldsymbol{S}_i \cdot \boldsymbol{S}_j \rangle \leqslant \sum_{w: i \to j} 3^{2-|w|}$$

To bound the number of (bond) self-avoiding walks on the square lattice, we divide such a walk into groups of four steps each. We then replace the constraint that the walk is (bond) self-avoiding by the constraint that the four bonds in each group are different from each other and are different from the last bond of the previous group of four bonds. The number of four-bond walks (with three possible initial directions) is 3^4. Of these, two walks have the property that the fourth bond overlaps the last bond from the previous group. Therefore the number of choices for each group of four bonds is equal to 3^4-2. Hence the number of bond self-avoiding walks of length l is bounded by $(3^4-2)^{l/4}$ times a constant. This result holds even if l is not divisible by 4 (simply by making the constant large enough). Therefore we get

$$\begin{aligned} 0 \leqslant (-1)^{|i-j|}\langle \boldsymbol{S}_i \cdot \boldsymbol{S}_j \rangle &\leqslant \sum_{l=|i-j|}^{\infty} \text{const} \cdot (3^4-2)^{l/4} 3^{-l} \\ &\leqslant \text{const} \cdot \left(1-\frac{2}{3^4}\right)^{|i-j|/4} \end{aligned}$$

which proves Theorem 3.1 for the square lattice.

The proof of Theorem 3.2 is essentially the same as the previous one. The only difference is in the treatment of the Néel boundary conditions in (3.2). The boundary function f in (3.5) is

$$f(\boldsymbol{\Omega}) = \prod_{i \in \Lambda_+ \cap \partial\Lambda} \left(\frac{1+\Omega_i^z}{2}\right)^{z-z(i)} \prod_{j \in \Lambda_- \cap \partial\Lambda} \left(\frac{1-\Omega_j^z}{2}\right)^{z-z(j)}$$

where Ω_i^z is the z component of $\boldsymbol{\Omega}_i$. We can again expand the "Boltzmann factor" $\prod (1-\boldsymbol{\Omega}_i \cdot \boldsymbol{\Omega}_j)$ and the product in $f(\boldsymbol{\Omega})$ to get the polymer representation (3.7) for Z with the constraint $\partial\gamma_i = \varnothing$ replaced by $\partial\gamma_i \subset \partial\Lambda$. Note that the (appropriately defined) statistical weights $W(\gamma)$ are still strictly positive, because the Néel boundary conditions are perfectly commensurate with the minus signs arising in the expansion. By developing the representation for $Z(S_i^3)$ and repeating the construction of the upper bound, we finally get the bound

$$0 \leqslant (-1)^i \langle S_i^z \rangle_{\text{Néel}} \leqslant (S+1) \sum_{w: i \to \partial\Lambda} 3^{-|w|}$$

where the sum runs over all the (bond) self-avoiding random walks which connect the site i to the boundary. Theorem 3.2 then follows by using the previous upper bounds for the number of walks of length l.

4. THE INFINITE-VOLUME LIMIT FOR THE HEXAGONAL LATTICE

Having found all the ground states for the finite hexagonal lattice with arbitrary boundary conditions in Section 2, we now turn our attention to the infinite-volume, or thermodynamic, limit. For the hexagonal lattice there is a spin 3/2 at each site and the Hamiltonian is

$$H = \sum_{(i,j) \in \mathbf{B}} P^3_{(i,j)} \tag{4.1}$$

The most important result in this section is a proof that this model has a unique infinite-volume ground state ω. This uniqueness implies that $\omega(\boldsymbol{S}_i) = 0$, i.e., the model does not have Néel order. We will also show that all truncated correlation functions for this ground state have exponential decay. Thus we have a rigorous example of a two-dimensional isotropic quantum antiferromagnet which has a *unique* ground state with exponentially decaying correlation functions.

In order to state our results as a theorem, we first recall some elementary definitions about the infinite system. A *local observable* A is any polynomial in the spin operators which involves only finitely many sites. (Examples include the identity operator and the operator $\boldsymbol{S}_i \cdot \boldsymbol{S}_j$.) The support of A is the set of sites which appear in A. A *state* ρ is a linear functional on the local observables such that $\rho(A^*A) \geqslant 0$ for all A and $\rho(1) = 1$.

One way to construct a state is the following. Let Ψ be the normalized ground state for a finite lattice Λ with periodic boundary conditions (which we have shown to be unique). For any local A we can define

$$\omega_\Lambda(A) = (\Psi_\Lambda, A\Psi_\Lambda) \tag{4.2}$$

provided Λ contains the support of A. We say that a sequence $\Lambda \to \infty$ if the Λ's are an increasing sequence and if every point in the infinite lattice is eventually contained in some Λ. Our next theorem asserts the existence of $\omega = \lim_{\Lambda \to \infty} \omega_\Lambda$ and asserts that ω is the only ground state.

Theorem 4.1 (Uniqueness of the Hexagonal Lattice Ground State). For every local observable A, the state $\omega(A) = \lim_{\Lambda \to \infty} \omega_\Lambda(A)$ exists and is independent of the sequence. This state ω is the only infinite-

volume ground state, that is, if ρ is a state which is a ground state in the sense that

$$\rho(P^3_{(i,j)}) = 0 \qquad \text{for every} \quad (i, j) \in \mathbf{B}$$

then $\rho = \omega$. Furthermore, $\omega(\boldsymbol{S}_i) = 0$ and

$$|\omega(\boldsymbol{S}_i \cdot \boldsymbol{S}_j)| \leqslant Ce^{-|i-j|/\xi} \tag{4.3}$$

for some positive C and ξ. In fact, for any two local observables A and B

$$|\omega(A; B)| = |\omega(AB) - \omega(A)\,\omega(B)| \leqslant C(A)\,C(B) \exp[-\mathrm{dist}(A, B)/\xi] \tag{4.4}$$

where $\mathrm{dist}(A, B)$ is the distance between the supports of A and B, i.e., the minimum number of bonds needed to go from a site in the support of A to a site in the support of B. Here $C(A)$ and $C(B)$ are constants which depend only on A and B.

Remarks. 1. There are other definitions of infinite-volume ground states. In general these definitions are not equivalent although we suspect that they are for this model. See the remark in Section 2.4 of ref. 2.

2. The assertion that ω is the unique infinite-volume ground state amounts, heuristically, to the assertion that if we take a sequence of planar lattices Λ_j tending to infinity and with boundary $\partial\Lambda_j$, then the choice of the state of $\partial\Lambda_j$ [i.e., the choice of Φ in (2.9)] eventually does not affect what happens in any finite subset of the infinite hexagonal lattice.

3. Our main tool to prove Theorem 4.1 is a convergent polymer expansion. There are no parameters, e.g., temperature, in our problem, so it is natural to ask how we can prove that our expansion converges without the luxury of a parameter which can be taken to be small. The answer is that the factor $1/3$ in Lemma 3.3 (with $n = 1$) is sufficiently small to prove convergence.

4. The reader may wonder why we do not prove an analogous theorem for the square lattice. The reason is that we are unable to show that the analogous polymer expansion for the square lattice model actually converges. In Theorem 3.1 we did show exponential decay of the two-point function for the square lattice with periodic boundary conditions, but, since that proof depended crucially on certain quantities being positive, it cannot extend to a proof of the uniqueness of the ground state. For the VBS models on lattices in sufficiently high dimension, we expect the ground states to have Néel order. If this is the case, the ground states are no longer unique.

We begin by developing an expansion for the finite-volume ground state ω_Λ. Consider the finite $L \times L$ lattice Λ with periodic boundary

conditions. Let Ψ_Λ be the unique, normalized ground state for this lattice. Then, by the representation of the previous section, for any local observable A there is a function $A(\mathbf{\Omega})$ of the solid angles $\mathbf{\Omega}_i$ for i in the support of A such that

$$(\Psi_\Lambda, A\Psi_\Lambda) = \frac{\int d\mathbf{\Omega} \prod_{(i,j)} (1 - \mathbf{\Omega}_i \cdot \mathbf{\Omega}_j)\, A(\mathbf{\Omega})}{\int d\mathbf{\Omega} \prod_{(i,j)} (1 - \mathbf{\Omega}_i \cdot \mathbf{\Omega}_j)} = \frac{Z_\Lambda(A)}{Z_\Lambda} \tag{4.5}$$

where the products are over all nearest neighbor pairs (i, j).

As before, we expand out $1 - \mathbf{\Omega}_i \cdot \mathbf{\Omega}_j$ to obtain

$$Z_\Lambda = \sum_{\{\gamma_1, \ldots, \gamma_n\}}^{\text{hc}} W(\gamma_1) \cdots W(\gamma_n) \tag{4.6}$$

Implicit in (4.6) is that sum over all $n = 0, 1, 2, \ldots$. In (4.6) each γ_i is a connected loop in Λ and $\gamma_i \cap \gamma_j = \varnothing$. This hard-core condition is indicated by the hc superscript on the sum. Recall from (3.13) that the statistical weight $W(\gamma)$ is

$$W(\gamma) = 3^{-|\gamma|+1} \tag{4.7}$$

Equation (4.6) is the partition function of a gas of loops on the hexagonal lattice with a hard core repulsion and an activity $W(\gamma)$. There is a convergent expansion for the logarithm of this partition function if $W(\gamma)$ is sufficiently small. The standard result is that if there is a positive function $a(\gamma)$ such that

$$\sup_{\gamma'} \frac{1}{a(\gamma')} \sum_{\gamma : \gamma \cap \gamma' \neq \varnothing} |W(\gamma)|\, e^{a(\gamma)} < 1 \tag{4.8}$$

then

$$Z_\Lambda = \exp\left[\sum_{\{\gamma_1, \ldots, \gamma_n\}} \psi_c(\gamma_1, \ldots, \gamma_n)\, W(\gamma_1) \cdots W(\gamma_n) \right] \tag{4.9}$$

Here, $\psi_c(\gamma_1, \ldots, \gamma_n)$ is the connected part of the hard-core interaction (for the definition of ψ_c see ref. 4). Note that the sum in (4.9) does not have the hard-core condition, which means that n can be arbitrarily large. It is not obvious that this sum converges, but (4.8) guarantees that it converges absolutely. The proof that condition (4.8) implies convergence of the expansion for the logarithm of the partition function may be found in ref. 9. In ref. 4 the cardinality of γ is used in place of a general function $a(\gamma)$. Nonetheless, the methods of ref. 4 may be used to prove that condition (4.8) with a general $a(\gamma)$ implies convergence.

We will let $a(\gamma) = \varepsilon|\gamma|$, where $|\gamma|$ is the number of bonds in γ and ε is a positive constant. Condition (4.8) then reduces to

$$\sum_{\gamma : b \in \gamma} |W(\gamma)| e^{\varepsilon|\gamma|} < \varepsilon \tag{4.10}$$

where b is some fixed bond in the lattice. (The translational invariance has been used.) We could bound the number of γ's of length l which contain b by 2^{l-1}. Then

$$\sum_{\gamma : b \in \gamma} |W(\gamma)| e^{\varepsilon|\gamma|} \leqslant \sum_{\substack{l=6 \\ l \text{ even}}}^{\infty} \left(\frac{1}{3}\right)^{l-1} e^{\varepsilon l} 2^{l-1}$$

After a little computation one discovers that this bound is too crude to prove that there is an $\varepsilon > 0$ for which (4.10) holds.

The bound can be improved by the following simple but useful strategem. For the first few values of l, we explicitly compute the number of γ's of length l which contain b. For $l=6$ there are two loops. For $l=8$ there are none, and for $l=10$ there are ten loops. Hence

$$\sum_{\gamma : b \in \gamma} |W(\gamma)| e^{\varepsilon|\gamma|} \leqslant \frac{2}{3^5} e^{6\varepsilon} + \frac{10}{3^9} e^{10\varepsilon} + \sum_{\substack{l=12 \\ l \text{ even}}}^{\infty} \left(\frac{2}{3}\right)^{l-1} e^{\varepsilon l} \tag{4.11}$$

The series can be summed, and one finds that the above bound is less than ε for ε in the range $0.0614 \leqslant \varepsilon \leqslant 0.0988$. One can greatly enlarge the range of ε for which (4.11) holds by computing the number of γ containing a fixed b for longer lengths. These numbers for lengths up to 28 may be found in Table I. Although they are not needed in this section, they will be needed in the Appendix.

There is a similar expansion for the numerator $Z_A(A)$ in Eq. (4.5),

$$Z_A(A) = \sum_{\gamma} \sum_{\{\gamma_1, \ldots, \gamma_n\}}^{\mathrm{hc}(\gamma, A)} W(\gamma; A)\, W(\gamma_1) \cdots W(\gamma_n) \tag{4.12}$$

Here γ is any subset of bonds of A (not necessarily a loop) with the property that every connected component of γ has nonempty intersection with the support of A. In the inner sum, the γ_i are closed loops with the properties that they do not intersect each other or γ or the support of A. This condition is abbreviated by $\mathrm{hc}(\gamma, A)$. The weight $W(\gamma, A)$ is defined by

$$W(\gamma; A) = \int d\boldsymbol{\Omega} \prod_{(i,j) \in \gamma} (-\boldsymbol{\Omega}_i \cdot \boldsymbol{\Omega}_j)\, A(\boldsymbol{\Omega}) \tag{4.13}$$

For a fixed γ, the sum over $\{\gamma_1,..., \gamma_n\}$ in (4.12) is the partition function for the volume obtained by deleting the sites in γ or in the support of A from the original volume. If condition (4.10) holds, then this partition function can be exponentiated,

$$Z_\Lambda(A) = \sum_\gamma W(A;\gamma) \exp\left[\sum_{\{\gamma_1,...,\gamma_n\}}^{(\gamma,A)} \psi_c(\gamma_1,..., \gamma_n)\, W(\gamma_1)\cdots W(\gamma_n) \right] \quad (4.14)$$

where the superscript (γ, A) means that each γ_i is a closed loop which is disjoint from γ and from the support of A. The γ_i do not have to be pairwise disjoint. Combining (4.9) and (4.14), we have

$$(\Psi_\Lambda, A\Psi_\Lambda) = \sum_\gamma W(A;\gamma) \exp\left[\sum_{\{\gamma_1,...,\gamma_n\}}^{[\gamma,A]} \psi_c(\gamma_1,..., \gamma_n)\, W(\gamma_1)\cdots W(\gamma_n) \right] \quad (4.15)$$

where the superscript $[\gamma, A]$ means that *at least one* of the γ_i must have nontrivial intersection with either γ or with the support of A.

Until now, in all our expressions γ and γ_i were sets of bonds in Λ. The limit as $L \to \infty$ is given by the right side of (4.15) without the constraint that the bonds are in Λ. The existence of this limit follows from the convergence of the polymer expansion by the usual arguments. The resulting infinite-volume state is denoted by ω. The final formula is given by (4.15) but without the restriction that the γ_i lie in any particular Λ. Since this formula is independent of the particular sequence of Λ's tending to infinity, the first sentence of Theorem 4.1 has been proved.

Condition (4.10) and standard arguments imply inequality (4.4) in Theorem 4.1. We refer the reader to ref. 9 or ref. 4 for these arguments. In ref. 9 the condition for convergence of the expansion [inequality (1) in ref. 9] contains the factor $\exp[a(\gamma) + d(\gamma)]$ rather than just $\exp[a(\gamma)]$ as in our (4.8). In ref. 9, $d(\gamma)$ is some positive function which is required for the proof of exponential decay of truncated correlations. In our (4.8) there is no $d(\gamma)$ present, but, since the inequality (4.10) is strict, we can replace the ε on the right side of (4.10) by $\varepsilon - \delta$ for some $\delta > 0$. It follows that (4.8) holds with $\mathrm{ep}[a(\gamma)]$ replaced by $\mathrm{ep}[a(\gamma) + d(\gamma)]$ if we let $a(\gamma) = (\varepsilon - \delta)\,|\gamma|$ and $d(\gamma) = \delta\,|\gamma|$.

To complete the proof of Theorem 4.1, our next task is to show that ω is the only infinite-volume ground state. Let ρ be an infinite-volume ground state as in the hypothesis of the theorem. We must show that $\rho(A) = \omega(A)$ for every local A.

If we restrict ρ to the algebra of observables with support in some

fixed, finite-volume V, then this restriction can be written as a density matrix which involves only ground states for V, i.e.,

$$\rho(A) = \sum_{\alpha} C_{\alpha}(\Psi_{\alpha}, A\Psi_{\alpha}) \tag{4.16}$$

where the C_{α} are nonnegative constants whose sum is 1, and each Ψ_{α} is a normalized ground state for the Hamiltonian

$$H_V = \sum_{(i,j) \in V} P^3_{(i,j)}$$

where $(i, j) \in V$ means $(i, j) \in \mathbf{B}$ and each of i and j belongs to V. To prove that $\omega = \rho$, it suffices to show that for all α

$$|(\Psi_{\alpha}, A\Psi_{\alpha}) - \omega(A)| \leqslant C \exp[-\mathrm{dist}(A, \partial V)/\xi] \tag{4.17}$$

where $\mathrm{dist}(A, \partial V)$ is the distance from the support of A to the boundary of V, and where $\xi > 0$ and C are constants.

For reasons which will become clear in the Appendix, we take V to be of the form shown in Fig. 2. The results of the previous section imply that in the u, v representation each Ψ_{α} is given by

$$\Psi_{\alpha}(u, v) = \prod_{(i,j) \in V} (u_i v_j - u_j v_i)\, \Phi_{\alpha}(u, v) \tag{4.18}$$

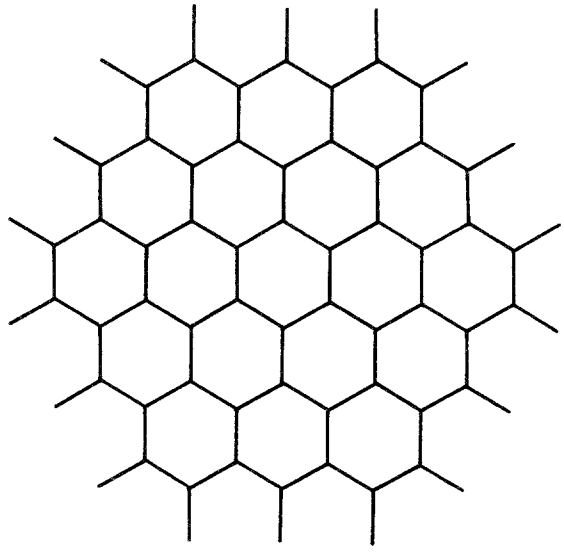

Fig. 2. The volume V used in the proof of the uniqueness of the infinite-volume ground state for the hexagonal lattice models. There is a spin 3/2 at each site including the endpoints of the boundary bonds.

where Φ_α is a polynomial in the u_i and v_i with $i \in \partial V$, the boundary sites in V. Furthermore, Φ_α must be jointly homogeneous of degree 2 in the variables u_i, v_i at each $i \in \partial V$.

In the $\mathbf{\Omega}$ representation, Eq. (4.18) implies

$$(\Psi_\alpha, A\Psi_\alpha) = \int d\mathbf{\Omega}\, |F_\alpha(\mathbf{\Omega})|^2 \prod_{(i,j)\in V} (1 - \mathbf{\Omega}_i \cdot \mathbf{\Omega}_j)\, A(\mathbf{\Omega}) \tag{4.19}$$

where $F_\alpha(\mathbf{\Omega})$ depends only on the $\mathbf{\Omega}_i$ with $i \in \partial V$. In the integration over the solid angles $\mathbf{\Omega}_i$, we will first integrate over the $\mathbf{\Omega}_i$ with i in the interior of V and then over the $\mathbf{\Omega}_i$ with $i \in \partial V$. We denote the former collection of $\mathbf{\Omega}_i$ by $\mathbf{\Omega}_{\text{int}}$ and the latter by $\mathbf{\Omega}_{\partial V}$. Hence,

$$\int d\mathbf{\Omega} = \int d\mathbf{\Omega}_{\partial V} \int d\mathbf{\Omega}_{\text{int}}$$

For any operator B, let us define

$$\| \langle B \rangle_{\mathbf{\Omega}_{\partial V}} \|_\infty = \sup_{\mathbf{\Omega}_{\partial V}} |\langle B \rangle_{\mathbf{\Omega}_{\partial V}}|$$

where

$$\langle B \rangle_{\mathbf{\Omega}_{\partial V}} = \frac{\int d\mathbf{\Omega}_{\text{int}}\, B(\mathbf{\Omega}) \prod_{(i,j)\in V} (1 - \mathbf{\Omega}_i \cdot \mathbf{\Omega}_j)}{\int d\mathbf{\Omega}_{\text{int}} \prod_{(i,j)\in V} (1 - \mathbf{\Omega}_i \cdot \mathbf{\Omega}_j)}$$

is the expectation value for fixed $\mathbf{\Omega}_{\partial V}$.

We then have

$$\begin{aligned}
&|(\Psi_\alpha, A\Psi_\alpha) - \omega(A)| \\
&= \left| \int d\mathbf{\Omega}_{\partial V}\, |F_\alpha(\mathbf{\Omega})|^2 \int d\mathbf{\Omega}_{\text{int}}\, \{A(\mathbf{\Omega}) - \omega(A)\} \prod_{(i,j)\in V} (1 - \mathbf{\Omega}_i \cdot \mathbf{\Omega}_j) \right| \\
&\leqslant \int d\mathbf{\Omega}_{\partial V}\, |F_\alpha(\mathbf{\Omega})|^2 \, \| \langle A - \omega(A) \rangle_{\mathbf{\Omega}_{\partial V}} \|_\infty \int d\mathbf{\Omega}_{\text{int}} \prod_{(i,j)\in V} (1 - \mathbf{\Omega}_i \cdot \mathbf{\Omega}_j) \\
&= \| \langle A - \omega(A) \rangle_{\mathbf{\Omega}_{\partial V}} \|_\infty (\Psi_\alpha, \Psi_\alpha) \\
&= \| \langle A - \omega(A) \rangle_{\mathbf{\Omega}_{\partial V}} \|_\infty
\end{aligned}$$

Therefore, in order to prove the bound (4.17), it suffices to check that for any choice of $\mathbf{\Omega}_{\partial V}$

$$|\langle A \rangle_{\mathbf{\Omega}_{\partial V}} - \omega(A)| \leqslant C \exp[-\text{dist}(A, \partial V)/\xi] \tag{4.20}$$

with C and $\xi > 0$ independent of $\mathbf{\Omega}_{\partial V}$. In what follows we omit the subscript $\mathbf{\Omega}_{\partial V}$ and denote by $\langle A \rangle$ the expectation value for some fixed $\mathbf{\Omega}_{\partial V}$.

We will prove (4.20) by developing a convergent polymer expansion for $\langle A \rangle$ and then comparing this with the expansion for $\omega(A)$. The expansion for $\langle A \rangle$ is developed in the same way as that already done for $\omega(A)$. The one important difference is that the expansion now contains polymers which are not loops. If γ is a walk which begins at a site i in ∂V and ends at a site j in ∂V, then $W(\gamma)$ will be nonzero. To compute $W(\gamma)$, we note that the integration over $\mathbf{\Omega}_k$ for k in γ with $k \neq i, j$ gives a factor of $1/3$. After the last such integration we are left with $\mathbf{\Omega}_i \cdot \mathbf{\Omega}_j$. Thus,

$$W(\gamma) = (1/3)^{|\gamma|-1} \mathbf{\Omega}_i \cdot \mathbf{\Omega}_j \tag{4.21}$$

Our polymer system consists of loops whose weight is given by (4.7), and of undirected walks between boundary sites whose weight is given by (4.21). The polymer expansion for this system converges if condition (4.8) holds. Our strategy for verifying (4.8) is the same as in the priodic boundary condition case. We explicitly calculate a finite number of terms in (4.8) and bound the rest. Unfortunately, we must now explicitly compute a rather large number of terms. These computations are relegated to the Appendix.

Finally we consider $\langle A \rangle - \omega(A)$. Our expansions (4.15) for the two quantities agree except for terms that reach all the way from the support of A to ∂V. [Recall that the presence of ψ_c in (4.15) requires that $\gamma, \gamma_1, \ldots, \gamma_n$ form one connected set.] The desired bound (4.20) follows by the usual techniques. The details are tedious, and therefore we omit them; similar arguments are given in ref. 13, Section 3, and in ref. 9, p. 494.

APPENDIX

The convergence of the polymer expansion developed in the last section is proved in this Appendix.

In this polymer gas there are two types of polymers—loops and self-avoiding walks which begin and end at sites in ∂V. We will refer to the later type simply as walks. In this Appendix, *walk* always means *bond self-avoiding walk*. The weight of a loop γ is

$$W(\gamma) = 3^{-|\gamma|+1}$$

where $|\gamma|$ is the number of bonds in γ. Recall from (4.21) that the weight of a walk γ from site i to site j is

$$W(\gamma) = 3^{-|\gamma|+1} \mathbf{\Omega}_i \cdot \mathbf{\Omega}_j$$

(For each site $i \in \partial \Lambda$ there is a fixed unit vector $\mathbf{\Omega}_i$.)

To check condition (4.8), we divide the polymers into various classes as follows:

$$\mathscr{L}_l = \{\gamma: \gamma \text{ is a loop with } |\gamma| = l\}$$

$$\mathscr{W}_l = \{\gamma: \gamma \text{ is a walk with } |\gamma| = l\}$$

$$\mathscr{L}_{>l} = \{\gamma: \gamma \text{ is a walk with } |\gamma| > l\}$$

$\mathscr{W}_{>l}$ is defined analogously.

We will prove (4.8) by considering the seven cases $\gamma' \in \mathscr{W}_3$, $\mathscr{W}_4$, $\mathscr{W}_5$, $\mathscr{W}_6$, $\mathscr{L}_6$, $\mathscr{W}_{>6}$, or $\mathscr{L}_{>6}$. In each of these cases we split up the sum in (4.8) into several sums according to whether γ belongs to $\mathscr{W}_3$, $\mathscr{W}_4$, $\mathscr{W}_5$,..., $\mathscr{W}_{20}$, $\mathscr{W}_{>20}$, $\mathscr{L}_6$, $\mathscr{L}_{10}$, $\mathscr{L}_{12}$,..., $\mathscr{L}_{26}$, or $\mathscr{L}_{>26}$. We should point out here that the shortest possible loop has six bonds. There are no loops with eight bonds, but beginning with $l = 10$ there are loops of length l for all even l. The shortest walk is of length 3 and can only occur at the corners of our region (see Fig. 2). Walks of all lengths $\geqslant 3$ are possible, but those with odd length must begin and end on opposite sides of a corner.

Our function $\alpha(\gamma)$ will only depend on $|\gamma|$, so we will write $a(l)$ for $\alpha(\gamma)$ with $|\gamma| = l$. We choose

$$a(3) = 0.52, \qquad a(4) = 0.56, \qquad a(5) = 0.66, \qquad a(6) = 0.70,$$
$$a(l) = 0.15l \qquad \text{for} \quad l > 6 \tag{A.1}$$

Let $N(l)$ denote the number of loops of length l in the infinite heagonal lattice which contain a fixed bond b.

$N(l)$, which is independent of b, can be found for small values of l by hand, and for larger values of l with the aid of a computer. Table I gives $N(l)$ for $l \leqslant 28$. For $l > 28$ we bound $N(l)$ as follows. Think of b as the first step of the loop. The remaining $l-1$ steps give at most 2^{l-1} loops. We can improve this bound by using the requirement that the loop must end at its starting point. Given all but the last two steps of the walk, this requirement uniquely determines the last two steps. Hence

$$N(l) \leqslant 2^{l-3}$$

The presence of the boundary can only reduce the number of loops of length l containing a fixed bond b, so $N(l)$ is always an upper bound for this number.

We now consider (4.8) for each of the seven cases of γ' and show that it is satisfied in each case.

Case 1. $\gamma' \in \mathscr{W}_3$. There are only six γ' with $|\gamma'| = 3$, one at each corner. The corners all look the same, so we need only consider one such

γ'. We can eplicitly calculate the number of walks γ of length l which intersect γ' for $l=3, 4,..., 20$ with the help of computer. The resulting integers will be denoted by $M(l, 3)$ and are shown in the first column of Table II.

The number of loops of length l which intersect γ' is denoted by $M(\bar{l}, 3)$ and is also shown in Table II for $l=6$ and 10.

Next we consider loops of length greater than 10. We will refer to bonds, both of whose endpoints are in the interior of V, as *interior bonds.* Bonds containing an endpoint in $\partial\Lambda$ will be called *boundary bonds.* γ' contains only $|\gamma'|-2=1$ interior bond, and any loop which intersects γ' must contain this bond. Thus, for $l>10$ we can bound the number of loops of length l which intersect γ' by $N(l)$.

Finally, we must consider walks of length $l>20$ which intersect γ'. We divide such walks γ into two classes according to whether γ contains an interior or a boundary bond in γ'. (Of course, these cases are not disjoint, so there is some overcounting here.)

Let $P_i(l)$ denote the supremum over interior bonds b of the number of walks of length l which intersect b. $P_b(l)$ is defined similarly, but with interior bond replaced by boundary bond.

Since γ' contains $|\gamma'|-2$ interior bonds and 2 boundary bonds, the number of walks of length $l>20$ intersecting γ' is at most

$$2P_b(l)+(|\gamma'|-2)\,P_i(l)$$

Table I. Number of Loops of a Fixed Length Containing a Fixed Bond[a]

l	$N(l)$
6	2
8	0
10	10
12	8
14	56
16	96
18	390
20	920
22	3,168
24	8,592
26	28,002
28	81,368

[a] The lattice is infinite.

Table II. Number of Polymers in the Class Represented by the Row Label which Intersect a fixed Polymer belonging to the Class Represented by the Column Label

Fixed polymer belongs to:	$\mathscr{W}_3$	$\mathscr{W}_4$	$\mathscr{W}_5$	$\mathscr{W}_6$	$\mathscr{L}_6$
Number of polymers in					
$\mathscr{W}_3$	1	1	1	1	1
$\mathscr{W}_4$	2	2	3	3	2
$\mathscr{W}_5$	2	2	2	2	2
$\mathscr{W}_6$	2	2	3	3	2
$\mathscr{W}_7$	6	7	7	7	7
$\mathscr{W}_8$	8	9	12	13	10
$\mathscr{W}_9$	14	18	19	20	20
$\mathscr{W}_{10}$	18	22	27	30	24
$\mathscr{W}_{11}$	38	50	55	62	60
$\mathscr{W}_{12}$	52	70	78	91	70
$\mathscr{W}_{13}$	106	140	156	179	174
$\mathscr{W}_{14}$	150	224	225	286	221
$\mathscr{W}_{15}$	296	404	454	511	547
$\mathscr{W}_{16}$	428	655	644	874	641
$\mathscr{W}_{17}$	868	1207	1337	1561	1657
$\mathscr{W}_{18}$	1284	2084	1940	2727	2066
$\mathscr{W}_{19}$	2530	3525	3985	4776	4965
$\mathscr{W}_{20}$	3818	6504	5793	8478	6578
$\mathscr{L}_6$	1	2	2	3	7
$\mathscr{L}_{10}$	3	7	6	10	30

Table III. Upper Bound on the Number of Walks of Length ℓ from a Fixed Site to the Boundary

l	$P(l)$
1	1
2	2
3	2
4	4
5	6
6	8
7	16
8	24
9	40
10	64

A crude bound on $P_b(l)$ and $P_i(l)$ is 2^{l-1}. Unfortunately, this bound is too crude, even for the cases $l > 20$. We obtain a better bound by using the restriction that a walk must start and end at a boundary site. For a site k in the interior of V and a positive integer l, let $p(k, l)$ be the number of walks of length l which begin at k and end at a site in ∂V. Then let

$$P(l) = \sup_k p(k, l)$$

$P(l)$ is computed with the help of a computer and shown in Table III.

We can now bound $P_b(l)$ as follows. Let b be a boundary bond. Let γ have length l and contain b. Since b is a boundary bond, we can think of b as the first step in γ. The next $l-11$ steps yield at most 2^{l-11} choices. The final 10 steps yield at most $P(10) = 64$ choices by the above. Consequently,

$$P_b(l) \leqslant 2^{l-11} \cdot 64 = 2^{l-5} \tag{A.2}$$

To bound $P_i(l)$, we fix an interior bond and arbitrarily designate one endpoint as the "left" endpoint and one as the "right" endpoint. For a walk γ which contains b, we let m be the number of bonds in the part of γ which attaches to the left endpoint. Then there are $l-m-1$ bonds in the part which attaches to the right endpoint. m must be summed from 1 to $l-1$. We now see that

$$P_i(l) \leqslant \sum_{m=1}^{l-1} P(m)\, P(l-m-1) \tag{A.3}$$

For $1 \leqslant m \leqslant 10$ we know $P(m)$ explicitly. For larger m we use $P(m) \leqslant 2^{m-10} P(10) = 2^{m-4}$. After a little computation we obtain

$$P_i(l) \leqslant (2l + 97) 2^{l-10} \tag{A.4}$$

Finally, we can write down a bound on (4.8) for $\gamma' \in \mathscr{W}_3$. To keep our expressions compact, we let

$$w(l) = 3^{-l+1} e^{a(l)}$$

so that $|W(\gamma)| e^{a(\gamma)} \leqslant w(|\gamma|)$. Then

$$\begin{aligned} &\sup_{\gamma' \in \mathscr{W}_3} \frac{1}{a(\gamma')} \sum_{\gamma : \gamma \cap \gamma' \neq \varnothing} |W(\gamma)| e^{a(\gamma)} \\ &\quad \leqslant \frac{1}{a(l')} \Bigg[\sum_{l = 3, 4, \ldots, 20, \overline{6}, \overline{10}} M(l, l')\, w(l) + \sum_{l = 12, 14, \ldots} (l' - 2)\, N(l)\, w(l) \\ &\qquad + \sum_{l=21}^{\infty} [2P_b(l) + (l'-2)\, P_i(l)]\, w(l) \Bigg] \end{aligned} \tag{A.5}$$

with $l' = 3$. Substituting our choice of $a(\gamma)$, Eq. (A.1), our bounds on $P_b(l)$ and $P_i(l)$, inequalities (A.2) and (A.4), and the values of $M(l, l')$ and $N(l)$ from Tables I and II, we obtain 0.8857 for the right side of (A.5). The various terms in this sum are shown in column 1 of Table IV.

Case 2. $\gamma' \in \mathcal{W}_4$. Unlike the previous case, there are now an infinite number of such walks γ'. Let $M(l, \gamma')$ denote the number of walks of length l which intersect γ'. For a fixed l, $M(l, \gamma')$ is independent of γ' if γ' is sufficiently far from the corners of V. Thus, finding all the $M(l, \gamma')$ for a fixed l is a finite computation. We would like to combine all the possibilities for γ' into a single "worst case." One way to do this would be to take the supremum over γ' of $M(l, \gamma')$. Unfortunately, this is too crude. We can do better by using the monotonicity of $w(l) = 3^{-l+1} \exp[a(l)]$. It suffices to find $M(l, 4)$ such that

$$\sup_{\gamma' \in \mathcal{W}_4} \sum_{l=3}^{20} M(l, \gamma')\, w(l) \leqslant \sum_{l=3}^{20} M(l, 4)\, w(l) \tag{A.6}$$

We claim that we can choose

$$M(l, 4) = \sup_{\gamma' \in \mathcal{W}_4} \sum_{k=3}^{l} M(k, \gamma') - \sup_{\gamma' \in \mathcal{W}_4} \sum_{k=3}^{l-1} M(k, \gamma') \tag{A.7}$$

Table IV. The Condition for Convergence of the Polymer Expansion Is That the Total for Each Column Be Less Than 1

Fixed polymer belongs to:	$\mathcal{W}_3$	$\mathcal{W}_4$	$\mathcal{W}_5$	$\mathcal{W}_6$	$\mathcal{L}_6$	$\mathcal{W}_{>6}$	$\mathcal{L}_{>6}$
Sum over							
$\mathcal{W}_3$	0.3594	0.3337	0.2832	0.2670	0.1780	0.1780	0.1246
$\mathcal{W}_4$	0.2494	0.2316	0.2947	0.2779	0.1235	0.2779	0.1297
$\mathcal{W}_5$	0.0919	0.0853	0.0724	0.0682	0.0455	0.0455	0.0318
$\mathcal{W}_6$	0.0319	0.0296	0.0377	0.0355	0.0158	0.0434	0.0221
$\mathcal{W}_7$	0.0452	0.0490	0.0416	0.0392	0.0261	0.0261	0.0183
$\mathcal{W}_8$	0.0234	0.0244	0.0276	0.0282	0.0145	0.0376	0.0324
$\mathcal{W}_9$	0.0158	0.0189	0.0169	0.0168	0.0112	0.0112	0.0078
$\mathcal{W}_{10}$	0.0079	0.0089	0.0093	0.0098	0.0052	0.0166	0.0137
$\mathcal{W}_{10<l<21}$	0.0169	0.0214	0.0197	0.0218	0.0131	0.0275	0.0208
$\mathcal{W}_{>20}$	0.0245	0.0386	0.0462	0.0562	0.0459	0.0591	0.0591
$\mathcal{L}_6$	0.0159	0.0296	0.0251	0.0355	0.0552	0.1105	0.1105
$\mathcal{L}_{10}$	0.0013	0.0028	0.0021	0.0033	0.0065	0.0152	0.0152
$\mathcal{L}_{>10}$	0.0022	0.0041	0.0052	0.0066	0.0055	0.0077	0.0077
Total	0.8857	0.8780	0.8817	0.8659	0.5460	0.8563	0.5937

for $l > 3$, while for $l = 3$

$$M(3, 4) = \sup_{\gamma' \in \mathscr{W}_4} M(3, \gamma')$$

The claim is proved as follows:

$$\sum_{l=3}^{20} M(l, 4)\, w(l)$$

$$= \sum_{l=3}^{19} \left\{ \sup_{\gamma' \in \mathscr{W}_4} \sum_{k=3}^{l} M(k, \gamma') \right\} [w(l) - w(l+1)]$$

$$+ \sup_{\gamma' \in \mathscr{W}_4} \sum_{k=3}^{20} M(k, \gamma')\, w(20) \tag{A.8}$$

Now fix some $\gamma' \in \mathscr{W}_4$. Since $w(l) - w(l+1) \geqslant 0$, the right side of (A.8) is

$$\geqslant \sum_{l=3}^{19} \sum_{k=3}^{l} M(k, \gamma')[w(l) - w(l+1)] + \sum_{k=3}^{20} M(k, \gamma')\, w(20)$$

$$= \sum_{l=3}^{20} M(l, \gamma')\, w(l) \tag{A.9}$$

With the help of a computer we first calculate $M(\gamma', 4)$ for all $\gamma' \in \mathscr{W}_4$ and then use (A.7) to calculate $M(l, 4)$. The result is shown in the second column of Table II.

The number of loops of lengths 6 and 10 which intersect γ' are shown in Table II. Bounding the other terms as in case 1, we get the bound (A.5) with $l' = 4$. Using (A.1) for $a(l)$, we find that the expression on the right side of (A.5) equals 0.8780.

Cases 3, 4, 5. $\gamma' \in \mathscr{W}_5$, $\mathscr{W}_6$, $\mathscr{L}_6$. These cases are all handled by the techniques used in the previous two cases. Table II contains the counting factors needed for these cases. The resulting bound is again given by (A.5) with $l' = 5$ for $\gamma' \in \mathscr{W}_5$, $l' = 6$ for $\gamma' \in \mathscr{W}_6$, and $l' = \bar{6}$ for $\gamma' \in \mathscr{L}_6$. The notation $l' = \bar{6}$ to denote the case of $\gamma' \in \mathscr{L}_6$ is also used in Table II.

Evaluating the right side of (A.5) for these three cases, we find

0.8817	for $\mathscr{W}_5$
0.8659	for $\mathscr{W}_6$
0.5460	for $\mathscr{L}_6$

Case 6. $\gamma' \in \mathscr{W}_{>6}$. We bound the number of $\gamma \in \mathscr{L}_l$ which intersect γ' by $N(l)$ times the number of interior bonds in γ', namely $|\gamma'| - 2$. We use this bound for $l = 6, 10, 12\ldots$. We then bound $|\gamma'| - 2 = l' - 2$ by l'.

Table V. Total Number of Lines of Length l for l Odd

l	$Q(l)$
3	1
5	2
7	7
9	20
11	64
13	202
15	647
17	2094
19	6803

Let $Q(l)$ denote the number of walks of length l for odd l. Recall that a walk of odd length must start and end on opposites sides of a corner. Consequently, the number of such walks is finite. In the definition of $Q(l)$ we only count walks which occur near one particular corner.

$Q(l)$ is found for $l=3, 5,..., 19$ with a computer and is shown in Table V. For odd l, $3 \leqslant l \leqslant 19$, the number of $\gamma \in \mathscr{L}_l$ which intersect γ' is bounded by $Q(l)$.

For $l > 20$ we bound the number of $\gamma \in \mathscr{L}_l$ which intersect γ' as before, i.e., by

$$2P_b(l) + (l'-2)\, P_i(l)$$

where $l' = |\gamma'|$. For $l > 20$, our bound on $P_i(l)$ is greater than our bound on $P_b(l)$. Thus, we can bound the above by $l'(2l+97)2^{l-10}$.

Finally, we must consider those γ in $\mathscr{L}_l$ for even l, $4 \leqslant l \leqslant 20$. We start with the case of $l=4$. If we fix l', then the γ' with $|\gamma'| = l'$ which intersects the largest number of γ's in $\mathscr{L}_4$ is that γ' which stays as close to ∂V as possible—as shown in Fig. 3. (The figure shows the case of even l'. When l'

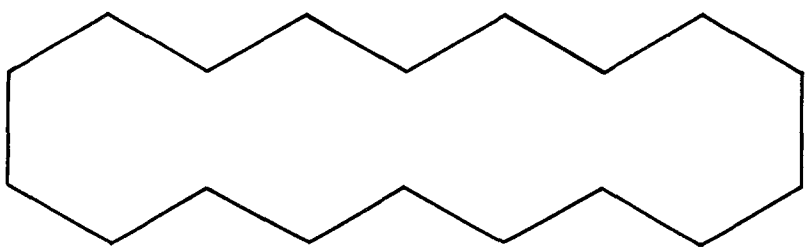

Fig. 3. The "worst" walk γ' which can occur in case 6.

is odd, γ' must go from one side of the corner to the other.) For such a γ' with l' even, the number of $\gamma \in \mathscr{L}_4$ intersecting γ' is $\frac{1}{2}l'+1$. If l' is odd, the number is bounded by $\frac{1}{2}l'+\frac{1}{2}$, which is $\leqslant \frac{1}{2}l'+1$. For $l=6$ the counting is similar since there is only one possible shape for γ with $|\gamma|=6$. In this case the number of $\gamma \in \mathscr{L}_6$ intersecting γ' is bounded by $\frac{1}{2}l'+2$.

To bound the cases of even l, $8 \leqslant l \leqslant 20$, fix a boundary bond b and let $R(l)$ be the number of $\gamma \in \mathscr{L}_l$ such that the rightmost boundary bond in γ is b. Given γ' and l, we consider how many such b's occur. The worst case occurs when γ' is stretched out as in Fig. 3. Bearing in mind that it takes two steps to go from one boundary bond to the next, we see from Fig. 4 that the number of such b is at most

$$\tfrac{1}{2}(l-2)+\tfrac{1}{2}(l'-2)+\tfrac{1}{2}(l-2)+1=\tfrac{1}{2}l'+l-2$$

Hence the number of $\gamma \in \mathscr{L}_l$ which intersect γ' is at most $(\frac{1}{2}l'+l-2)\,R(l)$.

The above bounds yield

$$\begin{aligned}
&\sup_{\gamma' \in \mathscr{W}_{>6}} \frac{1}{a(\gamma')} \sum_{\gamma:\gamma\cap\gamma'\neq\varnothing} |W(\gamma)|\, e^{a(\gamma)} \\
&\quad \leqslant \frac{1}{a(\gamma')}\Bigg[l' \sum_{l=6,\, l \text{ even}}^{\infty} N(l)\, w(l) + \sum_{l=3,\,5,\ldots,19} Q(l)\, w(l) \\
&\qquad + \sum_{l=21}^{\infty} l'(2l+97)2^{l'-10} w(l) + \left(\frac{1}{2}l'+1\right) w(4) \\
&\qquad + \left(\frac{1}{2}l'+2\right) w(6) + \sum_{l=8,\,10,\ldots,\,20} \left(\frac{1}{2}l'+l-2\right) R(l)\, w(l) \Bigg] \qquad \text{(A.10)}
\end{aligned}$$

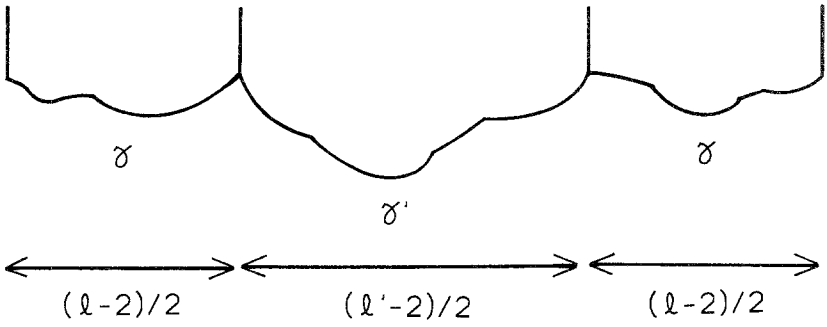

Fig. 4. Two possibilities for the location of a walk γ which intersects the walk γ'. The numbers shown lead to an upper bound on the number of possible locations for the boundary bonds in γ.

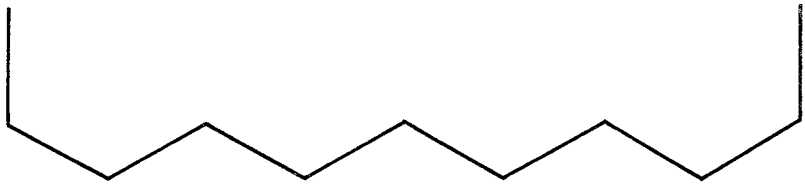

Fig. 5. The "worst" loop γ' which can occur in case 7.

Recall that $a(\gamma') = \varepsilon l'$, so factors of $l'/a(\gamma')$ equal $1/\varepsilon$. Since $l' \geqslant 7$, factors of $1/a(\gamma')$ are bounded by $1/7\varepsilon$. Then we e aluate our bound and find 0.8563 for the right side of (A.10).

Case 7. $\gamma' \in \mathscr{L}_{>6}$. The number of $\gamma \in \mathscr{L}_l$ which intersect γ' is bounded by $l'N(l)$ for $l = 6, 10, \ldots$.

For odd $l = 3, 5, \ldots, 19$ the number of $\gamma \in \mathscr{W}_l$ which intersect γ' is bounded by $Q(l)$. For $l > 20$, the number of $\gamma \in \mathscr{W}_l$ which intersect γ' is bounded by $l'P_i(l)$, since γ' contains only interior bonds.

In counting the number of $\gamma \in \mathscr{W}_l$ which intersect γ' for even γ, the worst γ' is shown in Fig. 5. For $l = 4$ and 6 the number of $\gamma \in \mathscr{W}_l$ which intersect γ' is bounded by $l'/4 + 1/2$ and by $l'/4 + 3/2$, respectively. As in the previous case, we consider the possible locations of the rightmost boundary bond in γ. The number of possible locations for this bond can be bounded by drawing a figure similar to Fig. 4. The resulting bound is

$$\tfrac{1}{2}(l-2) + \tfrac{1}{4}(l'-6) + \tfrac{1}{2}(l-2) + 1 = \tfrac{1}{4}l' + l - \tfrac{5}{2}$$

Table VI. Number of Lines Hitting a Fixed Bond in the Boundary and Returning to the Boundary to the Left of the Fixed Bond[a]

l	$R(l)$
4	1
6	1
8	4
10	9
12	26
14	75
16	215
18	649
20	1943

[a] The corner is infinitely for away.

Hence the number of $\gamma \in \mathscr{L}_l$ which intersect γ for even $l = 8, 10, ..., 20$ may be bounded by $(\frac{1}{4}l' + l - \frac{5}{2})\, R(l)$. Table VI shows values of $R(l)$.

Thus, we have

$$\begin{aligned}
&\sup_{\gamma' \in \mathscr{L}_{>7}} \frac{1}{a(\gamma')} \sum_{\gamma : \gamma \cap \gamma' \neq \varnothing} |W(\gamma)|\, e^{a(\gamma)} \\
&\quad \leqslant \frac{1}{a(\gamma)} \Bigg[l' \sum_{l=6, l \text{ even}} N(l)\, w(l) + \sum_{l=3,5,\ldots,19} Q(l)\, w(l) \\
&\qquad + l' \sum_{l=21}^{\infty} P_l(l)\, w(l) + \left(\frac{1}{4} l' + \frac{1}{2}\right) w(4) \\
&\qquad + \left(\frac{1}{4} l' + \frac{3}{2}\right) w(6) + \sum_{l=8,10,\ldots,20} \left(\frac{1}{4} l' + l - \frac{5}{2}\right) R(l)\, w(l) \Bigg]
\end{aligned}$$

which evaluates to 0.5937.

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