

Valence Bond Ground States in a Frustrated Two-Dimensional Spin-1/2 Heisenberg Antiferromagnet

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Abstract. We study a class of two-dimensional spin-1/2 Heisenberg antiferromagnets, introduced by Klein [1], in which the nearest-neighbor term is supplemented by next-nearest-neighbor pair and four-body interactions, producing additional frustration. For certain lattices, including e.g. the hexagonal lattice, we prove that any finite subset which admits a dimer covering has a ground state space spanned by valence bond states, each of which consists only of nearest-neighbor (dimer) singlet pairs. We also establish linear independence of these valence bond states. The possible relevance to resonating-valence-bond theories of high-temperature superconductors is briefly discussed. In particular, our results apply both to regular subsets of the lattice and to subsets with static holes.

I. Introduction

The purpose of this paper is to provide a concrete realization of short-ranged valence-bond state in a two-dimensional spin-1/2 Heisenberg antiferromagnet. Since this work is motivated by recent theories of high-temperature superconductivity, we will begin by presenting a brief review of the relevant theories, and, in particular, the resonating-valence-bond (RVB) approach [2]. We will then describe the model we consider and our results.

(a) *High-Temperature Superconductors and the RVB State.* The mechanism for high-temperature superconductivity in materials such as $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ and $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ is a subject of current interest. A host of theories have been proposed. These range from modifications of conventional, phonon-mediated BCS theory [3] to more exotic theories in which the electron-pairing mechanism is based not on phonons, but on excitons [4,5] or on antiferromagnetism

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[2, 6–31, 43–46, 48–51, 53–59]. Although many careful experiments have been performed, the interpretations are often contradictory and hence do not provide conclusive evidence for a particular mechanism.

Among the theories based on an antiferromagnetic mechanism, a good deal of work has concerned the resonating-valence-bond pictures [2, 6–9, 12–14, 16, 18–24, 29, 53, 56, 57]. Here one assumes that a typical copper-oxide plane of the undoped insulator (e.g. La_2CuO_4) is described by a (single-band) half-filled Hubbard model with large repulsion energy U . This is then roughly approximated [32, 33] by a two-dimensional spin-1/2 Heisenberg antiferromagnet with Hamiltonian

$$\mathcal{H} = \sum_{\langle i,j \rangle} J \mathbf{s}_i \cdot \mathbf{s}_j, \quad (1.1)$$

where the nearest-neighbor coupling is related to the standard Hubbard parameters via $J = 4t^2/U$. In the simplest version of the theory, planes of the doped material are described by a Hubbard model off half-filling; in the large U limit, one studies a Heisenberg antiferromagnet with (dynamic) holes.

The first step in this theory is a characterization of the ground state properties of the undoped insulator and hence of two-dimensional spin-1/2 Heisenberg antiferromagnets. Although much recent work has focused on the nature of the ground state in the pure nearest-neighbor model (1.1), it is useful to consider a larger class of short-ranged two-dimensional spin-1/2 Heisenberg antiferromagnets, with additional-neighbor couplings and possibly also local higher-body interactions. Such Hamiltonians can be obtained as the large U approximations to single-band Hubbard models with additional-neighbor couplings or as approximations to two-band Hubbard models. In the space of all such Hamiltonians, one can conceive of at least three distinct types of ground states. First, the ground state could be Néel-ordered, by which we mean a state with broken spin-rotational and translational symmetries. The Néel state is gapless to spin excitations. Second, the ground state could be what is called a quantum-spin-solid or spin-Peierls state: by this we mean a “crystalline” state with more than one spin per unit cell (i.e. a state with broken translational symmetry), but with spin-rotational symmetry. The quantum-spin-solid has a gap to spin excitations. Finally, the ground state could be a quantum-spin-liquid state, by which we mean a disordered state with both translational and spin-rotational symmetries. Some time ago, Anderson [34, 35] proposed a quantum-spin-liquid state in the form of a so-called resonating-valence-bond state: a superposition of wavefunctions in which each spin is singlet paired to another spin, this pair being represented graphically by a “valence bond.” Implicit in many RVB theories of high-temperature superconductivity is the assumption that there are short-ranged two-dimensional spin-1/2 Heisenberg antiferromagnets with quantum-spin-liquid ground states. In this paper, we take the first steps in addressing the question of existence of such states.

Let us briefly review what is known about one-dimensional spin-1/2 Heisenberg antiferromagnets. The exact solution of the nearest-neighbor spin chain gives a gapless ground state with power-law decay of correlations [67, 36, 68]. Due to some rather peculiar properties of one dimension, this state has been interpreted in various fashions. First, the state is in some sense as close to a Néel-ordered

state as is possible, given the constraints of one dimension; in particular, the magnetic susceptibility has been calculated [69] and is consistent with this interpretation. On the other hand, this state has recently been identified as a one-dimensional analogue of the quantum-spin-liquid states described above [2]. Finally, it is also worth noting that this state dimerizes—i.e. forms nearest-neighbor valence bonds—in a weak dimerizing field; the field exponent for the dimerization susceptibility has been calculated by a mapping to a continuum model [70, 71]. Another one-dimensional model, the Majumdar-Ghosh model [64], has antiferromagnetic next-nearest-neighbor and higher-body terms, in addition to the nearest-neighbor Heisenberg term (1.1). The ground states of this model have two spins per unit cell [64] and a gap to spin excitations [60], and thus may be interpreted as one-dimensional crystalline states.

In two dimensions, there is increasing evidence for a Néel-ordered ground state in the spin-1/2 nearest-neighbor Heisenberg antiferromagnet (1.1). Early diagonalizations [42] of small systems (16 sites) indicated long-range order. This result is supported by more recent work based on variational calculations [43–47], Monte Carlo simulations [48–50], and series expansions [51]. There is also recent evidence for two-dimensional order based on a sophisticated theoretical analysis [26] of the results of neutron scattering experiments on La_2CuO_4 .

The above evidence, of course, does not preclude quantum-spin-liquid ground states in two-dimensional spin-1/2 Heisenberg antiferromagnets with additional interactions, although, to our knowledge, there have been no previous attempts to rigorously identify such states. On the other hand, it is worth noting that two-dimensional *higher-spin* antiferromagnets, introduced by Klein [1] as generalizations of the Majumdar-Ghosh model [64], do have ground states which satisfy our definition of a quantum-spin-liquid. The ground state of the two-dimensional higher-spin Klein model has both spin-rotational and translational symmetries [1], and (on the hexagonal lattice) has recently been shown to have both a spectral gap and a gap to spin excitations [60]. Although the ground state appears ordered in the set of variables defined by Klein [1], it is disordered in the original spin variables.

In this work, we seek to identify RVB-type quantum-spin-liquid ground states in the space of two-dimensional spin-1/2 Heisenberg antiferromagnets. In this regard, it is important to note that the term RVB has been used to designate two macroscopically distinct quantum-spin-liquid states: 1) the original RVB state, or short-ranged RVB, and 2) the newer, long-ranged RVB. The short-ranged RVB consists of a linear superposition of short-ranged valence-bond states, of which a superposition of only nearest-neighbor valence-bond states is the prototypical example. This state corresponds closely to the chemist's notion of an RVB state [36, 37]. It has been studied in the context of magnetism by Anderson [34, 35] and others [38], and specifically in the context of superconductivity by several groups [6, 12, 16, 18–22, 29]; the present work concerns only the short-ranged RVB state. The majority of work on RVB superconductors is based on the longer-ranged RVB states [2, 7–9, 13, 14, 23, 24]. Here one begins with a superposition of wavefunctions in which states with valence bonds of all lengths make significant contributions. However, the relative coefficients of these wavefunctions are

generally not specified explicitly. Thus one often distinguishes short- and long-ranged RVB states not on the basis of the length of their valence bonds, but instead on the basis of the expected behaviors of their correlation functions: the former is believed to have exponentially falling spin–spin correlation functions and, presumably, a gap to spin excitations [29, 34, 35, 6, 12], while the latter is expected to be gapless and have power-law correlations [7].

It is worth noting that although the RVB state was proposed as an alternative to a Néel ordered state, it is not the case that RVB states and Néel ordered states are mutually exclusive. Indeed, it is rather clear (and, in fact, easy to prove) that all wavefunctions composed of valence bonds of arbitrary length span the singlet sector; since the ground state of the Hamiltonian (1.1) lies in this sector [39–41], it certainly can be expressed as a superposition of some set of valence-bond states. Thus, the question of a long-ranged RVB states vs. a Néel ordered state is rather subtle; it is not clear what restrictions on the distribution of long valence bonds ensure the absence of Néel order. On the other hand, the number of nearest-neighbor valence-bond states [62, 63] is substantially less than the total number of singlet states. Thus the statement that the ground state of a particular model consists only of nearest-neighbor valence-bond states is certainly a stronger statement than simply the fact that it is a singlet.¹ Of course, even this does not rigorously settle the question of a short-ranged RVB state vs. Néel order, although it is widely believed that a state composed exclusively of wavefunctions with finite-range valence bonds will not have long-range magnetic order.

Assuming that quantum-spin-liquid RVB states do exist, many workers agree that they provide a good starting point for the analysis of high-temperature superconductivity. As originally argued by Anderson [2], a quantum-spin-liquid of singlets provides a reservoir of preformed Cooper pairs; the charged vacancies corresponding to the dopant may have a natural tendency to undergo Bose condensation, yielding a superconducting state [6]. Beyond these basic points, there is controversy even among the proponents of an RVB picture: assuming the existence of an RVB ground state, there are serious disagreements concerning the nature of this state, as well as the exact mechanism for Bose condensation. In this regard, it should be noted that even a Néel ordered ground state does not preclude all RVB explanations: if Néel order exists but is tenuous, it can be broken either by factors which have not yet been incorporated in the ground state description of the insulator or by the introduction of dopant. For example, Anderson and collaborators [8] have argued that a small concentration of dopant would favor the RVB state, since according to the work of Brinkman and Rice [52], holes have low kinetic energy in the antiferromagnetic state (see, however, [53–59]).

Given the large body of work on resonating-valence-bond descriptions, it is of interest to know whether a (short-ranged) quantum-spin-liquid is an appropriate description of the ground state in some reasonable two-dimensional spin-1/2 Heisenberg antiferromagnet. For this purpose, it is useful to reconsider the

¹ In fact, it is not difficult to prove that the space spanned by all valence bonds states with valence bonds of any given finite range is a strict subset of the singlet sector

conclusions of the original work on the RVB state [34, 35]. The arguments presented there for an RVB ground state in the pure Heisenberg antiferromagnet (1.1) were rather cautious; on the other hand, it was strongly argued that if additional frustration is introduced into the system, e.g. in the form of next-nearest-neighbor interactions, then the ground state should be RVB. In this paper, we consider a Hamiltonian introduced by Klein [1] (and described in subsection I.b below) which contains additional frustration. On certain lattices, we show that this Hamiltonian has a valence-bond ground state in the strongest sense: the ground state space is spanned by wavefunctions composed exclusively of valence bonds of length one, the so-called dimer states.

It is important at the outset to make clear the underlying philosophy of studying this model. The Klein model provides an analyzable point in what we expect is a large region of the ground-state phase diagram of short-ranged spin-1/2 quantum antiferromagnets: namely a region characterized by short-range valence-bond ground states, presumably without Néel order. However, this special point possesses symmetries which are not shared by “nearby” models, and which we believe to be responsible for its extensive ground state entropy. Classes of perturbations which break this symmetry in different fashions will presumably lead to distinct behaviors—i.e., the spin-1/2 Klein model is presumably a multicritical point. Thus, we expect that the low-lying states of nearby models should lie largely in the ground state subspace of the Klein Hamiltonian, so that they can be studied using first-order degenerate perturbation theory; the resulting dimer Hamiltonian provides a concrete analyzable model (see e.g. [21, 22]). For certain types of perturbations, it is likely that the ground state will be a coherent superposition of short-ranged valence-bond states, i.e. an RVB state. We therefore feel that the results of this paper provide a good starting point for the study of spin-1/2 quantum-spin-liquids, and thus also provide circumstantial evidence for those aspects of an RVB picture which rely on the assumption of quantum-spin-liquid ground states.

(b) *The Spin-1/2 Klein Model.* In a remarkable paper [1], Klein introduced a class of antiferromagnetic Heisenberg models with short-range interactions. By expressing the Hamiltonians as sums of projection operators onto various spin states, Klein obtained exact ground states for his models. Some of the Klein Hamiltonians had large enough spin, depending on the coordination number, to produce (essentially) unique ground states; these were recently investigated in the work of [60] where it was not realized that Klein had previously introduced the models and obtained the relevant ground states. Further work on the higher-spin Klein models is contained in [61]. The spin-1/2 models have an entirely different character: the extreme quantum limit produces substantial frustration in the system which manifests itself in a large degeneracy of ground states. It is the latter models which are of relevance to the RVB theories of high-temperature superconductivity.

The spin-1/2 Klein models are defined in some detail in Sect. II, to which the reader should refer for a more precise discussion. For the purposes of this introduction, consider a quantum spin-1/2 magnet on a finite lattice. The Klein Hamiltonian may be written in the form

$$\mathcal{H} = \sum_i \hat{h}_i, \quad (1.2)$$

where \hat{h}_i projects the set of spins at i and in its immediate neighborhood onto their maximum possible spin state. If z_i is the local coordination number (which for many lattices is a constant except near the boundary), this maximum possible spin state is just $S = z_i + 1/2$.

Surprisingly enough, the spin-1/2 Klein Hamiltonian (1.2) is in some sense close to the pure nearest-neighbor spin-1/2 Heisenberg antiferromagnet (1.1). Indeed, a straightforward calculation shows that the Hamiltonian (1.1) is the leading term of the Klein Hamiltonian. This term is supplemented by other antiferromagnetic finite-ranged pair interactions and local higher-body terms, all of which have coefficients of order unity. (See Eq. (2.6) for an explicit calculation on the hexagonal lattice.)

Now consider the dimer states which, by definition, are wavefunctions where every spin is singlet-paired to one of its nearest neighbors. These are trivially in one-to-one correspondence with the dimer coverings of the lattice. Furthermore, it is easy to show that the number of dimer coverings of a regular subset of a regular lattice (e.g. the square or hexagonal lattice) and the number of distinct ground states grow exponentially with the size of the system.²

Klein [1] proved the simple, but very nice result that all dimer states are ground states of the Hamiltonian (1.2). Indeed, (1.2) is a sum of non-negative operators, so that the energy of any state is bounded below by zero. On the other hand, a singlet pair between the site i and one of its nearest neighbors ensures that the collection of spins at i and its immediate neighborhood cannot be in their maximum spin state. Hence, on any dimer state, each term in (1.2) vanishes individually and the total energy achieves its lower bound.

The major question we address in this paper is whether the dimer states are the only ground states of the Klein Hamiltonian: i.e. do they span the ground state space? Clearly, only an affirmative answer would allow us to assert that any ground state is expressible as a linear combination of dimer states and hence a (dimer) RVB state. For certain lattices, e.g. the two-dimensional hexagonal lattice, we will show that this dimer RVB picture is indeed correct. However, the question is somewhat more subtle than it might initially seem in that the answer depends not only on the spin-1/2 nature of the particles, but also quite sensitively on the lattice geometry.

In our proof, it was required that the lattice be devoid of triangles: that is, if a and b are neighbors, there is no point c which is a neighbor of both a and b . This condition is important in the sense that the result does not hold on e.g. the

² The existence and non-triviality of (exponential) growth constants for both the number of dimer coverings and the number of independent ground states of the Hamiltonian (1.2) is easy to demonstrate for regular lattices. Obviously one must not be so perverse as to choose shapes which do not have a dimer covering, e.g. shapes with an odd number of sites. Similarly, devious sequences of shapes can be arranged which allow some dimer coverings, but severely inhibit the thermodynamic growth of their total number. Exact growth constants for the number of dimer coverings of various lattices were obtained some time ago by Fisher [62] and Kasteleyn [63]

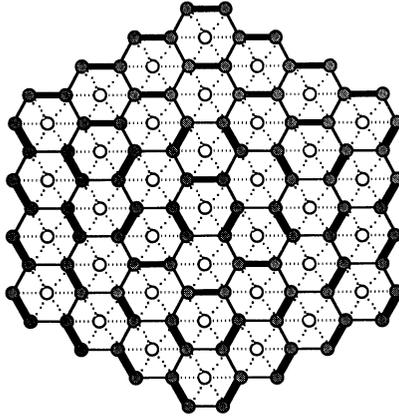


Fig. 1. A ground state of the triangular lattice

triangular lattice. To see this, regard the triangular lattice as a hexagonal lattice together with an extra site in the center of each hexagon, this site being connected to each of the six sites of the hexagon, thereby comprising a “hexagonal cell.” Now suppose that the lattice is generated in n stages by plating a single such cell with successive layers of cells. Then the n^{th} lattice can be viewed as n “rings” attached together by “spokes.” Each of these rings can be separately dimerized (in one of two ways), thus producing a complete dimer covering of the *hexagonal* portion of the lattice. (See Fig. 1.) However, the central spin of each hexagonal cell has at least one dimer in its neighborhood; thus, in the context of the Klein Hamiltonian is “free to do as it pleases.” In particular, these spins can be symmetrized—and thus we have a ferromagnetic ground state; or, perhaps even more disturbingly, they can be arranged to form a Néel state.

(c) *Results and Organization.* Our principal results concern the ground state space of the spin-1/2 Klein Hamiltonian (1.2) for arbitrary subsets of certain two-dimensional lattices, the most familiar example of which is the hexagonal lattice. Precise statements of our theorems for the hexagonal lattice are given at the end of Sect. II. Basically the results are:

- A) If the subset admits a dimer covering, then the set of all dimer states spans the ground state space.
- B) These dimer states are linearly independent (and hence form a basis for the ground state space).
- C) If the subset does not admit a dimer covering, then the ground state energy is strictly positive.

It should be noted that these results apply to arbitrary finite subsets, and therefore hold for the physically important case of lattices with (static) holes. Our conclusions make it seem plausible that the model has a gap to spin excitations, but we have not yet proved this. Another important open problem is the extension of result A to the infinite-volume system.

As explained earlier, results of the above type depend sensitively on lattice geometry. It is therefore not surprising that our proof is also tailored to the detailed lattice structure. The most important properties we use are relatively low coordination number and relatively large minimum loop size, although certain features are most easily handled on a case by case basis. In the Appendix, we extend the proofs of results A–C to other lattices including the two-dimensional octagonal-diamond lattice (depicted in Fig. 4) and the $2 \times N$ square strip. Although the strip is in some sense one-dimensional, it has many dimer coverings. In the Appendix, we also show that result B (linear independence of dimer states) holds for the two-dimensional square lattice.

Strictly one-dimensional results follow quite easily by our methods. In one dimension, the Klein Hamiltonian (1.2) reduces to the Majumdar-Ghosh (MG) model [64]. Here, the coordination number is sufficiently small that, even for spin-1/2, the ground state should be essentially unique (i.e. have at most a degeneracy of 0(1)). Such a result was recently proved for the open-chain MG model with particular boundary conditions [60]. Since both open chains and periodic chains are subsets of the hexagonal lattice, results A–C apply directly to these cases.

The remainder of this paper is organized as follows: In Sect. II, we give precise definitions and a statement of our results for the hexagonal lattice. In Sect. III, we provide a proof of these results, prefaced by a subsection on the strategy of the proof. Other lattices are treated in the Appendix.

II. Notation, Definitions and Statement of Results

Let Λ denote a finite lattice of points, which for most purposes we will take to be a subset of a regular two-dimensional lattice. In any case, certain pairs of points, $i, j \in \Lambda$, are deemed to be neighbors; this may be represented by drawing an edge joining the sites i and j . Without loss of generality, we will take Λ to be (edge) connected in the sense that if $i_1, i_k \in \Lambda$, there are points $i_2, \dots, i_{k-1} \in \Lambda$ such that $(i_1, i_2), (i_2, i_3), \dots, (i_{k-1}, i_k)$ are neighboring pairs. For each $i \in \Lambda$ we define the neighborhood of i , denoted by $\mathcal{N}(i)$, as the set consisting of i and all points which are neighbors of i . Thus if z_i is the local coordination number, then $|\mathcal{N}(i)| = z_i + 1$.

On each $i \in \Lambda$, we place a spin-1/2 particle: that is, a copy, \mathfrak{H}_i , of the two-dimensional vector space \mathbb{C}^2 . We will use the notation $\alpha(i)$ (spin up) and $\beta(i)$ (spin down) for an orthonormal basis of \mathfrak{H}_i . As a linear basis for the operators on \mathfrak{H}_i , we may take the unit operator and the usual Pauli spin matrices (generators of $SU(2)$) s_i^x, s_i^y and s_i^z . In this work, however, we will have essentially no need for an explicit representation of these quantities.

The Hilbert space associated with the full lattice is given by the tensor product

$$\mathfrak{H}_\Lambda \equiv \bigotimes_{i \in \Lambda} \mathfrak{H}_i. \quad (2.1)$$

Operators on \mathfrak{H}_Λ will be written as sums of products of various operators on the \mathfrak{H}_i ; necessary unit operators will be implicitly understood and omitted. For example, s_i^z is notation for the operator $\mathbb{1} \otimes \mathbb{1} \otimes \dots \otimes s_i^z \otimes \dots \otimes \mathbb{1}$.

A Hamiltonian on \mathfrak{H}_Λ is any self-adjoint operator. For the undoped magnet, the Hamiltonian has the translation symmetry of the underlying lattice (modulo boundary effects). However, in the presence of static holes, the appropriate Hamiltonian is not translationally invariant. Here we consider the general case.

Given a Hamiltonian \mathcal{H} , the energy of a $\psi \in \mathfrak{H}_\Lambda$ is given by

$$\frac{\langle \psi | \mathcal{H} \psi \rangle}{\langle \psi | \psi \rangle}. \quad (2.2)$$

A ground state is any $\psi \in \mathfrak{H}_\Lambda$ (usually already normalized) which minimizes (2.2).

The spin-1/2 Klein Hamiltonian [1] is constructed as follows: For any $\Phi \subset \Lambda$, let \mathbb{P}_Φ^\dagger denote the projection onto the maximum spin state of \mathfrak{H}_Φ . We take

$$\mathcal{H}_\Lambda = \sum_{i \in \Lambda} \mathbb{P}_{\mathcal{N}(i)}^\dagger \equiv \sum_{i \in \Lambda} \hat{h}_i \quad (2.3)$$

for the Hamiltonian on Λ .

As discussed in the introduction, \mathcal{H}_Λ is a sum of projection operators; thus it is clear that the energy of any $\psi \in \mathfrak{H}_\Lambda$ is non-negative. Indeed, for all i , the energy at i , $\langle \psi | \hat{h}_i \psi \rangle / \langle \psi | \psi \rangle$, is non-negative. However, if neighboring spins are in a singlet state, it is impossible that the total spin of the neighborhood assumes its maximum value. Thus the energy for both sites will vanish. For many lattices (those which admit a dimer covering) zero energy can be achieved in this fashion at all sites [1]. Hence it is possible to explicitly construct ground states for the Hamiltonian (2.3).

Remark. As is apparent, the ‘‘boundary conditions’’ we impose force each site to respect the local definition of neighborhood. It is for this and only this choice that we establish our results. In fact, when \mathcal{H}_Λ is of the form (2.3) but the lattice has periodic boundary conditions, one can often demonstrate the existence of additional ground states.

The above projections can, of course, be written explicitly in terms of the spin operators. Indeed, for general $\Phi \subset \Lambda$, let us denote by \mathbf{S}_Φ the spin vector

$$\mathbf{S}_\Phi = \left(\sum_{i \in \Lambda} s_i^x, \sum_{i \in \Lambda} s_i^y, \sum_{i \in \Lambda} s_i^z \right). \quad (2.4)$$

The operator S_Φ^2 has eigenvalues $(s)(s+1)$, $s = \frac{1}{2}|\Phi|, \frac{1}{2}|\Phi|-1, \dots$, according to the size of the spin. To project onto the maximum spin state, one need only kill off the lower sectors in succession. For example, if $|\Phi|$ is even, \mathbb{P}_Φ^\dagger is given by the expression

$$\mathbb{P}_\Phi^\dagger = \text{Const.} [S_\Phi^2] [S_\Phi^2 - 2] \cdots [S_\Phi^2 - \frac{1}{2}|\Phi| (\frac{1}{2}|\Phi| - 1)]. \quad (2.5)$$

Performing this calculation for the hexagonal lattice and resumming, the result for interior sites is:

$$C_1 \mathcal{H} = C_2 + \sum_{\langle i,j \rangle} \mathbf{s}_i \cdot \mathbf{s}_j + \frac{1}{2} \sum_{\langle\langle i,j \rangle\rangle} \mathbf{s}_i \cdot \mathbf{s}_j + \frac{2}{5} \sum_{\substack{\langle i,j \rangle: \\ \|i-k\| = \|j-r\| = 1; \\ j \neq k \neq r}} (\mathbf{s}_i \cdot \mathbf{s}_j)(\mathbf{s}_k \cdot \mathbf{s}_r), \quad (2.6)$$

with $C_1 > 0$ and C_2 irrelevant constants. Here, the first and third sums are over all

nearest-neighbor pairs $\langle i, j \rangle$, and the second is over all next-nearest neighbor pairs $\langle\langle i, j \rangle\rangle$. In the above, \mathcal{H} is exhibited as a familiar type of local Heisenberg Hamiltonian. It is highly frustrated and predominantly antiferromagnetic.

What is crucial to the mathematical analysis of this problem is not so much the size of the spin, but the degree of symmetry that various spin states enjoy. In particular, the highest spin state for a collection of particles is the state of complete symmetry. Thus, \hat{h}_i can also be expressed as the symmetrizer (i.e. sum over permutations) for the neighborhood of i . Since this perspective turns out to be useful, we will pause to introduce some relevant notation. Consider first the two-site problem, i.e. suppose that $\psi \in \mathfrak{H}_i \otimes \mathfrak{H}_j$. We use \mathbb{E}_{ij} to denote the exchange operator:

$$\mathbb{E}_{ij}\psi(i, j) = \psi(j, i). \quad (2.7)$$

(Thus ψ is symmetric if $\mathbb{E}_{ij}\psi = \psi$ and antisymmetric if $\mathbb{E}_{ij}\psi = -\psi$.) The symmetrizer for ψ is just

$$\mathbb{S}_{ij}\psi \equiv (1 + \mathbb{E}_{ij})\psi, \quad (2.8)$$

while

$$\mathbb{A}_{ij}\psi \equiv (1 - \mathbb{E}_{ij})\psi \quad (2.9)$$

is the antisymmetrizer. Notice that we have omitted the customary factor of $\frac{1}{2}$.

Usually one can symmetrize or antisymmetrize whole collections: The symmetrizer for three particles is simply

$$\mathbb{S}_{ijk} = \mathbb{S}_{ij}(1 + \mathbb{E}_{ik} + \mathbb{E}_{jk}), \quad (2.10)$$

and, in general,

$$\mathbb{S}_{\phi \cup \{k\}} = \mathbb{S}_{\phi} \left(1 + \sum_{j \in \phi} \mathbb{E}_{jk} \right). \quad (2.11)$$

For antisymmetrizers, analogous formulas may be written down with the \mathbb{E}_{nm} replaced by $-\mathbb{E}_{nm}$. However, for spin = 1/2, things can only go as far as two particles: for two particles, there is a unique antisymmetric function; antisymmetrization (sometimes called alternation) with additional particles will destroy the wavefunction.

The above notation allows yet another expression for the Hamiltonian (2.3):

$$\mathcal{H}_A = \sum_i \lambda_{\mathcal{N}(i)} \mathbb{S}_{\mathcal{N}(i)}, \quad (2.12)$$

where the $\lambda_{\mathcal{N}(i)} = 1/|\mathcal{N}(i)|!$ are unimportant constants. The obvious fact that wavefunctions which are antisymmetric on i and some $j \in \mathcal{N}(i)$ have zero energy at the site i can now be expressed in a different—but of course equivalent—language.

Since, as mentioned above, there is only one (independent) antisymmetric function between any pair of spin-1/2 sites, it pays to have explicit notation. We thus define

$$\zeta_{ij} \equiv \frac{1}{\sqrt{2}} [\alpha(i)\beta(j) - \beta(i)\alpha(j)]. \quad (2.13)$$

Evidently, if $\psi \in \mathfrak{S}_\Lambda$ is antisymmetric on $i, j \in \Lambda$, then ψ may be factored into

$$\psi = \zeta_{ij}\phi, \quad (2.14)$$

where $\phi \in \mathfrak{S}_{\Lambda \setminus (i,j)}$. Thus, it is seen that antisymmetrization of a wavefunction ψ —that is, operating on ψ with $\frac{1}{2}\mathbb{A}_{ij}$ —is a projection which amounts to the contraction of ψ with ζ_{ij} , thereby obtaining a $\phi \in \mathfrak{S}_{\Lambda \setminus (i,j)}$, and “multiplication” of said ϕ with ζ_{ij} . The latter perspective is not only of conceptual value; it is essential for performing calculations.

According to (2.14), we may (modulo a phase) graphically represent any wavefunction known to be antisymmetric on a pair (i, j) by drawing a bond between i and j ³. Fully bonded graphs, G , i.e. graphs where each i is paired to some j , are thus in one-to-one correspondence with the valence bond states, ψ_G , which are antisymmetric on all $(i, j) \in G$. It is also seen that these graphs have zero total spin. Bonds between neighbors will hereafter be called *dimers*. A fully bonded graph on Λ composed entirely of dimers will be called a dimerization of Λ , and will typically be denoted by Δ . The corresponding wavefunction, ψ_Δ , is a zero-energy state of the Hamiltonian \mathcal{H}_Λ defined in (2.3).

It is worth observing that if Δ is a dimerization of Λ , and b is any bond of Δ , then $\Delta \setminus b$ is a dimerization of $\Lambda \setminus b$. Writing ψ_Δ as $\zeta_b \phi_{\Delta \setminus b}$, it is seen that $\phi_{\Delta \setminus b}$ is a zero-energy wavefunction for the “reduced” Hamiltonian $\mathcal{H}_{\Delta \setminus b}$. The above turns out to be a general property of zero-energy wavefunctions of the \mathcal{H}_Λ on “untriangulated” lattices⁴: that is, for any zero-energy wave-function of \mathcal{H}_Λ which is antisymmetric on the bond b , the piece that lives on $\Delta \setminus b$ is also a zero-energy wavefunction according to the Hamiltonian $\mathcal{H}_{\Delta \setminus b}$. This will be proved in Lemma 2. Interestingly, such a property fails for triangulated lattices, as does our theorem. However, for e.g. the hexagonal lattice, this is strongly suggestive of the possibility that such wavefunctions *must* be composed of dimer graphs which contain the bond b —our principal result. We conclude this section with a formal statement of what we ultimately derive:

Theorem A. *Let \mathbb{H}_2 denote the two-dimensional hexagonal lattice and suppose that $\Lambda \subset \mathbb{H}_2$ is dimerizable. Let \mathcal{H}_Λ denote the Klein Hamiltonian (2.3) or (2.6), and define $\Omega_0 \equiv \Omega_0(\Lambda)$ to be the ground state subspace of \mathfrak{S}_Λ . Let $\mathcal{D} \equiv \mathcal{D}(\Lambda)$ denote the set of dimerizations of Λ and consider the space $\Omega_\mathcal{D}$ defined by*

$$\Omega_\mathcal{D} = \text{Span} \{ \psi_\Delta \mid \Delta \in \mathcal{D} \}.$$

Then $\Omega_0 = \Omega_\mathcal{D}$.

Theorem B. *For Λ , \mathcal{H}_Λ , $\mathcal{D}(\Lambda)$ defined as above, the functions*

$$\{ \psi_\Delta \mid \Delta \in \mathcal{D} \}$$

are linearly independent.

³ For the case of nearest-neighbor bonds on a bipartite lattice, a definite sign convention can be adopted by insisting that valence bonds “start” on red sites and “end” on black ones. Thus, a graphical representation of a wavefunction can be understood as a product of the corresponding ζ_{ij} with “ i ” the red site and “ j ” the black

⁴ An untriangulated lattice is a lattice with no triangles of nearest-neighbor sites

Theorem C. *If $\Lambda \subset \mathbb{H}_2$ does not admit a dimer covering, then the $\psi \in \Omega_0(\Lambda)$ have strictly positive energy.*

Remark. Note that even as stated, a special case of these results is a strictly one-dimensional chain, the so-called Majumdar-Ghosh (MG) model [64], with either free or periodic boundary conditions. Some results on the open-chain problem with different boundary conditions were obtained in [60] using different methods.

We believe that Theorems A–C hold under much more general circumstances. For certain reasons (some technical and others fundamental), we have had to focus on lattices with low coordination number and relatively long minimal loops. Although the hexagonal lattice is the most familiar lattice we can handle, in the Appendix we will establish Theorems A–C on the $2 \times N$ square strip and on the two-dimensional octogon-diamond lattice (depicted in Fig. 4). Unfortunately, due to various technical annoyances, we have, as yet, been unable to establish Theorems A and C for general subsets of the square lattice \mathbb{Z}^2 . (However, for this case, we can prove Theorem B.) At present, we are actively investigating this problem.

III. The Quantum Mechanics of Dimers

(a). *Strategy of the Proof.* As has been stated on several occasions, all dimer wavefunctions are ground states of the Hamiltonian (2.3), i.e. $\Omega_{\mathcal{D}} \subset \Omega_0$. Thus, to prove Theorem A, it is necessary to show that any zero-energy wavefunction has non-zero projection onto some dimer state. Formally: if $\psi \in \Omega_0$, $\psi \neq 0$, then $\exists \Delta \in \mathcal{D}$ such that $\mathbb{P}_{\Delta} \psi \neq 0$, where we have used the notation \mathbb{P}_{Δ} for projection onto ψ_{Δ} .

Due to the factorization property (2.14), it is seen that \mathbb{P}_{Δ} may be written as a product of commuting⁵ operators:

$$\mathbb{P}_{\Delta} = \prod_{b \in \mathcal{D}} \frac{1}{2} \mathbb{A}_b. \quad (3.1)$$

Thus a reasonable strategy is to project a $\psi \in \Omega_0(\Lambda)$ along some chosen bond and reduce the original problem to a similar one posed on a smaller lattice.

The initial step is straightforward. Indeed, if ψ has zero energy at some $i \in \Lambda$, then, by definition, ψ is not symmetric on $\mathcal{N}(i)$. It is therefore evident that one can find a $j \in \mathcal{N}(i)$ such that

$$\mathbb{A}_{ij} \psi \neq 0, \quad (3.2)$$

i.e. one can begin to dimerize any zero-energy wavefunction. After this first step, one may decompose:

$$\mathbb{A}_{ij} \psi = \zeta_{ij} \phi, \quad (3.3)$$

where ϕ is defined on the reduced lattice, and attempt to repeat the argument. In

⁵ If $b, b' \in \Delta$, $b \neq b'$, the projection operators which antisymmetrize on b and b' commute because they operate on disjoint coordinates

fact, if ψ had zero energy and $\psi \propto \mathbb{A}_{ij}\psi$, then ϕ would have zero reduced energy, i.e. $\mathcal{H}_{\Lambda \setminus \{i,j\}}\phi = 0$. (Cf. Lemma 2 for a proof.) Here one would be free to dimerize again.

Unfortunately, without substantial modification, the above program will soon run into trouble. Indeed, if ψ is not antisymmetric along the chosen bond, $\mathbb{A}_{ij}\psi$ will in general have positive energy at all the remaining neighbors of i and j . Let us illustrate this point with an explicit example. Consider a single hexagon and a wavefunction ψ given by

$$\psi = c_A \psi_A + c_B \psi_B \equiv c_A \begin{array}{c} 2 \\ \bullet \\ | \\ \bullet \\ 1 \end{array} + c_B \begin{array}{c} 2' \\ \bullet \\ / \quad \bullet \\ \bullet \quad \bullet \\ \backslash \quad \bullet \\ 3 \quad \bullet \\ 3' \end{array} + c_B \begin{array}{c} 2 \\ \bullet \\ / \quad \bullet \\ \bullet \quad \bullet \\ \backslash \quad \bullet \\ 1 \quad \bullet \\ 3 \quad \bullet \\ 3' \end{array} \quad (3.4)$$

where, as described in Sect. II, a bond between any pair of sites indicates antisymmetry of the wavefunction on that pair. Now any projection scheme must ultimately bond site 1 with one of its two nearest neighbors. However, it is easy to show that

$$\frac{1}{2} \mathbb{A}_{12} \psi = c_A \psi_A + \frac{1}{2} c_B \begin{array}{c} 2' \\ \bullet \\ | \\ \bullet \\ 3 \end{array} + \frac{1}{2} c_B \begin{array}{c} 2 \\ \bullet \\ | \\ \bullet \\ 3' \end{array} \quad (3.5)$$

while

$$\frac{1}{2} \mathbb{A}_{13} \psi = \frac{1}{2} c_A \begin{array}{c} 2 \\ \bullet \\ / \quad \bullet \\ \bullet \quad \bullet \\ \backslash \quad \bullet \\ 1 \quad \bullet \\ 3 \quad \bullet \\ 3' \end{array} + c_B \psi_B \quad (3.6)$$

In either case, the result is a positive energy wavefunction on the relevant reduced lattice. Thus an unadorned projection scheme in which the energy of the resulting wavefunction remains zero is not, in general, possible.

Nevertheless, projections of this sort are central to the problem at hand. The ultimate goal is to find a \mathbb{P}_Δ which does not destroy the candidate ψ . Given that any \mathbb{P}_Δ factors into its constituent bond operators, it is arguable that some form of a successive projection scheme must enter into a proof of Theorem A.

Positive energy does not, of course, preclude the possibility of continued projection; in fact, only unit energy (complete symmetry) at some site forces a halt to all these proceedings. However, unit energy will occur eventually (often on the last bond) if the candidate wavefunction is deviously constructed. In any case, a positive energy problem—even on a smaller lattice—is somewhat different than the original problem in which all site operators destroy the wavefunction.

Ideally, one would like to treat the problem of a zero-energy wavefunction on the reduced lattice, which as explained above will not, in general, occur after having antisymmetrized a $\psi \in \Omega_0(\Lambda)$ on any given bond. However, unless Theorem A is false, for each $j \in \Lambda$, there must be a bond b emanating from i such that $\mathbb{A}_b \psi$ is not orthogonal to all the zero-energy states of $\Lambda \setminus b$. Thus, defining $\mathcal{W}_{\Lambda \setminus b}^\circ$ to be the projection onto the zero-energy states of $\mathcal{H}_{\Lambda \setminus b}$ ⁶, one might consider using $\mathcal{W}_{\Lambda \setminus b}^\circ \mathbb{A}_b$ instead of \mathbb{A}_b as our fundamental bond projection operator. Indeed, such an operator would either

- i) destroy the wavefunction (indicating that a different bond should be tried); or
- ii) leave a zero-energy state (on $\mathfrak{S}_{\Lambda \setminus b}$), which is therefore in perfect condition for continued projection.

One can therefore envision finding a (sequential) dimerization (b_1, b_2, \dots, b_k) such that each of the successive operators of the above type does not destroy what remains of the wavefunction. Explicitly, let us define $\Lambda_1 \equiv \Lambda \setminus b_1$, $\Lambda_2 \equiv \Lambda_1 \setminus b_2, \dots, \Lambda_n \equiv \Lambda_{n-1} \setminus b_n$, etc. The above sentence amounts to the supposition that

$$\prod_n \mathcal{W}_{\Lambda_n}^\circ \mathbb{A}_{b_n} \psi \neq 0. \quad (3.7)$$

However, regardless of how plausible such a result may seem, it appears far removed from our original intention. Indeed, we had wanted to show

$$\mathbb{P}_\Delta \psi \equiv (\text{const}) \prod_n \mathbb{A}_{b_n} \psi \neq 0 \quad (3.8)$$

instead of (3.7), and the two expressions differ by the insertion of $\frac{1}{2}|\Lambda|$ highly nonlocal operators. Nevertheless, it can be shown (Proposition 1) that the two operators are identical; that is, if (b_1, b_2, \dots, b_k) is a dimerization Δ of Λ , then

$$2^{(1/2)|\Lambda|} \mathbb{P}_\Delta = \prod_n \mathcal{W}_{\Lambda_n}^\circ \mathbb{A}_{b_n}. \quad (3.9)$$

The spin-1/2 nature of this problem is essential in the proof of (3.9), since it enables us to decouple a singlet pair from the rest of the Hilbert space.

If the reader is prepared to accept Proposition 1 at face value, “all” that remains to be shown is that one can find a b such that $\Lambda \setminus b$ is dimerizable and that $\mathcal{W}_{\Lambda \setminus b}^\circ \mathbb{A}_b \psi \neq 0$. The question of dimerizability is easy for the lattices we consider (although it might require some work for lattices with large coordination number). The real issue is to show $\mathcal{W}_{\Lambda \setminus b}^\circ \mathbb{A}_b \psi \neq 0$; this is the subject of Propositions 3 and 4, with some help from Lemma 2. Roughly speaking, the key ingredient in these propositions is the construction of non-orthogonal projection operators which: (1) have non-zero projection onto the naively projected ψ , and (2) do not create positive energy. The latter property is demonstrated by considering all points in the vicinity of the antisymmetrized bond, and explicitly decomposing the wavefunction into

⁶ It is worth noting that this operator does not act on the coordinates of the bond b ; thus it has an interpretation as an operator on either the full or the reduced Hilbert space. We will use these two notions interchangeably in the hope that the relevant meaning will be clear from the context

its various symmetry types with respect to these points. The proof of Proposition 4 relies, technically, on certain properties of the hexagonal lattice.

After these results have been established, the formal proofs of Theorems A–C are easy corollaries.

(b) *The Dimer Ground State Space.* In this subsection, we prove Theorems A, B and C for arbitrary subsets of the hexagonal lattice. We will establish these results in a series of propositions, many of which hold in greater generality. Our starting point is to establish a fundamental result concerning the reaction of a zero-energy wavefunction to antisymmetrization. (See Sect. II for relevant notation and definitions.)

Proposition 1. *Let Λ denote any finite lattice which admits a dimer covering, and let Δ denote one such covering. Order the bonds of Δ in any desired fashion: (b_1, b_2, \dots, b_N) with $\bigcup_n b_n = \Delta$. Define $\Lambda_1 \equiv \Lambda \setminus b_1, \Lambda_2 \equiv \Lambda_1 \setminus b_2$, etc. Let \mathcal{H}_Λ denote the Klein Hamiltonian (2.3) on Λ and \mathcal{H}_{Λ_n} the (reduced) Klein Hamiltonian on Λ_n with boundary conditions as described in the Remark following (2.3). Finally, let $\mathcal{W}^\circ_{\Lambda_n}$ denote the projection onto $\Omega_0(\Lambda_n)$ (corresponding to the Hamiltonian \mathcal{H}_{Λ_n}). Then*

$$\prod_n \mathcal{W}^\circ_{\Lambda_n} \mathbb{A}_{b_n} = \prod_n \mathbb{A}_{b_n} \equiv 2^N \mathbb{P}_\Delta. \quad (3.10)$$

Proof. Observe that $\mathcal{W}^\circ_{\Lambda_n}$ and \mathbb{A}_{b_n} commute since they operate on disjoint coordinates. Indeed, for the same reason, whenever $m \geq n$,

$$[\mathcal{W}^\circ_{\Lambda_m}, \mathbb{A}_{b_n}] = 0, \quad (3.11)$$

since the Λ_m are even smaller than Λ_n . Thus we may bring all the antisymmetrizers to the rear, i.e.

$$2^{-N} \prod_n \mathcal{W}^\circ_{\Lambda_n} \mathbb{A}_{b_n} = 2^{-N} \prod_n \mathbb{A}_{b_n} \prod_n \mathcal{W}^\circ_{\Lambda_n} \equiv \mathbb{P}_\Delta \prod_n \mathcal{W}^\circ_{\Lambda_n}. \quad (3.12)$$

Hence if $\psi \in \mathfrak{H}_\Lambda$ is not destroyed by the above procedure, the result must be proportional to ψ_Δ .

Next observe that on ψ_Δ itself, all of the operators $\mathcal{W}^\circ_{\Lambda_n}$ and $2^{-1} \mathbb{A}_{b_n}$ act like the identity. Indeed, by definition, ψ_Δ is antisymmetric on each b_n , so these antisymmetrizers are tailor-made to do nothing. Furthermore, the restriction of Δ to any Λ_n (which may be regarded as $\Lambda \setminus (\{b_1, b_2, \dots, b_n\})$) is obviously a dimer covering of Λ_n . Hence the piece of ψ which lives on \mathfrak{H}_{Λ_n} represents a zero-energy state for \mathcal{H}_{Λ_n} , which implies $\mathcal{W}^\circ_{\Lambda_n} \psi_\Delta = \psi_\Delta$.

By the above reasoning, we have

$$2^{-N} \prod_n \mathcal{W}^\circ_{\Lambda_n} \mathbb{A}_{b_n} \psi_\Delta = \psi_\Delta, \quad (3.13)$$

so that

$$\left(2^{-N} \prod_n \mathcal{W}^\circ_{\Lambda_n} \mathbb{A}_{b_n} \right)^2 = 2^{-N} \prod_n \mathcal{W}^\circ_{\Lambda_n} \mathbb{A}_{b_n}. \quad (3.14)$$

Evidently, this operator is a projection with a one-dimensional range spanned by ψ_Δ . This does not yet prove that it is \mathbb{P}_Δ , because we have not established that it is an orthogonal (self-adjoint) projection. For the latter result, we need to show that for all ψ with $\psi \perp \psi_\Delta$, $\prod_n \mathcal{W}^\circ_{\Lambda_n} \mathbb{A}_{b_n} \psi$ is zero.

To this end, let $\psi \in \mathfrak{H}_\Lambda$ satisfy $\langle \psi | \psi_\Delta \rangle = 0$. Regardless of this condition, we know that

$$\prod_n \mathcal{W}^\circ_{\Lambda_n} \mathbb{A}_{b_n} \psi \propto \psi_\Delta; \quad (3.15)$$

let us call the constant of proportionality μ . Then

$$\mu = \left\langle \psi_\Delta \left| \prod_n \mathcal{W}^\circ_{\Lambda_n} \mathbb{A}_{b_n} \psi \right. \right\rangle = \left\langle \left(\prod_n \mathcal{W}^\circ_{\Lambda_n} \mathbb{A}_{b_n} \right)^\dagger \psi_\Delta \middle| \psi \right\rangle, \quad (3.16)$$

where “ \dagger ” denotes the Hermitian adjoint. However, the adjoint of $\prod_n \mathcal{W}^\circ_{\Lambda_n} \mathbb{A}_{b_n}$ is given by all the same factors written in reverse order (individually, they are all self-adjoint), each of which acts like the identity on ψ_Δ . Hence

$$\mu = \langle \psi_\Delta | \psi \rangle, \quad (3.17)$$

which vanishes by hypothesis. \square

Armed with this result, it is clear how we must proceed. Starting with our wavefunction ψ , we pick a site i and attempt to show that for some j which neighbors i , $\mathbb{A}_{ij} \psi$ is not orthogonal to the ground state space of the reduced lattice. Assuming this has been done, we denote the successful bond by b_1 , the reduced lattice, $\Lambda \setminus b_1$, by Λ_1 , define ψ_1 via

$$\mathcal{W}^\circ_{\Lambda_n} \mathbb{A}_{b_n} \psi = \zeta_{b_1} \psi_1, \quad (3.18)$$

and attempt to construct ψ_2 , etc.

This is obviously more manageable when the site i has as few neighbors as possible. In particular, the weak point of any subset of a regular lattice is found at the boundary. When $\Lambda \subset \mathbb{H}_2$, this is especially convenient since boundary sites are (by definition) not fully coordinated, and thus have at most two neighbors. (For the square lattice, we can also arrange a two-choice situation: we would choose, for example, the lowest, leftmost site, which clearly has no more than two neighbors.) Henceforth, we will only consider attacking in situations in which there are at most two bonds onto which we can project.

As we will see below, the easiest case is when the selected site has only a single neighbor in Λ —in these instances, our job is done. We will treat this case in two stages, since we will need the more substantive half (Lemma 2) for our later analysis.

Lemma 2. *Let Λ be any finite set which is devoid of triangles and let $\hat{h}_k \equiv \hat{h}_k(\Lambda)$ denote the site operators corresponding to the Klein Hamiltonian \mathcal{H}_Λ . Let (i, j) be a nearest-neighbor pair in Λ and suppose that $\psi \in \mathfrak{H}_\Lambda$ is antisymmetric on (i, j) . We write $\psi = \zeta_{ij} \phi$ with $\phi \in \mathfrak{H}_{\Lambda \setminus (i, j)}$. Consider the site operators \hat{h}_k , associated with the reduced Hamiltonian $\mathcal{H}_{\Lambda \setminus (i, j)}$. For those sites $k \in \Lambda \setminus (i, j)$ where ψ is annihilated by \hat{h}_k ,*

the corresponding reduced operators \hat{h}_k satisfy

$$\hat{h}_k \phi = 0.$$

Proof. The above is obvious unless $k \in \mathcal{N}(i)$ or $\mathcal{N}(j)$. Thus, we assume that $k \in \mathcal{N}(i)$, and consider only the non-trivial case $|A| > 3$.

We claim that the following identity is valid for spin-1/2: Let \mathbb{E}_{ij} , \mathbb{A}_{ij} etc. be exchangers and antisymmetrizers as defined in Sect. II. Then (for $i \neq j \neq k$)

$$\mathbb{A}_{ij} \mathbb{E}_{ik} \mathbb{A}_{ij} = \mathbb{A}_{ij}. \quad (3.19)$$

Indeed, observe that

$$\mathbb{A}_{ij} \mathbb{E}_{ik} \mathbb{A}_{ij} = -\mathbb{A}_{ij} \mathbb{E}_{ik} \mathbb{E}_{ij} \mathbb{A}_{ij}. \quad (3.20)$$

Now it is easy to verify that

$$\mathbb{E}_{ik} \mathbb{E}_{ij} = \mathbb{E}_{ij} \mathbb{E}_{jk}; \quad (3.21)$$

whence, substituting (3.21) into (3.20) and absorbing the $-\mathbb{E}_{ij}$ into the \mathbb{A}_{ij} on the left, we find that

$$\mathbb{A}_{ij} \mathbb{E}_{ik} \mathbb{A}_{ij} = \mathbb{A}_{ij} \mathbb{E}_{jk} \mathbb{A}_{ij}. \quad (3.22)$$

Thus, we may write

$$\mathbb{A}_{ij} \mathbb{E}_{ik} \mathbb{A}_{ij} = \frac{1}{2} \mathbb{A}_{ij} (\mathbb{E}_{ik} + \mathbb{E}_{jk}) \mathbb{A}_{ij}. \quad (3.23)$$

Adding and subtracting the identity from the term in the parentheses, we see that

$$\begin{aligned} \mathbb{A}_{ij} \mathbb{E}_{ik} \mathbb{A}_{ij} &= \frac{1}{2} \mathbb{A}_{ij}^2 - \frac{1}{2} \mathbb{A}_{ij} (1 - \mathbb{E}_{ik} - \mathbb{E}_{jk}) \mathbb{A}_{ij} \\ &\equiv \mathbb{A}_{ij} - \mathbb{A}_{ijk}. \end{aligned} \quad (3.24)$$

However, alternation on more than two particles results in the destruction of any spin-1/2 wavefunction; hence the identity (3.19).

Now for $k \in \mathcal{N}(i)$, the site operator of \mathcal{H}_A at k demands symmetrization on the full neighborhood of k —including i :

$$\hat{h}_k(A) \propto \mathbb{S}_{\mathcal{N}(k)}, \quad (3.25)$$

while on $A \setminus (i, j)$, i is no longer considered a neighbor of k :

$$\hat{h}_k(A \setminus (i, j)) \propto \mathbb{S}_{\mathcal{N}(k) \setminus i}. \quad (3.26)$$

Therefore our job is to show that $\mathbb{S}_{\mathcal{N}(k) \setminus i} \phi = 0$.

We start with the fact that ψ has zero energy for the original Hamiltonian, so that in particular

$$0 = \langle \psi | \mathbb{S}_{\mathcal{N}(k)} \psi \rangle. \quad (3.27)$$

Since ψ is assumed to be antisymmetric on i and j , (3.27) permits

$$0 = \langle \mathbb{A}_{ij} \psi | \mathbb{S}_{\mathcal{N}(k)} \mathbb{A}_{ij} \psi \rangle = \langle \psi | \mathbb{A}_{ij} \mathbb{S}_{\mathcal{N}(k)} \mathbb{A}_{ij} \psi \rangle. \quad (3.28)$$

Next, we use $\underline{\mathcal{N}}(k)$ as standing notation for the reduced neighborhood of $\mathcal{N}(k)$:

$$\underline{\mathcal{N}}(k) \equiv \mathcal{N}(k) \setminus i, \quad (3.29)$$

and rewrite the symmetrizer in Eq. (3.28):

$$0 = \left\langle \psi | \mathbb{A}_{ij} \left(\mathbb{1} + \sum_{m \in \mathcal{N}(k)} \mathbb{E}_{im} \right) \mathbb{S}_{\mathcal{N}(k)} \mathbb{A}_{ij} \psi \right\rangle. \quad (3.30)$$

Using the hypothesis that j does not belong to $\mathcal{N}(k)$, we may commute $\mathbb{S}_{\mathcal{N}(k)}$ and \mathbb{A}_{ij} ; this leaves us with

$$0 = \left\langle \psi | \mathbb{A}_{ij} \left(\mathbb{1} + \sum_{m \in \mathcal{N}(k)} \mathbb{E}_{im} \right) \mathbb{A}_{ij} | \mathbb{S}_{\mathcal{N}(k)} \psi \right\rangle. \quad (3.31)$$

However, by the formula derived previously (Eq. (3.19)), the term in the middle of (3.31) is proportional to \mathbb{A}_{ij} , which can be reabsorbed by $\langle \psi |$. Using the facts that $\mathbb{S}_{\mathcal{N}(k)}$ does not act (i.e. is the identity) on $\mathfrak{H}_i \otimes \mathfrak{H}_j$ and that ψ may be written as $\zeta_{ij} \phi$, the $\mathfrak{H}_{\Lambda \setminus (i,j)}$ statement of Eq. (3.31) may be expressed as

$$\langle \phi | \mathbb{S}_{\mathcal{N}(k)} \phi \rangle = 0. \quad (3.32)$$

Since $\mathbb{S}_{\mathcal{N}(k)}$ is (proportional to) an orthogonal projection operator, the above means $\mathbb{S}_{\mathcal{N}(k)} \phi = 0$, the desired result. \blacksquare

The single-choice scenario now follows easily:

Proposition 3. *Suppose that for some finite Λ there is an $i \in \Lambda$ which has only one neighbor, j . Then any $\psi \in \Omega_0(\Lambda)$ is antisymmetric on (i, j) . Furthermore, decomposing ψ according to*

$$\psi = \zeta_{ij} \phi$$

with $\phi \in \mathfrak{H}_{\Lambda \setminus (i,j)}$, ϕ has zero reduced energy, i.e.

$$\phi \in \Omega_0(\Lambda \setminus (i, j)).$$

Proof. If $\mathcal{N}(i)$ is simply the pair (i, j) , the site operator at i for \mathcal{H}_Λ is just a constant times \mathbb{S}_{ij} . Thus if ψ has zero energy, then in particular $\mathbb{S}_{ij} \psi = 0$, which means $\psi = \frac{1}{2} \mathbb{A}_{ij} \psi$. By Lemma 2, it is seen that all sites in $\Lambda \setminus (i, j)$ have zero reduced energy (i.e. as measured by the Hamiltonian $\mathcal{H}_{\Lambda \setminus (i, j)}$). We have evidently established, in these single choice situations,

$$\mathcal{W}_{\Lambda \setminus (i, j)}^\circ \frac{1}{2} \mathbb{A}_{ij} \psi = \psi,$$

as claimed. \blacksquare

Corollary. *For the open-chain Majumdar-Ghosh model with an even number of sites, the only dimer state is the only ground state.*

Proof. Applying Proposition 3, as we dimerize the chain from the left, it becomes evident that if ψ is a zero-energy state, then, up to a phase,

$$\psi = \prod_{j=1}^N \zeta_{2j-1, 2j}. \quad \blacksquare$$

As a consequence of Proposition 3, it is worthwhile, whenever possible, to rid the current lattice of any singly-connected sites and their neighbors. Assuming this

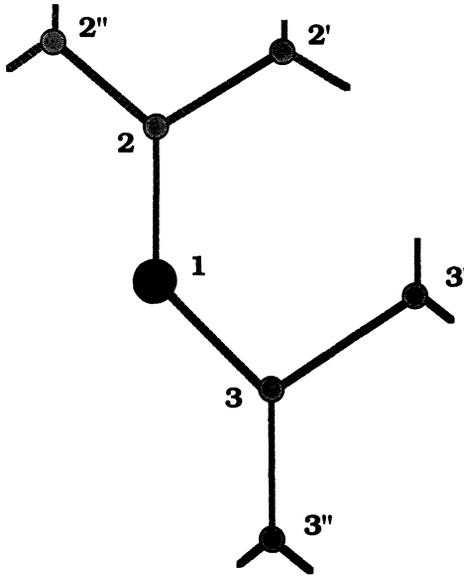


Fig. 2. Environment of site 1

has been done, we must face the two-choice problem: Here the result does not fall so easily.

Our procedure will be to define a pair of operators which allows us to decompose the current wavefunction into two pieces (one of which may vanish). These two quantities correspond to the two prospective directions in which we are allowed to project. Indeed, once Theorems A and B are rigorously established, the two wavefunctions can be identified as the dimer constituents of the current ψ which contain one or the other of the two possible bonds emanating from the chosen site. Regardless of this reinterpretation, Proposition 4 will establish that in the two-choice situations, we can define two functions, one for each of the choices, which:

- i) add up to the current wavefunction,
- ii) are antisymmetric along their respective bonds, and
- iii) have zero reduced energy on their respective reduced lattices.

From (i)–(iii), Theorem A is almost immediate. However the proof of (iii) is somewhat involved.

For the time being, we will drop the use of the word “current” when describing the partial wavefunction or what remains of the lattice; we will simply refer to these objects as ψ and Λ (and assume, of course that $\psi \in \Omega_0(\Lambda)$). To analyze the two-choice scenario on the hexagonal lattice, we will adopt the site labelling convention depicted in Fig. 2.

The two choices for the site 1 are, of course, the bonds (1, 2) and (1, 3). It need not be the case that all the secondary neighbors—2', 2'', 3' and 3''—are actually present. The other lattices we can treat (corresponding to the cases where $2' = 3'$

while 2'' and/or 3'' are absent) are in fact easier, but will nonetheless be dispensed with in the Appendix.

Proposition 4. *Let $\psi \in \Omega_0(\Lambda)$. Suppose that the site $1 \in \Lambda$ has the local configuration depicted in Fig. 2, with the possible absence of any of the secondary neighbors. Consider the operators $\mathbb{Y} \equiv \mathbb{A}_{12}\mathbb{S}_{13}$ and $\mathbb{Y}' \equiv \mathbb{A}_{13}\mathbb{S}_{12}$, and define the projected wavefunctions $\psi_{\mathbb{Y}} \equiv \frac{1}{3}\mathbb{Y}\psi$ and $\psi_{\mathbb{Y}'} \equiv \frac{1}{3}\mathbb{Y}'\psi$. Then*

$$(a) \quad \psi = \psi_{\mathbb{Y}} + \psi_{\mathbb{Y}'},$$

and either

$$\langle \mathbb{A}_{12}\psi | \psi_{\mathbb{Y}} \rangle \neq 0 \text{ or } \langle \mathbb{A}_{13}\psi | \psi_{\mathbb{Y}'} \rangle \neq 0$$

(or both).

(b) $\psi_{\mathbb{Y}}$ has zero reduced energy on $\Lambda \setminus (1, 2)$, while $\psi_{\mathbb{Y}'}$ has zero reduced energy on $\Lambda \setminus (1, 3)$. Explicitly, both of the relations

$$\mathcal{H}_{\Lambda \setminus (1,2)}\psi_{\mathbb{Y}} = 0$$

and

$$\mathcal{H}_{\Lambda \setminus (1,3)}\psi_{\mathbb{Y}'} = 0.$$

hold.

Remark. Observe that the \mathbb{Y} and \mathbb{Y}' are just the Young symmetrizers corresponding to the tableaux $\begin{array}{|c|c|} \hline 1 & 3 \\ \hline 2 & \\ \hline \end{array}$ and $\begin{array}{|c|c|} \hline 1 & 2 \\ \hline 3 & \\ \hline \end{array}$ respectively. This perspective is the cornerstone of our proof of Proposition 4.

Proof of Proposition 4(a). As is well-known [65, 66], the operators \mathbb{Y} and \mathbb{Y}' comprise the major part of a *resolution of the identity*; in general

$$\begin{aligned} \mathbb{1} &= \frac{1}{6} \begin{array}{|c|c|} \hline 1 & \\ \hline 2 & 3 \\ \hline \end{array} + \frac{1}{6} \begin{array}{|c|c|c|} \hline 1 & 2 & 3 \\ \hline \end{array} + \frac{1}{3} \begin{array}{|c|c|} \hline 1 & 3 \\ \hline 2 & \\ \hline \end{array} + \frac{1}{3} \begin{array}{|c|c|} \hline 1 & 2 \\ \hline 3 & \\ \hline \end{array} \\ &\equiv \frac{1}{6}\mathbb{A}_{123} + \frac{1}{6}\mathbb{S}_{123} + \frac{1}{3}\mathbb{Y} + \frac{1}{3}\mathbb{Y}', \end{aligned} \quad (3.35)$$

where $\frac{1}{6}$ and $\frac{1}{3}$ are unimportant constants. This particular resolution is constructed in [66]; it is simple enough to verify explicitly.

For spin-1/2, \mathbb{A}_{123} is zero. For $\psi \in \Omega_0$ we have, in particular, $\hat{h}_1\psi \propto \mathbb{S}_{123}\psi = 0$. Thus, we have established

$$\psi = \psi_{\mathbb{Y}} + \psi_{\mathbb{Y}'}. \quad (3.36)$$

Observe that if one of the \mathbb{Y} 's is the identity on ψ —which occurs when ψ is antisymmetric on the corresponding bond—then ψ is destroyed by the other symmetrizer. In general,

$$1 = \langle \psi | \psi_{\mathbb{Y}} \rangle + \langle \psi | \psi_{\mathbb{Y}'} \rangle, \quad (3.37)$$

so the terms cannot vanish simultaneously. Supposing e.g. that $\langle \psi | \psi_{\mathbb{Y}} \rangle \neq 0$, we have

$$\begin{aligned}
\langle \mathbb{A}_{12}\psi | \psi_{\mathbb{Y}} \rangle &\propto \langle \mathbb{A}_{12}\psi | \mathbb{A}_{12}\mathbb{S}_{13}\psi \rangle \\
&\propto \langle \psi | \mathbb{A}_{12}^2 \mathbb{S}_{13}\psi \rangle \\
&\propto \langle \psi | \psi_{\mathbb{Y}} \rangle \neq 0.
\end{aligned} \tag{3.38}$$

If $\langle \psi | \psi_{\mathbb{Y}} \rangle \neq 0$, the same reasoning holds. \blacksquare

The final job which lies ahead is to show that $\mathcal{H}_{\mathcal{A} \setminus (1,2)}\psi_{\mathbb{Y}}$ and $\mathcal{H}_{\mathcal{A} \setminus (1,3)}\psi_{\mathbb{Y}'}$ are both zero. For $|\mathcal{A}| \gg 1$, the majority of this statement is automatically true in the sense that for k not a neighbor of 1, 2, or 3, the energy operator (\hat{h}_k) has not changed in the lattice reduction and has not communicated with either of the Young operators. Hence, if $k \notin \mathcal{N}(1) \cup \mathcal{N}(2) \cup \mathcal{N}(3)$,

$$\hat{h}_k(\mathcal{A} \setminus (1, 2))\psi_{\mathbb{Y}} = \frac{1}{3}\hat{h}_k(\mathcal{A} \setminus (1, 2))\mathbb{Y}\psi = \frac{1}{3}\mathbb{Y}\hat{h}_k(\mathcal{A} \setminus (1, 2))\psi = \frac{1}{3}\mathbb{Y}\hat{h}_k(\mathcal{A})\psi = 0, \tag{3.39}$$

and the same applies for $\psi_{\mathbb{Y}'}$. There are, however, a modest number of sites which are potentially “hot”—including site 2 for $\psi_{\mathbb{Y}}$ and site 3 for $\psi_{\mathbb{Y}'}$. Since we can treat these primary cases fairly easily and without reference to the rest of the environment, we will attend to these sites immediately, and then deal with the secondaries.

Proof of Proposition (4b) for the sites 2 and 3. We define \hat{h}_3 to be the energy operator for site 3 associated with $\mathcal{H}_{\mathcal{A} \setminus (1,2)}$, and use an analogous definition for \hat{h}_2 . Here we will establish that

$$\hat{h}_3\psi_{\mathbb{Y}} = 0 \tag{3.40}$$

and

$$\hat{h}_2\psi_{\mathbb{Y}'} = 0. \tag{3.41}$$

However, only one of the above relations need be demonstrated explicitly since the two arguments are identical after relabelling.

We use the decomposition $\psi = \psi_{\mathbb{Y}} + \psi_{\mathbb{Y}'}$ and the fact that the original energy at site 3 is zero to obtain

$$\hat{h}_3\psi_{\mathbb{Y}} + \hat{h}_3\psi_{\mathbb{Y}'} = 0. \tag{3.42}$$

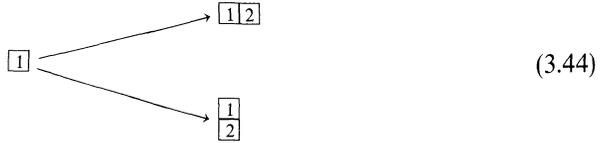
However, the leftmost operator of \mathbb{Y}' is antisymmetrization on the bond (1, 3), while the operator \hat{h}_3 contains the symmetrizer for the bond (1, 3), i.e.

$$\hat{h}_3 \propto \hat{h}_3 \mathbb{S}_{13}. \tag{3.43}$$

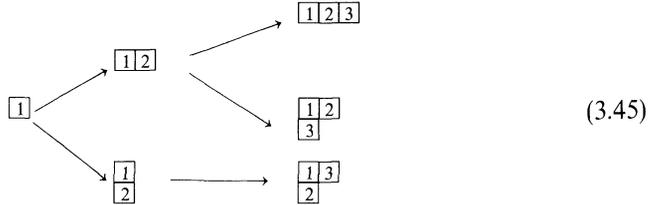
Thus $\hat{h}_3\psi_{\mathbb{Y}'} = 0$, which means that each term in (3.42) is individually zero.

We are now in a position to apply Lemma 2: $\psi_{\mathbb{Y}}$ is known to be antisymmetric on the sites 1 and 2 and has zero energy at site 3. It therefore has zero *reduced* energy at the site 3 and we have established (3.40). By the same reasoning, (3.41) holds. \blacksquare

An Interlude on Young Tableaux. It is tempting to write down a “complete set” of Young diagrams by ordering the relevant particles: (1, 2, 3, 4, ...) and constructing Young patterns via a binary tree. Explicitly, we start with \square , to which we can add \square in two ways:



Particle 3 can now be added in both possible ways on both possible diagrams; however, for spin-1/2, we cannot withstand more than two rows on any tableau:



At this stage, up to constants, we have achieved our previous three particle resolution. Continuing in this fashion, we develop a certain number of frames (that is, shapes) within which our particles have been placed in various patterns. The distinct frames correspond to different spin sectors and may be treated separately. (For example, we could decide on a different ordering of the particles.) However, within each sector, the various patterns do *not*, in general, sum up to a resolution of the identity (nor, in the context of the full space, to a projection onto the associated spin sector).

The reason for the above annoyance is completely obvious and relatively easy to fix up. In the authors' opinions, this deficiency is misleadingly understated in the standard textbooks. Let us illustrate in the case of interest, namely a collection of spin-1/2 particles. Suppose a given frame has K overhanging boxes on the top row. Then there are $(2K + 1)$ possible wavefunctions according to the possible values of S_z . Since the Young tableaux (as operators) preserve both S and S_z , we might just as well focus on a definite state of S_z (e.g. the maximal) within a given spin sector. Then there is a unique wavefunction which we can associate with a given pattern. This wavefunction (with $S_z = \frac{1}{2}K$) may be found either by directly reading the tableau—a singlet pairing on each column and an α for the remaining K particles which overhang—or, in what amounts to the same thing, operating on the entire $S = S_z = \frac{1}{2}K$ sector of the Hilbert space with the tableau and seeing what survives.

This procedure is satisfactory, in hindsight, because any given pattern (viewed as an operator) is a projection. It is not, however, an orthogonal projection. On the one hand, this necessitates the exercise of a certain amount of caution during manipulations; on the other, it makes these objects an appropriate vehicle for the valence bond descriptions of spin systems. Indeed, the valence bond wavefunctions are inherently non-orthogonal.

An elementary counting argument shows that, for a given sector, we have the right number of patterns. Let us call these patterns $\mathbb{Q}_1, \mathbb{Q}_2, \dots, \mathbb{Q}_L$, ordered from top to bottom as they emerged from the binary tree. We denote the associated wavefunctions by $\gamma_1, \gamma_2, \dots, \gamma_L$. It should be noted that, since the $\{\mathbb{Q}_j\}$ are not

orthogonal projections, even if they resolve the identity, it is not generally true that $\langle \gamma_i | \gamma_j \rangle = \delta_{ij}$. What we are looking for is the statement that

$$\mathbb{Q}_k \gamma_j = \delta_{jk} \gamma_j \quad (3.46a)$$

or, equivalently,

$$\mathbb{Q}_j \mathbb{Q}_k = \delta_{jk} \mathbb{Q}_j. \quad (3.46b)$$

If (3.46) were to hold, the $\{\mathbb{Q}_j\}$ would manifestly result in a resolution of the identity. Indeed, this would immediately establish linear independence of the $\{\gamma_j\}$ and, in particular, for ψ in the correct sector, one could write

$$\psi = \sum_j c_j \gamma_j \quad (3.47)$$

with

$$c_j = \langle \gamma_j | \mathbb{Q}_j \psi \rangle. \quad (3.48)$$

The $j = k$ piece of (3.46) is, of course, correct and it is not hard to see that for $k > j$, $\mathbb{Q}_j \mathbb{Q}_k = 0$. (The lower pattern will antisymmetrize some pair on which the upper pattern chose to symmetrize.) For $k < j$, $\mathbb{Q}_j \mathbb{Q}_k$ will in fact vanish for a small number of particles, but for five or more, $\mathbb{Q}_j \mathbb{Q}_k$ is usually non-zero.

However, given that (3.46) holds for $k \geq j$, it is not hard to construct operators which satisfy the desired relations for all k and j . These are:

$$\underline{\mathbb{Q}}_j = \mathbb{Q}_j \prod_{i < j} (1 - \mathbb{Q}_i), \quad (3.49)$$

where the product is ordered so that the operators of lower index operate first. It is easily verified that Eq. (3.46b) holds for the barred operators:

$$\underline{\mathbb{Q}}_j \underline{\mathbb{Q}}_k = \delta_{jk} \underline{\mathbb{Q}}_j, \quad (3.50)$$

while the original γ_j still enjoy $\underline{\mathbb{Q}}_j \gamma_j = \gamma_j$. The $\{\underline{\mathbb{Q}}_j\}$ will constitute our resolution of the identity.

Proof of Proposition (4b) for the secondary neighbors 2', 2'', 3' and 3''. We focus only on the site 3'; the fact that 3' does not include the site 2 in its neighborhood—a blessing of the hexagonal lattice—will enable a proof mutatis mutandis for the other secondaries. We denote by u and v the (possible) additional neighbors of the site 3'. As it turns out, the exact number of additional neighbors (if any) is quite unimportant. We are going to need a resolution of the identity for $\mathcal{N}(3')$ and sites 1 and 2, that is the set $\{1, 2, 3, 3', u, v\}$. However, the best ordering turns out to be $(1, 3, 2, 3', u, v)$.

As usual, it suffices to establish that $\hat{h}_3 \cdot \forall \psi = 0$ whenever $\psi \in \Omega_0(\Lambda)$, since this gets us the corresponding result on ψ_{\forall} , automatically. We do not, in the end, make use of the fact that ψ has zero energy at all sites. Indeed, we will prove the stronger statement that $\hat{h}_3 \cdot \forall \psi = 0$ whenever $\hat{h}_3 \cdot \psi = 0$ and $\hat{h}_1 \psi = 0$. Our method is as follows: We take any ψ in $\Omega_0(\Lambda)$ (or in what ultimately follows, with zero energy at sites 1 and 3') and resolve the identity of the collection $(1, 3, 2, 3', u, v)$ according to the previous discussion:

$$\psi = \sum_{j=1}^N \mathbb{Q}_j \psi. \tag{3.51}$$

We then demonstrate that for each j , $\hat{h}_3 \mathbb{Y} \mathbb{Q}_j \psi = 0$.

Many of the \mathbb{Q}_j will annihilate ψ because e.g. they lead off with symmetry operators that contain energy operators known to destroy ψ . On what remains, we hit, from the left, with $\hat{h}_3 \mathbb{Y}$. Armed with the hindsight of knowing which energy conditions are important—i.e. what particle groups to resolve—and how the particles must be ordered, the remaining $\mathbb{Q}_j \psi$ are taken out.

In contrast to the original tableaux, the composite operators are much too cumbersome to work with individually. However, if ψ belongs to some subspace \mathbb{G} and \mathbb{T} is any operator, it is easy to see that the relationship

$$0 = \mathbb{T} \mathbb{Q}_j \psi \tag{3.52}$$

is satisfied for all j when the following can be arranged:

- i) For $j = 1, 2, \dots, n$ each \mathbb{Q}_j destroys \mathbb{G} .
- ii) For $j = n + 1, \dots, N$ each \mathbb{Q}_j is destroyed by \mathbb{T} .

Our operator \mathbb{T} will, of course, be $\hat{h}_3 \mathbb{Y}$, and the relevant subspace will be wavefunctions with zero energy at sites 1 and 3'.

Let us begin by resolving up to the two particle stage:



We need not continue the bottom branch since all possible offspring operators contain (in the back) instructions to antisymmetrize on 1 and 3. When these are struck, from the left, with \mathbb{S}_{13} (the forefront of \mathbb{Y}), the consequence is zero. Continuing the top branch, we have:



By definition, $\overline{132}$ vanishes on any function with zero energy at site 1. Since all offspring of this diagram are at the beginning of the list, by i) we need not consider this branch any further. With regards to $\overline{13}$ and its future generations,

\mathbb{Y} acts like the identity and can no longer serve us. However, we still have \hat{h}_3 at our disposal.

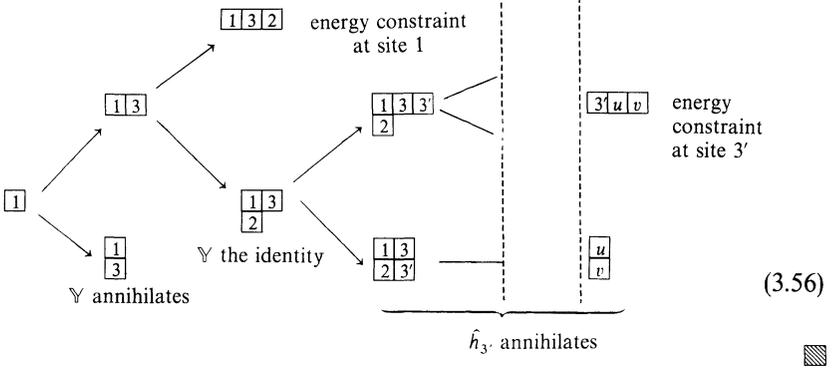
Adding $\overline{3}$ to what remains, we see



The lower branch contains a valence bond between 3 and 3' and is thus destroyed by \hat{h}_3 . The higher branch lives on. Continuing the argument, we see that as additional neighbors of 3' are injected, they either go symmetrically with 3', in which case the branch lives on, or end up pairing antisymmetrically with 3, whereby the operator gets destroyed by \hat{h}_3 from the back.

When we have exhausted all the neighbors of 3', the only diagram which has survived the onslaught from the left contains the entire neighborhood of 3' on the top row. The operator therefore first symmetrizes the neighborhood of 3' and thus destroys any ψ with $\hat{h}_3 \cdot \psi = 0$.

A summary (and complete proof of) the above can be found in equation (3.56).



Proof of Theorems A and C. Suppose $\Lambda \subset \mathbb{H}_2$ is finite and $\psi \in \Omega_0(\Lambda)$. We look for our first site, which we will denote by s_1 , on the boundary of Λ . If possible, we select an s_1 with only a single neighbor. In this case, by Proposition 3, ψ is automatically antisymmetric on s_1 and its neighbor, and has unit projection onto the zero-energy space of the reduced lattice. We rename the wavefunction ψ_1 and call the dimer b_1 . If s_1 has two neighbors, antisymmetrization on at least one of the two possible bond choices—which we would also denote by b_1 —followed by projection onto $\Omega_0(\Lambda \setminus b_1)$ produces a “ ψ_1 .” Observe that, in either case, ψ_1 is antisymmetric on b_1 , is in $\Omega_0(\Lambda)$ and (after factorization) in $\Omega_0(\Lambda \setminus b_1)$. We continue the procedure, selecting singly coordinated sites whenever possible, and produce the sequence $\psi_1, \psi_2, \psi_3, \dots$.

We claim that at every stage, the remaining lattice is dimerizable. Indeed, assume this is not the case and that, say, Λ itself has no dimer covering. By definition, this means that any attempt to dimerize Λ results in the isolation of sites. Suppose then that our procedure picks a sequence of sites, s_1, s_2, \dots and bonds, b_1, b_2, \dots (s_j being an endpoint of b_j), but that the n^{th} step results in an isolated point p . Obviously, just prior to the catastrophe, p had only one site in its neighborhood and this must have been one of the endpoints of b_n . If the sole neighbor of p was s_n , then s_n evidently possessed two neighbors which (at best) implies there was a programming error—the n^{th} site should have been p . On the other hand, if p was a neighbor of the other side of b_n (temporarily called \bar{s}_n) this implies that both s_n and p had as their sole neighbor the site \bar{s}_n . Now the wavefunction ψ_{n-1} was reported to be a zero-energy state of Λ_{n-1} which, by Proposition 3, implies the impossible (for spin-1/2) situation that ψ_{n-1} was

simultaneously antisymmetric on both (s_n, \bar{s}_n) and (p, \bar{s}_n) . Evidently, if Λ has no dimer covering, the only $\psi \in \Omega_0(\Lambda)$ is zero.

We have just proved Theorem C; let us finish off Theorem A. The above reasoning allows us to proceed until Λ has been covered by some dimer graph Δ . The final wavefunction that has been produced is, of course, proportional to ψ_Δ . It is also the projection of the original wavefunction onto ψ_Δ . \blacksquare

Proof of Theorem B. Let $\Lambda \subset \mathbb{H}_2$ be dimerizable and let $\Delta^{(1)}, \dots, \Delta^{(K)}$ denote the possible dimer coverings. For each $\Delta^{(j)}$ we may construct a dimer wavefunction; let us call this $\psi^{(j)}$. We need to demonstrate that whenever

$$0 = \sum_{j=1}^K c_j \psi^{(j)}, \quad (3.57)$$

all the c_j are zero. We start by focusing attention on c_1 and $\Delta^{(1)}$. Let us order the dimers of $\Delta^{(1)}$, $\Delta^{(1)} = (b_1, \dots, b_N)$, according to the strategy that was used in Theorem A: b_1 has an endpoint on the boundary of Λ , b_2 has an endpoint on the boundary of $\Lambda \setminus b_1$ etc. For each n , this means that there is a site, s_n , on the boundary of $\Lambda \setminus (b_1, \dots, b_{n-1})$ which belongs to the bond b_n . In addition to the other end of b_n , s_n has at most one other neighbor in $\Lambda \setminus (b_1, \dots, b_{n-1})$. In the cases where s_n has only one remaining neighbor, define an operator \mathbb{D}_n to be $\frac{1}{2} \mathbb{A}_{b_n}$. In the cases where s_n could give rise to an alternative bond in $\Lambda \setminus (b_1, \dots, b_{n-1})$, let us call this bond b'_n and define \mathbb{D}_n to be the Young symmetrizer associated with the choice of b_n over b'_n :

$$\mathbb{D}_n = \frac{1}{3} \mathbb{A}_{b_n} \mathbb{S}_{b'_n}. \quad (3.58)$$

Observe that each \mathbb{D}_n is the identity on $\psi^{(1)}$ —or any $\psi^{(j)}$ which contains the bond b_n —and, in the two-choice cases, \mathbb{D}_n destroys the $\psi^{(j)}$ that have a singlet pair along b'_n . In general, an individual \mathbb{D}_n will neither destroy nor act like the identity on a given $\psi^{(j)}$, but we have the right to apply the (\mathbb{D}_j) in succession: Operating on 0 in Eq. (3.57) with \mathbb{D}_1 , we obtain

$$0 = \sum_{j: b_1 \in \Delta_j} c_j \psi^{(j)}. \quad (3.59)$$

We are now in a position in which \mathbb{D}_2 destroys all *remaining* wavefunctions that are not antisymmetric on b_2 , and the process continues. Since eventually each $\Delta^{(j)}$, $j > 1$, disagrees with $\Delta^{(1)}$ on some bond, the inevitable conclusion is that $c_1 = 0$. Repeating the argument, Eq. (3.57) is seen to necessitate $c_j = 0$ for all j . \blacksquare

Appendix. Results on Other Lattices

(a) Linear Independence of Dimer States on the Square Lattice

Proof of Theorem B for the square lattice. The argument that was used for the hexagonal lattice applies almost directly to the square lattice, \mathbb{Z}^2 . The only apparent difficulty is that not all sites on the boundary of a $\Lambda \subset \mathbb{Z}^2$ are two-fold coordinated. However, for $|\Lambda| < \infty$, a certain subset of Λ is the “leftmost” portion:

$$\mathcal{L}_\Lambda \equiv \{x \in \Lambda \mid x_1 \leq y, \forall y \in \Lambda\}, \quad (\text{A.1})$$

which contains a unique lowest site, $x_{LL}(\Lambda)$. The site x_{LL} is manifestly two-fold coordinated.

We may repeat the previous proof by constructing the j^{th} “ \mathbb{D} ” operator for a given ψ_Δ along the bonds of Λ_{j-1} which emanate from $x_{LL}(\Lambda_{j-1})$, the (current) lowest, leftmost site. \blacksquare

(b) *The Ground State Space for Other Lattices.* The lattice-dependent aspects of the proofs of Theorems A–C concern the local configuration in the vicinity of the projected bond. The major simplification of the hexagonal lattice is that the neighbors of the focal site have no neighbor in common. Such a situation typically does occur on \mathbb{Z}^2 , and cannot, at present, be treated in full generality. Consider, however, the local configuration depicted in Fig. 3. The common secondary neighbor is the site 4. It is not difficult to see that the analysis of Proposition 4 holds for all sites *except* site 4. Here, however, the site 2 has no additional neighbors; for this special case, the result at site 4 is easily obtained.

Proposition 5. *Consider a finite lattice Λ with the local configuration at $1 \in \Lambda$ as depicted in Fig. 3, and define the operators \mathbb{Y} and \mathbb{Y}' as in Proposition 4. Suppose that $\psi \in \mathfrak{S}_\Lambda$ satisfies $\hat{h}_1\psi = \hat{h}_2\psi = \hat{h}_4\psi = 0$. Then*

$$\hat{h}_4\mathbb{Y}\psi = \hat{h}_4\mathbb{Y}'\psi = 0.$$

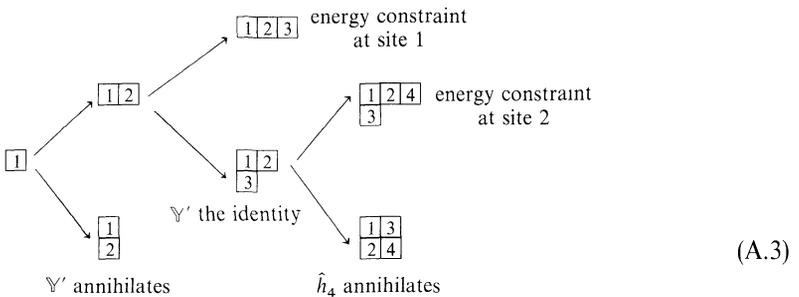
Furthermore, such a relationship holds with the \hat{h}_4 replaced by the appropriate reduced energy operators.

Proof. To prove the above, it is only necessary to establish that

$$\hat{h}_4\mathbb{Y}'\psi = 0. \tag{A.2}$$

Indeed, Eq. (A.2) and the fact that $\hat{h}_1\psi = 0$ immediately give us $\hat{h}_4\mathbb{Y}\psi = 0$; the desired results for the reduced operators then follow from Lemma 2.

To prove (A.2) we resolve the identity for the first four particles in canonical order. The branching diagram is:



which, by reasoning identical to that of Proposition 4, gives Eq. (A.2). \blacksquare

Corollary 1. *Theorems A, B and C hold for subsets of the $2 \times N$ square strips. (See Figure 4b.)*

Proof. It is easy to see that at any stage of a dimerization program, at the extreme left of the strip, a site is either singly coordinated or has a local neighborhood of the type described in Proposition 5. Supplemented with this result, the previous strategies may be employed. \blacksquare

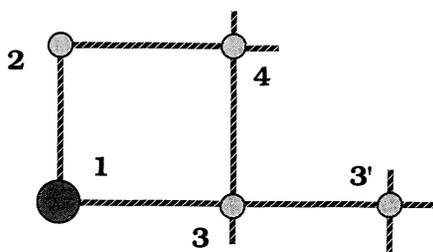


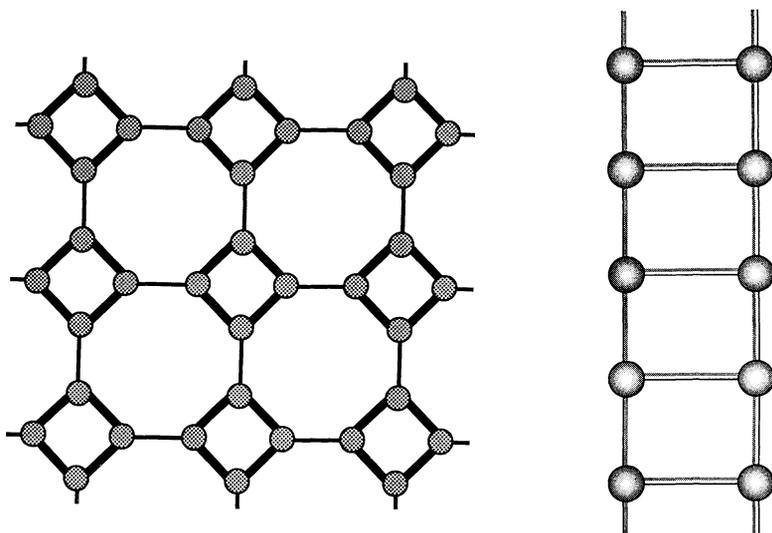
Fig. 3. Additional environment for site 1

Corollary 2. *Theorems A, B and C hold for subsets of the octagonal-diamond lattice. (See Fig. 4a).*

Proof. The octagonal-diamond lattice has coordination number 3, so any site on the boundary has at most two neighbors. From this, linear independence of the dimer states is easily established. However, not every boundary site has an environment of the type just treated or of the type encountered in the analysis of the hexagonal lattice.

Although site-wise the octagonal-diamond lattice is translation invariant, there are two types of edges. Indeed, one may regard this lattice as living above the square lattice with a diamond centered at each point. Thus, if Λ is a subset of the octagonal-diamond lattice, it may be regarded as a collection of partial or complete diamonds interconnected (often incompletely) as in \mathbb{Z}^2 .

If any diamond is incomplete (i.e. does not contain all four sites), it is easily seen that the analysis of Proposition 4 applies directly. Incomplete diamonds should be finished off whenever possible. What remains, if anything, is a partially connected collection of complete diamonds.

Fig. 4a and b. Other geometries. a The octagonal-diamond lattice. b The $2 \times N$ square strip

Since the lowest leftmost complete diamond is not connected to more than two other diamonds, it is seen that it possesses two sites satisfying the conditions of Proposition 5. It can therefore be dissected.

Theorems A and C now follow as before. \blacksquare

References

1. Klein, D. J.: Exact ground states for a class of antiferromagnetic Heisenberg models with short-range interactions. *J. Phys. A. Math. Gen.* **15**, 661–671 (1982)
2. Anderson, P. W.: The resonating-valence-bond state in La_2CuO_4 and superconductivity. *Science* **235**, 1196–1198 (1987)
3. Weber, W.: *Phys. Rev. Lett.* **58**, 1371 (1987)
4. Varma, C. M., Schmitt-Rink, S., Abrahams, E.: *Solid State Commun.* **62**, 681 (1987)
5. Ching, W. Y., Xu, Y., Zhou, G.-L., Wong, K. W., Zandiehnam: Electronic structure and exciton-enhanced superconducting mechanism in $\text{YBa}_2\text{Cu}_3\text{O}_{7-d}$. *Phys. Rev. Lett.* **59**, 1333–1336 (1987)
6. Kivelson, S. A., Rokhsar, D. S., Sethna, J. P.: Topology of the resonating-valence-bond ground state: Solitons and high T_c superconductivity. *Phys. Rev. B* **35**, 8865–8868 (1987)
7. Baskaran, G., Zou, Z., Anderson, P. W.: The resonating-valence-bond state and high- T_c superconductivity. *Solid State Commun.* **63**, 973–976 (1987)
8. Anderson, P. W., Baskaran, G., Zou, Z., Hsu, T.: Resonating-valence-bond theory of phase transitions and superconductivity in La_2CuO_4 -based compounds. *Phys. Rev. Lett.* **58**, 2790–2793 (1987)
9. Anderson, P. W.: Comment on “Two-dimensional antiferromagnetic quantum spin-fluid state in La_2CuO_4 .” *Phys. Rev. Lett.* **59**, 2497 (1987)
10. Emery, V. J.: *Phys. Rev. Lett.* **58**, 2794 (1987)
11. Hirsch, J. E.: Antiferromagnetism, localization and pairing in a two-dimensional model for CuO_2 . *Phys. Rev. Lett.* **59**, 228–231 (1987)
12. Kalmeyer, V., Laughlin, R. B.: Equivalence of the resonating-valence-bond and fractional quantum Hall ground states. *Phys. Rev. Lett.* **59**, 2095–2098 (1987)
13. Ruckenstein, A. E., Hirschfeld, P. J., Appel: *Phys. Rev. B* **36**, 857 (1987)
14. Gros, C., Joynt, R., Rice, T. M.: *Phys. Rev. B* **36**, 38 (1987)
15. Ioffe, L. B., Larkin, A. I.: The two-dimensional Hubbard model with strong electron repulsion, preprint (1987)
16. Kivelson, S. A.: Nature of the pairing in a resonating-valence-bond superconductor. *Phys. Rev. B* **36**, 7237–7240 (1987)
17. Zimanyi, G. T., Kivelson, S. A., Luther, A.: Superconductivity from predominantly repulsive interactions in quasi-one-dimensional systems, preprint (1987)
18. Kivelson, S. A., Rokhsar, D. S., Sethna, J. P.: $2e$ or not $2e$: Flux quantization in the resonating-valence-bond state, preprint (1987)
19. Sutherland, B.: The phase diagram of a lattice statistics problem associated with resonating-valence-bond ground states, preprint (1987)
20. Sutherland, B.: A novel mechanism for superconductivity in the resonating-valence-bond ground state, preprint (1987)
21. Rokhsar, D. S., Kivelson, S. A.: The short-ranged resonating-valence-bond superconductor, preprint (1988)
22. Kivelson, S. A., Rokhsar, D. S.: The low-temperature properties of a short-ranged resonating-valence-bond superconductor. Proceedings of the International Conference on High-Temperature Superconductors and Materials and Mechanisms of Superconductivity, Interlaken, to appear in *Physica B* (1988)
23. Kotliar, G.: Resonating-valence-bonds and d-wave superconductivity. *Phys. Rev. B* **37**, 3664–3666 (1988)
24. Inui, M., Doniach, S., Hirschfeld, P. J., Ruckenstein, A. E.: Coexistence of antiferromagnetism and superconductivity in a mean-field theory of high- T_c superconductors, preprint (1988)

25. Schrieffer, J. R., Wen, X.-G., Zhang, S.-C.: Spin-bag mechanism of high-temperature superconductivity. *Phys. Rev. Lett.* **60**, 944–947 (1988)
26. Chakravarty, S., Halperin, B. I., Nelson, D. R.: Low-temperature behavior of two-dimensional quantum antiferromagnets. *Phys. Rev. Lett.* **60**, 1057–1060 (1988)
27. Dzyaloshinski, I., Polyakov, A., Wiegmann, P.: Neutral fermions in paramagnetic insulators. *Phys. Lett. A* **127**, 112 (1988)
28. Wiegmann, P. B.: Superconductivity in strongly correlated electron systems and confinement vs. deconfinement phenomenon, preprint (1988)
29. Kohmoto, M., Shapir, Y.: preprint (1988)
30. Aharony, A., Birgeneau, R. J., Coniglio, A., Kastner, M. A., Stanley, H. E.: Magnetic phase diagram and magnetic pairing in doped La_2CuO_4 . *Phys. Rev. Lett.* **60**, 1330 (1988)
31. Loffe, L. B., Larkin, A. I.: Effective action of a two-dimensional antiferromagnet, preprint (1988)
32. Anderson, P. W.: *Solid State Phys.* **14**, 99 (1963)
33. Klein, D. J., Seitz, W. A.: Partially filled linear Hubbard model near the atomic limit. *Phys. Rev. B* **10**, 3217–3227 (1974)
34. Anderson, P. W.: *Mater. Res. Bull.* **8**, 153 (1973)
35. Fazekas, P., Anderson, P. W.: On the ground state properties of the anisotropic triangular antiferromagnet. *Philos. Mag.* **30**, 423–440 (1974)
36. Hulthén, L.: *Ark. Mat. Astr. Fys.* **26A**, 1 (1938)
37. Pauling, L.: *Proc. R. Soc. Lond.* **A196**, 343 (1949)
38. Thouless, D. J.: preprint, to appear in *Phys. Rev. B* (1987)
39. Marshall, W.: *Proc. R. Soc. Lond.* **A232**, 48 (1955)
40. Lieb, E., Schultz, T., Mattis, D.: Two soluble models of an antiferromagnetic chain. *Ann. Phys.* **16**, 407–466 (1961)
41. Lieb, E., Mattis, D.: *J. Math. Phys.* **3**, 749 (1962)
42. Oitmaa, J., Betts, D. D.: *Can. J. Phys.* **56**, 897 (1987)
43. Yokoyama, H., Shiba, H.: *J. Phys. Soc. Jpn.* **56**, 1490 and *ibid.* **56**, 3582 (1987)
44. Yokoyama, H., Shiba, H.: Variational Monte-Carlo studies of superconductivity in strongly correlated electron systems, preprint (1988)
45. Huse, D. A., Elser, V.: preprint (1988)
46. Horsch, P., von der Linden, W.: Spin-correlations of the spin-1/2 Heisenberg antiferromagnet on a square lattice, *Proceedings of the International Conference on High-Temperature Superconductors and Materials and Mechanisms of Superconductivity, Interlaken* (1988)
47. Fulde, P.: private communication
48. Reger, J. D., Young, A. P.: preprint, to appear in *Phys. Rev. B* (1988)
49. Barnes, T., Swanson, E.: Two two-dimensional Heisenberg antiferromagnet: A numerical study, preprint (1988)
50. Manousakis, E., Salvador, R.: Long-range correlations in the two-dimensional spin-1/2 antiferromagnetic Heisenberg model: A quantum Monte Carlo study. *Phys. Rev. Lett.* **60**, 840–843 (1988)
51. Huse, D. A.: *Phys. Rev.* **B37**, 2380 (1988)
52. Brinkman, W. F., Rice, T. M.: *Phys. Rev.* **B2**, 4302 (1970)
53. Lederer, P.: Kinetic energy of holes in the Hubbard model, preprint (1987)
54. Trugman, S.: *Phys. Rev.* **B37**, 1597 (1988)
55. Shraiman, B. I., Siggia, E. D.: Two-particle excitations in antiferromagnetic insulators. *Phys. Rev. Lett.* **60**, 740–743 (1988)
56. Lederer, P., Takahashi, Y.: Holon kinetic energy in the RVB state, preprint (1988)
57. Takahashi, Y.: The effect of zero-point spin wave motions on the hole propagation in the strongly correlated Hubbard model, preprint (1988)
58. Ogata, M., Shiba, H.: Holes in two-dimensional CuO_2 system—Pairing mechanism emerges from small cluster studies, preprint (1988)
59. Schmitt-Rink, S., Varma, C. M., Ruckenstein, A. E.: Spectral function of holes in a quantum antiferromagnet, preprint (1988)
60. Affleck, I., Kennedy, T., Lieb, E. H., Tasaki, H.: Rigorous results on valence bond ground states in antiferromagnets. *Phys. Rev. Lett.* **59**, 799–802 (1987); also: Valence bond ground states in isotropic quantum antiferromagnets. *Commun. Math. Phys.* **115**, 477–528 (1988)

61. Arovas, D. P., Auerbach, A., Haldane, F. D. M.: Extended Heisenberg models of antiferromagnetism: Analogies to the fractional quantum Hall effect. *Phys. Rev. Lett.* **60**, 531–534 (1988)
62. Fisher, M. E.: *Phys. Rev.* **124**, 1664–1672 (1961)
63. Kasteleyn, P. W.: *Physica* **27**, 1209–1225 (1961)
64. Majumdar, C. K., Ghosh, D. K.: On next-nearest-neighbor interactions in linear chain I, II. *J. Math. Phys.* **10**, 1388–1402 (1969)
65. Weyl, H.: *The classical groups*. Princeton, N.J: Princeton University Press 1939
66. Hamermesh, M.: *Group theory*. Reading, MA: Addison Wesley 1962
67. Bethe, H.: *Z. Phys.* **71**, 205 (1931)
68. Des Cloiseaux, J., Pearson: *Phys. Rev.* **128**, 2131 (1962)
69. Griffiths, R. B.: Magnetization curve at zero temperature for the antiferromagnetic Heisenberg linear chain. *Phys. Rev.* **133**, A768–A775 (1964)
70. Cross, M. C., Fisher, D. S.: *Phys. Rev.* **B19**, 402 (1979)
71. Black, J. L., Emery, V. J.: *Phys. Rev.* **B23**, 429 (1981)

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