Quadratic quantum antiferromagnets in the fermionic large-N limit

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We show that SU(N) Heisenberg Hamiltonians with arbitrary-range quadratic antiferromagnetic couplings (i.e., $\mathcal{H} = \sum_{(i,j)} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j$, with $J_{ij} > 0$) possess highly degenerate "dimerized" ground states in the fermionic infinite-N limit on a large class of lattices that includes all Bravais lattices in arbitrary dimension. These states break translational but not spin-rotational symmetry.

I. INTRODUCTION

Although it is now generally believed that the nearestneighbor, spin- $\frac{1}{2}$, square-lattice Heisenberg antiferromagnet has a ground state with long-range Néel order,¹ it has been argued² that further-neighbor frustrating couplings could lead to ground states with neither broken spinrotational nor broken translational symmetry. These so called "resonating-valence-bond" or "spin-liquid" insulators play important roles in various approaches to superconductivity,³ but unfortunately there are currently no soluble models (with short-ranged interactions) that exhibit such spin-liquid ground states. One promising tack⁴ involves generalizing the spin- $\frac{1}{2}$ SU(2) Heisenberg model to a version with an SU(N) spin at each site, where N is even. There are then N "flavors" of fermion (for N=2these correspond to "up" and "down") and the system is half-filled, i.e., each site is occupied by precisely N/2 fermions. This model was introduced by Affleck and Marston and has been called the "fermionic" SU(N) model, to distinguish it from other generalizations^{5,6} which utilize different representations of SU(N). The advantage of discussing SU(N) Heisenberg models is that they can be exactly solved by saddle point (i.e., mean-field) techniques in the large-N limit, and may provide insight into their less tractable (though physically relevant) SU(2) cousins.

The (arbitrary-range) antiferromagnetic SU(N) Heisenberg models we consider are defined for a network of spins by

$$\mathcal{H} = \sum_{(i,j)} J_{ij} S_i \cdot S_j, \quad J_{ij} > 0 , \qquad (1)$$

where $S_i = c_i^{\alpha^{\dagger}} \sigma_{\alpha}^{\beta} c_{i\beta}$ is the spin operator at site *i*, and the fermions created by $c_{i\alpha}^{\dagger}$ are subject to the constraint $c_i^{\alpha^{\dagger}} c_{i\alpha} = N/2$ at each site *i*. (Repeated Greek indices imply summation over flavors from 1 to *N*.) The summation in (1) is carried out over distinct pairs of sites on the network. We will consider model (1) in the infinite-*N* limit, where mean-field theory becomes exact.

We say that a network is "dimerizeable with respect to J_0 " if it is possible to partition the network into disjoint pairs of sites such that (a) every site belongs to one and only one pair, and (b) for each such pair (i, j) we have $J_{ij} = J_0$ (see Fig. 1). Let J_{max} denote the largest of the spin couplings J_{ij} . Our main result is that networks

which are dimerizeable with respect to J_{max} possess "spin-Peierls" states (i.e., states which are spin rotationally but not translationally invariant) which are among the ground states of (1) in the infinite-N limit. This is shown by finding equal upper and lower bounds on the infinite-N ground-state energy of (1) (thus precisely determining the ground-state energy) and demonstrating that spin-Peierls states with this energy exist. As a corollary, we show that in many cases states which respect the symmetries of the network have higher energies.

For most familiar networks, exponentially many dimerizations are possible, and the ground-state manifold of the corresponding infinite-N Heisenberg model (1) is highly degenerate. As shown by Read and Sachdev,⁶ this degeneracy is lifted to lowest order in 1/N. The ground state for large but finite N is then determined by the solution of a corresponding "dimer model"^{6,7} containing matrix elements between the different dimerized states. For the nearest-neighbor antiferromagnetic Heisenberg model on the square lattice, the 1/N corrections favor a state in which the dimers are arranged in columns.⁶ It has been shown⁷ in a special exactly soluble case that an appropriate dimer model can display a disordered phase, but the detailed connection between this result and a corresponding spin model remains undetermined. In exceptional cases, a network will possess a unique dimerized state, which implies a unique ground state⁸ of (1) for infinite- N. For other networks and choices of J_{ii} no dimerized states are possible (see Fig. 2). For this last class of Hamiltonians the lower bound on the energy determined below continues to hold, but no state saturating this bound can be simply constructed.

The reader should be cautioned that, despite its apparent generality, (1) by no means exhausts the set of SU(N) invariant Hamiltonians. It is not even the most general SU(N) invariant *pair* Hamiltonian: For N > 2, biquadratic [i.e., $(S_i \cdot S_j)^2$] and higher-order pair interactions are possible and can alter the nature of the ground state, as discussed by Affleck and Marston.⁴ Of course, SU(N) invariant *multispin* interactions are also possible, even for N=2: Wen, Wilczek, and Zee⁹ have recently emphasized the role that the three-spin interaction¹⁰— $(S_i \cdot S_j \times S_k)^2$ may play with regard to the breaking of time-reversal invariance. The usefulness of simple arbitrary-range quadratic Hamiltonians of the form (1) is

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FIG. 1. (a) Two-dimensional square lattice with first- and second-neighbor interactions, J_1 and J_2 . (b) The network of part (a) dimerized with respect to J_1 . (c) The network of part (a) dimerized with respect to J_2 .

that they are easily studied in the large-N limit. Unfortunately, we show below that for most familiar lattices the infinite-N ground state is not translationally invariant.

II. THE INFINITE-N LIMIT

Following Affleck and Marston,⁴ we can use identities involving the SU(N) generators σ_{α}^{β} to cast the Heisenberg Hamiltonian (1) in the pleasing and manifestly SU(N) invariant form



FIG. 2. This network, a decorated hexagonal net (also called the "expanded Kagome net" has two different couplings, J_1 (bold lines) and J_2 (thin lines). It is dimerizeable with respect to J_1 — the bold lines indicate the unique pairing of sites. The network is not, however, dimerizeable with respect to J_2 , and this system is not subject to the lower bound derived in the text. If the sites paired by bold lines are identified the network becomes a Kagome net, which is dimerizeable.

$$\mathcal{H} = \sum_{(i,j)} J_{ij} (c_i^{\alpha^{\dagger}} c_{j\alpha}) (c_j^{\beta^{\dagger}} c_{i\beta}) .$$
⁽²⁾

[In obtaining (2) from (1), constant terms have been dropped.] Next, introduce Hubbard-Stratonovich fields χ_{ij} for each pair of sites which are coupled by a nonzero J_{ij} (and define $\chi_{ij} \equiv 0$ whenever, $J_{ij} = 0$). For a given choice of fields χ_{ij} the mean-field Hamiltonian becomes

$$\mathcal{H}_{\rm MF} = N \sum_{(i,j)} \frac{|\chi_{ij}|^2}{J_{ij}} + \sum_{(i,j)} (\chi_{ij} c_i^{\alpha \dagger} c_{j\alpha} + {\rm H.c.}) .$$
(3)

Primed summations are carried out only over pairs of sites i and j which have nonzero J_{ij} .

The mean-field state corresponding to a given $\{\chi_{ij}\}$ is simply the Slater determinant obtained by placing N particles (one of each flavor) into each of the L/2 lowesteigenvalue eigenstates of the matrix χ_{ij} , where L denotes the number of spins (sites) in the network. Since the relative fluctuations in the number density at each site vary as $N^{-1/2}$ for such a state, the violation of the constraint of N/2 fermions per site becomes less and less important in the large-N limit, where the state can be considered exact. The energy of such a state is simply

$$E_{\rm MF} = N \sum_{(i,j)} \frac{|\chi_{ij}|^2}{J_{ij}} + N \sum_{\kappa \in \mathcal{L}} \varepsilon_{\kappa} , \qquad (4)$$

where the second summation is performed over the L/2lowest eigenvalues of χ_{ij} , which we denote $\{\varepsilon_{\kappa} | \kappa \in \mathcal{L}\}$. (It will also prove useful to define the set consisting of the L/2 highest eigenvalues, denoted $\{\varepsilon_{\kappa} | \kappa \in \mathcal{U}\}$.) We look for values of $\{\chi_{ii}\}$ such that the energy $E_{\rm MF}$ is minimized. This procedure is identical to a Hartree-Fock treatment of the Heisenberg Hamiltonian (2), with the fields $\{\chi_{ij}\}$ determined self-consistently via $\chi_{ij} = (J_{ij} / N) \langle c_j^{\alpha \dagger} c_{i\alpha} \rangle$.

Expressed in terms of the underlying fermions, SU(N)Heisenberg models possess a local U(1) gauge symmetry,¹¹ since the particle number on each site is conserved. This is relected in the invariance of the mean-field theory (3) with respect to the simultaneous multiplication of the fermion creation operators at site *i* by the phase factor $e^{i\phi_i}$, and χ_{ij} by the opposite phase factor $e^{-i\phi_i}$. All χ configurations related by such a gauge transformation therefore describe the same spin state. In characterizing a configuration χ , we must accordingly restrict ourselves to gauge-invariant quantities, i.e., the magnitudes $|\chi_{ii}|$ on each link and the products $\chi_{12}\chi_{23}\cdots\chi_{n1}$ for any set of sites $1, 2, 3, \ldots, n$. The phase of this complex product is called the "flux" of the closed path $1, 2, 3, \ldots, n, 1$.

III. FLUX, CHIRAL, SPIN-PEIERLS, AND BOX PHASES

Before searching for the optimal disposition of the fields χ , it is useful to classify possible configurations by symmetry.

(1) Translational and/or rotational invariance of the network is broken.12

(a) "Spin-Peierls" phase.⁴ χ_{ij} vanishes except on isolat-

ed links on the lattice. (b) "Box" phase.¹³ χ_{ij} vanishes except on isolated clusters of links on the lattice.

(2) Translational invariance of the network is preserved. For any two closed paths on the network which are related by a translation, the gauge-invariant product $\chi_{12}\chi_{23}\cdots\chi_{n1}$ is the same. Since we have not restricted ourselves to nearest-neighbor Heisenberg models, consecutive sites on these closed paths need not be nearest-neighbor sites. The translationally invariant states can be further classified according to the flux associated with closed paths on the lattice.

(a) "Uniform" phase.¹⁴ The flux through any closed path is zero, so that all of the χ_{ij} can be chosen to be real. (b) "Flux" phase.^{4,15} All fluxes are integer multiples of

 π , so that neither parity nor time-reversal invariance is broken. [Under either time reversal or parity, the flux through each closed path is negated, $mod(2\pi)$; only integer multiples of π are invariant under this operation.]

(c) "Chiral"⁹ phase. Parity and time-reversal invariance are broken, i.e., some fluxes are not integer multiples of π .

For Heisenberg models of the form (1), on all lattices which have been considered thus far, box and spin-Peierls phases have been found which are (a) degenerate and (b) appear to be the global minima of the mean-field Hamiltonian (3). In the following section we elevate this empirical observation to a theorem, by showing that for networks which are dimerizeable with respect to the largest spin-spin coupling J_{max} (a) spin-Peierls states are indeed global minima of the mean-field energy (4), and (b) all translationally invariant choices of χ have energies which are greater than or equal to the energy of the spin-Peierls-box phases in the infinite-N limit. A more descriptive definition of box states is obtained, and these state are seen to be among the degenerate ground states (along with spin-Peierls states) in this limit.

IV. THE LARGE-N GROUND STATE

Let J_{max} be the largest of the antiferromagnetic couplings $\{J_{ij}\}$. Consider the following "spin-Peierls" state on a network which is dimerizeable with respect to J_{max} . Let each site *i* have a nonzero χ_{ij} with one and only one site j for which $J_{ij} = J_{max}$. Assign the same (positive) value χ to all the corresponding matrix elements χ_{ii} . We note that while such a pairing of all sites ("dimerization") is possible for many familiar lattices and networks when the spin-spin couplings J_{ii} respect the symmetries of the network, this is not the generic case. "Dimerizeability" as defined above is a property of the network and the couplings on it, so that a network may be dimerizeable with respect to some couplings and not dimerizeable with respect to others. (See Fig. 2.)

Considered as a variational state, such a dimerized configuration provides an upper bound on the exact ground-state energy. Since each site is coupled to one and only one other site, the diagonalization of χ_{ii} reduces to the diagonalization of L/2 independent, identical two-site Hamiltonians. The spectrum of χ is then easily seen to consist of L/2 states of energy $-\chi$ and L/2states of energy $+\chi$. The mean-field energy (4) is

$$E_{\rm SP} = \frac{NL}{2} \frac{\chi^2}{J_{\rm max}} - \frac{NL}{2} \chi , \qquad (5)$$

which attains its minimum value of $-NLJ_{max}$ /8 when χ is equal to $J_{\text{max}}/2$. We now show that (a) this is the exact ground-state energy of (1) in the fermionic large-N limit, so that these spin-Peierls states are among the ground states of this model, and (b) except in special situations, translationally invariant states have higher energy.

As a preliminary exercise, we first bound the fermionic contribution to (4) by proving the following result.

Lemma. The average of the lowest L/2 eigenvalues $\{\varepsilon_{\kappa} | \kappa \in \mathcal{L}\}$ of a traceless Hermitian $L \times L$ matrix χ_{ii} satisfies the inequality

$$\langle \varepsilon_{\kappa} \rangle_{\mathcal{L}} \equiv \frac{1}{L/2} \sum_{\kappa \in \mathcal{L}} \varepsilon_{\kappa} \ge - \left[\frac{2}{L} \sum_{(i,j)} |\chi_{ij}|^2 \right]^{1/2}.$$
 (6)

Equality is attained only when all ε_{κ}^2 are identical, i.e., when χ^2 is proportional to the identity matrix.

Proof. Applying the Schwartz inequality (i.e., variances are positive) to each half of the spectrum yields the two inequalities

$$\langle \varepsilon_{\kappa} \rangle_{\perp}^2 \leq \langle \varepsilon_{\kappa}^2 \rangle_{\perp}$$
 (7a)

and

$$\langle \varepsilon_{\kappa} \rangle_{\mathcal{U}}^2 \leq \langle \varepsilon_{\kappa}^2 \rangle_{\mathcal{U}} . \tag{7b}$$

The equality (7a) is achieved when all ε_{κ} for κ belonging to \mathcal{L} are equal; similarly, (7b) becomes an equality when all ε_{κ} for κ belonging to \mathcal{U} are equal.

The tracelessness of χ_{ij} (along with the invariance of the trace under choice of basis) implies that

$$\langle \varepsilon_{\kappa} \rangle_{\mathcal{L}} = - \langle \varepsilon_{\kappa} \rangle_{\mathcal{U}} , \qquad (8)$$

so that inequality (7b) can be rewritten as

$$\langle \varepsilon_{\kappa} \rangle_{\mathcal{L}}^2 \leq \langle \varepsilon_{\kappa}^2 \rangle_{\mathcal{U}}$$
 (7b')

Adding (7a) and (7b') and dividing by two yields

$$\langle \varepsilon_{\kappa} \rangle_{\ell}^2 \leq \langle \varepsilon_{\kappa}^2 \rangle$$
, (9)

where the average on the right-hand side is over the entire spectrum of χ (both \mathcal{L} and \mathcal{U}). Again availing ourselves of the invariance of trace with respect to choice of basis, we see that

$$\langle \varepsilon_{\kappa}^2 \rangle = \frac{1}{L} \operatorname{Tr}(\chi^2) = \frac{1}{L} \sum_{i} \sum_{j} \chi_{ij} \chi_{ji} = \frac{2}{L} \sum_{(i,j)} |\chi_{ij}|^2 .$$
(10)

Substituting (10) into (9) and taking the square root of both sides (using the fact that $\langle \varepsilon_{\kappa} \rangle_{\ell}$ is less than or equal to zero) establishes the required bound (6). The bound is saturated when (7a) and (7b) become equalities, i.e., when χ^2 is proportional to the identity matrix.

Using the Lemma to bound the second term in the mean-field energy (4), we obtain a lower bound for the energy of a given χ configuration,

$$E_{\rm MF}(\chi) \ge N \sum_{(i,j)} \frac{|\chi_{ij}|^2}{J_{ij}} - N \left[\frac{L}{2} \sum_{(i,j)} |\chi_{ij}|^2 \right]^{1/2}$$
(11)

Minimizing this bound over all χ configurations then provides a lower bound for the large-N energy of (2). We extremize the right-hand side of (11) by setting its derivative with respect to $|\chi_{ij}|$ equal to zero for each pair of sites (i, j), which yields the conditions

$$\sum_{(k,l)} |\chi_{kl}|^2 = \frac{LJ_{lj}^2}{8}$$
(12a)

and/or

$$\chi_{ii} = 0 . (12b)$$

The left-hand side of (12a) is a fixed number independent of (i, j) so that for a given extremum of the bound (11), this equation can only hold for a particular numerical value of J_{ij} , which we call J_* . For pairs of sites (i, j) such that J_{ij} is not equal to J_* , (12b) must hold. Thus

$$E_{\rm MF}(\chi) \ge \frac{N}{J_{\star}} \frac{LJ_{\star}^2}{8} - N \left(\frac{L}{2} \frac{LJ_{\star}^2}{8}\right)^{1/2} = -\frac{NLJ_{\star}}{8} .$$
(13)

Since all extrema of (11) satisfy (12a) for some J_* , a general lower bound for $E_{\rm MF}$ is obtained with the largest J_* , i.e., $J_{\rm max}$. Therefore $-NLJ_{\rm max}/8$ is a *lower* bound for the large-N energy of an arbitrary configuration of χ_{ij} . The simple spin-Peierls states described above, however,

demonstrated that the same quantity is a variational *upper* bound whenever the network is dimerizeable. Therefore the large-N ground-state energy is then precisely equal to $-NLJ_{max}/8$. The spin-Peierls states described at the beginning of this section are therefore always among the exact large-N ground states of the SU(N) Heisenberg model.

V. FURTHER REMARKS

Until this point we have not ruled out the possibility that states other than the simple dimerized states may also be (degenerate) ground states of (1) on dimerizeable networks. Any state which is part of this degenerate manifold, however, must possess a gap and have dispersionless bands. For if a state is to be a ground state of (1), it must saturate the bound used in the Lemma, which requires that χ^2 be proportional to the identity matrix. The single-particle energies ε_{κ} are then simply $\pm \varepsilon$. We therefore seek matrices χ_{ij} such that $(\chi^2)_{ij} = \sum_k \chi_{ik} \chi_{kj}$ vanishes whenever $i \neq j$ and $(\chi^2)_{ii} = \sum_j |\chi_{ij}|^2$ is independent of *i*.

The matrix χ^2 describes two consecutive hops according to χ_{ii} . Double hops come in three classes (Fig. 3).

(a) Hop from site A to site B and then back to site A. These processes contribute to the diagonal matrix elements $(\chi^2)_{AA}$.

(b) Double hop from site A to site C via the unique intermediate site B. (For example, hopping two lattice spacings in the same direction on a Bravais lattice.) These processes always lead to a nonzero off-diagonal matrix element $(\chi^2)_{AC}$.

(c) Double hop from site A to site D via two different intermediate sites, B and B'. These contributions to $(\chi^2)_{AD}$ can cancel if

$$\chi_{AB}\chi_{BD} + \chi_{AB'}\chi_{B'D} = 0 , \qquad (14)$$

which implies

$$\chi_{AB}\chi_{BD}\chi_{DB'}\chi_{B'A} = -|\chi_{DB'}\chi_{B'A}|^2 .$$
(15)

According to (15), the off-diagonal contributions of these two paths can cancel only if the flux through the quadrilateral ABDB'A is an odd multiple of π . Here are some examples:



FIG. 3. Three types of "double hop" are possible on a square lattice with nearest-neighbor interactions: (a) $A \rightarrow B \rightarrow A$, (b) $A \rightarrow B \rightarrow C$, (c) $A \rightarrow B \rightarrow D + A \rightarrow B' \rightarrow D$. See text for details.



FIG. 4. "Box" phase on a square lattice with nearestneighbor interactions. Bold lines without arrows indicate $\chi_{ij} \neq 0$; bold lines with arrows indicate $\chi_{ij} = \chi e^{i\pi/4}$, where χ is real. The product of χ_{ij} around each box is negative, indicating a flux of π .

(1) Consider a hypercubic lattice (in arbitrary dimension) with equal nearest-neighbor spin-spin couplings. Arrange χ_{ii} such that isolated hypercubes include every lattice site, and the flux through all faces of the hypercubes is π . Then no pairs of sites are connected by type (b) double hops, and every type (c) double hop is canceled due to the π flux. These are generalizations of the box phase discovered by Dombre and Kotliar.¹³ Configurations with interspersed dimers and boxes also yield degenerate ground states. These considerations apply more generally to other lattices: Any cluster of sites and bonds which gives no net contribution from types (b) and (c) double hops yields a ground state (see Fig. 4).

(2) Flux states on hypercubic lattices with equal nearest-neighbor J_{ij} can be constructed in any dimension¹⁶ (Fig. 5). In the limit of infinite dimension these states become degenerate with spin-Peierls and box states. To construct these higher-dimensional flux states, set all nearest-neighbor $|\chi_{ij}|$ equal and arrange fluxes to be π through each square. It is easy to show that the eigenvalues of χ are given by

$$\varepsilon_{\mathbf{k}} = \pm 2|\chi| \left[\sum_{i} \cos^2(\mathbf{k} \cdot \mathbf{x}_i)\right]^{1/2}$$

The energy of such a state for dimensions 2, 3, 4, and 5 are -0.115, 0.119, -0.121, and -0.122, per site per



FIG. 5. A "flux" phase on a three-dimensional cubic lattice with nearest-neighbor interactions. On bold links, $\chi_{ij} = -\chi$. On thin links, $\chi_{ij} = \chi$. The product of the hopping matrix elements around each plaquette is $-\chi^4$ which is negative, indicating a flux of π .

flavor, respectively. In the limit of infinite dimension, the flux state becomes degenerate with the spin-Peierls and box states discussed above. (Note that our procedure corresponds to taking the $N \rightarrow \infty$ limit before the $d \rightarrow \infty$ limit.)

(3) Finally, consider the network formed by the edges of an icosahedron, with equal nearest-neighbor couplings. Arrange χ so that $|\chi_{ij}|$ is the same for all nearestneighbor pairs (i, j), and so that the flux through every triangular face of the icosahedron is $\pi/2$. Types (b) and (c) double hops are thereby eliminated, and the resulting chiral state (as well as its time reverse obtained with fluxes $-\pi/2$ through each triangle) belong to the degenerate ground-state manifold of the system. In addition, the icosahedron supports generalized box phases analogous to (1). Preliminary studies¹⁷ of the spin- $\frac{1}{2}$ nearestneighbor Heisenberg model on an icosahedral network, however, do not display the nearly degenerate low-lying states which would be expected if the infinite-N results were to continue to the case N=2.

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¹²It will be convenient to include in this class all states which

can be decomposed into isolated finite clusters of sites such that χ_{ij} is zero when *i* and *j* are in different clusters, even if this state has the translational symmetry of the network.

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