Balance and frustration in strongly correlated itinerant electron systems: An extension of Nagaoka's theorem

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We prove that Nagaoka's theorem, that the ground state of the large-U Hubbard model with exactly one hole is ferromagnetic, holds for any balanced Hamiltonian. We argue that, in itinerant electron systems, a balanced Hamiltonian, rather than bipartite lattice, defines an unfrustrated system. The proof is valid for multiorbital models with arbitrary two-orbital interactions provided that no exchange interactions are antiferromagnetic: a class of models including the Kanomori Hamiltonian.

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I. INTRODUCTION

Geometrical frustration plays a central role in the understanding of quantum magnetism [1]. The distinction between bipartite and geometrically frustrated lattices is fundamental for spin models of localized electrons. Itinerant electrons can also be frustrated in the sense that there may be no one-electron state that simultaneously minimizes every kinetic term in the Hamiltonian. Perhaps the simplest example of this is the three-site tight-binding model with the hopping integral $t < 0$. In the infinite-U Hubbard model on the same lattice this "kinetic frustration" leads to a triplet ground state for two electrons [2,3]. We argue below that in itinerant electron systems the bipartite/geometrically frustrated distinction is not relevant and balance [4] provides an appropriate definition of systems free of kinetic frustration.

Previous attempts to classify the frustration of itinerant electrons have focused on the reduced bandwidth in frustrated systems [3,5]. Therefore, these measures miss the fundamental role that the sign of the hopping integral plays in frustrated itinerant electron systems. Balance considers this. On the other hand, it is known that kinetic frustration can lead to antiferromagnetic states in the infinite-U limit [6–9]. A staggered magnetic flux can be used to control the degree of kinetic frustration, driving the ground state of certain models from magnetic to antiferromagnetic [9].

To ground the above claims we study one of the few exact results of strongly correlated itinerant electrons: Nagaoka's theorem. This theorem concerns the properties of the infinite-U Hubbard model—however, here we consider a larger class of Hamiltonians, which allows for arbitrary two-orbital interactions:

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_t + \hat{\mathcal{H}}_U + \hat{\mathcal{H}}_V + \hat{\mathcal{H}}_J + \hat{\mathcal{H}}_P + \hat{\mathcal{H}}_X, \tag{1}$$

where

$$\hat{\mathcal{H}}_t = -\sum_{ij\mu\nu\sigma} t_{ij\mu\nu}\hat{c}^\dagger_{i\mu\sigma}\hat{c}_{j\nu\sigma}, \tag{2a}$$

$$\hat{\mathcal{H}}_U = U\sum_{i\mu}\hat{n}_{i\mu\uparrow}\hat{n}_{i\mu\downarrow}, \tag{2b}$$

$$\hat{\mathcal{H}}_V = \hat{V}(\{\hat{n}_{i\mu}\}), \tag{2c}$$

$$\hat{\mathcal{H}}_J = \sum_{(i,\mu)\neq(j,\nu)}\sum_{\sigma\rho} J_{ij\mu\nu}\hat{c}^\dagger_{i\mu\sigma}\hat{c}^\dagger_{j\nu\rho}\hat{c}_{i\mu\rho}\hat{c}_{j\nu\sigma}$$

$$= \sum_{(i,\mu)\neq(j,\nu)} J_{ij\mu\nu}\left(\hat{\mathbf{S}}_{i\mu}\cdot\hat{\mathbf{S}}_{j\nu} + \frac{1}{4}\hat{n}_{i\mu}\hat{n}_{j\nu}\right), \tag{2d}$$

$$\hat{\mathcal{H}}_P = \sum_{(i,\mu)\neq(j,\nu)} P_{ij\mu\nu}\hat{c}^\dagger_{i\mu\uparrow}\hat{c}^\dagger_{i\mu\downarrow}\hat{c}_{j\nu\uparrow}\hat{c}_{j\nu\downarrow}, \tag{2e}$$

$$\hat{\mathcal{H}}_X = \sum_{(i,\mu)\neq(j,\nu)}\sum_{\sigma} X_{ij\mu\nu}\hat{c}^\dagger_{i\mu\sigma}\hat{c}_{j\nu\sigma}(\hat{n}_{i\mu\bar{\sigma}} + \hat{n}_{j\nu\bar{\sigma}} - 1), \tag{2f}$$

where $\hat{c}^{(\dagger)}_{i\mu\sigma}$ creates (annihilates) an electron with spin σ on the μth Wannier orbital centered on site i, $\bar{\sigma}\neq\sigma$, $\hat{n}_{i\mu\sigma} = \hat{c}^\dagger_{i\mu\sigma}\hat{c}_{i\mu\sigma}$, $\hat{n}_{i\mu} = \hat{n}_{i\mu\uparrow} + \hat{n}_{i\mu\downarrow}$, $\hat{\mathbf{S}}_{i\mu} = \frac{1}{2}\sum_{\alpha\beta}\hat{c}^\dagger_{i\mu\alpha}\boldsymbol{\sigma}_{\alpha\beta}\hat{c}_{i\mu\beta}$, and $\boldsymbol{\sigma}$ is the vector of Pauli matrices. Here $t_{ij\mu\nu}$ is the amplitude for hopping between the μth orbital on site i and the νth orbital on site j [10], U is the effective Coulomb interaction between two electrons on the same orbital, $\hat{V}(\{\hat{n}_{i\mu}\})$ is any potential that depends only on the orbital occupation numbers—obviously this includes arbitrary pairwise direct Coulomb interactions: $\sum_{ij\mu\nu} V_{ij\mu\nu}\hat{n}_{i\mu}\hat{n}_{j\nu}$. However, in fact the proofs below hold for arbitrary terms of this form, including multisite interactions, the $J_{ij\mu\nu}$ are the exchange couplings, the $P_{ij\mu\nu}$ are pair hopping amplitudes, and the $X_{ij\mu\nu}$ are correlated hopping amplitudes.

Note that, in the infinite-U limit, $\hat{\mathcal{H}}_P$ and the first two terms in $\hat{\mathcal{H}}_X$ are identically null. We stress that no assumption about the intrasite hopping has been made; in particular, $t_{ii\mu\nu}$ may be nonzero.

It is convenient below to differentiate between four versions of this model: (a) the multiorbital model—Eq. (1); (b) the single-orbital model—one orbital per site (henceforth we drop the orbital subscripts when discussing single-orbital models); (c) the extended Hubbard model—the single-orbital model with $J_{ij} = P_{ij} = X_{ij} = 0$ for all i, j, μ, and ν; and (d) the Hubbard model—the extended Hubbard model with $\hat{V}(\{\hat{n}_{i\mu}\}) = 0$.

Note that the hole-doped sector of each of these models ($N < L$, where N is the number of electrons and L is the number of orbitals on the entire lattice) is equivalent to the electron sector of that model ($N > L$) with the signs of all $t_{ij\mu\nu}$ reversed. A particle-hole transformation maps between the Hamiltonians, up to constants, even in the absence of particle-hole symmetry. Henceforth we only discuss the hole-doped problem; however it is implicit throughout that all results hold for the electron-doped problem if the signs of all $t_{ij\mu\nu}$ are reversed.

Nagaoka [11] showed that in the Nagaoka limit ($U \to \infty$ and $N = L - 1$) the ground state of the Hubbard model on certain lattices is a fully polarized ferromagnet—i.e., the magnetization $M = N/2$. Nagaoka showed that for nearest-neighbor hopping only ($t_{ij} = t$ for nearest neighbors, $t_{ij} = 0$ otherwise) and $t < 0$ [10] this result holds for simple cubic, body-centered cubic, face-centered cubic, and hexagonal close-packed lattices.

However, for $t > 0$ Nagaoka found that the theorem holds on the simple cubic and body-centered cubic lattices, but not for the face-centered cubic or hexagonal close-packed lattices. The former lattices are bipartite, while the latter are not. On a bipartite lattice the gauge transformation $\hat{c}_{i\sigma} \to -\hat{c}_{i\sigma}$ on one sublattice only changes the sign of all hopping integrals.

In 1989 Tasaki gave a more general proof of Nagaoka's theorem [12]. Specifically, Tasaki proved that Nagaoka's theorem holds for the extended Hubbard model on all lattices where $t_{ij} \leqslant 0$ for all i and j. Thus, one is moved to ask, which other Hamiltonians with some or all $t_{ij} > 0$ have ferromagnetic ground states? In particular, for which geometrically frustrated (non-bipartite) Hamiltonians can one prove Nagaoka's theorem? This is particularly important as for a simple covalent bonds one expects that $t_{ij} > 0$ [13].

In 1996 Kollar, Strack, and Vollhardt [14] extended Nagaoka's theorem in a different direction—discussing the role of other two-body interactions. Among other things they showed that Nagaoka's theorem holds for the infinite-U single-orbital model on periodic lattices if the hopping and all interactions are constrained to be between nearest neighbors only, exchange is ferromagnetic (or zero), and either $t < 0$ or the lattice is bipartite. It is therefore natural to ask, what other (e.g., longer range) two-orbital interactions admit a proof of Nagaoka's theorem?

Fully polarized Nagaoka ferromagnetism is importantly different from the partially polarized states observed in ferromagnetic metals such as iron, colbalt, and nickel. However, it should be possible to realize Nagaoka physics in atomic gases on optical lattices. Nevertheless, given that ferromagnetism is observed in many materials where multiple orbitals are relevant to the low-energy physics it is interesting to ask whether multiple orbital models exhibit Nagaoka-like ferromagnetism.

Below, we give partial answers to the above questions by proving the following:

Theorem 1. Consider the multiorbital model (1) with U being infinite; V and $\{P_{ij\mu\nu}\}$ being arbitrary; $J_{ij\mu\nu} \leqslant 0$ for all i, j, μ, and ν; and $N = L - 1$. If the signed graph $\mathcal{S}$ defined by the set of renormalized hopping integrals $\{t^*_{ij\mu\nu}\}$, where $t^*_{ij\mu\nu} \equiv t_{ij\mu\nu} + X_{ij\mu\nu}$, is balanced (defined below), then among the ground states there exist at least L states with $S = S_{\max} \equiv N/2$.

Theorem 2. Consider the multiorbital model (1) with U being infinite; V and $\{P_{ij\mu\nu}\}$ being arbitrary; $J_{ij\mu\nu} \leqslant 0$ for all i, j, μ, and ν; and $N = L - 1$. If the signed graph $\mathcal{S}$ defined by the set of renormalized hopping integrals $\{t^*_{ij\mu\nu}\}$ is balanced and $\hat{\mathcal{H}}_t + \hat{\mathcal{H}}_X$ satisfies the connectivity condition (defined below), then the ground state has $S = S_{\max} \equiv N/2$ and is unique up to the trivial N-fold degeneracy.

The remainder of the paper is laid out as follows. Having introduced balanced and unbalanced lattices in Sec. II, we prove that balance is a sufficient condition for the proof of Nagaoka's theorem in the Nagaoka limit (Sec. III). All of the lattices for which Nagaoka [11], Tasaki [12], or Kollar *et al.* [14] proved Nagaoka's theorem previously are balanced. Finally, in Sec. IV we discuss the implications of balance for the orbital part of the ground-state wave function, clarifying why balance favors ferromagnetism.

II. BALANCE

The sign of the hopping between a pair of orbitals, $t^*_{ij\mu\nu}$, is not gauge invariant: the transformation $\hat{c}_{j\nu\sigma} \to e^{-i\theta_{j\nu}}\hat{c}_{j\nu\sigma}$ takes $t^*_{ij\mu\nu} \to t^*_{ij\mu\nu}e^{i\theta_{j\nu}}$. Nevertheless, gauge-invariant information is contained in the signs of the set $\{t^*_{ij\mu\nu}\}$ associated with a particular Hamiltonian.

This is a topological problem—the magnitudes of the $t^*_{ij\mu\nu}$ values are unimportant; only their signs matter. Thus, rather than considering every $\{t^*_{ij\mu\nu}\}$ separately, it is sufficient to instead study a related "signed graph." We define this signed graph as follows. We introduce a vertex of the graph corresponding to each orbital in the physical Hamiltonian, $\{\aleph\} = \{(i,\mu)\}$ (throughout this paper we use Latin characters for sites in the Hamiltonian, Greek characters for orbitals, and Hebrew characters for vertices in the signed graph). Furthermore, we introduce a set of edges defined by $\{\tau_{(i,\mu),(j,\nu)}\}$, where $\tau_{(i,\mu),(j,\nu)} \equiv -\mathrm{sgn}(t^*_{ij\mu\nu})$ if and only if $t^*_{ij\mu\nu} \neq 0$. We now ask whether there exists a series of gauge transformations that make all $\tau_{\aleph\beth} = 1$. If so, the gauge transformation makes all $t^*_{ij\mu\nu} \leqslant 0$.

A *walk* on a signed graph is defined as a sequence of vertices such that consecutive vertices in the sequence are connected by an edge, e.g., $\aleph \to \beth \to \gimel \to \cdots \to \resh \to \shin \to \tav$. A walk in which all the vertices that are visited are distinct (i.e., a self-avoiding walk) is called a *path*. A path that visits at least three vertices and is closed (e.g., $\aleph = \tav$, in the example above) is called a *cycle*. The sign of a path or cycle on a signed graph is defined as the product of signs $(\tau_{\aleph\beth}\tau_{\beth\gimel}\ldots\tau_{\resh\shin}\tau_{\shin\tav})$ of the edges forming the path or cycle. Thus every positive cycle has an even number (including zero) of negative edges. A signed graph is *balanced* if all cycles in the corresponding signed graph are positive (cf. Fig. 1). We call a Hamiltonian balanced if it maps onto a balanced signed graph in the sense described above.

The fundamental theorem of signed graphs [15] states that for a signed graph, $\mathcal{S}$, the following three conditions are equivalent:

(i) $\mathcal{S}$ is balanced, i.e., all cycles within $\mathcal{S}$ are positive.

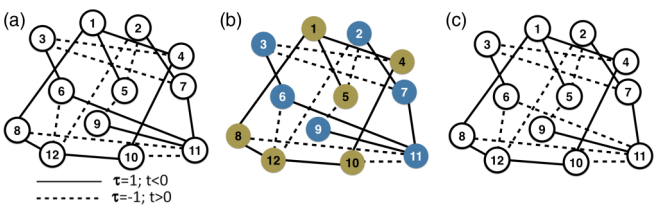

FIG. 1. Balanced and unbalanced signed graphs. In all panels solid lines indicate $\tau_{\aleph\beth} = 1$ [$t_{ij\mu\nu} < 0$, where $\aleph = (i,\mu)$ and $\beth = (j,\nu)$] and dashed lines indicate $\tau_{\aleph\beth} = -1$ ($t_{ij\mu\nu} > 0$). (a) A balanced lattice. (b) As in panel (a) with a choice of the subsets $\mathcal{S}_a$ and $\mathcal{S}_b$ indicated by the shading of the vertices. (c) An unbalanced lattice: The path $6 \to 11 \to 10 \to 12 \to 6$ is negative ($\tau_{6,11}\tau_{11,10}\tau_{10,12}\tau_{12,6} = -1$).

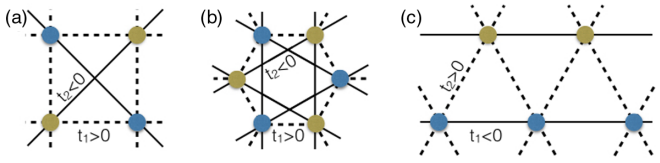

FIG. 2. Three geometrically frustrated but balanced periodic lattices. (a) The square lattice with nearest-neighbor hopping $t_1 > 0$ and next-nearest-neighbor hopping $t_2 < 0$. (b) The honeycomb lattice with $t_1 > 0$ and $t_2 < 0$. (c) The anisotropic triangular lattice, relevant to organic superconductors and magnets [16], with $t_1 < 0$ and $t_2 > 0$. In each case two sublattices are marked; all hopping integrals are made positive by the transformation $\hat{c}_{i\sigma} \to -\hat{c}_{i\sigma}$ on one sublattice only.

(ii) For any pair of vertices א and ב in $\mathcal{S}$ all paths joining א and ב have the same sign.

(iii) There exists a partition of $\mathcal{S}$ into two subsets, $\mathcal{S}_a$ and $\mathcal{S}_b$ (one of which may be empty), such that $\tau_{\text{אב}} \geqslant 0$ for all א and ב within the same subset, but $\tau_{\text{בא}} = \tau_{\text{אב}} \leqslant 0$ for א $\in \mathcal{S}_a$ and ב $\in \mathcal{S}_b$.

Thus, for example, bipartite lattices with only nearest-neighbor hopping (and the same sign of hopping between all neighbors) are balanced. Some simple examples of geometrically frustrated but balanced lattices are shown in Fig. 2.

III. BALANCE IS SUFFICIENT FOR NAGAOKA

In the Nagaoka limit all states with finite energy can be written as a superposition of "single-hole states" of the form

$$|i,\mu,\tau\rangle = (-1)^{\rho(i,\mu)} \prod_{(j,\nu)\neq(i,\mu)} \hat{c}^{\dagger}_{j\nu\sigma_j}|0\rangle, \tag{3}$$

where $\tau = \{\sigma_j\}_{j\neq i}$ is a binary vector describing the spins of all of the electrons; $|0\rangle$ is the vacuum state defined by $\hat{c}_{i\mu\sigma}|0\rangle = 0$ for all i, μ, and σ; and $\rho(i,\mu) \in [0, L-1]$ is an arbitrary ordering of the orbitals. $\rho(i,\mu)$ need have no correlation to the structure of the lattice, but is required to enforce the correct antisymmetrization of the hole states—the operators in the product are to be ordered by $\rho(i,\mu)$ with lower values to the left.

We describe two states as "directly connected" if $\langle i,\mu,\tau|\hat{\mathcal{H}}_t + \hat{\mathcal{H}}_X|j,\nu,\upsilon\rangle \neq 0$. We denote direct connection by $(i,\mu,\tau) \leftrightarrow (j,\nu,\upsilon)$. For directly connected states

$$\langle i,\mu,\tau|\hat{\mathcal{H}}_t + \hat{\mathcal{H}}_X|j,\nu,\upsilon\rangle = t^{*}_{ij\mu\nu}. \tag{4}$$

A Hamiltonian is said to satisfy the connectivity condition if there exists an integer n for which $\langle i,\mu,\tau|(\hat{\mathcal{H}}_t + \hat{\mathcal{H}}_X)^n|j,\nu,\upsilon\rangle \neq 0$ for every pair of states with the same S^z. Notably, one-dimensional single-orbital models with only nearest-neighbor hopping are not connected in this sense [11,12].

A. Proof of Theorem 1

Compare the arbitrary superposition of states of single-hole states,

$$|A_h\rangle = \sum_{i\mu\tau} \alpha_{i\mu\tau}|i,\mu,\tau\rangle, \tag{5}$$

with a fully spin polarized superposition,

$$|\Phi_h\rangle = \sum_{i\mu} \phi_{i\mu}|i,\mu,\Uparrow\rangle, \tag{6}$$

where $\tau = \Uparrow$ indicates that all the electrons are up and $\phi_{i\mu} = \sqrt{\sum_\tau |\alpha_{i\mu\tau}|^2}$. We have

$$\begin{aligned}\langle A_h|\hat{\mathcal{H}}_V|A_h\rangle &= \sum_{i\mu\tau} |\alpha_{i\mu\tau}|^2 \langle i,\mu,\tau|\hat{\mathcal{H}}_V|i,\mu,\tau\rangle \\ &= \sum_{i\mu\tau} |\alpha_{i\mu\tau}|^2 \langle i,\mu,\Uparrow|\hat{\mathcal{H}}_V|i,\mu,\Uparrow\rangle \\ &= \sum_{i\mu} |\phi_{i\mu}|^2 \langle i,\mu,\Uparrow|\hat{\mathcal{H}}_V|i,\mu,\Uparrow\rangle \\ &= \langle \Phi_h|\hat{\mathcal{H}}_V|\Phi_h\rangle. \end{aligned} \tag{7}$$

That is, because U is infinite and $V(\{\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}\})$ only depends on the site occupation numbers, $\langle\hat{\mathcal{H}}_V\rangle$ is independent of the spin degrees of freedom for single-hole states.

Now note that

$$\begin{aligned}&\langle i,\mu,\Uparrow|\big(\hat{\mathbf{S}}_{i'\mu'}\cdot\hat{\mathbf{S}}_{j'\nu'} + \tfrac{1}{4}\hat{n}_{i'\mu'}\hat{n}_{j'\nu'}\big)|j,\nu,\Uparrow\rangle \\ &\quad\geqslant \langle i,\mu,\tau|\big(\hat{\mathbf{S}}_{i'\mu'}\cdot\hat{\mathbf{S}}_{j'\nu'} + \tfrac{1}{4}\hat{n}_{i'\mu'}\hat{n}_{j'\nu'}\big)|j,\nu,\upsilon\rangle \geqslant 0 \end{aligned} \tag{8}$$

for all i, i', j, j', μ, μ', ν, ν', τ, and υ. Thus, if $J_{ij\mu\nu} \leqslant 0$ for all i, j, μ, and ν, then

$$0 \geqslant \langle j,\nu,\upsilon|\hat{\mathcal{H}}_J|i,\mu,\tau\rangle \equiv K^{j\nu\upsilon}_{i\mu\tau} \geqslant K^{j\nu\Uparrow}_{i\mu\Uparrow} \tag{9}$$

for all i, j, μ, ν, τ, and υ. Therefore,

$$\begin{aligned}\langle A_h|\hat{\mathcal{H}}_J|A_h\rangle &= \sum_{ij\mu\nu\tau\upsilon} K^{j\nu\upsilon}_{i\mu\tau}\alpha^{*}_{j\mu\tau}\alpha_{i\nu\upsilon} \\ &\geqslant \sum_{ij\mu\nu} K^{j\nu\Uparrow}_{i\mu\Uparrow}\sum_{\tau\upsilon}\alpha^{*}_{j\mu\tau}\alpha_{i\nu\upsilon} \\ &\geqslant \sum_{ij\mu\nu} K^{j\nu\Uparrow}_{i\mu\Uparrow}\phi^{*}_{j\mu}\phi_{i\nu} = \langle\Phi_h|\hat{\mathcal{H}}_J|\Phi_h\rangle, \end{aligned} \tag{10}$$

where the second inequality follows from the Cauchy-Schwartz inequality.

Because double occupancy is forbidden in the infinite-U limit, $\langle i,\mu,\tau|\hat{\mathcal{H}}_P|j,\nu,\upsilon\rangle = 0$.

Finally, we specialize to the case of a balanced lattice. Property (iii) of the fundamental theorem of signed graphs implies that we can construct a gauge transformation that maps the Hamiltonian onto one where all $t^{*}_{ij\mu\nu} \leqslant 0$. An explicit example of such a gauge transformation is

$$\begin{aligned}\hat{c}_{i\mu\sigma} &\to -\hat{c}_{i\mu\sigma} \quad \text{for all} \quad (i,\mu) \in \mathcal{S}_a, \\ \hat{c}_{i\mu\sigma} &\to \hat{c}_{i\mu\sigma} \quad \text{for all} \quad (i,\mu) \in \mathcal{S}_b. \end{aligned} \tag{11}$$

Furthermore,

$$\begin{aligned}\langle A_h|\hat{\mathcal{H}}_t + \hat{\mathcal{H}}_X|A_h\rangle &= t^{*}_{ij\mu\nu}\sum_{\tau\leftrightarrow\upsilon}\alpha^{*}_{j\mu\tau}\alpha_{i\nu\upsilon} \\ &\geqslant t^{*}_{ij\mu\nu}\phi^{*}_{j\mu}\phi_{i\nu} = \langle\Phi_h|\hat{\mathcal{H}}_t + \hat{\mathcal{H}}_X|\Phi_h\rangle, \end{aligned} \tag{12}$$

where we have again made use of the Cauchy-Schwartz inequality and $\sum_{\tau\leftrightarrow\upsilon}$ indicates that the sum is restricted to run only over τ and υ such that $(i,\mu,\tau)\leftrightarrow(j,\nu,\upsilon)$, as the overlap integral vanishes otherwise. Thus, there are no states with energy lower than $|\Phi_h\rangle$. Theorem 1 follows immediately from the SO(3) symmetry of the model. ■

B. Proof of Theorem 2

The Perron-Frobenius theorem [17] states (among other things) that if all the elements of an irreducible real square matrix are non-negative then it has a unique largest real eigenvalue and that the corresponding eigenvector has strictly positive components. A Hermitian matrix is reducible if and only if it can be block diagonalized by a permutation matrix. Let use write the Hamiltonian (1) in the form

$$\hat{\mathcal{H}}=\sum_{m=(1-N)/2}^{(N-1)/2}\mathcal{H}_m, \tag{13}$$

where m labels the z component of the total spin of the system. Each of the N matrices $M_m=-\mathcal{H}_m$ is irreducible provided the Hamiltonian satisfies the connectivity condition. Furthermore, we have seen above that all of the matrix elements of $\mathcal{H}_m\leqslant 0$. Therefore each of the M_m satisfy the Perron-Frobenius theorem.

The SO(3) symmetry of the Hamiltonian means that $|\Phi_h\rangle$ must be N-fold degenerate. As no states have lower energy than $|\Phi_h\rangle$, this means that the lowest energy states of the S_z sectors are necessarily degenerate and that, up to this required N-fold degeneracy, $|\Phi_h\rangle$ is unique. ■

It is interesting to note that there exist matrices with some negative elements for which the dominant eigenvector is non-negative and corresponds to a positive eigenvector [18,19]. This suggests that, while sufficient, balance and/or connectivity may not be necessary conditions for Nagaoka's theorem.

IV. FRUSTRATION AND THE ORBITAL PART OF THE GROUND-STATE WAVE FUNCTION

For the Hubbard model the explicit wave function can be straightforwardly constructed. Of course one could simply take Eq. (6) as a variational wave function and minimize all of the ϕ_i. However, a more elegant approach is to introduce an ancillary model of noninteracting spinless fermions on the same lattice:

$$\hat{\mathcal{H}}_a=-\sum_{ij}t_{ij}\hat{c}_i^\dagger\hat{c}_j, \tag{14}$$

and then make a particle-hole transformation $\hat{h}_i^\dagger=\hat{c}_i$. As this is a single-particle Hamiltonian the ground state can be written in the form

$$|\Psi_h\rangle=\sum_i\psi_i\hat{h}_i^\dagger|vac\rangle, \tag{15}$$

where the vacuum for holes, $|vac\rangle$, is the state for which $\hat{h}_i|vac\rangle=0$ for all i. Note that

$$|i,\Uparrow\rangle=\hat{c}_{i\uparrow}\prod_j\hat{c}_{j\uparrow}^\dagger|0\rangle=\hat{h}_{i\uparrow}^\dagger|\Uparrow\rangle, \tag{16}$$

where $\hat{h}_{i\sigma}^\dagger=\hat{c}_{i\sigma}$ and $|\Uparrow\rangle=\prod_j\hat{c}_{j\uparrow}^\dagger|0\rangle$, where the ordering of the operators in the products is as in Eq. (3).

Recalling Eqs. (4) and (6) one finds that $\phi_i=\psi_i$ for all i, which means that we can calculate the ground-state wave function of the Hubbard model from the ancillary noninteraction model. Often, directly minimizing Eq. (15) is not the most efficient approach; for example, if the lattice is periodic, a Fourier transformation leads directly to the solution.

If all $t_{ij}<0$, the ground state must have $\phi_i=\psi_i>0$ for all i. That is, the wave function is bonding between all sites. In this sense, the ground-state wave function is unfrustrated. Note that, in a periodic system, it always possible to construct a wave function that is strictly positive at high-symmetry points with wave vectors $\boldsymbol{k}$, satisfying $2\boldsymbol{k}=n\boldsymbol{G}$, where $\boldsymbol{G}$ is a reciprocal lattice vector for any $n\in\mathbb{Z}$. The set of all such high-symmetry points always includes the Γ point (origin of the unit cell).

Returning to the multiorbital model, the Perron-Frobenius theorem guarantees the existence of a gauge for which all $\phi_{i\mu}$ are strictly positive. Thus again the ground-state wave function is unfrustrated.

In this context it is interesting to note the recent discovery that on some kinetically frustrated lattices antiferromagnetic states with magnetization near the classical limit occur in the Nagaoka limit [6–9]. Again here releasing the frustration in the orbital part of the wave function appears to play a crucial role [7].

V. CONCLUSIONS

We have shown that balance and the absence of antiferromagnetic exchange are sufficient to prove that the ground state of the infinite-U multiorbital model, Eq. (1), with arbitrary pairwise interactions is ferromagnetic.

Balance implies the absence of kinetic frustration—therefore, for itinerant electrons, balance is the natural definition of an unfrustrated lattice. While bipartite lattices (with no hopping within the sublattices) are always balanced, many non-bipartite lattices are also balanced (see Fig. 2 for some examples). An interesting question, beyond the scope of this paper, is the role of balance to other problems involving frustration and itinerant electrons.

Balance is important because it allows for an unfrustrated orbital part of the ground-state wave function. This is consistent with the general insight that Nagaoka's theorem arises from the minimization of the hole's kinetic energy.

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[10] Note the negative sign on the right-hand-side of Eq. (2a). Though now standard it is not included in some older papers, e.g., Refs. [11,12]. This is potentially confusing when discussing the signs of the t_{ij}. Note that throughout this paper all such signs are those using the sign convention employed in Eq. (2a).

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