Exact Results for Itinerant Ferromagnetism in Multiorbital Systems on Square and Cubic Lattices

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We study itinerant ferromagnetism in multiorbital Hubbard models in certain two-dimensional square and three-dimensional cubic lattices. In the strong coupling limit where doubly occupied orbitals are not allowed, we prove that the fully spin-polarized states are the unique ground states, apart from the trivial spin degeneracies, for a large region of filling factors. Possible applications to p-orbital bands with ultracold fermions in optical lattices, and electronic $3d$-orbital bands in transition-metal oxides, are discussed.

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Itinerant ferromagnetism (FM) is one of the central topics in condensed matter physics [1–18]. Historically, it had been thought that exchange energy, which is a perturbation-theoretic idea, favors FM, but that is opposed by the kinetic energy increase required by the Pauli exclusion principle to polarize a fermionic system. Interactions need to be sufficiently strong to drive FM transitions, and hence FM is intrinsically a strong correlation problem. In fact, the Lieb-Mattis theorem [1] for one-dimensional (1D) systems shows that FM never occurs, regardless of how large the exchange energy might be. Even with very strong repulsion, electrons can remain unpolarized while their wave functions are nevertheless significantly far from the Slater-determinant type.

Strong correlations are necessary for itinerant FM, but the precise mechanism is subtle. An early example is Nagaoka's theorem about the infinite U Hubbard model, fully filled except for one missing electron, called a hole. He showed [3], and Tasaki generalized the result [19], that the one hole causes the system of itinerant electrons to be fully spin polarized—i.e., saturated FM. However, Nagaoka's theorem is not relevant in 1D because no nontrivial loops are possible in this case. For infinite U, ground states are degenerate, regardless of spin configurations along the chain. As U becomes finite, as shown in Ref. [20], the degeneracy is lifted and the ground state is a spin singlet. Another set of exact results is the flatband FM models on line graphs [12–14,21,22]. On such graphs, there exist Wannier-like localized single particle eigenstates, which eliminate the kinetic energy cost of spin polarization. Later, interesting metallic ferromagnetic models without flatband structures were proposed by Tasaki [23], and then by Tanaka and Tasaki [24]. FM in realistic flatband systems has been proposed in the p orbitals in honeycomb lattices with ultracold fermions [25].

In this Letter, we prove a theorem about FM in the two-dimensional (2D) square and three-dimensional (3D) cubic lattices with *multiorbital* structures. We can even do this in 1D, as shown in Corollary 2 in the Supplemental Material [26], where we reproduce, by our method, Shen's result [27] that the multiorbital 1D system is FM. Our result differs from that of Nagaoka in that it is valid for a large region of filling factors in both 2D and 3D. It is also different from flatband FM, in which fermion kinetic energy differences are suppressed.

We emphasize that our result is robust in that the translation invariance is not really required. The hopping magnitudes can vary along chains and from chain to chain. We confine our attention here to the translation invariant Hamiltonian purely for simplicity of exposition.

Our band Hamiltonians behave like decoupled, perpendicular 1D chains, which are coupled by the standard on-site, multiorbital Hubbard interactions that are widely used in the literature [4,5,28,29]. In the limit of infinite intraorbital repulsion, we prove that the interorbital Hund's rule coupling at each site drives the ground states to fully spin-polarized states. Furthermore, the ground states are nondegenerate except for the obvious spin degeneracy, and the wave functions are nodeless in a properly defined basis. This theorem is generalized here to multicomponent fermions with $\mathrm{SU}(N)$ symmetries. This itinerant FM theorem is not just of academic interest because it may be relevant to the p-orbital systems with ultracold atoms [30] and to the $LaAlO_3/SrTiO_3$ interface of $3d$-orbital transition-metal oxides [31–33].

Let us first very briefly give a heuristic overview of our model in 2D. Think of the square lattice $\mathbb{Z}^2$ as consisting of horizontal lines and vertical lines, and imagine two kinds of electrons, one of which can move with hard-core interactions along the horizontal lines and the other of which can move along the vertical lines. No transition between any two lines is allowed. When two electrons of different type meet at a vertex, Hund's rule requires them to prefer to be in a triplet state. Our theorem is that this interaction forces the whole system to be uniquely FM. The two kinds

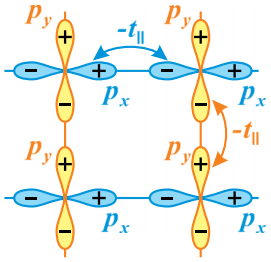

FIG. 1 (color online). The square lattice with the quasi-1D band structure of the p-orbital bands. Particles in the p_x (p_y) orbital can only move along the x (y) direction, respectively. The sign of $t_\parallel$ can be changed by a gauge transformation on the square lattice.

of electrons in this picture are the p_x-orbital and p_y-orbital electrons. The p_x orbitals overlap only in the x direction and thus can allow motion only in that direction—and similarly for p_y orbitals.

Now, let us describe multiorbital systems for spin-1/2 fermions on 2D square and 3D cubic lattices with quasi-1D band structures. The p-orbital systems are used, but this is only one possible example of atomic orbitals that could be considered, another example being d_{xz} and d_{yz} orbitals. Nearest-neighbor hoppings can be classified as either σ bonding with hopping amplitude $t_\parallel$ or π bonding with hopping amplitude $t_\perp$, which describe the hopping directions parallel or perpendicular to the orbital orientation, respectively. Typically, $t_\perp$ is much smaller than $t_\parallel$ and thus will be neglected here, leading to the following quasi-1D band Hamiltonian (see Fig. 1):

$$H_{\rm kin}^{\rm 2D(3D)} = \sum_{\mu=x,y,(z)} H_{\rm kin}^{{\rm 1D},\mu} - \mu_0 \sum_{\mathbf{r}} n(\mathbf{r}),$$
$$H_{\rm kin}^{{\rm 1D},\mu} = -t_\parallel \sum_{\mathbf{r},\sigma=\uparrow,\downarrow} p_{\mu,\sigma}^\dagger(\mathbf{r}+\hat{\mathbf{e}}_\mu) p_{\mu,\sigma}(\mathbf{r}) + \text{H.c.} \quad (1)$$

Here, $p_{\mu,\sigma}(\mathbf{r})$ is the annihilation operator in the p_μ orbital $[\mu = x, y, (z)]$ on site $\mathbf{r}$ with the spin eigenvalue σ; $n(\mathbf{r})$ is the total particle number on site $\mathbf{r}$, and $\hat{\mathbf{e}}_\mu$ is the unit vector in the μ direction. Since the lattice is bipartite, the sign of $t_\parallel$ can be flipped by a gauge transformation. Without loss of generality, it is taken to be positive. The generic multiorbital on-site Hubbard interactions [34,35] are as follows:

$$H_{\rm int} = U \sum_{\mu,\mathbf{r}} n_{\mu,\uparrow}(\mathbf{r}) n_{\mu,\downarrow}(\mathbf{r}) + \frac{V}{2} \sum_{\mu\neq\nu,\mathbf{r}} n_\mu(\mathbf{r}) n_\nu(\mathbf{r})$$
$$- \frac{J}{2} \sum_{\mu\neq\nu,\mathbf{r}} \left\{ \vec{S}_\mu(\mathbf{r}) \cdot \vec{S}_\nu(\mathbf{r}) - \frac{1}{4} n_\mu(\mathbf{r}) n_\nu(\mathbf{r}) \right\}$$
$$+ \Delta \sum_{\mu\neq\nu,\mathbf{r}} p_{\mu\uparrow}^\dagger(\mathbf{r}) p_{\mu\downarrow}^\dagger(\mathbf{r}) p_{\nu\downarrow}(\mathbf{r}) p_{\nu\uparrow}(\mathbf{r}), \quad (2)$$

where $n_{\mu,\sigma} = p_{\mu,\sigma}^\dagger p_{\mu,\sigma}$ and $\vec{S}_\mu = p_{\mu,\alpha}^\dagger \vec{S}_{\alpha\beta} p_{\mu,\beta}$ represent the spin operators in the p_μ orbital. The U and V terms are intra- and interorbital Hubbard interactions, respectively; the J term represents the Hund's rule coupling; the Δ term describes the pair hopping process between different orbitals. The expressions of U, V, J, and Δ in terms of integrals of Wannier orbital wave functions and their physical meaning are provided in Sec. I of the Supplemental Material [26].

We consider the limit $U \to +\infty$ and start with the 2D version of the Hamiltonian $H_{\rm kin} + H_{\rm int}$. States with double occupancy in a *single* orbital $(1/\sqrt{2})\{p_{x\uparrow}^\dagger p_{x\downarrow}^\dagger \pm p_{y\uparrow}^\dagger p_{y\downarrow}^\dagger\}|0\rangle$ are projected out. The projected Fock space on a single site is a tensor product of that on each orbital spanned by three states as $\mathcal{F}_{\mathbf{r}} = \bigotimes_{\mu=x,y} \mathcal{F}_{\mathbf{r}}^\mu$ with $\mathcal{F}_{\mathbf{r}}^\mu = \{|0\rangle, p_{\mu,\uparrow}^\dagger(\mathbf{r})|0\rangle, p_{\mu,\downarrow}^\dagger(\mathbf{r})|0\rangle\}$. The projected Fock space $\mathcal{F}$ of the system is a tensor product of $\mathcal{F}_{\mathbf{r}}$ on each site.

We state three lemmas before presenting the FM Theorem 1. The proofs of Lemmas 2 and 3 are provided in Sec. II of the Supplemental Material [26]. We shall always assume henceforth the following two conditions, which are essential for Lemmas 2 and 3, respectively.

(i) The boundary condition [36] on each row and column is periodic (respectively, antiperiodic) when the particle number in the row or column is odd (respectively, even). The fact that the particle number in each row or column is fixed is contained in Lemma 1 below.

(ii) There is at least one particle and one hole in each chain. "Hole" means an empty orbital.

The following lemma is obvious.

Lemma 1. *In the projected Fock space $\mathcal{F}$ for the Hamiltonian $H = H_{\rm kin} + H_{\rm int}$ [see Eqs. (1) and (2)], the particle numbers of each row and each column are separately conserved.*

Based on Lemma 1, we can specify a partition of particle numbers into rows $\mathcal{X} = \{r_i = 1, \ldots, L_y\}$ and columns $\mathcal{Y} = \{c_i = 1, \ldots, L_x\}$ as

$$\mathcal{N}_\mathcal{X} = \{N_{r_i}\}, \qquad \mathcal{N}_\mathcal{Y} = \{N_{c_i}\}, \quad (3)$$

where N_{r_i} and N_{c_i} are the particle numbers conserved in the r_ith row and the c_ith column, respectively. Altogether, $\sum_{r_i=1}^{L_y} N_{r_i} + \sum_{c_i=1}^{L_x} N_{c_i} = N_{\rm tot}$ is the total particle number. The physical Hilbert space $\mathcal{H}_{\mathcal{N}_\mathcal{X},\mathcal{N}_\mathcal{Y}}$ is spanned by states in $\mathcal{F}$ satisfying Eq. (3). A many-body basis in $\mathcal{H}_{\mathcal{N}_\mathcal{X},\mathcal{N}_\mathcal{Y}}$ can be defined using the following convention: we first order p_x-orbital particles in each row by successively applying the creation operators of p_x orbitals, starting with the leftmost occupied site x_1^r and continuing to the right until $x_{N_r}^r$ in the rth row. The operator creating the whole collection of N_r p_x-orbital particles in the row r is denoted as

$$\mathcal{P}_{x,r}^\dagger = \prod_{i=1,\mathbf{r}_i\in \text{row } r}^{N^r} p_{x,\alpha_i^r}^\dagger(\mathbf{r}_i)$$
$$= p_{x,\alpha_{N_r}^r}^\dagger(\mathbf{r}_{N_r}) \cdots p_{x,\alpha_2^r}^\dagger(\mathbf{r}_2) p_{x,\alpha_1^r}^\dagger(\mathbf{r}_1). \quad (4)$$

Here, i is the particle index in row r. $\mathbf{r}_i = (x_i^r, r)$ and α_i^r are, respectively, the coordinate and s_z eigenvalue for the ith

particle in the rth row; similarly, the creation operator for the N^c p_y-orbital particles in the cth column can be defined, following an order from top to bottom, as $\mathcal{P}^\dagger_{y,c} = \prod_{i=1,\mathbf{r}_i\in\text{column }c}^{N^c} p^\dagger_{y,\beta^c_i}(\mathbf{r}_i) = p^\dagger_{y,\beta^c_{N_c}}(\mathbf{r}_{N_c})\cdots p^\dagger_{y,\beta^c_2}(\mathbf{r}_2)p^\dagger_{y,\beta^c_1}(\mathbf{r}_1)$. Here, similar definitions apply to $\mathbf{r}_i = (c, y^c_i)$ in column c and β^c_i. These coordinates for particles in each chain are ordered as $1 \le x^r_1 < x^r_2 < \cdots < x^r_{N_r} \le L_x$ and $1 \le y^c_1 < y^c_2 < \cdots < y^c_{N_c} \le L_y$.

Based on the above ordering within each row and each column, the many-body basis can be set up by further ordering them by rows and columns and applying the following creation operators to the vacuum $|0\rangle$ as

$$|\mathcal{R},\mathcal{S}\rangle_{\mathcal{N}_\mathcal{X},\mathcal{N}_\mathcal{Y}} = \prod_{j=1}^{L_x}\mathcal{P}^\dagger_{y,c_j}\prod_{j=1}^{L_y}\mathcal{P}^\dagger_{x,r_j}|0\rangle = \mathcal{P}^\dagger_{y,c_{L_x}}\cdots\mathcal{P}^\dagger_{y,c_2}\mathcal{P}^\dagger_{y,c_1}\mathcal{P}^\dagger_{x,r_{L_y}}\cdots\mathcal{P}^\dagger_{x,r_2}\mathcal{P}^\dagger_{x,r_1}|0\rangle. \quad (5)$$

Here, j denotes the index of columns and rows. Given a partition of the particle number $\mathcal{N}_\mathcal{X}$, $\mathcal{N}_\mathcal{Y}$, the many-body basis is specified by the coordinates of occupied sites $\mathcal{R} = \{\mathbf{r}^{r_j}_i; \mathbf{r}^{c_j}_i\}$ and the corresponding spin configuration $\mathcal{S} = \{\alpha^{r_j}_i; \beta^{c_j}_i\}$ for all i's and j's.

Lemma 2 ***(Nonpositivity).*** *The off-diagonal matrix elements of the Hamiltonian $H_{\text{kin}} + H_{\text{int}}$ with respect to the bases defined in Eq. (5) are nonpositive.*

Since the Hamiltonian is spin invariant, its eigenstates can be labeled by the total spin S and its z component S_z. The Hilbert space $\mathcal{H}_{\mathcal{N}_\mathcal{X},\mathcal{N}_\mathcal{Y}}$ can be divided into subspaces with different values of total S_z, denoted as $\mathcal{H}^{S_z}_{\mathcal{N}_\mathcal{X},\mathcal{N}_\mathcal{Y}}$. The many-body basis in this subspace is denoted as $|\mathcal{R},\mathcal{S}\rangle^{S_z}$. The smallest non-negative value of S_z is denoted as $S^{\min}_z$, which equals 0 ($\frac{1}{2}$) for even (odd) values of N_{tot}. The corresponding subspace is denoted as $\mathcal{H}^{\min}_{\mathcal{N}_\mathcal{X},\mathcal{N}_\mathcal{Y}}$. Every set of eigenstates with total spin S has one representative in $\mathcal{H}^{\min}_{\mathcal{N}_\mathcal{X},\mathcal{N}_\mathcal{Y}}$, and thus the ground states in this subspace are also the ground states in the entire Hilbert space.

Lemma 3 ***(Transitivity).*** *Consider the Hamiltonian matrix in the subspace $\mathcal{H}^M_{\mathcal{N}_\mathcal{X},\mathcal{N}_\mathcal{Y}}$ with $S_z = M$. Under condition (ii), for any two basis vectors $|u\rangle$ and $|u'\rangle$, there exits a series of basis vectors with nonzero matrix elements $|u_1\rangle, |u_2\rangle, \ldots, |u_k\rangle$ connecting them, i.e.,*

$$\langle u|H|u_1\rangle\langle u_1|H|u_2\rangle\cdots\langle u_k|H|u'\rangle \ne 0. \quad (6)$$

Based on the above lemmas, we now establish the following theorem about FM, which is the main result of this Letter.

Theorem 1 ***(2D FM ground state).*** *Consider the Hamiltonian $H_{\text{kin}} + H_{\text{int}}$ with boundary condition (i) in the limit $U \to +\infty$. The physical Hilbert space is $\mathcal{H}_{\mathcal{N}_\mathcal{X},\mathcal{N}_\mathcal{Y}}$. For any value of $J > 0$, the ground states include the fully spin-polarized states. If condition (ii) is also satisfied, the ground state is unique apart from the trivial spin degeneracy. The ground state $|\Psi^M_G\rangle$ in $\mathcal{H}^M_{\mathcal{N}_\mathcal{X},\mathcal{N}_\mathcal{Y}}$ for all values of $-N_{\text{tot}}/2 \le M \le N_{\text{tot}}/2$ forms a set of spin multiplets with $S = N_{\text{tot}}/2$, which can be expressed as*

$$|\Psi^M_G\rangle = \sum_{\mathcal{R},\mathcal{S}} c_{\mathcal{R},\mathcal{S}}|\mathcal{R},\mathcal{S}\rangle^M, \quad (7)$$

with all the coefficients strictly positive.

Proof. Lemma 2 together with the Perron-Frobenius theorem [37,38] (see Sec. III of the Supplemental Material [26]) implies that there is a ground state $|\Psi^M_G\rangle$ in $\mathcal{H}^M_{\mathcal{N}_\mathcal{X},\mathcal{N}_\mathcal{Y}}$ that can be expanded as

$$|\Psi^M_G\rangle = \sum_{\mathcal{R},\mathcal{S}} c_{\mathcal{R},\mathcal{S}}|\mathcal{R},\mathcal{S}\rangle^M, \quad (8)$$

with all coefficients non-negative, i.e., $c_{\mathcal{R},\mathcal{S}} \ge 0$. Because of the possible degeneracy, $|\Psi^M_G\rangle$ may not be an eigenstate of total spin. We define a reference state by summing over all the bases in $\mathcal{H}^M_{\mathcal{N}_\mathcal{X},\mathcal{N}_\mathcal{Y}}$ with equal weight as $|\Psi^M_{\text{FM}}\rangle = \sum_{\mathcal{R},\mathcal{S}}|\mathcal{R},\mathcal{S}\rangle^M$, which is symmetric under the exchange of spin configurations of any two particles and thus is one of the multiplet of the fully polarized states $S = (N_{\text{tot}}/2)$. Define a projection operator P_S for the subspace spanned by states with total spin S. Clearly, $\langle\Psi^M_G|\Psi^M_{\text{FM}}\rangle = \sum_{\mathcal{R},\mathcal{S}} c_{\mathcal{R},\mathcal{S}} > 0$ up to normalization factors; thus, $P_{N_{\text{tot}}/2}|\Psi^M_G\rangle \ne 0$. We have

$$HP_{N_{\text{tot}}/2}|\Psi^M_G\rangle = P_{N_{\text{tot}}/2}H|\Psi^M_G\rangle = E^M_G P_{N_{\text{tot}}/2}|\Psi^M_G\rangle. \quad (9)$$

For $M = S^{\min}_z$, $P_{S=N_{\text{tot}}/2}|\Psi^M_G\rangle$ lies in $\mathcal{H}^{\min}_{\mathcal{N}_\mathcal{X},\mathcal{N}_\mathcal{Y}}$ and thus is a ground state in the entire Hilbert space.

Further, if condition (ii) is satisfied, Lemma 3 of transitivity is also valid. In that case, the Hamiltonian matrix in the subspace $\mathcal{H}^M_{\mathcal{N}_\mathcal{X},\mathcal{N}_\mathcal{Y}}$ is irreducible. According to the Perron-Frobenius theorem, the ground state $|\Psi^M_G\rangle$ in this subspace is nondegenerate, and thus it must be an eigenstate of total spin which should be $S = N_{\text{tot}}/2$. Otherwise, $\langle\Psi^M_G|\Psi^M_{\text{FM}}\rangle = 0$, which would contradict the fact that $\langle\Psi^M_G|\Psi^M_{\text{FM}}\rangle > 0$. Furthermore, the coefficients in the expansion of Eq. (7) are strictly positive, i.e., $c_{\mathcal{R},\mathcal{S}} > 0$, as explained in Sec. III of the Supplemental Material [26]. ∎

Remark. Theorem 1 does not require translation symmetry and thus remains true in the presence of on-site disorders.

Theorem 1 is a joint effect of the 1D band structure and the multiorbital Hund's rule (i.e., $J > 0$). In the usual 1D case, if U is infinite, fermions cannot pass each other. With periodic boundary conditions, only order-preserving cyclic permutations of spins can be realized through hopping terms, and thus the Hamiltonian matrix is *not transitive*. The

ground states are degenerate. For $H_{\rm kin}+H_{\rm int}$, particles in orthogonal chains meet each other at the crossing sites, and their spins are encouraged to align by the J term, which also promotes the transitivity of the Hamiltonian matrix. This removes the degeneracy and selects the fully polarized FM state. If condition (ii) is not met, Lemma 3 of transitivity may not be valid, and thus the ground states could be degenerate. On the other hand, condition (ii) is not necessary for transitivity and can be relaxed to a weaker condition, as described in Sec. III D of the Supplemental Material [26].

Unlike Nagaoka's FM state, the particles in our FM states still interact with each other through the V term even though they are fully polarized. Conceivably, it could further lead to Cooper pairing instability and other strong correlation phases within the fully polarized states. Owing to the nodeless structure of the ground state wave function [Eq. (7)], these states can be simulated by quantum Monte Carlo simulations free of any sign problem.

Theorem 1 can be further generalized from the SU(2) systems to those with SU(N) symmetry. These high-spin symmetries are not just of academic interest. It is proposed to use ultracold alkali and alkaline-earth fermions to realize SU(N) and Sp(N) symmetric systems [39–42]. Recently, the SU(6) symmetric ^{173}Yb fermions have been loaded into optical lattices to form a Mott-insulating state [43,44]. The SU(N) kinetic energy $H_{\rm kin}^{\rm SU}$ can be obtained by simply increasing the number of fermion components in $H_{\rm kin}^{{\rm 1D},\mu}$ defined in Eq. (1), i.e., $\sigma=1,2,\ldots,N$. The SU(N) interaction term can be expressed as

$$\begin{aligned}H_{\rm int}^{\rm SU}=&\frac{U}{2}\sum_{\mu,\sigma\neq\sigma',\mathbf{r}}n_{\mu,\sigma}(\mathbf{r})n_{\mu,\sigma'}(\mathbf{r})+\frac{V}{2}\sum_{\mu\neq\nu,\mathbf{r}}n_{\mu}(\mathbf{r})n_{\nu}(\mathbf{r})\\&-\frac{J}{4}\sum_{\mu\neq\nu,\mathbf{r}}\{P_{\mu\nu}(\mathbf{r})-n_{\mu}(\mathbf{r})n_{\nu}(\mathbf{r})\}\\&+\frac{\Delta}{2}\sum_{\mu\neq\nu,\sigma\neq\sigma',\mathbf{r}}p_{\mu\sigma}^{\dagger}(\mathbf{r})p_{\mu\sigma'}^{\dagger}(\mathbf{r})p_{\nu\sigma'}(\mathbf{r})p_{\nu\sigma}(\mathbf{r}),\end{aligned}\tag{10}$$

where $n_{\mu}(\mathbf{r})=\sum_{\sigma}n_{\mu,\sigma}(\mathbf{r})$; $P_{\mu\nu}(\mathbf{r})$ is the exchange operator defined as $P_{\mu\nu}(\mathbf{r})=\sum_{\sigma\sigma'}p_{\mu\sigma}^{\dagger}(\mathbf{r})p_{\nu\sigma'}^{\dagger}(\mathbf{r})p_{\mu\sigma'}(\mathbf{r})p_{\nu\sigma}(\mathbf{r})$.

For the SU(N) Hamiltonian $H_{\rm kin}^{\rm SU}+H_{\rm int}^{\rm SU}$, not only is the particle number of each chain separately conserved, but also the total particle number of each component σ is separately conserved. We still use $\mathcal{N}_{\mathcal{X}}$ and $\mathcal{N}_{\mathcal{Y}}$ to denote particle number distribution in rows and columns, and use $\mathcal{N}_{\sigma}$ to represent the distribution of particle numbers among different components. The corresponding subspace is denoted as $\mathcal{H}^{\mathcal{N}_\sigma}_{\mathcal{N}_{\mathcal{X}},\mathcal{N}_{\mathcal{Y}}}$. By imitating the proof of Theorem 1, we arrive at the following theorem. The proof is shown in Sec. IV of the Supplemental Material [26].

Theorem 2 [SU(N) *ground state FM].* *Consider the* SU(N) *Hamiltonian* $H_{\rm kin}^{\rm SU}+H_{\rm int}^{\rm SU}$ *in the limit* $U\to\infty$, *whose physical Hilbert space is* $\mathcal{H}_{\mathcal{N}_{\mathcal{X}},\mathcal{N}_{\mathcal{Y}}}$. *Under condition (i), for any value of* $J>0$, *the ground states include those belonging to the fully symmetric rank-*$N_{\rm tot}$ *tensor representation. If condition (ii) is further satisfied, the ground states are unique apart from the trivial* $(N+N_{\rm tot}-1)!/(N-1)!N_{\rm tot}!$*-fold* SU($N$) *spin degeneracy. In each subspace* $\mathcal{H}^{\mathcal{N}_\sigma}_{\mathcal{N}_{\mathcal{X}},\mathcal{N}_{\mathcal{Y}}}$, $|\Psi_G^{\mathcal{N}_\sigma}\rangle=\sum_u c_u|u\rangle$, *with* $c_u>0$ *for all basis vectors of* $|u\rangle$ *in the subspace* $\mathcal{H}^{\mathcal{N}_\sigma}_{\mathcal{N}_{\mathcal{X}},\mathcal{N}_{\mathcal{Y}}}$.

We turn now to the 3D and 1D cases. As proved in Sec. V of the Supplemental Material [26], Lemmas 1, 2, and 3 are still valid under conditions (i) and (ii). We then arrive at the following corollary. (The 1D case is discussed in Sec. VI of the Supplemental Material [26].)

Corollary 1 ***(3D FM ground state).*** *The statements in Theorems 1 and 2 of FM are also valid for the 3D version of* $H_{\rm kin}+H_{\rm int}$ *defined in Eqs. (1) and (2) under the same conditions.*

So far, we have considered the case of $J>0$. In certain systems with strong electron-phonon coupling, such as alkali-doped fullerenes, Hund's rule may be replaced by an anti-Hund's rule, i.e., $J<0$ [45]. In this case, we obtain the following Theorem 3 in 2D.

Theorem 3. *Consider the 2D Hamiltonian* $H_{\rm kin}+H_{\rm int}$ *in the limit* $U\to+\infty$ *with* $J<0$. *If conditions (i) and (ii) are satisfied, then the ground state in each subspace* $\mathcal{H}^{M}_{\mathcal{N}_{\mathcal{X}},\mathcal{N}_{\mathcal{Y}}}$, *denoted as* $|\Psi_G^M\rangle$, *is nondegenerate and obeys the following sign rule:*

$$|\Psi_G^M\rangle=\sum_{\mathcal{R},\mathcal{S}}(-)^{\Gamma}c_{\mathcal{R},\mathcal{S}}|\mathcal{R},\mathcal{S}\rangle^M,\tag{11}$$

where all coefficients are strictly positive, i.e., $c_{\mathcal{R},\mathcal{S}}>0$; *the sign* $(-)^{\Gamma}$ *is defined by* $\Gamma=\sum_{1\le c_j\le L_x,1\le i\le N_{c_j}}(\frac{1}{2}-\beta_i^{c_j})$. *The total spin of* $|\Psi_G^M\rangle$ *is* $S=|M|$ *for* $|M|>\frac{1}{2}\Delta N$ *and* $S=\Delta N/2$ *for* $\Delta N/2\le M\le\Delta N/2$, *respectively, where* ΔN *is the difference between total particle numbers in the* p_x *and* p_y *orbitals.*

Theorem 3 can be proved following the proof of the Lieb-Mattis theorem [20] and of Lieb's theorem [46] for antiferromagnetic Heisenberg models in bipartite lattices. Here, p_x and p_y orbitals play the roles of two sublattices. However, the system here is itinerant, not of local spin moments. Because of the quasi-1D geometry, fermions do not pass each other, and thus their magnetic properties are not affected by the mobile fermions. The detailed proof is presented in Sec. VII of the Supplemental Material [26]. However, this theorem cannot be generalized to the 3D case and the SU(N) case, even in 2D, because in both cases, the antiferromagnetic coupling $J<0$ leads to intrinsic frustrations.

The search for FM states has become a research focus in cold atoms [25,47–53]. Both the 2D and 3D Hamiltonians $H_{\rm kin}+H_{\rm int}$ can be realized in the p-orbital band in optical lattices. With a moderate optical potential depth $V_0/E_R=15$, where E_R is the recoil energy, it was

calculated that $t_\perp/t_\parallel \approx 5\%$ [54], and thus the neglect of $t_\parallel$ in Eq. (1) is justified. A Gutzwiller variational approach has been applied to the 2D Hamiltonian of $H_{\rm kin} + H_{\rm int}$ [30]. Furthermore, many transition-metal oxides possess t_{2g}-orbital bands with quasi-2D layered structures, such as the (001) interface of $3d$-orbital transition-metal oxides [31–33]. Its $3d_{xz}$ and $3d_{yz}$ bands are quasi-1D, as described by Eq. (1), with $p_{x(y)}$ there corresponding to $d_{x(y)z}$. Also, strongly correlated $3d$ electrons possess the large U physics. Further discussion on the physics of finite U and V is given in Sec. VIII of the Supplemental Material [26].

Summary.—We have shown—contrary to the normal situation in 1D without orbital degrees of freedom—that fully saturated ferromagnetism is possible in certain tight-binding lattice models with several orbitals at each site. This holds for 2D and 3D models and for SU(N) models as well as SU(2) models. Hard-core interactions in 1D chains, together with the Hund's rule coupling, stabilize the effect and result in unique ground states with saturated ferromagnetism. The result also holds for a large region of electron densities in both 2D and 3D, or in 1D with two or three p orbitals at each site. Our theorems might provide a reference point for the study of itinerant FM in experimental orbitally active systems with ultracold optical lattices and transition-metal oxides.

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