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

Yi Li,[1,2] Elliott H. Lieb,[3] and Congjun Wu[2]

[1]*Princeton Center for Theoretical Science, Princeton University, Princeton, New Jersey 08544, USA*
[2]*Department of Physics, University of California, San Diego, La Jolla, California 92093, USA*
[3]*Departments of Mathematics and Physics, Princeton University, Princeton, New Jersey 08544, USA*

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.

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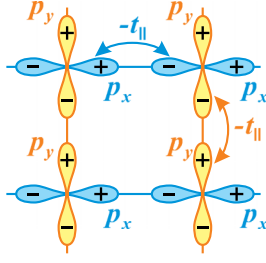
FIG. 1 (color online).  The square lattice with the quasi-1D band structure of the $p$-orbital bands. Particles in the $p_x$ ($p_y$) orbital can only move along the $x$ ($y$) direction, respectively. The sign of $t_\parallel$ can be changed by a gauge transformation on the square lattice.

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 $\sigma$ bonding with hopping amplitude $t_\parallel$ or $\pi$ 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):

$$H_{\text{kin}}^{\text{2D(3D)}} = \sum_{\mu=x,y,(z)} H_{\text{kin}}^{\text{1D},\mu} - \mu_0 \sum_{\mathbf{r}} n(\mathbf{r}),$$

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

Here, $p_{\mu,\sigma}(\mathbf{r})$ is the annihilation operator in the $p_\mu$ orbital $[\mu = x, y, (z)]$ on site $\mathbf{r}$ with the spin eigenvalue $\sigma$; $n(\mathbf{r})$ is the total particle number on site $\mathbf{r}$, and $\hat{\mathbf{e}}_\mu$ is the unit vector in the $\mu$ 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:

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

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 $p_\mu$ orbital. The $U$ and $V$ terms are intra- and interorbital Hubbard interactions, respectively; the $J$ term represents the Hund's rule coupling; the $\Delta$ term

describes the pair hopping process between different orbitals. The expressions of $U$, $V$, $J$, and $\Delta$ 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 $H_{\text{kin}} + H_{\text{int}}$. 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 $H = H_{\text{kin}} + H_{\text{int}}$ [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 $r_i$th row and the $c_i$th column, respectively. Altogether, $\sum_{r_i=1}^{L_y} N_{r_i} + \sum_{c_i=1}^{L_x} N_{c_i} = N_{\text{tot}}$ 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 $r$th 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 $\alpha_i^r$ are, respectively, the coordinate and $s_z$ eigenvalue for the $i$th

particle in the $r$th row; similarly, the creation operator for the $N^c$ $p_y$-orbital particles in the $c$th 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 $\beta^c_i$. 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 $N_{\text{tot}}$. 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

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

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 $H_{\text{kin}} + H_{\text{int}}$, 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 $H_{\text{kin}}^{\text{SU}}$ can be obtained by simply increasing the number of fermion components in $H_{\text{kin}}^{\text{1D},\mu}$ defined in Eq. (1), i.e., $\sigma = 1, 2, \ldots, N$. The SU($N$) interaction term can be expressed as

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

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 $H_{\text{kin}}^{\text{SU}} + H_{\text{int}}^{\text{SU}}$, not only is the particle number of each chain separately conserved, but also the total particle number of each component $\sigma$ 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 $\mathcal{H}_{\mathcal{N}_{\mathcal{X}},\mathcal{N}_{\mathcal{Y}}}^{\mathcal{N}_\sigma}$. 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 $H_{\text{kin}}^{\text{SU}} + H_{\text{int}}^{\text{SU}}$ 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-$N_{\text{tot}}$ tensor representation. If condition (ii) is further satisfied, the ground states are unique apart from the trivial $(N + N_{\text{tot}} - 1)!/(N - 1)!N_{\text{tot}}!$-fold SU($N$) spin degeneracy. In each subspace $\mathcal{H}_{\mathcal{N}_{\mathcal{X}},\mathcal{N}_{\mathcal{Y}}}^{\mathcal{N}_\sigma}$, $|\Psi_G^{\mathcal{N}_\sigma}\rangle = \sum_u c_u |u\rangle$, with $c_u > 0$ for all basis vectors of $|u\rangle$ in the subspace $\mathcal{H}_{\mathcal{N}_{\mathcal{X}},\mathcal{N}_{\mathcal{Y}}}^{\mathcal{N}_\sigma}$.*

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

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

*where all coefficients are strictly positive, i.e., $c_{\mathcal{R},\mathcal{S}} > 0$; the sign $(-)^\Gamma$ is defined by $\Gamma = \sum_{1 \leq c_j \leq L_x, 1 \leq i \leq N_{c_j}} (\frac{1}{2} - \beta_i^{c_j})$. The total spin of $|\Psi_G^M\rangle$ is $S = |M|$ for $|M| > \frac{1}{2}\Delta N$ and $S = \Delta N/2$ for $\Delta N/2 \leq M \leq \Delta N/2$, respectively, where $\Delta N$ 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 $H_{\text{kin}} + H_{\text{int}}$ 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 $H_{kin} + H_{int}$ [30]. Furthermore, many transition-metal oxides possess $t_{2g}$-orbital bands with quasi-2D layered structures, such as the (001) interface of 3$d$-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 3$d$ 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 ferro-magnetism. 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 exper-imental orbitally active systems with ultracold optical lattices and transition-metal oxides.

[1] E. H. Lieb and D. Mattis, Phys. Rev. **125**, 164 (1962).

[2] D. C. Mattis, *The Theory of Magnetism Made Simple* (World Scientific, Singapore, 2006).

[3] Y. Nagaoka, Phys. Rev. **147**, 392 (1966).

[4] L. M. Roth, Phys. Rev. **149**, 306 (1966).

[5] K. Kugel and D. Khomskii, Zh. Eksp. Teor. Fiz. **64**, 1429 (1973).

[6] J. A. Hertz, Phys. Rev. B **14**, 1165 (1976).

[7] T. Moriya, in *Spin Fluctuations in Itinerant Electron Magnetism*, edited by P. Fulde, Springer Series in Solid-State Sciences Vol. 56 (Springer, Berlin, 1985).

[8] J. Torrance, S. Oostra, and A. Nazzal, Synth. Met. **19**, 709 (1987).

[9] W. Gill and D. J. Scalapino, Phys. Rev. B **35**, 215 (1987).

[10] J. E. Hirsch, Phys. Rev. B **40**, 2354 (1989).

[11] B. S. Shastry, H. R. Krishnamurthy, and P. W. Anderson, Phys. Rev. **100**, 675 (1955).

[12] A. Mielke, J. Phys. A **24**, L73 (1991).

[13] A. Mielke, J. Phys. A **24**, 3311 (1991).

[14] H. Tasaki, Phys. Rev. Lett. **69**, 1608 (1992).

[15] A. J. Millis, Phys. Rev. B **48**, 7183 (1993).

[16] D. Belitz, T. R. Kirkpatrick, and T. Vojta, Rev. Mod. Phys. **77**, 579 (2005).

[17] H. v. Löhneysen, A. Rosch, M. Vojta, and P. Wölfle, Rev. Mod. Phys. **79**, 1015 (2007).

[18] L. Liu, H. Yao, E. Berg, S. R. White, and S. A. Kivelson, Phys. Rev. Lett. **108**, 126406 (2012).

[19] H. Tasaki, Phys. Rev. B **40**, 9192 (1989).

[20] E. H. Lieb and D. C. Mattis, J. Math. Phys. (N.Y.) **3**, 749 (1962).

[21] A. Mielke, J. Phys. A **25**, 4335 (1992).

[22] A. Mielke, Phys. Lett. A **174**, 443 (1993).

[23] H. Tasaki, Commun. Math. Phys. **242**, 445 (2003).

[24] A. Tanaka and H. Tasaki, Phys. Rev. Lett. **98**, 116402 (2007).

[25] S. Zhang, H. H. Hung, and C. Wu, Phys. Rev. A **82**, 053618 (2010).

[26] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevLett.112.217201 for the ex-pression for the interaction matrix elements; proofs and discussion of Lemmas 2 and 3, Theorems 2 and 3, Corollary 1, and the one dimensional case; estimation of the FM energy scale and the effect of finite $U$.

[27] S. Q. Shen, Phys. Rev. B **57**, 6474 (1998).

[28] M. Cyrot and C. Lyon-Caen, J. Phys. (France) **36**, 253 (1975).

[29] A. M. Oleś, Phys. Rev. B **28**, 327 (1983).

[30] L. Wang, X. Dai, S. Chen, and X. C. Xie, Phys. Rev. A **78**, 023603 (2008).

[31] L. Li, C. Richter, J. Mannhart, and R. Ashoori, Nat. Phys. **7**, 762 (2011).

[32] J. A. Bert, B. Kalisky, C. Bell, M. Kim, Y. Hikita, H. Y. Hwang, and K. A. Moler, Nat. Phys. **7**, 767 (2011).

[33] G. Chen and L. Balents, Phys. Rev. Lett. **110**, 206401 (2013).

[34] J. Hubbard, Proc. R. Soc. A **276**, 238 (1963).

[35] J. C. Slater, *Quantum Theory of Molecules and Solids* (McGraw-Hill, New York, 1963), Vol. I, Appendix 6.

[36] This condition is taken to simplify the proof. Our results also hold for open boundary conditions without the constraint on odd or even particle numbers in each row and column. With open boundary conditions, Theorem 1 remains correct when both the on-site potentials and nearest-neighbor hoppings are disordered.

[37] O. Perron, Math. Ann. **64**, 248 (1907).

[38] F. G. Frobenius, Sitzungsber. Akad. Wiss. Berlin, Phys. Math. Kl. 471 (1908).

[39] C. Wu, J. P. Hu, and S. C. Zhang, Phys. Rev. Lett. **91**, 186402 (2003).

[40] C. Wu, Mod. Phys. Lett. B **20**, 1707 (2006).

[41] A. Gorshkov, M. Hermele, V. Gurarie, C. Xu, P. S. Julienne, J. Ye, P. Zoller, E. Demler, M. D. Lukin, and A. M. Rey, Nat. Phys. **6**, 289 (2010).

[42] C. Wu, Nat. Phys. **8**, 784 (2012).

[43] S. Taie, Y. Takasu, S. Sugawa, R. Yamazaki, T. Tsujimoto, R. Murakami, and Y. Takahashi, Phys. Rev. Lett. **105**, 190401 (2010).

[44] S. Taie, R. Yamazaki, S. Sugawa, and Y. Takahashi, Nat. Phys. **8**, 825 (2012).

[45] O. Gunnarsson, *Alkali-Doped Fullerides: Narrow-Band Solids with Unusual Properties* (World Scientific, Singapore, 2004).

[46] E. H. Lieb, Phys. Rev. Lett. **62**, 1201 (1989).

[47] R. A. Duine and A. H. MacDonald, Phys. Rev. Lett. **95**, 230403 (2005).

[48] I. Berdnikov, P. Coleman, and S. H. Simon, Phys. Rev. B **79**, 224403 (2009).

[49] G. J. Conduit and B. D. Simons, Phys. Rev. A **79**, 053606 (2009).

[50] L. J. LeBlanc, J. H. Thywissen, A. A. Burkov, and A. Paramekanti, Phys. Rev. A **80**, 013607 (2009).

[51] G. B. Jo, Y. R, Lee, J. H. Choi, C. A. Christensen, T. H. Kim, J. H. Thywissen, D. E. Pritchard, and W. Ketterle, Science **325**, 1521 (2009).

[52] D. Pekker, M. Babadi, R. Sensarma, N. Zinner, L. Pollet, M. W. Zwierlein, and E. Demler, Phys. Rev. Lett. **106**, 050402 (2011).

[53] X. Cui and T. L. Ho, Phys. Rev. A **89**, 023611 (2014).

[54] A. Isacsson and S. M. Girvin, Phys. Rev. A **72**, 053604 (2005).

# Supplemental Material to "Exact Results for Itinerant Ferromagnetism in Multiorbital Systems on Square and Cubic Lattices"

Yi Li,[1,2] Elliott H. Lieb,[3] and Congjun Wu[2]

[1]*Princeton Center for Theoretical Science, Princeton University, Princeton, New Jersey 08544, USA*
[2]*Department of Physics, University of California, San Diego, La Jolla, California 92093, USA*
[3]*Departments of Mathematics and Physics, Princeton University, Princeton, New Jersey 08544, USA*

## I. EXPRESSIONS FOR $U, V, J$ AND $\Delta$

In this section, we present the expression for the interaction matrix elements $U$, $V$, $J$ and $\Delta$ in $H_{int}$ defined in Eq. (2) in the body text. We assume that the bare interaction between two particles in free space is $V(\mathbf{r}_1 - \mathbf{r}_2)$. For example, it can be the Coulomb interaction between electrons, or a short-range $s$-wave scattering interaction between two ultra-cold fermion atoms. Let us consider one site with degenerate $p_x$ and $p_y$ orbitals whose Wannier orbital wave functions are $\phi_x(\mathbf{r})$ and $\phi_y(\mathbf{r})$, respectively. Then $U$, $V$, $J$ and $\Delta$ can be represented [1, 2] as

$$U = \int d\mathbf{r}_1 d\mathbf{r}_2 \phi_x(\mathbf{r}_1)\phi_x(\mathbf{r}_2)V(\mathbf{r}_1 - \mathbf{r}_2)\phi_x(\mathbf{r}_2)\phi_x(\mathbf{r}_1),$$

$$V = \int d\mathbf{r}_1 d\mathbf{r}_2 \phi_x(\mathbf{r}_1)\phi_y(\mathbf{r}_2)V(\mathbf{r}_1 - \mathbf{r}_2)$$
$$\times \left\{ \phi_y(\mathbf{r}_2)\phi_x(\mathbf{r}_1) - \phi_x(\mathbf{r}_2)\phi_y(\mathbf{r}_1) \right\},$$

$$J = 2\int d\mathbf{r}_1 d\mathbf{r}_2 \phi_x(\mathbf{r}_1)\phi_y(\mathbf{r}_2)V(\mathbf{r}_1 - \mathbf{r}_2)\phi_x(\mathbf{r}_2)\phi_y(\mathbf{r}_1),$$

$$\Delta = \int d\mathbf{r}_1 d\mathbf{r}_2 \phi_x(\mathbf{r}_1)\phi_x(\mathbf{r}_2)V(\mathbf{r}_1 - \mathbf{r}_2)\phi_y(\mathbf{r}_2)\phi_y(\mathbf{r}_1).$$

The physical meanings of $U, V, J$ and $\Delta$ can be explained as follows. Consider a single site with two orbitals and put two fermions on the site. There are four states in which each orbital is singly occupied, including the triplet states $p_{x\uparrow}^\dagger p_{y\uparrow}^\dagger |0\rangle$, $\frac{1}{\sqrt{2}}\left\{ p_{x\uparrow}^\dagger p_{y\downarrow}^\dagger + p_{x\downarrow}^\dagger p_{y\uparrow}^\dagger \right\}|0\rangle$, and $p_{x\downarrow}^\dagger p_{y\downarrow}^\dagger |0\rangle$, and the singlet state $\frac{1}{\sqrt{2}}\left\{ p_{x\uparrow}^\dagger p_{y\downarrow}^\dagger - p_{x\downarrow}^\dagger p_{y\uparrow}^\dagger \right\}|0\rangle$ with energies $V$ and $J + V$, respectively. Their energy difference is the Hund's rule coupling energy. The other two states are singlets involving doubly occupied orbitals, namely $\frac{1}{\sqrt{2}}\left\{ p_{x\uparrow}^\dagger p_{x\downarrow}^\dagger \pm p_{y\uparrow}^\dagger p_{y\downarrow}^\dagger \right\}|0\rangle$, whose energies are $U \pm \Delta$, respectively.

## II. PROOFS OF LEMMAS 2 AND 3

In this section, we present the detailed proofs to Lemmas 2 and 3 which are used in proving Theorem 1. Lemma 1, as we noted, is obvious.

### A. Proof of Lemma 2

Let us start with the general basis $|\mathcal{R}, \mathcal{S}\rangle$ defined in Eq. (5) in the body text, and check the hopping matrix elements. It suffices to consider hoppings along the $x$-direction, because the $y$-direction is similar. The following hopping along row $r$, denoted as

$$H_{x,\pm}(\mathbf{r}_i; \alpha_i^r) = -t_\parallel p_{x,\alpha_i^r}^\dagger(\mathbf{r}_i \pm \hat{e}_x)p_{x,\alpha_i^r}(\mathbf{r}_i), \qquad (1)$$

generate non-zero off-diagonal matrix elements if $x_i^r + 1 < x_{i+1}^r$, or, $x_i^r - 1 > x_{i-1}^r$, where the boundary condition (i) for coordinates is assumed and the particle indices $i \pm 1$ are defined on row $r$ modulo $N_r$. Without loss of generality, we only need to consider $H_{x,+}$. If this hopping is not between the ends of the row, when $H_{x,+}$ acts on $|\mathcal{R}, \mathcal{S}\rangle = |\{\mathbf{r}_i^{r_j} \alpha_i^{r_j}; \mathbf{r}_i^{c_j} \beta_i^{c_j}\}\rangle$, it just replaces $p_{x,\alpha_i^r}^\dagger(\mathbf{r}_i)$ by $p_{x,\alpha_i^r}^\dagger(\mathbf{r}_i + \hat{e}_x)$ in the sequence of creation operators in Eq. (5) in the body text without affecting the ordering; thus its matrix element is just $-t_\parallel$. If this hopping goes from one end to another end, i.e., $x_i^r = L_x$, and then $x_i^r + 1 \equiv 1$ mod $(L_x)$, it replaces the operator $p_{x,\alpha_i^r}^\dagger(\mathbf{r}_i)$ with $\mathbf{r}_i = (L_x, r)$ by that with $\mathbf{r}_i = (1, r)$ together with a minus sign if $N_r$ is even. To fit the ordering of creation operators in Eq. (6) in the body text, we move the operator $p_{x,\alpha_i^r}^\dagger(\mathbf{r}_i)$ with $\mathbf{r}_i = (1, a)$ to its right location after passing $N_r - 1$ operators in the $a$-th row. If $N_r$ is even or odd, no additional sign is generated and the matrix element is still $-t_\parallel$. The same reasoning applies to the hopping operator $H_{x,-}$, and for those along the $y$-direction.

Next we check matrix elements associated with the interaction terms in Eq. (2) in the body text. On the physical Hilbert space $\mathcal{H}_{\mathcal{N}_\mathcal{X}, \mathcal{N}_\mathcal{Y}}$, only the following term, denoted as

$$H_J(\mathbf{r}) = -\frac{J}{2}\left\{ p_{x\uparrow}^\dagger(\mathbf{r})p_{x\downarrow}(\mathbf{r})p_{y\downarrow}^\dagger(\mathbf{r})p_{y\uparrow}(\mathbf{r}) + H.c. \right\}, \quad (2)$$

generates non-zero off-diagonal matrix elements. When $H_J(\mathbf{r})$ acts on $|\mathcal{R}, \mathcal{S}\rangle = |\{\mathbf{r}_i^{r_j} \alpha_i^{r_j}; \mathbf{r}_i^{c_j} \beta_i^{c_j}\}\rangle$, it updates the creation operators without affecting the ordering in Eq. (5) in the body text, and thus the corresponding matrix elements are just $-J/2$. In summary, all the off-diagonal matrix elements are either zero or negative, i.e., non-positive.                    Q.E.D.
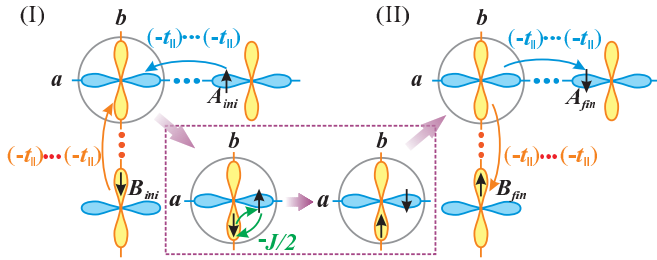
FIG. 2: The scheme of exchanging any two given opposite spins in orthogonal chains. Starting from configuration (I), two particles, marked with black arrows for spin up and down, arrive at the crossing site (as circled) by successively hopping along each chain. Then their spins are flipped by the on-site $J$ term. Finally, they hop back to the initial locations with spins configuration flipped as in (II).

## B. Proof of Lemma 3

We denote two general basis vectors $|u\rangle$ and $|u'\rangle$ in $\mathcal{H}^M_{\mathcal{N}_\mathcal{X},\mathcal{N}_\mathcal{Y}}$ as $|u\rangle = |\mathcal{R},\mathcal{S}\rangle^M = |\{\mathbf{r}_i^{r_j}\alpha_i^{r_j};\mathbf{r}_i^{c_j}\beta_i^{c_j}\}\rangle^M$ and $|u'\rangle = |\mathcal{R}',\mathcal{S}'\rangle^M = |\{\mathbf{r}'^{r_j}_i\alpha'^{r_j}_i;\mathbf{r}'^{c_j}_i\beta'^{c_j}_i\}\rangle^M$. First, we can successively apply the hopping terms to rearrange the spatial locations of particles from $\mathcal{R}$ in $|u\rangle$ to be $\mathcal{R}'$. We arrive at an intermediate state $|v\rangle = |\mathcal{R}',\mathcal{S}\rangle^M = |\{\mathbf{r}'^{r_j}_i\alpha_i^{r_j};\mathbf{r}'^{c_j}_i\beta_i^{c_j}\}\rangle^M$ as

$$|v\rangle = \prod_{c_j,i}p^\dagger_{y,\beta_i^{c_j}}(\mathbf{r}'^{c_j}_i)\prod_{r_j,i}p^\dagger_{x,\alpha_i^{r_j}}(\mathbf{r}'^{r_j}_i)|0\rangle. \quad (3)$$

Compared to the final state $|u'\rangle = |\{\mathbf{r}'^{r_j}_i\alpha'^{r_j}_i;\mathbf{r}'^{c_j}_i\beta'^{c_j}_i\}\rangle^M$, defined as

$$|u'\rangle = \prod_{c_j,i}p^\dagger_{y,\beta'^{c_j}_i}(\mathbf{r}'^{c_j}_i)\prod_{r_j,i}p^\dagger_{x,\alpha'^{r_j}_i}(\mathbf{r}'^{r_j}_i)|0\rangle, \quad (4)$$

the locations of particles in $|v\rangle$ and in $|u'\rangle$ are equal, but the spin configuration in $|v\rangle$ are the same as that in $|u\rangle$. This arrangement can be decomposed into independent hops within each chain without interference among chains, because particle numbers in each row and each column are conserved separately.

Next we prove that it is possible to adjust the sequence of spin indices in the chain of creation operators in Eq. (3) for $|v\rangle$ to be the same as that in Eq. (4) for $|u'\rangle$. Two sequences of spin indices are the same up to a permutation. Since any permutation can be decomposed into a product of exchanges, we only need to prove that any exchange can be realized by successively applying off-diagonal Hamiltonian matrix elements of the hopping and $J$ terms. Obviously, we only need consider the exchange of two opposite spins.

First, we consider the exchange between two particles $A$ and $B$ in orthogonal chains. Without loss of generality, we assume $A$ to be in the $p_x$-orbital of the $a$-th row and $B$ to be in the $p_y$-orbital of the $b$-th column as shown in Figure 2. Their configuration is denoted as $A_{ini}$:$(\mathbf{r}_A;p_x\uparrow)$ and $B_{ini}$:$(\mathbf{r}_B;p_y\downarrow)$ with $\mathbf{r}_A = (x,a)$

and $\mathbf{r}_B = (b,y)$. Since there is at least one hole in each chain, cyclic permutations of particle locations along the chain can be realized by applying only hopping terms along it. We move these two particles to the crossing site $\mathbf{r}_c = (b,a)$ and flip their spins by using the $J$ term. We can then restore the spatial locations of particles in the $a$-th row and the $b$-th column to be the same as those in $|v\rangle$ by applying only hopping terms. The net effect is the exchange of spin indices into $A_{fin}$:$(\mathbf{r}_A;p_x\downarrow)$ and $B_{fin}$:$(\mathbf{r}_B;p_y\uparrow)$.

Second, we consider the exchange between two particles with opposite spin indices in the same chain, or, in two parallel chains. Without loss of generality, they may be assumed to be in the $p_x$-orbitals in row $a_1$ and $a_2$ respectively. Their coordinates and spins are denoted as $A_{ini}(\mathbf{r}_A;p_x\uparrow)$ and $B_{ini}(\mathbf{r}_B;p_x\downarrow)$ with $\mathbf{r}_A = (m,a_1)$ and $\mathbf{r}_B = (n,a_2)$, respectively. Let us choose an arbitrary $p_y$ particle and, without loss of generality, assume its configuration to be $C(\mathbf{r}_C;p_y\downarrow)$ with $\mathbf{r}_C = (b,y)$. Then we first exchange particles $A$ and $C$ following the method described above, and then exchange particles $B$ with the updated configuration of $C$. The net effect is the exchange between $A_{ini}$ and $B_{ini}$ with the new configuration of $A_{fin}(\mathbf{r}_A;p_x\downarrow)$ and $B_{fin}(\mathbf{r}_B;p_x\uparrow)$, while $C$ is restored to its initial configuration. Thus we have proved the transitivity of the Hamiltonian matrix in the subspace $\mathcal{H}^M_{\mathcal{N}_\mathcal{X},\mathcal{N}_\mathcal{Y}}$. $\hspace{1cm}$ Q.E.D.

## C. More extensions

In fact, Theorem 1 can be made even more general by adding off-site interactions such as

$$H'_{int} = \sum_{\mathbf{r}\mathbf{r}';\mu\nu}\left(V_{\mathbf{r}\mathbf{r}';\mu\nu}n_\mu(\mathbf{r})n_\nu(\mathbf{r}') - J_{\mathbf{r}\mathbf{r}';\mu\nu}\vec{S}_\mu(\mathbf{r})\cdot\vec{S}_\nu(\mathbf{r}')\right),$$
$$(5)$$

where $\mu,\nu$ represent orbital indices. In order to satisfy the hypothesis of the Perron-Frobenius theorem, the spin channel interaction parameters should be ferromagnetic, i.e., $J_{\mathbf{r}\mathbf{r}';\mu\nu} > 0$, while the charge channel interactions $V_{\mathbf{r}\mathbf{r}';\mu\nu}$ can be arbitrary.

## D. Discussion of Lemma 3 of transitivity

If the transitivity condition of the Hamiltonian matrix is not satisfied, then Theorem 1 may not be valid, i.e., the ground state might be degenerate. We consider below a concrete example in which all the rows of $p_x$-orbitals are empty except in the first row where all the $p_x$-orbitals are filled. Thus particles in the first row cannot hop. For the first row, all the different spin configurations are degenerate because of the absence of hopping. Let us assume that all other columns contain at least one hole. Following Hund's rule, for every column of the $p_y$-orbital, say, the $r$-th one, we align all the particles therein to

be the same as the one in the $p_x$-orbital at site $(r, 1)$. Although the total spin for each column is fully polarized, no coupling exists between adjacent columns, and thus the 2D system overall is still paramagnetic. Nevertheless, if we just add one particle in the 2nd row of the $p_x$-orbital which is otherwise empty, it connects different columns through multiple spin-flip processes from the $J$ term, and realizes the transitivity condition. The ground state is again unique and fully-polarized.

*Condition* (ii) is sufficient but not necessary for Lemma 3 of transitivity. It would be interesting to figure out the necessary condition. In fact, condition (ii) can be further weakened as follows: There is at least one hole in *one* of the chains along any one direction and one hole in *each* chain along other directions. At the same time, there must be at least one particle in *one* of the columns and another particle in *one* of the rows.

In particular, the situation is more complicated for the open boundary condition. Although Lemma 2 of non-positivity is valid regardless of the oddness of filling numbers in every chain, it is more difficult to effect the connectivity with open boundary conditions. Nevertheless, we expect that in the thermodynamic limit the effects of boundary conditions vanish, and the ground state ferromagnetism remains robust for generic fillings.

## III. THE PERRON-FROBENIUS THEOREM AND TRANSITIVITY

To keep the paper self-contained, we explain how transitivity gives rise to a unique ground state in the Perron-Frobenius set up [3, 4]. Suppose $M$ is a real symmetric matrix with all off-diagonal elements non-positive. Let $V$ be a ground state. Then, by the variational principle, $|V| = \{|V_j|\}$ is also a ground state. If the ground state is unique, then $V = |V|$, *i.e.*, $V_j \geq 0$ for all $j$.

Suppose now that $W$ is another ground state. Clearly, there is a real number $\alpha$ so that the ground state $\widetilde{V} = V + \alpha W$ has at lease one component, say $\widetilde{V}_1$, equals zero. Then $\hat{V} = |\widetilde{V}|$ is a ground state with non-negative components and at least one component zero, namely $\hat{V}_1$. Without loss of generality we may assume that the ground state eigenvalue $\lambda$ is not zero and the diagonal elements $M_{ii}$'s are all negative, for otherwise, we can replace $M$ by $M - cI$. We thus have, for $p \in \mathbb{N}$, $M^p \hat{V} = \lambda^p \hat{V} \neq 0$, but $(M^p \hat{V})_1 = 0$.

Assuming transitivity now, we have that for some $p$, $(M^p)_{1j}$ has a strictly non-zero entry for some $j$ such that $\hat{V}_j \neq 0$. This contradicts the fact that $(M^p \hat{V})_1 = 0$.

Thus, transitivity implies that every ground state has only non-zero components. This means that there is no other ground state $W$, for otherwise the ground state $(V + \alpha W)_j = 0$ for some $\alpha$ and some $j$.

## IV. EXTENSION OF THEOREM 1 TO SU($N$) SYMMETRIC SYSTEMS

In this section, we extend Theorem 1 from the SU(2) systems to those with SU($N$) symmetry.

The physical meanings of the $U$, $V$, $J$ and $\Delta$ in the SU($N$) *multi-orbital* interaction defined in Eq. (10) in the body text are similar to the case of $SU(2)$. Again for simplicity, we consider the 2D case with $p_x$ and $p_y$ orbitals. If we load two fermions in a single site, there are $\binom{2N}{2} = N(2N - 1)$ states which are SU($N$) rank-2 tensor states. They can be classified into a) one set of symmetric tensor states, b) one set of anti-symmetric tensor states with singly occupied orbitals, c) two sets of anti-symmetric tensor states with doubly occupied orbitals. Their energies are $V$, $V + J$ and $U \pm \Delta$, respectively. The dimensions for the rank-2 SU($N$) symmetric and anti-symmetric tensor representations are $N(N \pm 1)/2$, respectively.

Again Lemma 1 for the SU(2) case remains valid for the SU($N$) Hamiltonian in the limit $U \rightarrow +\infty$. The many-body basis for the SU($N$) case can still be set up in a manner similar to that defined in Eq. (5) in the body text. The only difference is that fermion spins can take $N$ different values. The off-diagonal elements of the Hamiltonian matrix in $\mathcal{H}_{N_A, N_B}$ are also non-positive, and thus Lemma 2 remains valid. Following essentially the same method as in the proof of Lemma 3 with slight variations, any two bases in the subspace $\mathcal{H}_{\mathcal{N}_\mathcal{X}, \mathcal{N}_\mathcal{Y}}^{\mathcal{N}_\sigma}$ can be connected by successively applying the hopping and $J$ terms under *condition* (ii). Thus the Hamiltonian matrix is also transitive in each subspace $\mathcal{H}_{\mathcal{N}_\mathcal{X}, \mathcal{N}_\mathcal{Y}}^{\mathcal{N}_\sigma}$.

The SU(2) fully polarized FM state with total spin $S = N_{tot}/2$ can be easily generalized to the SU($N$) case. These SU($N$) FM states belong to the representation denoted by the Young pattern with one row of $N_{tot}$ boxes, *i.e.*, the fully symmetric rank-$N_{tot}$ tensor representation. Its dimension, $\binom{N + N_{tot} - 1}{N_{tot}} = \frac{(N + N_{tot} - 1)!}{(N - 1)! N_{tot}!}$, is the number of partition of $N_{tot}$ particles into $N$ different components, which is just the number of different subspaces $\mathcal{H}_{\mathcal{N}_\mathcal{X}, \mathcal{N}_\mathcal{Y}}^{\mathcal{N}_\sigma}$ with respect to the configurations of $\mathcal{N}_\sigma$. Any state of this representation is fully symmetric with respect to exchange spin components of any two particles.

Since Lemmas 1, 2, and 3 are generalized to the SU($N$) case, we obtain Theorem 3. $Q.E.D.$

## V. FM IN THE 3D CUBIC LATTICE

In this section, we generalize Theorem 1 to the 3D Hamiltonian $H_{kin} + H_{int}$ in the same limit $U \rightarrow \infty$ with $J > 0$.

The generalization is easy. The particle number in each chain along any of the three directions is separately conserved because of the vanishing of transverse hoppings and the absence of doubly occupied orbitals. We can further set up the many-body basis in a manner simi-

lar to Eq. (5) in the body text by ordering particles in each chain and ordering one chain after another. The non-positivity of the off-diagonal elements of the many-body Hamiltonian matrix is still valid under *condition*(i). Next, we generalize Lemma 3 of transitivity to 3D.

**Lemma 4 (Transitivity of the 3D Hamiltonian)** *The many-body Hamiltonian matrix of the 3D version of $H_{kin} + H_{int}$ is transitive under condition (ii) in the Hilbert subspace characterized by the particle number distributions in each chain and the z-component of total spin.*

**Proof:** The proof is very similar to that of Lemma 3. We only need to show that spin configurations of any two particles $A$ and $B$, if different, can be exchanged by applying hopping and $J$ terms. Lemma 3 has already proved that it is true if the two particles are coplanar. Now we consider the non-coplanar case, and denote particle locations as $\mathbf{r}_A$ and $\mathbf{r}_B$, respectively. If they lie in parallel orbitals, say, $p_x$-orbital, we can find an $x$-directional chain with its $yz$ coordinates $(r_{A,y}, r_{B,z})$; if they lie in orthogonal orbitals, say, particle $A$ lying in the $p_x$-orbital and particle $B$ lying in the $p_y$-orbital, we can find a $z$-directional chain with the $xy$ coordinates $(r_{B,x}, r_{A,y})$. In both cases, the third chain defined above is coplanar with each of the two particles $A$ and $B$.

We then choose a particle $C$ in the third chain. Let us consider the general SU($N$) case. If the spin component of particle $C$ is the same as one of the two particles, say, particle $B$, owing to Lemma 3, we can first switch the spin configuration between $A$ and $C$, and then that between $B$ and $C$. If the spin component of particle $C$ is different from both that of $A$ and $B$, we first switch the spin configuration between $A$ and $C$, then that between $B$ and $C$, and at last that between $A$ and $C$. The net result is that the spin configuration between $A$ and $B$ is switched while that of $C$ is unchanged.      Q.E.D.

Since all the three lemmas have been generalized to the 3D case, we arrive at Corollary 1 of ferromagnetism in 3D in the main text.      Q.E.D.

## VI.  FM IN THE 1D LATTICE

As a byproduct, our results can be extended to 1D multi-orbital systems. As illustrated in Fig. 3, in addition to the $\sigma$-bonding with hopping amplitude $t_\parallel$, a nonzero $\pi$-bonding with hopping amplitude $t_\perp$ is needed in the kinetic Hamiltonian, to satisfy Lemma 3. Unique FM ground states in this 1D system can be proved under the same *conditions* (i) and (ii) as the following corollary. We emphasize that this result was already obtained by Shen [5] using the Bethe Ansatz.

**Corollary 2 (1D FM Ground State)** *The statements in Theorems 1 and 2 of FM are also valid for the 1D multi-orbital systems $H'_{kin} + H_{int}$ under the same condi-*
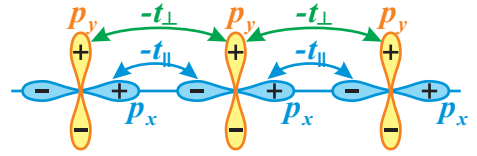


FIG. 3: The 1D lattice along $x$ direction with $p_x$- and $p_y$-orbitals at each site. Different from Fig. 1 in the main text, here, particles in $p_x$- and $p_y$-orbitals can all move along the $x$-direction with hopping amplitudes $t_\parallel$ and $t_\perp$ respectively. The signs of $t_\parallel$ and $t_\perp$ can be changed independently by gauge transformations.

*tions. Here,*

$$H'_{kin} = \sum_{x=1,\sigma=\uparrow,\downarrow}^{L_x} \Big[ -t_\perp \sum_{\mu=y,(z)} p^\dagger_{\mu,\sigma}(x+1)p_{\mu,\sigma}(x)$$
$$-t_\parallel p^\dagger_{x,\sigma}(x+1)p_{x,\sigma}(x) + h.c. \Big] - \mu_0 \sum_{x=1}^{L_x} n(x). \quad (6)$$

## VII.  PROOF OF THEOREM 3 ON THE ABSENCE OF FM

In this section, we will consider the opposite situation with $J < 0$, *i.e.*, anti-Hund's rule coupling.

### A.  FM states as the highest energy states

A direct result of the anti-Hund's rule coupling is the following corollary.

**Corollary 3** *Consider the same Hamiltonian in the same limits as those in Theorem 1 but in the case of $J < 0$. Under condition (i), the many-body eigenstates with the highest energy include the fully polarized states. If condition (ii) is also satisfied, the highest energy states are non-degenerate except for the trivial spin degeneracy.*
**Proof:** As we discussed before, the sign of the hopping integral $t_\parallel$ can be flipped by the gauge transformation $p_{\mu,\sigma}(\mathbf{r}) \to (-)^{r_\mu} p_{\mu,\sigma}(\mathbf{r})$. We denote the resultant Hamiltonian as $H'$, whose eigenstates have the same energy and the same physical properties as those of $H$. The negative of $H'$, *i.e.*, $-H'$, satisfies all conditions of Theorem 1. The ground states of $-H'$ are the highest energy states of $H'$, and thus correspond to the highest energy states of $H$ up to a gauge transformation, which proves this corollary.      Q.E.D.

### B.  Proof of Theorem 3

Following the same strategy in the proof of Lieb-Mattis' Theorem [6] and Lieb's Theorem [7] for antiferromagnetic Heisenberg models on bipartite lattices, we

first perform a gauge transformation on the operators for $p_y$-orbitals and keep those of $p_x$-orbitals unchanged

$$p'_{x,\alpha}(\mathbf{r}) = p_{x,\alpha}(\mathbf{r}), \quad p'_{y,\alpha}(\mathbf{r}) = (-)^{\alpha-\frac{1}{2}} p_{y,\alpha}(\mathbf{r}). \quad (7)$$

After this transformation, $H$ is transformed to $H'$, which is identical to $H$ except that the $xy$-components of the Hund's coupling term flip the sign as

$$H'_J = -|J| \sum_{\mathbf{r}} \left\{ S_x^x(\mathbf{r})S_y^x(\mathbf{r}) + S_x^y(\mathbf{r})S_y^y(\mathbf{r}) - S_x^z(\mathbf{r})S_y^z(\mathbf{r}) \right\}, \quad (8)$$

and the many-body bases defined in Eq. (5) in the body text transform as

$$|\mathcal{R}, \mathcal{S}\rangle' = (-)^{\Gamma} |\mathcal{R}, \mathcal{S}\rangle, \quad (9)$$

with

$$\Gamma = \sum_{1 \le c_j \le L_x, 1 \le i \le N_{c_j}} \left( \frac{1}{2} - \beta_i^{c_j} \right). \quad (10)$$

For each subspace $\mathcal{H}^M_{\mathcal{N}_\mathcal{X}, \mathcal{N}_\mathcal{Y}}$, the matrix element of $H'$ satisfies Lemma 2 of non-positivity under *condition* (i), and Lemma 3 of transitivity under *condition* (ii). Again, the Perro-Frobenius theorem ensures that the ground state $|\Psi_G^M\rangle$ in each subspace $\mathcal{H}^M_{\mathcal{N}_\mathcal{X}, \mathcal{N}_\mathcal{Y}}$ is non-degenerate, and

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

with $c_{\mathcal{R}, \mathcal{S}} > 0$.

Next we study the spin quantum number for the state $|\Psi_G^M\rangle$. Following the method in Ref. [8], we define a reference Hamiltonian,

$$H^R = |J| \left\{ \sum_{\mathbf{r}} \vec{S}_x(\mathbf{r}) \right\} \cdot \left\{ \sum_{\mathbf{r}} \vec{S}_y(\mathbf{r}) \right\}. \quad (12)$$

The spectra of Eq. (12) can be easily solved as

$$E(S_x, S_y; S) = |J| \left\{ S(S+1) - S_x(S_x+1) - S_y(S_y+1) \right\}/2, \quad (13)$$

where $S_x$ ($S_y$) is the total spin of all the particles in the $p_x$ ($p_y$)-orbital, respectively; $S$ is the total spin of the system which takes value from $|S_x - S_y|, |S_x - S_y| + 1, \cdots, S_x + S_y$. For any fixed values of $S_x$ and $S_y$, the minimization of $E(S_x, S_y; S)$ is reached at $S = |S_x - S_y|$ which yields the result:

$$E_{min}(S_x, S_y) = -|J| \left\{ S_x S_y + \min(S_x, S_y) \right\}. \quad (14)$$

Define $N_x = \sum_{1 \le r_i \le L_y} N_{r_i}$ and $N_y = \sum_{1 \le c_i \le L_x} N_{c_i}$, and thus $S_x \le N_x/2$ and $S_y \le N_y/2$. The absolute ground state energy for $H^R$ is reached with

$$S_x = N_x/2, \quad S_y = N_y/2, \quad S = \Delta N/2. \quad (15)$$

Thus in all the subspaces of $\mathcal{H}^M_{N_A, N_B}$ with $M \le \Delta N/2$, the ground states of $H^R$, $|\Psi_G^{M,R}\rangle$, possess the spin quantum number $S = \Delta N/2$. In comparison, for $M > \Delta N/2$, the spin quantum number of $|\Psi_G^{M,R}\rangle$ is $S = M$. Clearly, by the same transformation given in Eq. (7), the $H^R$-matrix satisfies Lemma 2 in each subspace $\mathcal{H}^M_{\mathcal{N}_\mathcal{X}, \mathcal{N}_\mathcal{Y}}$. Since the Lemma 3 of transitivity is not satisfied for $H^R$, its ground states $|\Psi_G^{M,R}\rangle$ are expressed as

$$|\Psi_G^{M,R}\rangle = \sum_{\mathcal{R}, \mathcal{S}} (-)^{\Gamma} c_{\mathcal{R}, \mathcal{S}}^R |\mathcal{R}, \mathcal{S}\rangle^M \quad (16)$$

with $c_{\mathcal{R}, \mathcal{S}}^R \ge 0$. Nevertheless $|\Psi_G^{M,R}\rangle$ carries a unique spin quantum number as analyzed above.

Now we are ready to prove Theorem 3. Obviously $\langle \Psi_G^{M,R} | \Psi_G^M \rangle > 0$, thus $\Psi_G^M$ shares the same spin quantum number $S$ as that of $|\Psi_G^{M,R}\rangle$. In short, $|\Psi_G^M\rangle$ is the non-degenerate ground state in the subspace $\mathcal{H}^M_{\mathcal{N}_\mathcal{X}, \mathcal{N}_\mathcal{Y}}$. For the series of subspaces $\mathcal{H}^M_{\mathcal{N}_\mathcal{X}, \mathcal{N}_\mathcal{Y}}$ with $M \le \Delta N/2$, $|\Psi_G^M\rangle$'s form spin multiplets with $S = \Delta N/2$. Thus we conclude that the ground state energies $E_G^M$ in each subspace $\mathcal{H}^M_{\mathcal{N}_\mathcal{X}, \mathcal{N}_\mathcal{Y}}$ satisfy $E_G^M < E_G^{M'}$ for $\Delta N/2 < M < M'$, and $E_G^M = E_G^{\Delta N/2}$ for $M \le \Delta N/2$. *Q.E.D.*

### C. More extensions

Theorem 3 implies strong ferromagnetic correlation inside and among parallel chains. Consider the special case in which there is only one particle in each column, while in all the rows particle densities are positive in the thermodynamic sense. Then the ground states are nearly fully polarized. Even though the inter-orbital coupling $J$ is antiferromagnetic, the particles in the column mediate FM coupling among those in the rows. If particle numbers in rows and columns are equal, the ground state is a spin singlet. Although we cannot prove it, a spontaneous symmetry breaking spin-nematic ground state conceivably occurs in the thermodynamic limit. All the rows and columns are FM ordered, but the polarizations of rows and columns are opposite to each other. The possibility of spin-nematic phase also applies to the 3D version of the SU(2) Hamiltonian $H_{kin} + H_{int}$. In this case, similar to the frustration in the 2D triangular lattice, the FM polarizations in the three types of orthogonal chains may form a 120° angle with respect to each other.

### VIII. FURTHER DISCUSSION

In this section, we estimate the FM energy scale $J_{FM}$ and the effect of finite values of $U$ which result in an antiferromagnetic (AFM) energy scale $J_{AFM}$ (See Sect. B below).

## A. The FM energy scale $J_{FM}$

We assume that the electron filling in every chain is the same. The average density per orbital (not per site) is $x$ which satisfies $0 < x < 1$, and then the average distance between two adjacent fermions in the same chain is $d = 1/x$. The FM energy scale $J_{FM}$ is estimated as the energy cost of flipping the spin of one fermion while keeping all other fermions spin polarized. $J_{FM}$ determines the spin-wave stiffness and sets up the energy scale of Curie temperature. For simplicity, we only consider the 2D spin-$\frac{1}{2}$ case as an example.

Let us first consider the *low filling* limit $x \ll 1$, and start with the fully spin polarized ground state as a background. Without loss of generality, we choose the first row of $p_x$-orbital, and pick up the $i$-th $p_x$-orbital fermion in this row. We consider the motion of the $i$-th fermion while fixing positions of all other fermions. The locations of the $i \pm 1$-th fermions are the wavefunction nodes of the $i$-th one, and the typical distance between the $i$-th and $i \pm 1$-th fermions is $d$. In fact, typically speaking, before the $i$-th fermion sees these nodes, it feels the scattering potential of $V$ from two $p_y$-orbital fermions intersecting this row with the average distance of $d$. If we flip the spin of the $i$-th fermion, then the scattering potential from it-s adjacent $p_y$-orbital fermions increases to the order of $J + V$. Under the condition that $xt/V \ll 1$, we can estimate from strong coupling analysis that the energy cost of is the order of $J_{FM} \sim x^3 \frac{t^2}{V} \frac{J}{J+V}$. In the limit of $J \gg V$, $J_{FM}$ saturates to the order of $x^3 \frac{t^2}{V}$.

On the other hand, at the *high filling* limit, *i.e.*, $1 - x \ll 1$, although on most sites two fermions are spin polarized by the Hund's rule coupling $J$, the intersite FM coherence is mediated by the motion of holes, and thus, the FM energy scale is much smaller than $J$. In fact, in the absence of holes, i.e., $x = 1$, all the spin configurations are degenerate which suppresses $J_{FM} \to 0$. The average distance between holes along the same chain is $d_h = 1/(1-x)$. Again let us start with a fully spin polarized background. Without loss of generality, we pick up a spin-1 site at the intersection of the $i$-th row and

$j$-th column. This site is filled by two fermions coupled by Hund's rule and we flip its spin. This process generates a new scattering center to adjacent holes in the $i$-th row and in the $j$-th column, and the scattering potential is at the order of $J$. In case of $(1-x)t/J \ll 1$, this spin flipped site effectively blocks the motion of holes, which costs kinetic energy at the order of $J_{FM} \propto t(1-x)^2$.

Conceivably, $J_{FM}$ is optimized at certain intermediate filling $x$. While generally evaluating $J_{FM}$ in this regime is difficult, we can consider a special case of $x = 1/2$, such that the FM state coexists with the antiferro-orbital ordering. The ideal Néel orbital configuration is that $p_x$ and $p_y$-orbitals are alternatively occupied with spin polarized fermions. In the case of $V \gg t$, the orbital superexchange is at the order of $t^2/V$, and flipping the spin of one fermion reduces the orbital superexchange energy to $t^2/(V + J)$. The difference is the FM energy scale $J_{FM} \propto \frac{t^2}{V} \frac{J}{J+V}$.

## B. The AFM energy scale $J_{AFM}$

So far, we have only considered the case of infinite $U$ which suppresses the AFM energy scale $J_{AFM}$ to zero. At large but finite values of $U$, fermions in the same chain with opposite spins can pass each other. This process lowers the kinetic energy and sets up $J_{AFM}$. In the low filling limit $x \ll 1$, the probability of two fermions with opposite spins sitting on two neighboring sites s-cales as $x^3$ under the condition that $xt/U \ll 1$, and thus $J_{AFM} \sim x^3 \frac{t^2}{U}$. At high fillings, $x \to 1$, the above probability simply scales as $x$, and thus $J_{AFM} \sim x\frac{t^2}{U}$.

Let us compare the energy scales of $J_{FM}$ vs $J_{AFM}$. At low filling limit, since usually $U \gg V$ and $J,V$ are at the same order, $J_{FM}$ wins over $J_{AFM}$. Nevertheless, $J_{AFM}$ increases with $x$ monotonically, and thus it wins over $J_{FM}$ as $x \to 1$. The FM ground states are expected to be stable in the low and intermediate filling regimes until $J_{AFM}$ becomes comparable with $J_{FM}$.

[1] J. Hubbard, Proc. R. Soc. Lond. A **276**, 238 (1963).
[2] J. C. Slater, Quantum Theory of Molecules and Solids (McGraw-Hill, New York, 1963), Vol. I, Appendix 6.
[3] O. Perron, Mathematische Annalen **64**, 248 (1907).
[4] F. G. Frobenius, Sitzungsber. Akad. Wiss. Berlin, Phys. Math. Kl., 471 (1908).
[5] S. Q. Shen, Phys. Rev. B **57**, 6474 (1998).
[6] E. H. Lieb and D. C. Mattis, J. Math. Phys **3**, 749 (1962).
[7] E. H. Lieb, Phys. Rev. Lett. **62**, 1201 (1989).
[8] E. H. Lieb and D. Mattis, Phys. Rev. **125**, 164 (1962).