Exact results for itinerant ferromagnetism in a t_{2g}-orbital system on cubic and square lattices

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(Received 8 January 2015; revised manuscript received 25 February 2015; published 11 March 2015)

We study itinerant ferromagnetism in a t_{2g} multiorbital Hubbard system in the cubic lattice, which consists of three planar oriented orbital bands of d_{xy}, d_{yz}, and d_{zx}. Electrons in each orbital band can only move within a two-dimensional plane in the three-dimensional lattice parallel to the corresponding orbital orientation. Electrons of different orbitals interact through the on-site multiorbital interactions including Hund's coupling. The strong-coupling limit is considered in which there are no doubly occupied orbitals but multiple on-site occupations are allowed. We show that in the case in which there is one and only one hole for each orbital band in each layer parallel to the orbital orientation, the ground state is a fully spin-polarized itinerant ferromagnetic state, which is unique apart from the trivial spin degeneracy. When the lattice is reduced into a single two-dimensional layer, the d_{zx} and d_{yz} bands become quasi-one-dimensional while the d_{xy} band remains two-dimensional. The ground-state ferromagnetism also appears in the strong-coupling limit as a generalization of the double-exchange mechanism. Possible applications to the systems of $SrRuO_3$ and $LaAlO_3/SrTiO_3$ interface are discussed.

DOI: 10.1103/PhysRevB.91.115122 PACS number(s): 71.10.Hf, 71.10.Fd, 71.20.Be

I. INTRODUCTION

Itinerant ferromagnetism (FM) is not only a representative strong-correlation problem, but also a highly nonperturbative one [1–18]. It is widely known as a long-standing problem of condensed matter physics, and also a current research focus in ultracold-atom physics [19–26]. The Stoner mechanism states that polarized electron systems can save the exchange interaction energy. Nevertheless, because of the associated cost of kinetic energy, FM is not guaranteed even in the presence of very strong repulsions. For example, in rigorously one-dimensional (1D) systems, no matter how strong the repulsive interactions are, the ground state is always a spin singlet, which is known as the famous Lieb-Mattis theorem [1]. In other words, electrons can remain unpolarized but avoid each other to reduce interaction; nevertheless, their wave functions are strongly correlated. Certainly the Lieb-Mattis theorem in 1D only applies for spin-independent systems. Ferromagnetism in 1D is still possible if the interaction is spin dependent.

Because of the strong-correlation nature of itinerant FM, exact theorems are important to provide reference points. Nagaoka's theorem is an early example, which applies to the infinite U Hubbard model with a single hole in the half-filled background [3,27,28]. The fully polarized FM state facilitates the hole's coherent motion, which minimizes the kinetic energy of the hole and is therefore selected as the ground state. Another class of FM theorems is based on the flat-band structure on line graphs [12–14,29,30]. Because of the divergence of density of states in the flat band, the kinetic energy cost because of spin polarization is suppressed. Metallic FM states with a dispersive band structure have also been proved [31,32].

Recently, a ground-state FM theorem has been proved in both two-dimensional (2D) square and three-dimensional (3D) cubic lattices systems with multiorbital structures [33]. The band structure behaves like decoupled orthogonal 1D chains, while different chains are coupled at their crossing site through multiorbital Hubbard interactions. In particular, spins of each chain are not conserved but coupled by Hund's interaction. Hence, the ground-state FM ordering is genuinely 2D or 3D. Different from Nagaoka's theorem, the result of multiorbital FM allows a stable FM phase over a large region of filling factors in both 2D and 3D. An important consequence of this theorem is that the sign structure of the many-body Hamiltonian matrix leads to the absence of the quantum Monte Carlo (QMC) sign problem [33]. Consequently, QMC simulations on finite-temperature thermodynamic properties of itinerant FM have been performed [34], which yield asymptotically exact results and shed light on the mechanism of magnetic phase transitions in the strong-coupling limit.

In this article, we generalize Nagaoka's theorem of itinerant FM from the single-orbital system to multiorbital systems. We consider the 3D cubic lattice and each site consists of three t_{2g} orbitals: d_{xy}, d_{yz}, and d_{zx}. Each orbital has a planar orientation, and the associated band structure is quasi-2D-like. Electrons of different orbitals interact through the on-site multiorbital interactions including Hund's coupling. In the limit of intraorbital interaction $U \to \infty$, states with doubly occupied orbitals are projected out. When each plane of the cubic lattice has one and only one hole in the in-plane orbital band, this system can be be viewed as crossing layers of Nagaoka FM states. We prove that, in this limit, the ground state of this system is the fully spin-polarized itinerant ferromagnetic state, and it is nondegenerate apart from the trivial spin degeneracy. Furthermore, when this system is reduced to a single 2D layer system of t_{2g} orbitals, the d_{zx}- and d_{yz}-orbital bands become quasi-1D and coupled to the quasi-2D band of d_{xy} through Hund's coupling. The ground-state FM is still valid, where the quasi-1D d_{zx} and d_{yz} bands are allowed to take general values of filling, while the d_{xy} band can possess a single hole or be fully filled. Although the above exact results require an idealized strong-coupling limit, the strong-correlation physics that they imply sheds important light on the mechanism of itinerant FM in transition-metal oxides.

The rest of this paper is organized as follows: In Sec. II, the multiorbital Hubbard model for the t_{2g} orbital in the 3D cubic lattice is defined. In Sec. III, Theorem 1 of the ground-state itinerant FM in the 3D t_{2g}-orbital system is proved. In Sec. IV,

Theorem 2 of the ground-state itinerant FM for the reduced 2D layered system is proved. Discussion on connections to experiment systems is provided in Sec. V. Conclusions are presented in Sec. VI.

II. THE MODEL HAMILTONIAN: A 3D MULTIORBITAL HUBBARD MODEL

In this section, we define a 3D multiorbital Hubbard model in the 3D cubic lattice, which will be shown to possess itinerant FM ground states under conditions I and II in Sec. III.

We consider a t_{2g}-orbital system filled with spin-1/2 electrons; i.e., each site possesses d_{xy}, d_{yz}, and d_{zx} orbitals. The Wannier wave function of the t_{2g} orbitals is planar-like as shown in Fig. 1. The kinetic energy of each orbital band exhibits a 2D structure: Say, for electrons in the d_{xy} orbital, they can only move in the xy plane with a hopping amplitude $t_\parallel$. However, their hopping amplitude $t_\perp$ along the transverse direction of the z axis is very small. Usually, the in-plane hopping $t_\parallel$ is assisted by the p orbitals of oxygen anions lying at the middle point of the bond, which leads to large hopping amplitudes, while the transverse hopping $t_\perp$ can only be attributed to the direct overlap between two d_{xy} orbitals offset along the z axis. Since d-orbital Wannier functions are nearly localized and the z axis is perpendicular to the orbital plane, $t_\parallel$ is negligible in realistic transition-metal oxides. Similarly, electrons in the d_{yz} and d_{zx} orbitals only hop along the yz and zx planes, respectively.

Because of the different parity eigenvalues of these three t_{2g} orbitals with respect to the xy, yz, and zx planes, they do not hybridize by the nearest-neighbor hopping. If we neglect the longer range hopping terms, the kinetic energy part can simply be written as

$$H^K = H^K_{xy} + H^K_{yz} + H^K_{zx}, \tag{1}$$

where H^K_{xy}, H^K_{yz}, and H^K_{zx} are the kinetic energies of electrons in the xy-, yz-, and zx-orbital bands, respectively. The kinetic energy for the xy-orbital band is expressed as

$$H^K_{xy} = \sum_{\mathbf{r}} t_\parallel (d^\dagger_{xy,\sigma}(\mathbf{r}) d_{xy,\sigma}(\mathbf{r} + a_0\hat{x}) + d^\dagger_{xy,\sigma}(\mathbf{r}) d_{xy,\sigma}(\mathbf{r} + a_0\hat{y}) + \text{H.c.}), \tag{2}$$

where a_0 is the lattice constant; $d_{xy,\sigma}(\mathbf{r})$ is the annihilation operator in the d_{xy} orbital on site $\mathbf{r}$ with the spin index $\sigma = \uparrow$ or $\downarrow$. For convenience later, we choose $t_\parallel$ positive. For the bipartite lattice such as the cubic one, the sign of $t_\parallel$ can be flipped by a gauge transformation, which does not affect any physical observable. The transverse hopping $t_\perp$ term is neglected in Eq. (2). Similarly, $H^K_{yz(zx)}$ can also be defined by permuting the indices of orbitals and hopping directions in H^K_{xy}, whose expressions are not repeated here.

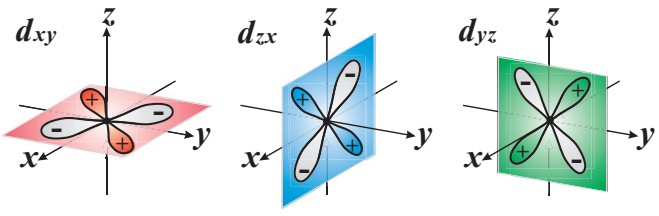

FIG. 1. (Color online) The Wannier orbital wave functions of t_{2g} orbitals: d_{xy}, d_{yz}, and d_{zx}. For electrons in the d_a orbitals ($a = xy, yz, zx$), they can only move along the xy, yz, or zx plane, respectively, but not perpendicular to the orbital orientation plane.

The interaction term is the standard multiorbital Hubbard interaction [4,5,35,36] defined on-site as

$$H^I = U \sum_{\mathbf{r},a} n_{a,\uparrow}(\mathbf{r}) n_{a,\downarrow}(\mathbf{r}) - J \sum_{\mathbf{r},a\neq b} \left(\vec{S}_a(\mathbf{r}) \cdot \vec{S}_b(\mathbf{r}) - \frac{1}{4} n_a(\mathbf{r}) n_b(\mathbf{r}) \right) + V \sum_{\mathbf{r},a\neq b} n_a(\mathbf{r}) n_b(\mathbf{r}) + \Delta \sum_{\mathbf{r},a\neq b} (d^\dagger_{a,\uparrow}(\mathbf{r}) d^\dagger_{a,\downarrow}(\mathbf{r}) d_{b,\downarrow}(\mathbf{r}) d_{b,\uparrow}(\mathbf{r}) + \text{H.c.}), \tag{3}$$

where $a = xy, yz, zx$ is the orbital index; $n_{a,\sigma}(\mathbf{r})$ is the number of electrons occupying the a orbital at site $\mathbf{r}$ with spin index σ; $n_a = n_{a,\uparrow} + n_{a,\downarrow}$; $\vec{S}_a(\mathbf{r})$ is the spin operator of the ath orbital at site $\mathbf{r}$.

Equation (3) contains all the possible terms satisfying the spin SU(2) symmetry and the lattice cubic symmetry. The U term is the usual intraorbital Hubbard interaction; the V term is the interorbital Hubbard interaction; the J term is Hund's coupling with $J > 0$; and the Δ term describes the singlet pairing hopping process among different orbitals. The expressions of U, V, J, and Δ are presented in Appendix A following the standard physical meaning of two-body Coulomb interactions.

III. FERROMAGNETISM IN THE 3D t_{2g}-ORBITAL SYSTEM

In this section, we consider the 3D t_{2g}-orbital systems in the cubic lattice of size $L_x \times L_y \times L_z$. We also assume the following two conditions:

(I) $U \to +\infty$, Δ is finite.

(II) For each orbital band, there is one and only one hole in every layer parallel to the orbital plane. For example, there is one and only one hole in every xy plane in the d_{xy}-orbital band, and similarly for the d_{yz}- and d_{zx}-orbital bands.

Condition II can be well defined because of the following lemma whose proof is obvious.

Lemma 1. The Hamiltonian of Eqs. (2) and (3) conserves particle number in each orbital band in each plane parallel to the orbital orientation.

Accordingly, the Hilbert space of the system can be factorized as the tensor product of the Hilbert space of each orbital band in each layer as

$$\mathcal{H} = \bigotimes_{l_z=1}^{L_z} \mathcal{H}^{xy}_{l_z} \bigotimes_{l_x=1}^{L_x} \mathcal{H}^{yz}_{l_x} \bigotimes_{l_y=1}^{L_y} \mathcal{H}^{zx}_{l_y}, \tag{4}$$

where $l_{z,x,y}$ are the indices of the xy, yz, and zx planes, respectively. Under condition I, states with doubly occupied orbitals are projected out, and each orbital can only be occupied at most by one particle. Further, condition II restricts one and only one hole for each orbital band in a layer. In each given

Hilbert space $\mathcal{H}^a_{l_i}$, each state is determined by the location of the hole and the spin configuration at other sites. For example, in the Hilbert space of the d_{xy} orbital of the l_zth layer, we can label all the d_{xy} orbitals of this layer in an arbitrary order by the index $i_{l_z} = 1, \ldots, L_x L_y$. Then, the states in this layer can be represented as

$$\left|h^{xy}_{l_z}; \{\sigma\}_{l_z}\right\rangle = (-)^{h^{xy}_{l_z}} \prod_{i_{l_z}}{}' d^\dagger_{xy,\sigma}(i_{l_z})|0\rangle, \tag{5}$$

where $h^{xy}_{l_z}$ labels the location of the hole; $\{\sigma\}_{l_z}$ represents the spin configuration; $\prod'$ means the ordered product of the creation operators except the one at the location of the hole; $\prod'_{i_{l_z}} d^\dagger_{xy,\sigma}(i_{l_z})|0\rangle = d^\dagger_{xy,\sigma_1}(1)\cdots d^\dagger_{xy,\sigma_{h-1}}(h^{xy}_{l_z} - 1)\widehat{d^\dagger_{xy,\sigma_h}(h^{xy}_{l_z})} d^\dagger_{xy,\sigma_{h+1}}(h^{xy}_{l_z}+1)\cdots d^\dagger_{xy,\sigma_{L_xL_y}}(L_xL_y)|0\rangle$ with the "hat" means the operator below it does not appear. Then, we can define the bases of the product Hilbert space for our entire system as

$$|\{h\},\{\sigma\}\rangle = \bigotimes_{l_z=1}^{L_z} \left|h^{xy}_{l_z}; \{\sigma\}_{l_z}\right\rangle \bigotimes_{l_x=1}^{L_x} \left|h^{yz}_{l_x}; \{\sigma\}_{l_x}\right\rangle \bigotimes_{l_y=1}^{L_y} \left|h^{zx}_{l_y}; \{\sigma\}_{l_y}\right\rangle, \tag{6}$$

where $\{h\}$ represents the locations of all the holes in a given state and $\{\sigma\}$ represents the spin configuration of this state with the labels of orbitals and layers omitted,. Because of the spin conservation, we can decompose the Hilbert space into different sectors $\mathcal{H}^{S_z}$ by the value of the z component of total spin S_z, denoted as $\mathcal{H} = \bigoplus \mathcal{H}^{S_z}$. Nevertheless, $\mathcal{H}^{S_z}$ cannot be further factorized as the product space of different orbital bands and layers.

Next, let us prove two lemmas as the preparation of the FM Theorem 1.

Lemma 2 (nonpositivity). Under the bases $|\{h\},\{\sigma\}\rangle$ defined above for the Hilbert space $\mathcal{H}$ with total spin S_z, the off-diagonal matrix elements of the many-body Hamiltonian $H = H_{\rm kin} + H_{\rm int}$ [see Eqs. (2) and (3)] are nonpositive.

Proof. The off-diagonal matrix elements are contributed by the hopping part and Hund's interaction part. The pairing hopping term does not exist in the limit of $U \to +\infty$ since states with doubly occupied orbitals have been projected out. For the hopping term, because of the sign convention of the many-body bases defined in Eq. (6) inherited from Eq. (5), it is easy to check that

$$\langle\{h\},\{\sigma\}|H_t|\{h'\},\{\sigma'\}\rangle = -t \quad \text{or} \quad 0. \tag{7}$$

This step is the same as that in the proof of the usual Nagaoka theorem for a 2D single-orbital Hubbard model [27]: Although there are $(L_x + L_y + L_z)$ holes in our system, the fermion ordering does not change under hopping because of Lemma 1. For the xy component of Hund's interaction $H_{J_{xy}} = -J/2\sum_{a\neq b}(S^+_a S^-_b + S^-_a S^+_b)$ with $S^\pm_a = S^x_a \pm i S^y_a$, it does not change the fermion ordering either, and thus, its matrix elements read

$$\langle\{h\},\{\sigma\}|H_{J_{xy}}|\{h'\},\{\sigma'\}\rangle = -J/2 \text{ or } 0, \tag{8}$$

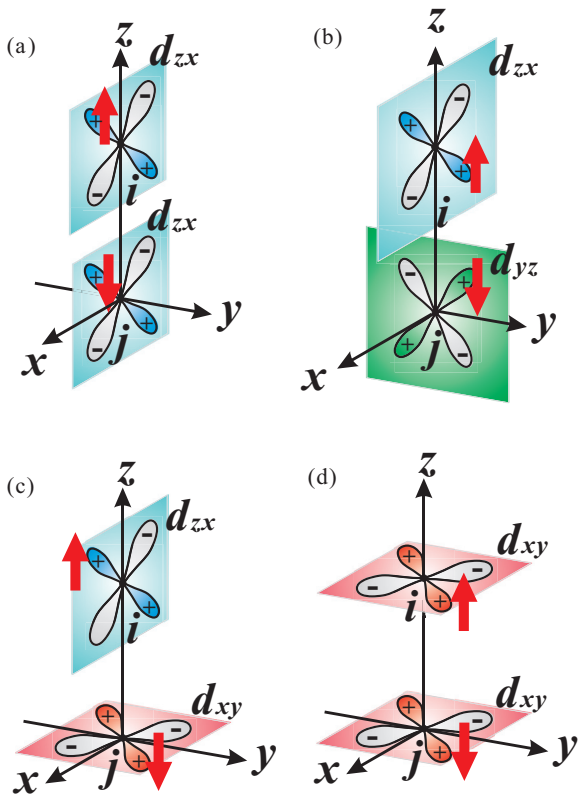

FIG. 2. (Color online) Representative orbital configurations along a bond $\langle ij\rangle$ with two orbitals at sites i and j initially occupied by spins $\uparrow$ and $\downarrow$, respectively. Case (a): $[d_{zx,\uparrow}(i); d_{zx,\downarrow}(j)]$, case (b): $[d_{zx,\uparrow}(i); d_{yz,\downarrow}(j)]$, case (c): $[d_{zx,\uparrow}(i); d_{xy,\downarrow}(j)]$, case (d): $[d_{xy,\uparrow}(i); d_{xy,\downarrow}(j)]$. Any two cases of (a)–(d) are nonequivalent under the lattice symmetry transformation.

which are also nonpositive. The V term and the z component of Hund's interaction only contribute to the diagonal part of the many-body matrix. *Q.E.D.*

Let us consider a general hole and spin configuration satisfying conditions I and II. We pick up a bond $\langle ij\rangle$ and consider the d_a orbital of site i and the d_b orbital of site j. If they are occupied by spin σ and σ', respectively, let us denote this bond configuration as $[d_{a,\sigma}(i); d_{b,\sigma'}(j)]$. We have the following lemma:

Lemma 3. The spin configuration in $[d_{a,\sigma}(i); d_{b,\sigma'}(j)]$ can be flipped to $[d_{a,\sigma'}(i); d_{b,\sigma}(j)]$ by applying a series of hopping and Hund's interaction processes without finally affecting spin and hole configurations in the rest of the system.

Proof. Without loss of generality, we assume the bond $\langle ij\rangle$ is along the z axis, and only discuss how to flip $[d_{a,\uparrow}(i); d_{b,\downarrow}(j)]$ to $[d_{a,\downarrow}(i); d_{b,\uparrow}(j)]$. Since a and b can take any of the xy, yz, and zx, there are 9 possible orbital configurations for a bond. Nevertheless, they can be classified into 4 nonequivalent classes because of the lattice geometry as shown in Figs. 2(a) to 2(d).

For later convenience, the single-hole assisted spin flipping in the 2D single-orbital infinite U Hubbard model is reviewed in Appendix B, which plays an important role in the proof of the Nagaoka FM ground state and will be employed repeatedly below.

Class (a): Let us consider $a = b = zx$. The same reasoning can also apply to the case of $a = b = yz$. Since two orbitals and the bond are coplanar and there is one hole in this plane, we can directly use the result in Appendix B to exchange their spins $[d_{zx,\uparrow}(i); d_{zx,\downarrow}(j)] \rightarrow [d_{zx,\downarrow}(i); d_{zx,\uparrow}(j)]$.

Class (b): Let us consider $a = zx$ and $b = yz$, i.e., the configuration $[d_{zx,\uparrow}(i); d_{yz,\downarrow}(j)]$. The reasoning below also applies to the case of $a = yz$ and $b = zx$. Let us use another orbital, d_{yz}, at site i. First, we assume that it is occupied since we can always move an electron from other neighboring sites and return it back afterwards. If it is occupied by spin-↑, a familiar bond configuration $[d_{yz,\uparrow}(i); d_{yz,\downarrow}(j)]$ appears. As already shown in class (a), their spins can be exchanged to give an intermediate configuration $[d_{yz,\downarrow}(i); d_{yz,\uparrow}(j)]$ for class (b). Then, on site i, we have both $d_{zx,\uparrow}(i)$ and $d_{yz,\downarrow}(i)$, whose spins can be further exchanged by the $H_{J_{xy}}$ term to become $d_{zx,\downarrow}(i)$ and $d_{yz,\uparrow}(i)$. Combining these two steps of spin exchange, the initial configuration $[d_{zx,\uparrow}(i); d_{yz,\downarrow}(j)]$ is flipped to $[d_{zx,\downarrow}(i); d_{yz,\uparrow}(j)]$ and the third $d_{yz}(i)$ orbital remains spin-↑ finally. If the $d_{yz}(i)$ orbital is occupied by spin-↓, we can first apply Hund's interaction to exchange spins between the $d_{zx}(i)$ and $d_{yz}(i)$ orbitals, and then apply the process in class (a) to further exchange the spins between two d_{yz} orbitals on sites i and j.

Class (c) contains four equivalent configurations $a = d_{zx}$, $b = d_{xy}$; $a = d_{yz}$, $b = d_{xy}$; $a = d_{xy}$, $b = d_{zx}$; $a = d_{xy}$, $b = d_{yz}$. Class (d) only contains one configuration $a = b = d_{xy}$. The proof for these two classes is similar to that of class (b) by combining Hund's interaction and the hole's hopping. The detailed proofs are given in Appendix C. $Q.E.D.$

Based on Lemma 3, we can have an important property of transitivity for the many-body matrix in any sub-Hilbert space $\mathcal{H}^{S_z}$.

Lemma 4 (transitivity). Consider the Hamiltonian matrix in the subspace $\mathcal{H}^{S_z}$. For any two basis vectors, $|\{h\},\{\sigma\}\rangle$ and $|\{g\},\{\alpha\}\rangle$, there always exists a series of basis vectors $|\{h_1\},\{\sigma_1\}\rangle$, $|\{h_2\},\{\sigma_2\}\rangle$, ..., $|\{h_k\},\{\sigma_k\}\rangle$ connected with nonzero matrix elements of H, such that

$$\langle\{g\},\{\alpha\}|H|\{h'_1\},\{\sigma_1\}\rangle\langle\{h_1\},\{\sigma_1\}|H|\{h_2\},\{\sigma_2\}\rangle \times ...\langle\{h_k\},\{\sigma_k\}|H|\{h\},\{\sigma\}\rangle \neq 0. \quad (9)$$

Proof. First, we can always apply the hopping term to $|\{h\},\{\sigma\}\rangle$ to rearrange the locations of holes of each orbital band in each layer. Then we reach an intermediate state $|\{g'\},\{\alpha'\}\rangle$ in which the locations of holes are the same as that in $|\{g\},\{\alpha\}\rangle$. Since the two states $|\{g\},\{\alpha\}\rangle$ and $|\{g'\},\{\alpha'\}\rangle$ have the same z component of the total spin S_z, they only differ by their spin configurations with a permutation of spins.

Since any permutation can be generated by exchanges, it suffices to show as below that in $|\{g'\},\{\alpha'\}\rangle$ two opposite spins in any two orbitals can be exchanged by consecutively applying hoppings and Hund's interactions without finally affecting the configuration of the rest of the system.

If the two orbitals are on the same site, it is easy to exchange their spins by applying Hund's interaction with $H_{J_{xy}}$ once. If they are located at different sites, we can always find a path of successive bonds connecting these two sites, and passing through nonempty sites [here are at most a number of $\min(L_x, L_y, L_z)$ sites with all three orbitals empty]. Then, we can have a sequence of occupied orbitals in which every two adjacent orbitals are located on two nearest-neighbor sites. We can exchange the two spins at two ends of this path as follows: Following Lemma 3, we can flip different spins at occupied orbitals on two neighboring sites. Then, by successively applying this operation, we are able to exchange the spins of two ends without affecting other parts of the system. $Q.E.D.$

Now we are ready to prove the following theorem.

Theorem 1 (3D FM ground state). Consider the Hamiltonian $H_{\rm kin} + H_{\rm int}$ satisfying conditions I and II. The physical Hilbert space is $\mathcal{H}^{S_z}$. For any values of V and $J > 0$, the ground states are spin fully polarized and are unique apart from the trivial spin degeneracy. They can be expressed as

$$\left|\Psi_G^{S_z}\right\rangle = \sum{}' c_{\{h\},\{\sigma\}}|\{h\},\{\sigma\}\rangle, \quad (10)$$

where all the coefficients are strictly positive and $\sum'$ means the summation over states in $\mathcal{H}^{S_z}$.

Proof. Because of Lemma 2 of nonpositivity and Lemma 4 of transitivity, the Hamiltonian matrix within $\mathcal{H}^{S_z}$ satisfies the prerequisites of the Perron-Frobenius theorem theorem. The importance of the transitivity to the nondegenerate ground state is also explained in Sec. III of the Supplementary Material of Ref. [33]. Then it is straightforward to conclude that Eq. (10) is true which is nondegenerate within each $\mathcal{H}^{S_z}$.

To show that $|\Psi_G^{S_z}\rangle$ in Eq. (10) is a fully spin-polarized state, we introduce a reference state in $\mathcal{H}^{S_z}$ by summing over all its bases with equal weights,

$$\left|\Psi_{\rm ref}^{S_z}\right\rangle = \sum{}' |\{h\},\{\sigma\}\rangle. \quad (11)$$

Since $|\Psi_{\rm ref}^{S_z}\rangle$ is symmetric under exchanging spins of any two orbitals, it is a fully spin-polarized state with the total spin $S = N_{\rm tot}/2$ and its z component S_z. Apparently, $\langle\Psi_G^{S_z}|\Psi_{\rm ref}^{S_z}\rangle \neq 0$. Since $|\Psi_G^{S_z}\rangle$ is the unique ground state in $\mathcal{H}^{S_z}$, these two nonorthogonal states must share the same good quantum numbers of S and S_z. $Q.E.D.$

Because of the spin SU(2) symmetry, all ground states $|\Psi_G^{S_z}\rangle$ in different $\mathcal{H}^{S_z}$ with $-N_{\rm tot}/2 \leqslant S_z \leqslant N_{\rm tot}/2$ are degenerate, and form a set of spin multiplets with the maximal total spin $S = N_{\rm tot}/2$.

Remark. Theorem 1 is true for both the periodic and open boundary conditions.

Based on Theorem 1, we have the following two corollaries with their proofs presented in Appendix D.

Corollary 1. Under condition I and a modified condition II: There is one and only one doubly occupied orbital for each orbital band in each layer; we have that the Hamiltonian of Eqs. (2) and (3) also possesses the fully spin-polarized FM ground state which is unique up to the trivial spin degeneracy.

Corollary 2. If there is one and only one particle in each orbital band in each layer, we also have that the ground state is fully spin polarized and unique up to the trivial spin degeneracy for any values of $J > 0$ and V.

IV. FERROMAGNETISM IN THE 2D t_{2g}-ORBITAL LAYER

In this section, we will consider the same multiorbital Hubbard Hamiltonian of Eqs. (2) and (3) but in a single layer

along the xy plane. The d_{xy}-orbital band remains 2D, while the d_{zx} and d_{yz} orbitals form crossed 1D bands with dispersion perpendicular to each other. The FM ground state of this system will be discussed when both 1D and 2D bands present.

When only the two quasi-1D bands are considered, the FM ground state has been proved in Ref. [33] under condition I and the following two conditions:

(III) Open boundary condition or periodic (antiperiodic) boundary condition with odd (even) number of particles in each row or column.

(IV) Arbitrary filling with at least one hole and one particle in each row and each column.

To describe the d_{zx} and d_{yz} bands with general fillings, let us first recapture the many-body bases constructed for the quasi-1D system in Ref. [33] and rewrite them in terms of d_{zx} and d_{yz} bands. By Lemma 1, for any generic filling, we can always 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 $\mathcal{N}_\mathcal{X}=\{N_{r_i}\},\mathcal{N}_\mathcal{Y}=\{N_{c_i}\}$, where N_{r_i} and N_{c_i} are the particle numbers of d_{zx} and d_{yz} orbitals conserved in the r_ith row and the c_ith column, respectively. We can order electrons in each row from the leftmost particle to the rightmost one, followed by the ordering in each column from the top to bottom. The corresponding many-body basis can be set up as

$$\begin{aligned}|\mathcal{R},\mathcal{S}\rangle_{\mathcal{N}_\mathcal{X},\mathcal{N}_\mathcal{Y}} &= \prod_{j=1}^{L_x} d^\dagger_{yz,c_j}\prod_{j=1}^{L_y} d^\dagger_{zx,r_j}|0\rangle \\ &= d^\dagger_{yz,c_{L_x}}\cdots d^\dagger_{yz,c_2}d^\dagger_{yz,c_1}d^\dagger_{zx,r_{L_y}}\cdots d^\dagger_{zx,r_2}d^\dagger_{zx,r_1}|0\rangle,\end{aligned} \tag{12}$$

where j denotes the index of columns and rows; $\mathcal{R}=\{\mathbf{r}_i^{r_j};\mathbf{r}_i^{c_j}|$ all i's and j's$\}$ represents the coordinates of occupied sites; $\mathcal{S}=\{\alpha_i^{r_j};\beta_i^{c_j}|$ all i's and j's$\}$ represents their the spin configurations. The operator $d^\dagger_{zx,r_j}$ ($d^\dagger_{yz,c_j}$) creates a whole line of N_{r_j} (N_{c_j}) d_{zx} (d_{yz}) electrons in the row r_j (column c_j) ordered from left to right (from top to bottom), $d^\dagger_{zx,r_j}=\prod_{\mathbf{r}_i\in \mathrm{row}_{r_j}} d^\dagger_{zx}(\mathbf{r}_1)d^\dagger_{zx}(\mathbf{r}_2)\cdots d^\dagger_{zx}(\mathbf{r}_{N_{r_j}})$, and $d^\dagger_{yz,c_j}$ can be similarly defined.

Now, let us consider the additional quasi-2D d_{xy} band with one and only one hole. The basis for this layer of d_{xy} orbital $|h^{xy},\{\sigma\}\rangle$ is defined following Eq. (5) but without the layer index. Then, the basis for the Hilbert space of this 2D system $\mathcal{H}_{2D}$ can be constructed by the direct product of the basis for the 1D bands and that for the 2D band,

$$|\mathcal{R},\mathcal{S}\rangle_{\mathcal{N}_\mathcal{X},\mathcal{N}_\mathcal{Y}}\otimes|h^{xy},\{\sigma\}\rangle. \tag{13}$$

Again, because of the conservation of the z component of the total spin, this Hilbert space can be decomposed as $\mathcal{H}_{2D}=\bigoplus\mathcal{H}_{2D}^{S_z}$. Following the same steps in Ref. [33] and in Sec. III, it is straightforward to show that for the basis defined in Eq. (13), and under condition III for 1D bands, the off-diagonal matrix elements of the many-body Hamiltonian are nonpositive.

Below, we further show the transitivity of the Hamiltonian matrix in the sub-Hilbert space $\mathcal{H}_{2D}^{S_z}$ under condition IV for d_{zx} and d_{yz} bands. Since the locations of electrons can be easily adjusted by applying hopping terms, it suffices to show the transitivity between two bases only differ by spin configurations $|u\rangle=|\mathcal{R},\mathcal{S}\rangle_{\mathcal{N}_\mathcal{X},\mathcal{N}_\mathcal{Y}}\otimes|h^{xy},\{\sigma\}\rangle$ and $|v\rangle=|\mathcal{R},\mathcal{S}'\rangle_{\mathcal{N}_\mathcal{X},\mathcal{N}_\mathcal{Y}}\otimes|h^{xy},\{\sigma'\}\rangle$. Again, we only need to show that for the state of $|u\rangle$, we can exchange any two different spins by applying hopping and Hund's interaction terms. If these two electrons are both in quasi-1D bands d_{zx} and d_{yz}, this situation has been proved in Ref. [33]. If these two electrons are both in the d_{xy} band, it is reduced to the usual case of the Nagaoka system.

Now let us consider the case of one electron in the quasi-1D bands, without loss of generality, in the d_{zx}-orbital band with spin-$\uparrow$, and another electron in the d_{xy} band with spin-$\downarrow$. We denote their locations as $\mathbf{r}_{zx}$ and $\mathbf{r}_{xy}$, respectively. Let us identify the site $\mathbf{r}_c$ which is in the same row of the d_{zx} electron and in the same column of the d_{xy} electron, and consider the d_{yz} orbital at this site. We assume that there is an electron of the d_{yz} orbital at $\mathbf{r}_c$. If not, because of condition IV, we can always move a d_{yz} electron of that column to $\mathbf{r}_c$ by hopping. And the configuration in this column can be restored by reversing the hopping afterward. If the electron of the d_{yz} orbital at $\mathbf{r}_c$ has spin-$\uparrow$, it can first be moved to $\mathbf{r}_{xy}$ by hoppings. Then, it can exchange the spins with the d_{xy} electron at $\mathbf{r}_{xy}$ by Hund's interaction. After reversing the hopping, this d_{yz} electron can be moved back to $\mathbf{r}_c$ but with spin-$\downarrow$. Further, it can be moved to $\mathbf{r}_{zx}$ to exchange the spins with the d_{zx} electron and be moved back to $\mathbf{r}_c$ again with its original spin-$\uparrow$ recovered. The net effect is the exchange of spin configurations between the d_{xy} and d_{zx} electrons without affecting other configurations. The case of the d_{yz} electron at $\mathbf{r}_c$ with spin-$\downarrow$ can be similarly proved.

So far, we have shown both the nonpositivity of off-diagonal matrix elements and the transitivity of the Hamiltonian matrix in the sub-Hilbert space $\mathcal{H}_{2D}^{S_z}$. Then, following the same reasoning in the proof of Theorem 1, it is straightforward to have the following theorem

Theorem 2 (2D FM ground state). Consider the case in which there is one and only one hole in the d_{xy} band. Under conditions I, III, and IV, for any values of V and $J>0$, the ground states are fully spin polarized which is unique apart from the trivial spin degeneracy.

Next, we consider the situation in which the d_{xy} band is half filled, i.e., there is no hole. In this case, the d_{xy} band by itself is not ferromagnetic. Because of the coupling to the quasi-1D band, we have the following theorem.

Corollary 3. If the d_{xy} band is half filled, under the same conditions in Theorem 2, for any values of V and $J>0$, the ground states are fully spin polarized which is unique apart from the trivial spin degeneracy.

Proof. We first define the basis for the local moments for the half-filled d_{xy} band, which can be ordered in an arbitrary way as

$$|\{\sigma\}\rangle=\prod_i d^\dagger_{xy,\sigma}(i)|0\rangle, \tag{14}$$

where $\langle\sigma\rangle$ is an arbitrary spin distribution. Then for the combined system, the basis is defined as

$$|\mathcal{R},\mathcal{S}\rangle_{\mathcal{N}_\mathcal{X},\mathcal{N}_\mathcal{Y}}\otimes|\{\sigma\}\rangle. \tag{15}$$

Again because of spin conservation, the Hilbert space in this case $\mathcal{H}'_{2D}$ can be further decomposed into the direct sum of different sectors of S_z's as $\mathcal{H}'_{2D}=\oplus\mathcal{H}_{2D}^{S_z\prime}$.

Similarly to Theorem 2, the off-diagonal elements of the Hamiltonian matrix are nonpositive. We next show the transitivity of the Hamiltonian matrix in each physical sub-Hilbert space $\mathcal{H}_{2D}^{S_z'}$. Again, we only need to show that for any state in $\mathcal{H}_{2D}^{S_z'}$, opposite spins of any two electrons can be exchanged by applying hopping and Hund's interaction without affecting other parts of the system. The proof is very similar to that of Theorem 2. Nevertheless, a new situation needs to be addressed: both electrons are in the d_{xy} band with spin-↑ and spin-↓, respectively. Their locations are denoted as $\mathbf{r}$ and $\mathbf{r}'$, respectively. Then we can choose an electron in the d_{zx} band, and, without loss of generality, assume its spin-↑. Then according to the proof of Theorem 2, we can first flip the pair of electrons $d_{zx,\uparrow}$ and $d_{xy,\downarrow}(\mathbf{r}')$, then their spins become $d_{zx,\downarrow}$ and $d_{xy,\uparrow}(\mathbf{r}')$. Next, we consider the pair of $d_{zx,\downarrow}$ and $d_{xy,\uparrow}(\mathbf{r})$ and exchange their spins. The net result is the exchange of the spins of two d_{xy} electrons.

With both results of nonpositivity and transitivity, it is also straightforward to arrive at Corollary 3 by similar proof of Theorem 1. *Q.E.D.*

V. DISCUSSION ON EXPERIMENTS

Although Theorems 1 and 2 are under ideal conditions and limits, they do have close connections to realistic systems of transition-metal oxides. For the multiorbital Hubbard Hamiltonian of Eqs. (2) and (3), they are actually a good approximation of the t_{2g}-orbital systems of transition-metal oxides in 3D. For example, the itinerant FM $SrRuO_3$ belongs to this class of materials [37–39], which is a t_{2g}-active material of $4d$ electrons in a cubic lattice. Even though typical interaction strength in the $4d$ electron systems are intermediately strong, it already exhibits the FM phase with $T_c = 165$ K. Furthermore, the magnetic moment of this system is observed as $1.6\mu_B$ per site with the electron filling in $SrRuO_3$ as four electrons per site. Therefore, the FM ground state stated in Theorem 1 would possibly persist to the intermediate interaction regime and with finite electron or hole density away from half filling. Nevertheless, the magnetization would be no longer fully polarized but partially polarized to save the kinetic energy cost.

Another important system is the $LaAlO_3/SrTiO_3$ interface between two component insulators. This interface is experimentally found metallic and ferromagnetic with large magnetization [40,41]. This is a t_{2g}-orbital active material with $3d$ electrons in 2D layered systems, whose d_{zx} and d_{yz} are quasi-1D orbital bands while its d_{xy} orbital forms the quasi-2D band. For $3d$ electrons, the interaction strength is stronger than that of $4d$ materials. The RKKY, itinerant, and double-exchange mechanisms were proposed to explain the FM in this system [42–44]. Here, we have shown that the ground-state itinerant FM is fully spin polarized and robust for general densities in the d_{zx} and d_{yz} bands under strong intraorbital interactions.

VI. CONCLUSIONS

In summary, we have investigated the Nagaoka-type itinerant FM in t_{2g}-orbital systems in a 3D cubic lattice. The hole motion in each orbital band is constrained in the plane parallel to the orbital orientation. Effectively, this system behaves as crossing planes of 2D Nagaoka FM coupled by on-site interorbital Hund's coupling. Consequently, 3D itinerant FM ground states are developed, which are proved fully polarized and unique apart from the trivial spin multiplet degeneracy. Also, we have considered the 2D layer of t_{2g}-orbital systems: the quasi-1D bands are itinerant with arbitrary generic fillings and the quasi-2D band can have a single hole or be half filled. Its ground state is shown remaining the fully spin-polarized itinerant FM. The theorems established in this article can be helpful for further understanding the mechanism of FM in $SrRuO_3$ and the transition-metal oxides interface.

ACKNOWLEDGMENTS

Y.L. is grateful to Elliott H. Lieb and Congjun Wu for their helpful discussion and encouragement. Y.L. thanks the Princeton Center for Theoretical Science at Princeton University for support.

APPENDIX A: EXPRESSIONS AND PHYSICAL MEANING OF U, V, J, AND Δ

The expressions of U, V, J, and Δ in Eq. (3) are standard two-body Coulomb integrals under the t_{2g}-orbital basis. We assume the bare Coulomb interaction as $V(\mathbf{r}_1 - \mathbf{r}_2)$, and express the Wannier t_{2g}-orbital wave functions $\phi_a(\mathbf{r})$ with $a = xy, yz$, and zx, respectively. Then U, V, J, and Δ can be represented [45,46] as

$$\begin{aligned} U &= \int d\mathbf{r}_1 d\mathbf{r}_2 \phi_a^*(\mathbf{r}_1)\phi_a^*(\mathbf{r}_2)V(\mathbf{r}_1-\mathbf{r}_2)\phi_a(\mathbf{r}_2)\phi_a(\mathbf{r}_1), \\ V &= \int d\mathbf{r}_1 d\mathbf{r}_2 \phi_a^*(\mathbf{r}_1)\phi_b^*(\mathbf{r}_2)V(\mathbf{r}_1-\mathbf{r}_2) \\ &\quad \times \{\phi_b(\mathbf{r}_2)\phi_a(\mathbf{r}_1) - \phi_a(\mathbf{r}_2)\phi_b(\mathbf{r}_1)\}, \\ J &= 2\int d\mathbf{r}_1 d\mathbf{r}_2 \phi_a^*(\mathbf{r}_1)\phi_b^*(\mathbf{r}_2)V(\mathbf{r}_1-\mathbf{r}_2)\phi_a(\mathbf{r}_2)\phi_b(\mathbf{r}_1), \\ \Delta &= \int d\mathbf{r}_1 d\mathbf{r}_2 \phi_a^*(\mathbf{r}_1)\phi_a^*(\mathbf{r}_2)V(\mathbf{r}_1-\mathbf{r}_2)\phi_b(\mathbf{r}_2)\phi_b(\mathbf{r}_1), \end{aligned} \tag{A1}$$

where $a \neq b$ and no summation over repeated indices is assumed.

Let us explain the physical meanings of U, V, J, and Δ by considering a single-site problem filled with only two fermions. In total there are 15 states, which can be classified as 3 sets of spin triplets and 6 spin singlets. The three sets of spin triplet states can be expressed as

$$\begin{aligned} &d_{a,\uparrow}^\dagger d_{b,\uparrow}^\dagger|0\rangle, \quad d_{a,\downarrow}^\dagger d_{b,\downarrow}^\dagger|0\rangle, \\ &\times\frac{1}{\sqrt{2}}\{d_{a,\uparrow}^\dagger d_{b,\downarrow}^\dagger + d_{a,\downarrow}^\dagger d_{b,\uparrow}^\dagger\}|0\rangle \end{aligned} \tag{A2}$$

with $a \neq b$, and their energy is V. The 6 spin singlets can be further classified as the orbital angular momentum (OAM) singlet, doublet, and triplet as follows. The splitting between the OAM doublet and triplet states is because of the cubic symmetry, which is a two-particle analogy to the single-particle version of the t_{2g} and e_g level splitting.

The orbital angular momentum singlet state is expressed as

$$\frac{1}{\sqrt{3}}\{d^\dagger_{xy,\uparrow}d^\dagger_{xy,\downarrow}+d^\dagger_{yz,\uparrow}d^\dagger_{yz,\downarrow}+d^\dagger_{zx,\uparrow}d^\dagger_{zx,\downarrow}\}|0\rangle, \quad \text{(A3)}$$

whose energy is $U+2\Delta$. The orbital angular momentum doublet states have the energy $U-\Delta$, and they are expressed as

$$\frac{1}{\sqrt{6}}\{d^\dagger_{yz,\uparrow}d^\dagger_{yz,\downarrow}+d^\dagger_{zx,\uparrow}d^\dagger_{zx,\downarrow}-2d^\dagger_{xy,\uparrow}d^\dagger_{xy,\downarrow}\}|0\rangle,$$
$$\times\frac{1}{\sqrt{2}}\{d^\dagger_{yz,\uparrow}d^\dagger_{yz,\downarrow}-d^\dagger_{zx,\uparrow}d^\dagger_{zx,\downarrow}\}|0\rangle. \quad \text{(A4)}$$

The orbital angular momentum triplet states have energy $J+V$, whose wave functions are expressed as

$$\frac{1}{\sqrt{2}}\{d^\dagger_{yz,\uparrow}d^\dagger_{zx,\downarrow}-d^\dagger_{yz,\downarrow}d^\dagger_{zx,\uparrow}\}|0\rangle,$$
$$\frac{1}{\sqrt{2}}\{d^\dagger_{zx,\uparrow}d^\dagger_{xy,\downarrow}-d^\dagger_{zx,\downarrow}d^\dagger_{xy,\uparrow}\}|0\rangle, \quad \text{(A5)}$$
$$\frac{1}{\sqrt{2}}\{d^\dagger_{xy,\uparrow}d^\dagger_{yz,\downarrow}-d^\dagger_{xy,\downarrow}d^\dagger_{yz,\uparrow}\}|0\rangle.$$

Clearly, the energy difference between the interorbital singlet and triplet states is J as comes from Hund's coupling.

APPENDIX B: SPIN FLIPPING IN A SINGLE-ORBITAL 2D HUBBARD MODEL IN THE SQUARE LATTICE

To keep this paper self-contained, we review an important step showing the transitivity in the single-orbital Nagaoka system [31]. We only consider the case of the 2D Hubbard model in the square lattice with $U=+\infty$ with a single hole [3]. The Hamiltonian can be written as

$$H=t\sum_{\langle ij\rangle}P\{c^\dagger_i c_j+\text{H.c.}\}P, \quad \text{(B1)}$$

where P is the projection operator projecting out the doubly occupied state.

Consider a bond $\langle ij\rangle$ with its two sites i and j occupied by spins σ and σ' in orbitals d_a and d_b, respectively. This configuration is denoted as $[d_{a,\sigma}(i),d_{b,\sigma'}(j)]$. As shown below, the spins in this configuration can be exchanged to be $[d_{a,\sigma'}(i),d_{b,\sigma}(j)]$ by applying a series of hoppings in Eq. (B1) without affecting hole and spin configurations of other sites.

Obviously, we only need to consider the case of $s_z\neq s'_z$. Spin flipping can be realized by the following motion of the single hole. We can choose a plaquette unit containing the bond $\langle ij\rangle$. If here is a hole in this plaquette, without loss of generality, we can assume that here are two spin-$\uparrow$'s and one spin-$\downarrow$ in the rest 3 sites of this plaquette. They can form in total 12 possible combinatorial configurations. As shown in Fig. 3, they can be connected to each other by simply applying hole hoppings clockwise in the plaquette for at most three rounds. Therefore, it is possible to exchange the spins on the bond $\langle ij\rangle$ without affecting other sites.

If this plaquette does not contain a hole, we can first apply the hopping process to move the hole to this plaquette. During this process, we require that the hole should not pass sites i and j, which is possible because even when we remove all the bonds connecting i and j, the remaining part of the lattice is still connected. Following the conclusion above, we can flip the spin configuration on the bond $\langle ij\rangle$ without affecting other sites. Afterwards, we can restore the rest of the spin configuration by reversing the hole's motion along the same path on which it was brought to the plaquette before. Finally, the spin configuration on $\langle ij\rangle$ becomes flipped, i.e., $[d_{a,\sigma}(i),d_{b,\sigma'}(j)]\rightarrow[d_{a,\sigma'}(i),d_{b,\sigma}(j)]$. Meanwhile, the hole returns to its original location and spin configurations on other sites are restored.

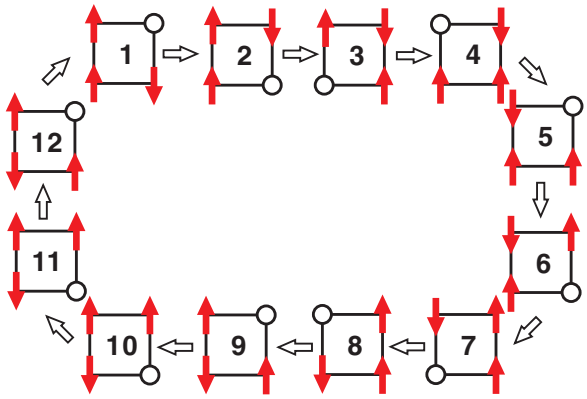

FIG. 3. (Color online) The 12 configurations with three electrons (2 spin-$\uparrow$ and 1 spin-$\downarrow$) and a single hole in a square plaquette. The hole's motion builds up transitivity among all these states. From Ref. [3].

APPENDIX C: EXCHANGING SPINS IN CLASSES (c) AND (d)

In this section, we complete the proof of Lemma 3 for the orbital configurations of classes (c) and (d) below.

Proof. Class (c): We consider the case of $a=zx$ and $b=xy$, i.e., the configuration $[d_{zx,\uparrow}(i);d_{xy,\downarrow}(j)]$. The reasoning below also applies to the other 3 situations of $a=yz, b=xy$; $a=xy, b=zx$; and $a=xy, b=yz$. Here, the spin exchange between $d_{zx,\uparrow}(i)$ and $d_{xy,\downarrow}(j)$ can be aided by the $d_{zx}(j)$ orbital. Following the reasoning in the main text, $d_{zx}(j)$ can always be assumed occupied. If it has spin-$\uparrow$, on site j, we have $d_{zx,\uparrow}(j)$ and $d_{xy,\downarrow}(j)$, whose spins can be exchanged by Hund's interaction to be $d_{zx,\downarrow}(j)$ and $d_{xy,\uparrow}(j)$. Then bond $\langle ij\rangle$ has a new spin configuration $[d_{zx,\uparrow}(i);d_{zx,\downarrow}(j)]$, which can be flipped as shown in class (a). As a result, the initial configuration of $[d_{zx,\uparrow}(i);d_{xy,\downarrow}(j)]$ is flipped to $[d_{zx,\downarrow}(i);d_{xy,\uparrow}(j)]$ without affecting $d_{zx,\uparrow}(j)$. Similarly, if the $d_{zx}(j)$ orbital is occupied by spin-$\downarrow$, we can first apply the process in class (a) to flip the spin configuration of d_{zx} orbitals on sites i and j, and then apply Hund's interaction to flip spins on the $d_{zx}(j)$ and $d_{xy}(j)$ orbitals.

Class (d): We consider the case in which both orbitals on $\langle ij\rangle$ are transverse, i.e., the configuration $[d_{xy,\uparrow}(i);d_{xy,\downarrow}(j)]$. This time we check the $d_{zx}(i)$ orbital, and first assume it is occupied. If its configuration is $d_{zx,\uparrow}(i)$, then along the bond $\langle ij\rangle$ we have $[d_{zx,\uparrow}(i);d_{xy,\downarrow}(j)]$, which can be flipped to $[d_{zx,\downarrow}(i);d_{xy,\uparrow}(j)]$ following the steps in class (c). Then on site i, the spin configuration is changed to $[d_{zx,\downarrow}(i);d_{xy,\uparrow}(i)]$, which can be flipped to $[d_{zx,\uparrow}(i);d_{xy,\downarrow}(i)]$ by Hund's interaction. As a

result, the initial configuration of $[d_{xy,\uparrow}(i);d_{xy,\downarrow}(j)]$ is flipped to $[d_{xy,\downarrow}(i);d_{xy,\uparrow}(j)]$ and $d_{zx,\uparrow}(i)$ is maintained. If $d_{zx}(i)$ is occupied by spin-$\downarrow$, we can first apply Hund's interaction on site i and then apply the steps presented in class (c). Finally, if the $d_{zx}(i)$ orbital is empty, we can move this hole to a neighboring site, and perform the above process, and then move the hole back.

APPENDIX D: THE PROOFS OF COROLLARIES 1 AND 2

In this part, we prove the two corollaries in Sec. III.

Proof of Corollary 1. We perform a particle-hole transformation, i.e., $d_{a,\sigma} \to d^{\dagger}_{a,\sigma}$. Under this transformation, the hopping Hamiltonian Eq. (2) remains the same except for the reversed sign of $t_{\|}$. Nevertheless, for the bipartite lattice, the sign of $t_{\|}$ can be reversed by a gauge transformation, which will not change the physics. The physical quantities transform as follows:

$$n_{a,\sigma} \to 1 - n_{a,\sigma}, \quad \vec{S}_a \to -\vec{S}_a. \tag{D1}$$

It is easy to check that for the interaction part $H_{\rm int}$, U, V, J, and Δ remain the same apart from a constant and a term proportional to electron density. In the case of fixing particle numbers, the difference is just a constant which does not affect real physics. Under this transformation, the doubly occupied orbitals are mapped to holes. According to Theorem 1, the ground states are FM states with the total spin $S = N_{\rm tot}/2 - L_x - L_y - L_z$ and are unique up to spin degeneracy.

Proof of Corollary 2. We order the d_{xy} electrons layer by layer and define

$$|\{r_{xy}\},\{\sigma\}_{xy}\rangle = \prod_{l_z=1}^{L_z} d^{\dagger}_{xy,\sigma}\left(\mathbf{r}^{xy}_{l_z},l_z\right)|0\rangle, \tag{D2}$$

where $\mathbf{r}_{xy}$ is the in-plane location of the electron in the l_zth layer. Similar bases can also be defined for d_{yz} and d_{zx} electrons as $|\{r_{yz}\},\{\sigma\}_{yz}\rangle$ and $|\{r_{zx}\},\{\sigma\}_{zx}\rangle$, respectively. The many-body bases for the entire system can be defined as

$$|\{r\},\{\sigma\}\rangle = |\{e_{xy}\},\{\sigma\}_{xy}\rangle \otimes |\{e_{yz}\},\{\sigma\}_{yz}\rangle \otimes |\{e_{zx}\},\{\sigma\}_{zx}\rangle, \tag{D3}$$

where $\{r\}$ and $\{\sigma\}$ represent the distributions of electron coordinates and spins in each orbital band in each layer.

We also need to perform a gauge transformation to flip the sign of $t_{\|}$ to be negative. Then in this case, the off-diagonal matrix elements of hopping are negative because hopping does not change the ordering of electrons in the definition of Eq. (D3). Because each orbital band of each layer only contains one electron, only J and V terms contribute. Again the off-diagonal matrix elements arise from J, which are also negative.

Next, we show the transitivity. Since we can also move the positions of electrons freely, we only need to consider two bases with the same electron locations but different spin configurations, denoted as $|\{r\},\{\sigma\}\rangle$ and $|\{r\},\{\sigma'\}\rangle$. Then, it suffices to show that for any two electrons in $|\{r\},\{\sigma\}\rangle$, we can flip their spin configuration. If these two electrons live in different orbitals, say, d_{xy} and d_{yz}, then the planes of their motions cross and share a common line parallel to the y axis. We can move these two electrons to any site of this line, and then apply Hund's interaction to flip their spins, and then move back to their original locations. If these two electrons live in the same orbital with opposite spins, say, two d_{xy} electrons but in two parallel layers, then we can find another electron in d_{zx} orbitals. We first choose the d_{xy} electron with the spin opposite to that of d_{zx}, and switch their spins. Then combine the new configuration of the d_{zx} and the other d_{xy} electron, and switch their spins. The net effect is that two d_{xy}-electron spins are flipped, and the d_{zx}-electron spin is restored.

Having proved nonpositivity and transitivity, we can follow the same steps in Theorem 1 to prove this corollary, which will not be repeated here.

[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, *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, Syn. 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. B **41**, 2375 (1990).
[12] A. Mielke, J. Phys. A: Math. Gen. **24**, L73 (1991).
[13] A. Mielke, J. Phys. A: Math. Gen. **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] R. A. Duine and A. H. MacDonald, Phys. Rev. Lett. **95**, 230403 (2005).
[20] 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).
[21] S. Zhang, H.-h. Hung, and C. Wu, Phys. Rev. A **82**, 053618 (2010).
[22] I. Berdnikov, P. Coleman, and S. H. Simon, Phys. Rev. B **79**, 224403 (2009).
[23] D. Pekker and E. Demler, arXiv:1107.3930.
[24] C.-C. Chang, S. Zhang, and D. M. Ceperley, Phys. Rev. A **82**, 061603 (2010).
[25] X. Cui and T.-L. Ho, Phys. Rev. A **89**, 023611 (2014).
[26] S. Pilati, I. Zintchenko, and M. Troyer, Phys. Rev. Lett. **112**, 015301 (2014).
[27] H. Tasaki, Phys. Rev. B **40**, 9192 (1989).
[28] G.-S. Tian, Phys. Rev. B **44**, 4444 (1991).

[29] A. Mielke, J. Phys. A: Math. Gen. **25**, 4335 (1992).
[30] A. Mielke, Phys. Lett. A **174**, 443 (1993).
[31] H. Tasaki, Commun. Math. Phys. **242**, 445 (2003).
[32] A. Tanaka and H. Tasaki, Phys. Rev. Lett. **98**, 116402 (2007).
[33] Y. Li, E. H. Lieb, and C. Wu, Phys. Rev. Lett. **112**, 217201 (2014).
[34] S. Xu, Y. Li, and C. Wu, arXiv:1411.0340.
[35] M. Cyrot and C. Lyon-Caen, J. Phys. (France) **36**, 253 (1975).
[36] A. M. Oleś, Phys. Rev. B **28**, 327 (1983).
[37] G. Koster, L. Klein, W. Siemons, G. Rijnders, J. Dodge, C.-B. Eom, D. Blank, and M. Beasley, Rev. Mod. Phys. **84**, 253 (2012).
[38] G. Cao, S. McCall, M. Shepard, J. E. Crow, and R. P. Guertin, Phys. Rev. B **56**, 321 (1997).
[39] D. W. Jeong, H. C. Choi, C. H. Kim, S. H. Chang, C. H. Sohn, H. J. Park, T. D. Kang, D.-Y. Cho, S. H. Baek, C. B. Eom, J. H. Shim, J. Yu, K. W. Kim, S. J. Moon, and T. W. Noh, Phys. Rev. Lett. **110**, 247202 (2013).
[40] L. Li, C. Richter, J. Mannhart, and R. Ashoori, Nat. Phys. **7**, 762 (2011).
[41] J. A. Bert, B. Kalisky, C. Bell, M. Kim, Y. Hikita, H. Y. Hwang, and K. A. Moler, Nat. Phys. **7**, 767 (2011).
[42] K. Michaeli, A. C. Potter, and P. A. Lee, Phys. Rev. Lett. **108**, 117003 (2012).
[43] G. Chen and L. Balents, Phys. Rev. Lett. **110**, 206401 (2013).
[44] S. Banerjee, O. Erten, and M. Randeria, Nat. Phys. **9**, 626 (2013).
[45] J. Hubbard, Proc. R. Soc. London, Ser. A **276**, 238 (1963).
[46] J. C. Slater, H. Statz, and G. F. Koster, Phys. Rev. **91**, 1323 (1953).