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

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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 $d_{xy}$ and $d_{yz}$ bands become quasi-one-dimensional while the $d_{zx}$ 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.

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I. INTRODUCTION

Itinerant ferromagnetism (FM) is not only a representative strong-correlation problem, but also a highly non-perturbative one$^{1-18}$. It is widely known as a long-standing problem of condensed matter physics, and also a current research focus in ultra-cold 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$^{1,27,28}$. 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 intra orbital 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 non-degenerate apart from the trivial spin degeneracy. Furthermore, when this system is reduced to a single 2D layer system of $t_{2g}$ orbitals, the $d_{xx}$ 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 $d_x$ and $d_y$ 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 layer 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 wavefunction 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 $\hat{d}$ orbital Wannier functions are nearly localized and the $z$ axis is perpendicular to the orbital plane, $t_{\perp}$ is negligible in realistic transition metal oxides. Similarly, electrons in the $d_{yz}$ and $d_{zx}$ orbitals hop only 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

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

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

$$H^K_{xy} = \sum_{\mathbf{r}} t_{\parallel}(d_{xy,\sigma}^{\dagger}(\mathbf{r})d_{xy,\sigma}(\mathbf{r} + a_0\hat{x})$$

$+ d_{xy,\sigma}^{\dagger}(\mathbf{r})d_{xy,\sigma}(\mathbf{r} + a_0\hat{y}) + \text{h.c.}),$$

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, $H^K_{yz(xz)}$ can also be defined by permuting the indices of orbitals and hopping directions in $H^K_{xy}$, whose expressions are not repeated here.

The interaction term is the standard multiorbital Hubbard interaction $^{4,5,35,36}$ defined on-site as

$$H^I = \sum_{\mathbf{r},a} n_{a,\uparrow}(\mathbf{r})n_{a,\downarrow}(\mathbf{r})$$

$- J \sum_{\mathbf{r},a \neq b} \left( \hat{S}_{a}(\mathbf{r}) \cdot \hat{S}_{b}(\mathbf{r}) - \frac{1}{4} n_{a}(\mathbf{r})n_{b}(\mathbf{r}) \right)$

$+ V \sum_{\mathbf{r},a \neq b} n_{a}(\mathbf{r})n_{b}(\mathbf{r})$

$+ \Delta \sum_{\mathbf{r},a \neq b} (d_{a,\uparrow}^{\dagger}(\mathbf{r})d_{a,\downarrow}^{\dagger}(\mathbf{r})d_{b,\downarrow}(\mathbf{r})d_{b,\uparrow}(\mathbf{r}) + \text{h.c.}),$ (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 $\sigma$; $n_{a} = n_{a,\uparrow} + n_{a,\downarrow}$; $\hat{S}_{a}(\mathbf{r})$ is the spin operator of the $a$-th 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 intra orbital Hubbard interaction; the $V$ term is the inter orbital Hubbard interaction; the $J$ term is Hund’s coupling with $J > 0$; and the $\Delta$ term describes the singlet pairing hopping process among different orbitals. The expressions of $U$, $V$, $J$, and $\Delta$ are presented in Appendix A following the standard physical meaning of two-body Coulomb interactions.

![FIG. 1. The Wannier orbital wavefunctions of $t_{2g}$ orbitals: $d_{xy}$, $d_{yz}$, and $d_{zx}$. For electrons in the $d_x$ 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.](image-url)
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) $U \to +\infty$, $\Delta$ is finite;

(II) For each orbital band, there is one and only one hole in every layer parallel to the orbital plane. E.g., 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

$$
\mathcal{H} = \bigotimes_{i_z=1}^{L_z} \mathcal{H}_{i_z}^{xy} \bigotimes_{i_z=1}^{L_z} \mathcal{H}_{i_z}^{yz} \bigotimes_{i_z=1}^{L_z} \mathcal{H}_{i_z}^{zx},
$$

where $i_z, x, y, z$ are the indices of the $xy, yz, z$-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 $\mathcal{H}_{i_z}^q$, 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 $i_z$-th layer, we can label all the $d_{xy}$ orbitals of this layer in an arbitrary order by the index $i_{xz} = 1, \cdots, L_x L_y$. Then, the states in this layer can be represented as

$$
|h_{i_{xz}}^{xy}; \{\sigma\}_{i_z}\rangle = (-)^{n_{i_{xz}}} \prod_{i_{xz}}' d_{i_{xz}y, \sigma}(i_{xz}) \{\sigma\}_{i_z}\rangle,
$$

where $h_{i_{xz}}^{xy}$ labels the location of the hole; $\{\sigma\}_{i_z}$ represents the spin configuration; $\prod'$ means the ordered product of the creation operators except the one at the location of the hole, $\prod_{i_{xz}}' d_{i_{xz}y, \sigma}(i_{xz})\{\sigma\}_{i_z}\rangle = d_{i_{xz}y, \sigma_1}(1) \cdots d_{i_{xz}y, \sigma_{n_{i_{xz}}}}(1) \cdots d_{i_{xz}y, \sigma_{n_{i_{xz}}-1}}(1) \cdots d_{i_{xz}y, \sigma_{n_{i_{xz}}+1}}(1) \cdots d_{i_{xz}y, \sigma_{n_{i_{xz}}+1}}(1)(L_x L_y)|0\rangle$ 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

$$
\{|h\}, \{\sigma\}\rangle = \bigotimes_{i_z=1}^{L_z} |h_{i_z}^{xy}; \{\sigma\}_{i_z}\rangle \bigotimes_{i_z=1}^{L_z} |h_{i_z}^{yz}; \{\sigma\}_{i_z}\rangle \bigotimes_{i_z=1}^{L_z} |h_{i_z}^{zx}; \{\sigma\}_{i_z}\rangle,
$$

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 (Non-positivity)** 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 $H = H_{\text{kin}} + H_{\text{int}}$ (see Eqs. (2) and (3)) are non-positive.

**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

$$
\langle\{h\}, \{\sigma\}|H_{xy}|\{h'\}, \{\sigma'\}\rangle = -t \text{ or } 0.
$$

This step is the same as that in the proof of the usual Nagaoka theorem for a 2D single orbital Hubbard model. Although here we have $(L_x + L_y + L_z)$ holes in our system, the fermion ordering does not change under hopping because of Lemma 1. For the $xy$ component of Hund’s interaction $H_{xy} = -J/2 \sum_{a \neq b}(S^a_x S^b_y + S^a_y S^b_x)$ with $S^a_x = S^x \pm i S^y$, it does not change the fermion ordering either, and thus, its matrix elements read

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

which are also non-positive. 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 $(ij)$ and consider the $d_a$ orbital of site $i$ and the $d_b$ orbital of site $j$. If they are occupied by spin $\sigma$ and $\sigma'$, respectively, let us denote this bond configuration as $|d_{a, \sigma}(i); d_{b, \sigma'}(j)\rangle$. We have the following lemma:

**Lemma 3** The spin configuration in $|d_{a, \sigma}(i); d_{b, \sigma'}(j)\rangle$ can be flipped to $|d_{a, \sigma'}(i); d_{b, \sigma}(j)\rangle$ 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 $(ij)$ is along the $z$ axis, and only discuss how to flip $|d_{a, \uparrow}(i); d_{b, \downarrow}(j)\rangle$ to $|d_{a, \downarrow}(i); d_{b, \uparrow}(j)\rangle$. Since $a$ and $b$ can take any of the $xy$, $yz$, and $zx$ sites, there are 9 possible orbital configurations for a bond. Nevertheless, they can be classified into 4 non-equivalent classes because of the lattice geometry as shown in Figs. 2 (a) to (d).
FIG. 2. Representatives 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): \( [d_{xy,\uparrow}(i); d_{xy,\downarrow}(j)] \), case (d): \( [d_{xy,\uparrow}(i); d_{yz,\downarrow}(j)] \). Any two cases of (a)-(d) are nonequivalent under the lattice symmetry transformation.

For later convenience, the single hole assisted spin-flipping in the 2D single orbital infinite \( U \) Hubbard model is reviewed in Appendix B, which played 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-\( \uparrow \), 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 \( d_{yz,\downarrow}(t) \), 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-\( \uparrow \) finally. If the \( d_{yz}(i) \) orbital is occupied by spin-\( \downarrow \), 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 \( a = d_{zx}, b = d_{xy}; a = d_{x}, b = d_{y}, a = d_{y}, b = d_{x} \). The proof for these two classes are similar to that of class (b) by combining Hund’s interaction and 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, \( \{|\{h\},\{\sigma\}\} \) and \( \{|\{g\},\{\alpha\}\} \), there always exists a series of basis vectors \( \{|\{h_1\},\{\sigma_1\}\}, \{|\{h_2\},\{\sigma_2\}\}, \ldots, \{|\{h_k\},\{\sigma_k\}\} \) connected with nonzero matrix elements of \( H \), such that

\[
\langle\{g\},\{\alpha\}|H|\{h_1\},\{\sigma_1\}\rangle \langle\{h_1\},\{\sigma_1\}|H|\{h_2\},\{\sigma_2\}\rangle \cdots \langle\{h_2\},\{\sigma_2\}|H|\{h_k\},\{\sigma_k\}\rangle \neq 0.
\]

**Proof:** Firstly, we can always apply the hopping term to \( \{|\{h\},\{\sigma\}\} \) to rearrange the locations of holes of each orbital band in each layer. Then we reach an intermediate state \( \{|\{g'\},\{\alpha'\}\} \) in which the locations of holes are the same as that in \( \{|\{g\},\{\alpha\}\} \). Since the two states \( \{|\{g\},\{\alpha\}\} \) and \( \{|\{g'\},\{\alpha'\}\} \) 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 \( \{|\{g'\},\{\alpha'\}\} \) two opposite spins in any two orbitals can be exchanged by consecutively applying Hund’s and hole’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 site, 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 \( H_{kin} + H_{int} \) 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 fully spin-polarized and are unique apart from the trivial spin degeneracy.
They can be expressed as
\[ |\Psi^S_G\rangle = \sum_{\{h\},\{\sigma\}} c_{\{h\},\{\sigma\}} |\{h\},\{\sigma\}\rangle \] (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 non-positivity 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 non-degenerate 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 non-degenerate within each \( \mathcal{H}^{S_z} \).

To show that \( |\Psi^S_G\rangle \) 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,
\[ |\Psi^S_{ref}\rangle = \sum' |\{h\},\{\sigma\}\rangle. \] (11)

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

**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 \( d_{xz} \) 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:

1. **Open boundary condition or periodic (anti-periodic)** boundary condition with odd (even) number of particles in each row or column;
2. **Arbitrary filling** with at least one hole and one particle in each row and each column.

To describe the part of \( d_{xz} \) and \( d_{yz} \) bands with general fillings, let us first recapitulate the many-body bases constructed for the quasi-1D system in Ref. [33] and rewrite them in terms of \( d_{xz} \) and \( d_{yz} \) bands. By Lemma 1, for any generic filling, we can always specify a partition of particle numbers into rows \( \mathcal{X} = \{ r_1, \cdots, L_y \} \) and columns \( \mathcal{Y} = \{ c_1, \cdots, L_x \} \), where \( N_{r_1} \) and \( N_{c_1} \) are the particle numbers of \( d_{xz} \) and \( d_{yz} \) orbitals conserved in the \( r_1 \)-th row and the \( c_1 \)-th column, respectively. We can order electrons in each row from the left most particle to the right most one, followed by the ordering in each column from the top to bottom. The corresponding many-body basis can be set up as
\[
|\mathcal{R},\mathcal{S}\rangle_{N_x, N_y} = \prod_{j=1}^{L_y} d_{y_{zx}, r_j}^\dagger \prod_{r_j} d_{x_{zx}, r_j} \prod_{j=1}^{L_x} d_{y_{yz}, c_j}^\dagger \prod_{c_j} d_{y_{yz}, c_j} \{|0\rangle \}
\] (12)

where \( j \) denotes the index of columns and rows; \( \mathcal{R} = \{ r_j \}^j \) all \( i \)'s and \( j \)'s represents the coordinates of occupied sites; \( \mathcal{S} = \{ c_j \}^j \) all \( i \)'s and \( j \)'s represents their the spin configurations. The operator \( d_{x_{zx}, r_j} \) (\( d_{y_{yz}, c_j} \)) creates a whole line of \( N_{r_j} (N_{c_j}) \) \( d_{xz} \) (\( d_{yz} \)) electrons in the row \( r_j \) (column \( c_j \)) ordered from left to right (from top to bottom), and \( d_{y_{zx}, r_j} \) 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,
\[
|\mathcal{R},\mathcal{S}\rangle_{N_x, N_y} \otimes |h_{xy},\{\sigma\}\rangle.
\] (13)

Again, because of the conservation of the \( z \) component of the total spin, this Hilbert space can be decomposed as \( \mathcal{H}_{2D} = \bigoplus \mathcal{H}^{S_z}_{2D} \). 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 non-positive.

Below, we further show the transitivity of the Hamiltonian matrix in the sub-Hilbert space \( \mathcal{H}^{S_z}_{2D} \) under condition (IV) for \( d_{xz} \) 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, 

\[ |u\rangle = |R,S\rangle_{N_x,N_y} \otimes |h_{xy}, \{ \sigma \} \rangle \quad \text{and} \quad |v\rangle = |R,S'\rangle_{N_x,N_y} \otimes |h_{xy}, \{ \sigma' \} \rangle. \]

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 \(d_{x^2} \) 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 \(d_{xz}\) orbital band with spin-\(\uparrow\); and another electron in the \(d_{xy}\) band with spin-\(\downarrow\). We denote their locations as \(r_{zx}\) and \(r_{xy}\), respectively. Let us identify the site \(r_c\) 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 \(r_c\). If not, because of condition (IV), we can always move a \(d_{yz}\) electron of that column to \(r_c\) 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 \(r_c\) has spin-\(\uparrow\), it can first be moved to \(r_{xy}\) by hoppings. Then, it can exchange the spins with the \(d_{xy}\) electron at \(r_{xy}\) by Hund’s interaction. After reversing the hopping, this \(d_{yz}\) electron can be moved back to \(r_c\) but with spin-\(\downarrow\). Further, it can be moved to \(r_{zx}\) to exchange the spins with the \(d_{zx}\) electron and be moved back to \(r_c\) again with its original spin-\(\uparrow\) recovered. The net effect is the exchange of spin configurations between the \(d_{xy}\) and \(d_{xz}\) electrons without affecting other configurations. The case of the \(d_{yz}\) electron at \(r_c\) with spin-\(\downarrow\) can be similarly proved.

So far, we have shown both the non-positivity of off-diagonal matrix elements and the transitivity of the Hamiltonian matrix in the sub-Hilbert space \(H_{2D}^{S_2D'}\). 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

\[ |\{ \sigma \} \rangle = \prod_i d_{xy,\sigma}^\dagger (i) |0\rangle, \quad (14) \]

where \(\{ \sigma \} \) is an arbitrary spin distribution. Then for the combined system, the basis is defined as

\[ |R,S\rangle_{N_x,N_y} \otimes |\{ \sigma \} \rangle. \quad (15) \]

Again because of spin conservation, the Hilbert space in this case \(H_{2D}^D\) can be further decomposed into the direct sum of different sectors of \(S_z\) as \(H_{2D}^D = \boxplus H_{2D}^{S_z'}\).

Similarly to Theorem 2, the off-diagonal elements of the Hamiltonian matrix is non-positive. We next show the transitivity of the Hamiltonian matrix in each physical sub-Hilbert space \(H_{2D}^{S_z'}\). Again, we only need to show that for any state in \(H_{2D}^{S_z'}\), 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-\(\uparrow\) and -\(\downarrow\), respectively. Their locations are denoted as \(r\) and \(r'\), respectively. Then we can choose an electron in the \(d_{zx}\) band, and, without loss of generality, assume its spin-\(\uparrow\). Then according to the proof of Theorem 2, we can first flip the pair of electrons \(d_{zx,\uparrow}\) and \(d_{xy,\downarrow}(r')\), then their spins become \(d_{zx,\downarrow}\) and \(d_{xy,\uparrow}(r')\). Next, we consider the pair of \(d_{zx,\downarrow}\) and \(d_{xy,\uparrow}(r)\) and exchange their spins. The net result is the exchange of the spins of two \(d_{xy}\) electrons. With both results of non-positivity 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 intermediate strong, it already exhibits the FM phase with \(T_c = 165K\). 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 \(d_{xz}\) and \(d_{yz}\) are quasi-1D orbital bands while its \(d_{xy}\) orbital
forms the quasi-2D band. For 3\textit{d} electrons, the interaction strength is stronger than that of 4\textit{d} materials. The RKKY, itinerant, and double-exchange mechanisms were proposed to explain the FM in this system\textsuperscript{12–44}. Here, we have shown that the ground state itinerant FM is fully spin polarized and robust for general densities in the \textit{d}\textsubscript{zx} and \textit{d}\textsubscript{yz} bands under strong intra orbital interactions.

\section{Conclusions}

In summary, we have investigated the Nagaoka type itinerant FM in \textit{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 inter orbital 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 the trivial spin multiplet degeneracy. Also, we have considered the 2D layer of \textit{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\textsubscript{3} and the transition-metal oxides interface.

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\section*{Appendix A: Expressions and physical meaning of \textit{U}, \textit{V}, \textit{J} and \textit{\Delta}}

The expressions of \textit{U}, \textit{V}, \textit{J} and \textit{\Delta} in Eq. (3) are standard two-body Coulomb integrals under the \textit{t}_{2g} orbital basis. We assume the bare Coulomb interaction as \textit{V}(\textit{r}_1 - \textit{r}_2), and express the Wannier \textit{t}_{2g} orbital wavefunctions \textit{\phi}_a(\textit{r}) with \textit{a} = \textit{xy}, \textit{yz} and \textit{zx}, respectively. Then \textit{U}, \textit{V}, \textit{J} and \textit{\Delta} can be represented\textsuperscript{45,46} as

\begin{equation}
\begin{aligned}
\textit{U} &= \int \text{d}\textit{r}_1 \text{d}\textit{r}_2 \phi^*_a(\textit{r}_1) \phi_a(\textit{r}_2) \textit{V}(\textit{r}_1 - \textit{r}_2) \phi_a(\textit{r}_2) \phi_a(\textit{r}_1), \\
\textit{V} &= \int \text{d}\textit{r}_1 \text{d}\textit{r}_2 \phi^*_a(\textit{r}_1) \phi_b(\textit{r}_2) \textit{V}(\textit{r}_1 - \textit{r}_2) \\
&\quad \times \left\{ \phi_a(\textit{r}_2) \phi_a(\textit{r}_1) - \phi_a(\textit{r}_2) \phi_b(\textit{r}_1) \right\}, \\
\textit{J} &= 2 \int \text{d}\textit{r}_1 \text{d}\textit{r}_2 \phi^*_a(\textit{r}_1) \phi_b(\textit{r}_2) \textit{V}(\textit{r}_1 - \textit{r}_2) \phi_b(\textit{r}_2) \phi_b(\textit{r}_1), \\
\textit{\Delta} &= \int \text{d}\textit{r}_1 \text{d}\textit{r}_2 \phi^*_a(\textit{r}_1) \phi_b(\textit{r}_2) \textit{V}(\textit{r}_1 - \textit{r}_2) \phi_b(\textit{r}_2) \phi_b(\textit{r}_1).
\end{aligned}
\end{equation}

(A1)

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

Let us explain the physical meanings of \textit{U}, \textit{V}, \textit{J} and \textit{\Delta} 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{equation}
\begin{aligned}
d_{a,\uparrow}^\dagger d_{b,\uparrow}^\dagger |0\rangle, & \quad d_{a,\downarrow}^\dagger d_{b,\downarrow}^\dagger |0\rangle \\
\frac{1}{\sqrt{2}} \left\{ d_{a,\downarrow}^\dagger d_{b,\uparrow}^\dagger + d_{a,\uparrow}^\dagger d_{b,\downarrow}^\dagger \right\} |0\rangle
\end{aligned}
\end{equation}

with \(a \neq b\), and their energy is \textit{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 \textit{t}_{2g} and \textit{e}_g level splitting. The orbital angular momentum singlet state is expressed as

\begin{equation}
\frac{1}{\sqrt{3}} \left\{ d_{xy,\uparrow}^\dagger d_{xy,\downarrow}^\dagger + d_{yz,\uparrow}^\dagger d_{yz,\downarrow}^\dagger + d_{zx,\uparrow}^\dagger d_{zx,\downarrow}^\dagger \right\} |0\rangle,
\end{equation}

(A3)

whose energy is \(\textit{U} + 3\textit{\Delta}\). The orbital angular momentum doublet states have the energy \(\textit{U} - \textit{\Delta}\), and they are expressed as

\begin{equation}
\begin{aligned}
\frac{1}{\sqrt{6}} \left\{ d_{yz,\uparrow}^\dagger d_{yz,\downarrow}^\dagger + d_{zx,\uparrow}^\dagger d_{zx,\downarrow}^\dagger - 2d_{xy,\uparrow}^\dagger d_{xy,\downarrow}^\dagger \right\} |0\rangle, \\
\frac{1}{\sqrt{2}} \left\{ d_{yz,\uparrow}^\dagger d_{yz,\downarrow}^\dagger - d_{zx,\uparrow}^\dagger d_{zx,\downarrow}^\dagger \right\} |0\rangle.
\end{aligned}
\end{equation}

(A4)

The orbital angular momentum triplet states have energy \(\textit{J} + \textit{\Delta}\), whose wavefunctions are expressed as

\begin{equation}
\begin{aligned}
\frac{1}{\sqrt{2}} \left\{ d_{yz,\uparrow}^\dagger d_{yz,\downarrow}^\dagger - d_{yz,\downarrow}^\dagger d_{yz,\uparrow}^\dagger \right\} |0\rangle, \\
\frac{1}{\sqrt{2}} \left\{ d_{zx,\uparrow}^\dagger d_{zx,\downarrow}^\dagger - d_{zx,\downarrow}^\dagger d_{zx,\uparrow}^\dagger \right\} |0\rangle, \\
\frac{1}{\sqrt{2}} \left\{ d_{xy,\uparrow}^\dagger d_{xy,\downarrow}^\dagger - d_{xy,\downarrow}^\dagger d_{xy,\uparrow}^\dagger \right\} |0\rangle.
\end{aligned}
\end{equation}

(A5)

Clearly, the energy difference between the inter orbital singlet and triplet states is \(\textit{J}\) as comes from Hund’s coupling.

\section*{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\textsuperscript{31}. We only consider the case of the 2D Hubbard model in the square lattice with \(\textit{U} = +\infty\) with a single hole [3]. The Hamiltonian can be written as

\begin{equation}
\textit{H} = t \sum_{\langle\textit{ij}\rangle} \textit{P} \left\{ \textit{c}_i^\dagger \textit{c}_j^\dagger + \text{h.c.} \right\} \textit{P},
\end{equation}

(B1)
Finally, the spin configuration on the bond $\langle ij \rangle$ 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.

Appendix C: Exchanging spins in Classes (c) an (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 $a = xz$ and $b = xy$, i.e., the configuration $[d_{xz\uparrow}(i); d_{xy\downarrow}(j)]$. The reasoning below also applies to the other 3 situations of $a = yz, b = xy, a = xy, b = zz$; and $a = xy, b = yz$. Here, the spin exchange between $d_{xz\uparrow}(i)$ and $d_{xy\downarrow}(j)$ can be aided by the $d_{xz\downarrow}(j)$ orbital. Following the reasoning in the main text, $d_{xz}(j)$ can always be assumed occupied. If it has spin-$\uparrow$, on site $j$, we have $d_{xz\uparrow}(j)$ and $d_{xy\downarrow}(j)$, whose spins can be exchanged by Hund’s interaction to be $d_{xz\downarrow}(j)$ and $d_{xy\uparrow}(j)$. Then bond $\langle ij \rangle$ has a new spin configuration $[d_{xz\uparrow}(i); d_{xz\downarrow}(j)]$, which can be flipped as shown in class (a). As a result, the initial configuration of $[d_{xz\uparrow}(i); d_{xy\downarrow}(j)]$ is flipped to $[d_{xz\downarrow}(i); d_{xy\uparrow}(j)]$ without affecting $d_{xz\uparrow}(j)$. Similarly, if the $d_{xz}(j)$ orbital is occupied by spin-$\downarrow$, we can first apply the process in class (a) to flip the spin configuration of $d_{xz}$ orbitals on sites $i$ and $j$, and then apply Hund’s interaction to flip spins on $d_{xz}(j)$ 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 $d_{xz}(i)$ orbital, and first assume it is occupied. If its configuration is $d_{xz\uparrow}(i)$, then along the bond $\langle ij \rangle$ we have $[d_{xz\uparrow}(i); d_{xy\downarrow}(j)]$, which can be flipped to $[d_{xz\downarrow}(i); d_{xy\uparrow}(j)]$ following the steps in class (c). Then on site $i$, the spin configuration is changed to $[d_{xz\downarrow}(i); d_{xy\uparrow}(i)]$, which can be flipped to $[d_{xz\uparrow}(i); d_{xy\downarrow}(i)]$ 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 $d_{xz\uparrow}(i)$ is maintained. If $d_{xz}(i)$ 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 $d_{xz}(i)$ 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 proof of Corollaries I and II

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

**(Corollary 1)** **Proof:** We perform a particle-hole transformation, i.e., $d_{a,\sigma} \rightarrow d_{b,\sigma}^{\dagger}$. Under this transformation, the hoppings Hamiltonian Eq. (2) remains the same except for the reversed sign of $t_1$. Nevertheless, for the bipartite lattice, the sign of $t_1$ can be reversed by a gauge transformation, which will not change the physics. The physical quantities transform as follows:

$$n_{a,\sigma} \rightarrow 1 - n_{a,\sigma}, \quad \vec{S}_{a} \rightarrow -\vec{S}_{a}. \quad (D1)$$

It is easy to check that for the interaction part $H_{int}, U, V, J$, and $\Delta$ 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 $S = N_{tot}/2 - L_x - L_y - L_z$ and are unique up to spin degeneracy.

(Corollary 2) Proof: We order the $d_{xy}$ electrons layer by layer and define

$$\{|r_{xy}\}, \{|\sigma\}_{xy}\} = \frac{L_x}{l_x=1} d_{xy,\sigma}(r_{xy}^l, l_z)\langle 0 \rangle,$$  \hspace{1cm} (D2)

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

$$\{|r\}, \{|\sigma\| = \{|e_{xy}\}, \{|\sigma\}_{xy}\} \otimes \|\{|e_{yz}\}, \{|\sigma\}_{yz}\| \otimes \|\{|e_{zx}\}, \{|\sigma\}_{zx}\|,$$  \hspace{1cm} (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 $t_{ij}$ 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 bands 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 basis with the same electron locations but different spin configurations, denoted as $\{|\sigma\}_{xy}, \{|\sigma\}_{yz}$ and $\{|\sigma\}_{zx}$. Then, it suffices to show that for any two electrons in $\{|r\}, \{|\sigma\}$, 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 plane 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 non-positivity and transitivity, we can follow the same steps in Theorem 1 to prove this corollary, which will not be repeated here.

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