Constraints on the possible pairing symmetry of iron arsenide superconductors in a two-orbital model

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In this work, we establish a few exact identities through commutation of intraorbital and interorbital on-site pairings with a two-orbital model describing the FeAs-based superconductors. Applying the conclusion drawn from rigorous relation and physical interpretation, we give constraints on the possible symmetries of the superconducting pairing of the model. Hence the favorable pairings in high-temperature oxypnictide superconductors are proposed.

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I. INTRODUCTION

The family of FeAs-based $ReFeAsO_{1-x}F_x$ (Re=La, Nd, Ce, Pr, etc.) high-temperature superconductors (SCs) (Refs. 1 and 2) has sparked great interest both experimentally[3–15] and theoretically.[16–36] So far the transition temperature T_c has gone up as high as above 50 K.[3–5] This family of materials provides another platform to explore high-T_c superconductivity besides cuprate superconductors. Both FeAs-based materials and cuprate superconductors are transition-metal compounds on a two-dimensional (2D) square lattice, and their parent compounds are magnetically ordered. However, there are several significant differences in their electronic properties. First, the undoped oxypnictides are bad metals,[5] while cuprates are Mott/charge-transfer insulators. Second, neutron-scattering experiments have shown that the magnetic structure in undoped oxypnictides is not a simple antiferromagnetic order as in cuprates but instead a collinear spin-density wave along the $(\pi,0)$ direction.[5,6] Third, probably the most important, the multiorbital nature of the oxypnictides has been emphasized, in contrast to the single-orbital cuprates. From the band-structure point of view, it seems likely that all 3*d* orbitals of the Fe atoms contribute to the low-energy electronic properties.[16,17]

Meanwhile, the pairing symmetry remains controversial. Based on the fermionic nature of the gap function, the possible superconducting order parameters can be classified according to group theory.[18–21] There are surveys that support either *s* or extended *s* wave,[22–26] or *p* wave,[27,28] or *d* wave,[29–34] or even mixture of s_{xy} and $d_{x^2-y^2}$.[35,36] Nevertheless, none of them has been confirmed, although *s* wave seems to have more support. Recently, superconductivity in either electron-doped or hole-doped oxypnictides with multiple-gap structure was suggested by specific-heat measurements,[7] nuclear-magnetic-resonance (NMR) experiments,[10–12] point-contact spectroscopy,[13] and angle-resolved photoelectron spectroscopy (ARPES).[14] Therefore, the investigation of possible coexistence of various superconducting orders is highly desired and is the motivation of this work.

In the following, we investigate the coexistence of different superconducting pairing symmetries in a multiorbital model. An important result which we would like to emphasize is that different hopping amplitudes in a multiorbital system can greatly enhance the coexistence of various kinds of pairing orders, such as *d*- and extended *s*-wave pairings. Theoretically, the simultaneous existence of these pairing orders has been speculated about for a single-band system such as the single-band Hubbard model. However, its stability generally requires the introduction of additional interactions, e.g., electron-phonon interactions, which give rise to different hopping amplitudes. While in the multiorbital system, the extra orbital degrees of freedom generally create the anisotropic hopping integrals of interorbital hopping and intraorbital hopping. The peculiarity in the multiorbital systems may lead to the simultaneous existence of pairing orders.

II. HAMILTONIAN

The Fe atoms in a Fe-As plane form a 2D square lattice. Due to the buckling of the As atoms, the real unit cell contains two Fe atoms. As shown in crystal-field splitting and simple valence counting as well as more reliable local-density-approximation (LDA) calculations,[16] it is reasonable to assume that only the lowest 2 or 3 *d* orbitals of Fe play an important role in the low-energy physics of these materials. LDA results show the presence of small Fermi surfaces (FS).[25] In the unfolded Brillouin zone (BZ), corresponding to one Fe per unit cell, electron and hole pockets exist around *M* and Γ points, respectively.[15] The Fermi surfaces are holelike around the Γ point and electronlike around the *M* point of the Brillouin zone. Upon electron doping, the holelike FS shrinks, while the electronlike FS expands, as shown in Fig. 1. The leftmost figures schematically represent the hole doping region (less than electron half-filling), in which holelike FS resides clearly around Γ point. The middle figures correspond to the half-filling case, in which electronlike FS around *M* point appears, while holelike FS is slightly scaled down. The rightmost figures indicate the electron doping region (more than electron half-filling), in which the electronlike FS spreads out and holelike FS shrinks further. The dominant contributions to the superconductivity clearly arise from the surroundings of the Γ and *M* points. Therefore, we consider a 2D square lattice with "d_{xz}, d_{yz}" orbitals per site as a starting model to describe FeAs-based superconductors[37]

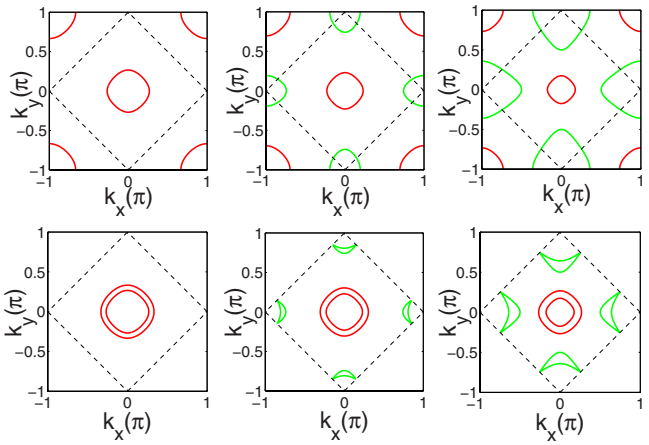

FIG. 1. (Color online) Top: The Fermi surface of the two-orbital model on the large one Fe per cell BZ at $\mu=1.00$, $\mu=1.45$, and $\mu=2.00$ from left to right. The dashed square indicates the BZ of two Fe per cell. Bottom: The Fermi surface folded into the two Fe per cell BZ at $\mu=1.00$, $\mu=1.45$, and $\mu=2.00$ from left to right. Here the hopping integrals of the tight-binding model are set as $t_1=-1$, $t_2=1.3$, and $t_3=t_4=0.85$, which are shown in Fig. 2. In this case, $\mu=1.45$ for the middle two figures corresponds to half-filling. The leftmost two figures correspond to hole doping, and Fermi surfaces (red lines) reside around Γ point. Upon doping, the hole Fermi surfaces shrink, while the electron Fermi surfaces around M point (green lines) expand.

for the oxypnictide compounds. The reason will be discussed later;

$$H = H_0 + H_I, \tag{1}$$

$$H_0 = -\sum_{ij\sigma} t^{cc}_{ij,\sigma}(c^\dagger_{i,\sigma}c_{j,\sigma} + \text{H.c.}) - \sum_{ij\sigma} t^{dd}_{ij,\sigma}(d^\dagger_{i,\sigma}d_{j,\sigma} + \text{H.c.}) - \sum_{(ij)\sigma} t^{cd}_{ij,\sigma}(c^\dagger_{i,\sigma}d_{j,\sigma} + \text{H.c.}) - \mu\sum_{i\sigma}(n_{i,c,\sigma} + n_{i,d,\sigma}), \tag{2}$$

$$H_I = \sum_i (U_c n_{i,c,\uparrow}n_{i,c,\downarrow} + U_d n_{i,d,\uparrow}n_{i,d,\downarrow} + U_{cd}n_{i,c}n_{i,d} - J_H S_{i,c}S_{i,d}). \tag{3}$$

Here c (d) labels d_{xz} (d_{yz}) orbitals, $c^\dagger_{i,\sigma}$ ($d^\dagger_{i,\sigma}$) is the creation operator for electrons of spin σ, orbital d_{xz} (d_{yz}) at site i, $n_{i,c,\sigma}=c^\dagger_{i,\sigma}c_{i,\sigma}$, $n_{i,d,\sigma}=d^\dagger_{i,\sigma}d_{i,\sigma}$, and the hopping integrals are

$$t^{cc}_{ij,\sigma} = t_1\delta(i-j+\hat{x}) + t_2\delta(i-j+\hat{y}) + t_3\delta(i-j+\hat{x}+\hat{y}) + t_3\delta(i-j-\hat{x}+\hat{y}), \tag{4}$$

$$t^{dd}_{ij,\sigma} = t_2\delta(i-j+\hat{x}) + t_1\delta(i-j+\hat{y}) + t_3\delta(i-j+\hat{x}+\hat{y}) + t_3\delta(i-j-\hat{x}+\hat{y}), \tag{5}$$

$$t^{cd}_{ij,\sigma} = t_4\delta(i-j+\hat{x}-\hat{y}) + t_4\delta(i-j-\hat{x}+\hat{y}) - t_4\delta(i-j+\hat{x}+\hat{y}) - t_4\delta(i-j-\hat{x}-\hat{y}), \tag{6}$$

which are illustrated in Fig. 2. U_c and U_d are intraband Coulomb repulsions with the relation $U_c=U_d\equiv U$, U_{cd} denotes interband Coulomb repulsion, and J_H is Hund's rule coupling. For later convenience, we set $t_\perp=(t_1+t_2)/2$ and $t_\parallel=(t_1-t_2)/2$. The space group of LaFeAsO is $P4/nmm$ and it is characterized by point group D_4 and lattice translation group T. Therefore, the basis matrix functions belong to different irreducible representations of point group D_4, which has five irreducible representations, including four one-dimensional (1D) representations (A_1, A_2, B_1, and B_2) and one two-dimensional representation (E). Typical bases in each 1D representation are listed in Table I. The orbital part of the pairing matrix Ω is in the space spanned by two-component vectors, i.e., d_{xz} and d_{yz} (like a spinor), which is the irreducible representation E of the point group D_4, and $\tau_{0,1,2,3}$ in Table I are transformed as A_1, B_2, A_2, and B_1, respectively, with τ_i as the Pauli matrices.[19,21]

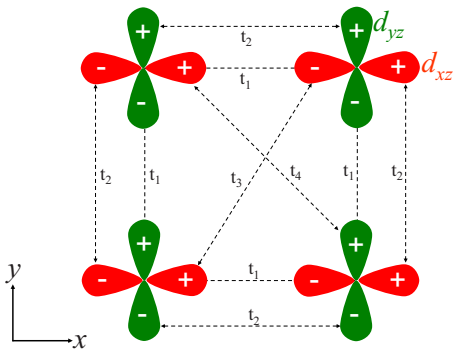

FIG. 2. (Color online) The schematic illustration for the hopping parameters of the two-orbital d_{xz},d_{yz} model on a square lattice. The projections of the d_{xz} (d_{yz}) orbitals onto the xy plane are depicted in red (green). Here t_1 represents the nearest-neighbor hopping integral between σ orbitals and t_2 the nearest-neighbor hopping integral between π orbitals; t_3 denotes next-nearest-neighbor hopping between similar orbitals and t_4 the next-nearest-neighbor hopping integral between different orbitals.

In the following, we will establish sum rules for various pairings by exploiting the commutation relations between the Hamiltonian and the on-site pairing operators. Suppose $A_\mathbf{i}$, $B_\mathbf{i}$, $C_\mathbf{i}$, and $D_\mathbf{i}$ are some localized operators defined on lattice Λ and they satisfy the commutation relation

$$[H_\Lambda, A_\mathbf{i}] = \alpha B_\mathbf{i} + \beta C_\mathbf{i} + \gamma D_\mathbf{i}, \tag{7}$$

where $\alpha\neq 0$, $\beta\neq 0$, and $\gamma\neq 0$ are some constants. Since

$$\langle\Psi_0|[H_\Lambda, A_\mathbf{i}]|\Psi_0\rangle = (E_0 - E_0)\langle\Psi_0|A_\mathbf{i}|\Psi_0\rangle = 0, \tag{8}$$

where Ψ_0 is the ground state of H_Λ, we have

TABLE I. One-dimensional irreducible representations (IRs) of D_4 group in spatial and orbital spaces.

IR	Spatial basis functions	Bases in orbital space Ω
A_1	x^2+y^2	τ_0
B_2	xy	τ_1
A_2	$xy(x^2-y^2)$	τ_2
B_1	x^2-y^2	τ_3

$$\alpha\langle\Psi_0|B_{\mathbf{i}}|\Psi_0\rangle + \beta\langle\Psi_0|C_{\mathbf{i}}|\Psi_0\rangle + \gamma\langle\Psi_0|D_{\mathbf{i}}|\Psi_0\rangle = 0. \quad (9)$$

It implies that the orders of $B_{\mathbf{i}}$, $C_{\mathbf{i}}$, and $D_{\mathbf{i}}$ should be either absent altogether or at least two of them should exist simultaneously in the ground state.[38] The rigorous proof will be presented in Sec. V.

III. INTRAORBITAL PAIRING

We consider intraorbital pairing first and define the on-site pairing operator on site r

$$\Delta_r^{cc} = c_{r,\uparrow}c_{r,\downarrow}, \quad \Delta_r^{dd} = d_{r,\uparrow}d_{r,\downarrow}, \quad (10)$$

the nearest-neighbor (NN) or the next-nearest-neighbor (NNN) spin singlet intraorbital pairing operators

$$\Delta_{r+\vec{\delta}}^{cc} = c_{r,\uparrow}c_{r+\vec{\delta},\downarrow} - c_{r,\downarrow}c_{r+\vec{\delta},\uparrow},$$

$$\Delta_{r+\vec{\delta}}^{dd} = d_{r,\uparrow}d_{r+\vec{\delta},\downarrow} - d_{r,\downarrow}d_{r+\vec{\delta},\uparrow}, \quad (11)$$

and NN or NNN spin singlet interorbital pairing operators

$$\Delta_{r+\vec{\delta}}^{cd} = c_{r,\uparrow}d_{r+\vec{\delta},\downarrow} - c_{r,\downarrow}d_{r+\vec{\delta},\uparrow},$$

$$\Delta_{r+\vec{\delta}}^{dc} = d_{r,\uparrow}c_{r+\vec{\delta},\downarrow} - d_{r,\downarrow}c_{r+\vec{\delta},\uparrow}. \quad (12)$$

By calculating the commutation relations between the Hamiltonian and the on-site pairing operators, we find that results can be expressed as linear combinations of s- and d-wave symmetry operators involving NN and NNN electrons, such as the on-site s-wave pairing operators, extended s^*-wave pairing operators, s_{xy}-wave pairing operators, $d_{x^2-y^2}$-wave pairing operators, and d_{xy}-wave pairing operators with the definition

$$\text{on-site } s \text{ wave}: \Delta_s = \frac{1}{N}\sum_r \Delta_r,$$

$$\text{extended } s^* \text{ wave}: \Delta_{s*} = \frac{1}{N}\sum_r (\Delta_{r-\hat{x}} + \Delta_{r+\hat{x}} + \Delta_{r-\hat{y}} + \Delta_{r+\hat{y}}),$$

$$s_{xy} \text{ wave}: \Delta_{s_{xy}} = \frac{1}{N}\sum_r (\Delta_{r+\hat{x}+\hat{y}} + \Delta_{r-\hat{x}-\hat{y}} + \Delta_{r+\hat{x}-\hat{y}} + \Delta_{r-\hat{x}+\hat{y}}),$$

$$d_{xy} \text{ wave}: \Delta_{d_{xy}} = \frac{1}{N}\sum_r (\Delta_{r+\hat{x}+\hat{y}} + \Delta_{r-\hat{x}-\hat{y}} - \Delta_{r+\hat{x}-\hat{y}} - \Delta_{r-\hat{x}+\hat{y}}),$$

$$d_{x^2-y^2} \text{ wave}: \Delta_{d_{x^2-y^2}} = \frac{1}{N}\sum_r (\Delta_{r-\hat{x}} + \Delta_{r+\hat{x}} - \Delta_{r-\hat{y}} - \Delta_{r+\hat{y}}). \quad (13)$$

The respective pair coordinates are shown in Fig. 3.

Thus, we have

$$[H, \Delta_s^{cc}] = t_\perp \Delta_{s*}^{cc} + t_\parallel \Delta_{d_{x^2-y^2}}^{cc} + t_3 \Delta_{s_{xy}}^{cc} - t_4 \Delta_{d_{xy}}^{cd} - (U - 2\mu + 2U_{cd}n_{r,d})\Delta_s^{cc}, \quad (14)$$

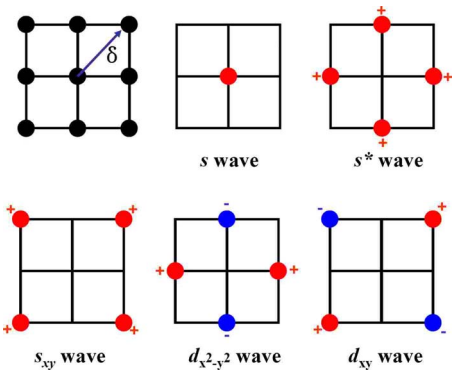

FIG. 3. (Color online) The pair coordinates $\vec{\delta}$ used to define $\Delta_{\vec{\delta}}$, the range over five positions including (0,0).

$$[H, \Delta_s^{dd}] = t_\perp \Delta_{s*}^{dd} - t_\parallel \Delta_{d_{x^2-y^2}}^{dd} + t_3 \Delta_{s_{xy}}^{dd} - t_4 \Delta_{d_{xy}}^{dc} - (U - 2\mu + 2U_{cd}n_{r,c})\Delta_s^{dd}. \quad (15)$$

Since there is interorbital hopping in the original Hamiltonian (1), interorbital pairings appear on the right side of Eqs. (14) and (15). Furthermore, we treat the quartic terms such as $n_{r,d}\Delta_s^{cc}$ in the mean-field sense by taking number operators n_r as their average $\langle n_r\rangle$, assuming that there is no charge-density wave (CDW). Even if CDW occurs, the Coulomb repulsion will suppress the on-site s-wave pairing, i.e., $\Delta_s = 0$, and it will not affect our conclusion. Thus, in the following, we treat the number operators for the two orbitals as $\langle n_{r,d}\rangle = \langle n_{r,c}\rangle \equiv \langle n\rangle$ in all quartic terms. Defining $U_1 = U - 2\mu + 2U_{cd}\langle n\rangle$, we consider linear combinations of Eqs. (14) and (15),

$$[H, \Delta_s^{cc} + \Delta_s^{dd}] = t_\perp(\Delta_{s*}^{cc} + \Delta_{s*}^{dd}) + t_\parallel(\Delta_{d_{x^2-y^2}}^{cc} - \Delta_{d_{x^2-y^2}}^{dd}) + t_3(\Delta_{s_{xy}}^{cc} + \Delta_{s_{xy}}^{dd}) - t_4(\Delta_{d_{xy}}^{cd} + \Delta_{d_{xy}}^{dc}) - U_1(\Delta_s^{cc} + \Delta_s^{dd}), \quad (16)$$

$$[H, \Delta_s^{cc} - \Delta_s^{dd}] = t_\perp(\Delta_{s*}^{cc} - \Delta_{s*}^{dd}) + t_\parallel(\Delta_{d_{x^2-y^2}}^{cc} + \Delta_{d_{x^2-y^2}}^{dd}) + t_3(\Delta_{s_{xy}}^{cc} - \Delta_{s_{xy}}^{dd}) - U_1(\Delta_s^{cc} - \Delta_s^{dd}). \quad (17)$$

To write the formulas in a more compact way, with the help of the Nambu representation $\phi_\sigma(k) = (c_{-k,\sigma}, d_{-k,\sigma})$, the pairing gap in momentum and orbital spaces can be expressed as $\Sigma_{k\alpha\beta}\phi_{\alpha,\sigma}(-k)f(k)(\tau_i)_{\alpha\beta}\phi_{\beta,\bar{\sigma}}(k)$, where τ_i is the basis of orbital space and $f(k)$ is the pairing function in momentum space. $f(k)$ for different pairing symmetries is given by

$$\text{on-site } s \text{ wave}: f_s(k) = 1,$$

$$\text{extended } s^* \text{ wave}: f_{s*}(k) = \cos k_x + \cos k_y,$$

$$s_{xy} \text{ wave}: f_{s_{xy}}(k) = \cos k_x \cos k_y,$$

$$d_{xy} \text{ wave}: f_{d_{xy}}(k) = \sin k_x \sin k_y,$$

TABLE II. Potential pairing basis matrices under different irreducible representations of the model, which are classified into three groups in the table. The first column is the index number, the second and the third columns denote the representations and the basis matrix functions, respectively. The parities of spins [singlet (S) or triplet (T)] and orbitals [symmetric (s) or antisymmetric (a)] are shown in the fourth and the last columns, respectively.

No. (i)	IR	Pairing function $f_i(k)$	Spin	Orbital
1	A_1	$(\cos k_x+\cos k_y)\tau_0$	S	s
2	A_1	$(\cos k_x-\cos k_y)\tau_3$	S	s
3	A_1	$(\cos k_x \cos k_y)\tau_0$	S	s
4	A_1	$(\sin k_x \sin k_y)\tau_1$	S	s
5	A_1	τ_0	S	s
6	B_1	$(\cos k_x+\cos k_y)\tau_3$	S	s
7	B_1	$(\cos k_x-\cos k_y)\tau_0$	S	s
8	B_1	$(\cos k_x \cos k_y)\tau_3$	S	s
9	B_1	τ_3	S	s
10	B_2	$(\cos k_x+\cos k_y)\tau_1$	S	s
11	B_2	$(\cos k_x \cos k_y)\tau_1$	S	s
12	B_2	$(\sin k_x \sin, k_y)\tau_0$	S	s
13	B_2	τ_1	S	s
14	A_2	$(\cos k_x+\cos k_y)i\tau_2$	T	a
15	A_2	$(\cos k_x \cos k_y)i\tau_2$	T	a
16	A_2	$i\tau_2$	T	a

$$d_{x^2-y^2} \text{ wave:} f_{d_{x^2-y^2}}(k) = \cos k_x - \cos k_y. \tag{18}$$

Then, in another representation, Eqs. (16) and (17) can be written as

$$[H,\tau_0] \sim t_\perp(\cos k_x + \cos k_y)\tau_0 + t_\parallel(\cos k_x - \cos k_y)\tau_3 + t_3(\cos k_x \cos k_y)\tau_0 + t_4 \sin k_x \sin k_y \tau_1 - U_1\tau_0, \tag{19}$$

$$[H,\tau_3] \sim t_\perp(\cos k_x + \cos k_y)\tau_3 + t_\parallel(\cos k_x - \cos k_y)\tau_0 + t_3(\cos k_x \cos k_y)\tau_3 - U_1\tau_3, \tag{20}$$

There are five types of pairing patterns on the right side of Eq. (19) and four in Eq. (20), listed as Nos. 1–9 in Table II.

IV. INTERORBITAL PAIRING

When interorbital pairing is taken into consideration, more pairings are involved. Defining the on-site interorbital pairing operator as

$$\Delta_r^{cd} = c_{r,\uparrow}d_{r,\downarrow}, \quad \Delta_r^{dc} = d_{r,\uparrow}c_{r,\downarrow}, \tag{21}$$

and NN or NNN interorbital pairing operators in a similar manner with $U_2=(U-2\mu+2U_{cd}-3J_H/4)\langle n\rangle+3J_H/4$, we get

$$[H,\Delta_s^{cd}+\Delta_s^{dc}] = t_\perp(\Delta_{s*}^{cd}+\Delta_{s*}^{dc}) + t_3(\Delta_{s_{xy}}^{cd}+\Delta_{s_{xy}}^{dc}) - t_4(\Delta_{d_{xy}}^{cc}+\Delta_{d_{xy}}^{dd}) - U_2(\Delta_s^{cd}+\Delta_s^{dc}). \tag{22}$$

The pairing operators can be expressed in momentum and orbital space as

$$[H,\tau_1] \sim t_\perp(\cos k_x + \cos k_y)\tau_1 + t_3(\cos k_x \cos k_y)\tau_1 - t_4(\sin k_x \sin k_y)\tau_0 - U_2\tau_1. \tag{23}$$

Similarly, with the definition of spin triplet pairing operators

$$\bar{\Delta}_{\vec{\delta}}^{cd} = c_{r\uparrow}d_{r+\vec{\delta}\downarrow} + c_{r\downarrow}d_{r+\vec{\delta}\uparrow},$$

$$\bar{\Delta}_{\vec{\delta}}^{dc} = d_{r\uparrow}c_{r+\vec{\delta}\downarrow} + d_{r\downarrow}c_{r+\vec{\delta}\uparrow}, \tag{24}$$

and $U_3=(U-2\mu+2U_{cd}+J_H/4)\langle n\rangle-J_H/4$, we have

$$[H,\Delta_s^{cd}-\Delta_s^{dc}] = t_\perp(\bar{\Delta}_{s*}^{cd}-\bar{\Delta}_{s*}^{dc}) + t_3(\bar{\Delta}_{s_{xy}}^{cd}-\bar{\Delta}_{s_{xy}}^{dc}) - U_3(\Delta_s^{cd}-\Delta_s^{dc}). \tag{25}$$

The formula in our momentum and orbital representation is

$$[H,i\tau_2] \sim t_\perp(\cos k_x + \cos k_y)i\tau_2 + t_3(\cos k_x \cos k_y)i\tau_2 + U_3 i\tau_2. \tag{26}$$

There are four types of pairing on the right side of Eq. (23) and three in Eq. (26), which are listed as Nos. 10–16 in Table II.

V. INEQUALITIES AND ANALYSIS

With the use of the above commutation relations, let us establish the sufficient condition for the coexistence of two long-range orders rigorously. We should take advantage of the theory of off-diagonal long-range order[39] and generalize the approach of Ref. 40 to obtain a strict proof. Interested readers may also find similar treatments to the single-band Hubbard model and the t-J model.[41,42]

Let $G_\mathbf{i}$ be a general localized operator centered at site $\mathbf{i}$ defined on lattice Λ. We define a reduced density matrix $\mathcal{M}(G_\mathbf{i})=(\mathcal{M}_\mathbf{ij})$ by

$$\mathcal{M}_\mathbf{ij} \equiv \langle\Psi_0(\Lambda)|G_\mathbf{i}^\dagger G_\mathbf{j}|\Psi_0(\Lambda)\rangle. \tag{27}$$

Then, $\Psi_0(\Lambda)$ has a long-range order of $G_\mathbf{i}$ if and only if the largest eigenvalue $\zeta_{\max}$ of $\mathcal{M}(G_\mathbf{i})$ satisfies the condition[39]

$$\zeta_{\max} \geq \lambda N_\Lambda, \tag{28}$$

where $\lambda>0$ is a constant independent of N_Λ, as $N_\Lambda\to\infty$ with fixed density.

The presence of a long-range order of $G_\mathbf{i}$ in the ground state $\Psi_0(\Lambda)$ can be also thought as a Bose-Einstein condensation of the G operator at a certain reciprocal vector $k=k_0$, which is characterized by

$$\langle\Psi_0(\Lambda)|G_k^\dagger G_k|\Psi_0(\Lambda)\rangle \geq \lambda N_\Lambda, \quad \lambda>0, \tag{29}$$

where G_k is the reciprocal operator of $G_\mathbf{i}$ in k space.

Assuming that such an operator $A_\mathbf{i}$ satisfies the following commutation relation:

$$[H_\Lambda, A_{\mathbf{i}}] = \sum_\mu \lambda_\mu G_{\mathbf{i}}^\mu, \tag{30}$$

which is a general formula of Eq. (7). We replace Eq. (30) in k space with

$$[H_\Lambda, A_k] = \sum_\mu \lambda_\mu G_k^\mu \equiv Q_k. \tag{31}$$

Let us consider the correlation function of Q_k. Clearly, we can have

$$\begin{aligned} 0 &\le \langle \Psi_0(\Lambda)|Q_k^\dagger Q_k|\Psi_0(\Lambda)\rangle \\ &\le \langle \Psi_0(\Lambda)|Q_k^\dagger Q_k|\Psi_0(\Lambda)\rangle + \langle \Psi_0(\Lambda)|Q_k Q_k^\dagger|\Psi_0(\Lambda)\rangle \\ &\equiv S_Q. \end{aligned} \tag{32}$$

Introducing a complete set of the eigenvectors $\{\Psi_n(\Lambda)\}$ of H_Λ, S_Q can be further written as

$$\begin{aligned} S_Q &= \sum_n (|\langle \Psi_n(\Lambda)|Q_k^\dagger|\Psi_0(\Lambda)\rangle|^2 + |\langle \Psi_n(\Lambda)|Q_k|\Psi_0(\Lambda)\rangle|^2) \\ &= \sum_n \left\{ \frac{|\langle \Psi_n(\Lambda)|Q_k^\dagger|\Psi_0(\Lambda)\rangle|}{\sqrt{E_n - E_0}} (|\langle \Psi_n(\Lambda)|Q_k^\dagger|\Psi_0(\Lambda)\rangle \right. \\ &\quad \left. \times |\sqrt{E_n - E_0}) + \frac{|\langle \Psi_n(\Lambda)|Q_k|\Psi_0(\Lambda)\rangle|}{\sqrt{E_n - E_0}} \right. \\ &\quad \left. \times (|\langle \Psi_n(\Lambda)|Q_k|\Psi_0(\Lambda)\rangle| \sqrt{E_n - E_0}) \right\}. \end{aligned} \tag{33}$$

Since $\Psi_0(\Lambda)$ is the ground state of H_Λ, $\sqrt{E_n - E_0}$ is well defined. We should notice that the fraction terms in Eq. (33) seem ill defined because the complete set of eigenvectors includes the ground state and some eigenvectors $\Psi_n(\Lambda)$ may be degenerate with $\Psi_0(\Lambda)$. However, these seemingly ill-defined fraction terms in Eq. (33) can be eliminated by substituting the commutation relation (31) into the numerators of the fractions. When $E_n - E_0 = 0$, we have

$$\langle \Psi_n(\Lambda)|Q_k|\Psi_0(\Lambda)\rangle = (E_n - E_0)\langle \Psi_n(\Lambda)|A_k|\Psi_0(\Lambda)\rangle = 0. \tag{34}$$

Consequently, this gives

$$\frac{|\langle \Psi_n(\Lambda)|Q_k|\Psi_0(\Lambda)\rangle|}{\sqrt{E_n - E_0}} = \sqrt{E_n - E_0}\langle \Psi_n(\Lambda)|A_k|\Psi_0(\Lambda)\rangle = 0. \tag{35}$$

Similarly, we can also show that $\langle \Psi_n(\Lambda)|Q_k^\dagger|\Psi_0(\Lambda)\rangle = 0$. Therefore, we do not have to exclude these specific cases from the summation in Eq. (33).

Next, we apply the Cauchy-Schwarz inequality to the right side of Eq. (33). We obtain

$$\begin{aligned} S_Q \le & \sqrt{\left[\sum_n (|\langle \Psi_n(\Lambda)|Q_k^\dagger|\Psi_0(\Lambda)\rangle|^2 + |\langle \Psi_n(\Lambda)|Q_k|\Psi_0(\Lambda)\rangle|^2)(E_n - E_0) \right]} \\ & \times \sqrt{\left[\sum_n \frac{(|\langle \Psi_n(\Lambda)|Q_k^\dagger|\Psi_0(\Lambda)\rangle|^2 + |\langle \Psi_n(\Lambda)|Q_k|\Psi_0(\Lambda)\rangle|^2)}{(E_n - E_0)} \right]}. \end{aligned} \tag{36}$$

The first square brackets on the right side of inequality (36) is equal to

$$\sqrt{\left[\sum_n (|\langle \Psi_n(\Lambda)|Q_k^\dagger|\Psi_0(\Lambda)\rangle|^2 + |\langle \Psi_n(\Lambda)|Q_k|\Psi_0(\Lambda)\rangle|^2)(E_n - E_0) \right]} = \sqrt{\langle \Psi_0(\Lambda)|[Q_k^\dagger, [H_\Lambda, Q_k]]|\Psi_0(\Lambda)\rangle} \equiv m(Q_k). \tag{37}$$

On the other hand, by using commutation relation (31), the second factor on the right side of inequality (36) can be simplified as

$$\begin{aligned} \sqrt{\sum_n \frac{(|\langle \Psi_n(\Lambda)|Q_k^\dagger|\Psi_0(\Lambda)\rangle|^2 + |\langle \Psi_n(\Lambda)|Q_k|\Psi_0(\Lambda)\rangle|^2)}{(E_n - E_0)}} &= \sqrt{\sum_n (|\langle \Psi_n(\Lambda)|A_k^\dagger|\Psi_0(\Lambda)\rangle|^2 + |\langle \Psi_n(\Lambda)|A_k|\Psi_0(\Lambda)\rangle|^2)(E_n - E_0)} \\ &= \sqrt{\langle \Psi_0(\Lambda)|[A_k^\dagger, [H_\Lambda, A_k]]|\Psi_0(\Lambda)\rangle} \equiv m(A_k). \end{aligned} \tag{38}$$

Therefore, we have proved that

$$\langle \Psi_0(\Lambda)|Q_k^\dagger Q_k|\Psi_0(\Lambda)\rangle \le m(Q_k)m(A_k). \tag{39}$$

Here $m(Q_k)$ and $m(A_k)$ are quantities of order $O(1)$ as N_Λ tends to infinity. Therefore, the correlation function of Q_k is at most a quantity of order $O(1)$.

Replacing Q_k in inequality (39) with Eq. (31) and expanding the inequality, we find

$$\begin{aligned} &\sum_\mu |\lambda_\mu|^2 \langle \Psi_0(\Lambda)|G_k^{\mu\dagger} G_k^\mu|\Psi_0(\Lambda)\rangle \\ &\quad + \sum_{\mu \ne \nu} 2\lambda_\mu^* \lambda_\nu \langle \Psi_0(\Lambda)|G_k^{\mu\dagger} G_k^\nu|\Psi_0(\Lambda)\rangle \le m(Q_k)m(A_k). \end{aligned} \tag{40}$$

By shifting the mixing terms to the right side of inequality

(40) and applying the Cauchy-Schwarz inequality to these terms, we can further derive the inequality

$$\sum_{\mu} |\lambda_{\mu}|^2 \langle \Psi_0(\Lambda)|G_k^{\mu\dagger} G_k^{\mu}|\Psi_0(\Lambda)\rangle \leq m(Q_k)m(A_k) + \sum_{\mu\neq\nu} 2|\lambda_{\mu}| \times |\lambda_{\nu}| \sqrt{\langle \Psi_0(\Lambda)|G_k^{\mu\dagger} G_k^{\mu}|\Psi_0(\Lambda)\rangle \langle \Psi_0(\Lambda)|G_k^{\nu\dagger} G_k^{\nu}|\Psi_0(\Lambda)\rangle}. \tag{41}$$

Now, let us assume that $\Psi_0(\Lambda)$ has a long-range order in only one of the operators in Eq. (31), say for some $G_k^{\mu} \equiv B_k$, then

$$\langle \Psi_0(\Lambda)|B_k^{\dagger} B_k|\Psi_0(\Lambda)\rangle \geq \lambda_B N_{\Lambda}, \quad \lambda_B > 0, \tag{42}$$

as $N_{\Lambda} \to \infty$. Since the left side of inequality (41) is a quantity of order $O(N_{\Lambda})$ and the correlation functions of other operators are, at most, of order $O(1)$ in the thermodynamic limit by assumption, the right side of the inequality (41) can be, at most, a quantity of order $O(\sqrt{N_{\Lambda}})$. In this case, inequality (41) becomes contradictory. Therefore, $\Psi_0(\Lambda)$ must have a long-range order of an additional operator, say $G_k^{\nu} \equiv C_k$, that is,

$$\langle \Psi_0(\Lambda)|C_k^{\dagger} C_k|\Psi_0(\Lambda)\rangle \geq \lambda_C N_{\Lambda}, \quad \lambda_C > 0. \tag{43}$$

The conclusion is that either all orders are absent or at least two long-range orders must be present simultaneously in the ground state $\Psi_0(\Lambda)$ of the Hamiltonian H_{Λ}. Obviously, it is easy to generalize the conclusion to the case where there are more than three operators on the right side of Eq. (31).

Applying the above rigorous result to Hamiltonian (1), we have a basic conclusion that orders of the same group listed in Table II, say Nos. 1–5, either should be all absent or at least two of them should coexist. Specifically, we can refine this conclusion as follows. Since group A_1 is quite similar to group B_1, we focus on group B_1.

First, having two electrons located on the same site is energetically unfavorable due to the on-site Coulomb repulsion, so the probability of forming an on-site electron pair is low, let alone coherent pair condensation. This argument does not rely much on the strength of the on-site Coulomb interaction. As long as there are on-site Coulomb repulsions and considering the fact that on-site Coulomb repulsions are always stronger than off-site Coulomb repulsions, the probabilities of off-site pairings are far greater than those of on-site pairing. Therefore, all the states involving s-wave pairing are suppressed. In other words, Nos. 5 and 9 (symmetric intraorbital s), 13 (symmetric interorbital s), and 16 (antisymmetric interorbital s) will be unfavorable.

Second, Eq. (20) shows that all order parameters in the second group B_1 of Table II have spin singlet, intraorbital, and even parity pairing symmetry. Nevertheless, our rigorous results [Eqs. (42) and (43)] require that orders of Nos. 6–8 should either vanish simultaneously or at least two of them should coexist. If two of them coexist, the magnitudes of the two order parameters are determined by the product of their pairing functions $[f_6(k), f_7(k)]$. So if s^* and s_{xy} coexist, $f_6(k) = (\cos k_x + \cos k_y)$ and $f_8(k) = \cos k_x \cos k_y$. Their overlap becomes dominant around the hole pocket about the Γ point in the Brillouin zone but is very small around the electron pocket of the M point. While if $d_{x^2-y^2}$ and s_{xy} coexist, $f_7(k) = (\cos k_x - \cos k_y)$ and $f_8(k) = \cos k_x \cos k_y$. Their product has an enhanced contribution from the electron pocket about the M point but is suppressed from the hole pocket about the Γ point. However, the coexistence of s^* and $d_{x^2-y^2}$ is not favorable because their overlap is very tiny around both M and Γ points.

Third, in the group B_2 of Table II, there are Nos. 10 (symmetric interorbital s^*), 11 (symmetric interorbital s_{xy}), and 12 (intraorbital d_{xy}) left on the right side of Eq. (23). Since $f_{12}(k) = \sin k_x \sin k_y$ is peaked around $(\pi/2, \pi/2)$, if No. 12 coexists with No. 10 or No. 11, $f_{12}(k)$ has a tiny contribution at M and Γ points and does support the current Fermi-surface topology; therefore, No. 12 is not favored. So the remaining s^* and s_{xy} of the spin singlet must either be absent together or coexist simultaneously. According to the behavior of pairing function $f_{10(11)}(k)$, the coexistence of s^* and s_{xy} is compatible only around hole pocket about Γ point but not favored in electron pocket about M point.

Fourth, regarding pairings No. 14 (antisymmetric interorbital s^*) and No. 15 (antisymmetric interorbital s_{xy}) on the right side of Eq. (26), which belong to group A_2 of Table II, our rigorous results [Eqs. (42) and (43)] impose that both of them should either be absent or coexist. Besides, both of these two pairings carry antisymmetric orbital parity, and their excitation spectra will become gapless, which is inconsistent with experimental evidence showing either nodal gap or full gap.[12,13] Therefore, the chance of their coexistence seems slim.

Finally, in the weak coupling limit, two orbitals' energy splitting might lead to a mismatch of interorbital pairing in momentum space with opposite sign instead of pairing between two different $|k|$'s. That is, the piling up of low-energy density of states in the gapless SC state will lead to a Fulde-Ferrel-Larkin-Ovchinnikov (FFLO) state with magnetic ordering and will not create SC instability. In this sense, the orbital antisymmetric pairing state such as Nos. 14 and 15 might be ruled out. Moreover, other interband pairings, such as Nos. 10 and 11 in Table II, are also not favorable according to the analysis based on the FFLO state. Thus we arrive at our further conclusion that, around half filling, in the electron doping region, the system will favor coexistence of $d_{x^2-y^2}$ and s_{xy} waves pairing, while in the hole doping region, the system might prefer to have s^* and s_{xy} waves pairing.

VI. SUMMARY

To summarize, we have built some identities based on a two-orbital model and obtained constraints on a few possible pairings. Our results provide more information than the group theory classification. According to the sufficient condition for coexistence of two superconducting orders and resorting to physical consideration, we propose the most favorable pairings around half-filling. Although our discussion is based on a two-orbital model, it is straightforward to generalize the strategy to Hamiltonians involving more orbitals. For example, we can construct similar commutation relation in three-orbital model with the notations defined in Ref. 27,

$$[H_{3\text{-orbital}}, \Delta_s^{xz} + \Delta_s^{yz} - \Delta_s^{xy}]$$
$$= \sum_k [-2\epsilon_{xz}(k) c_{k,\uparrow}^{xz} c_{-k,\downarrow}^{xz} - 2\epsilon_{yz}(k) c_{k,\uparrow}^{yz} c_{-k,\downarrow}^{yz}$$
$$+ 2\epsilon_{xy}(k) c_{k,\uparrow}^{xy} c_{-k,\downarrow}^{xy} - 4t'_{xz,yz} \sin(k_x)\sin(k_y)(c_{k,\uparrow}^{yz} c_{-k,\downarrow}^{xz}$$
$$+ c_{k,\uparrow}^{xz} c_{-k,\downarrow}^{yz})] - (U_1/2 + 2U_2\langle n\rangle/3)(\Delta_s^{xz} + \Delta_s^{yz} - \Delta_s^{xy}), \quad (44)$$

and we will come to the similar conclusion from this identity. In principle, we have not ruled out spatial odd parity pairing, e.g., p wave, which can be achieved by commutation between an odd parity pairing operator and the Hamiltonian, or other combination of the commutation operators, and the sufficient condition of coexistence of the odd parity pairings is still applicable. Nevertheless, they do not get along well with our Fermi-surface topology analysis given above. In addition, it is worth mentioning that, even though the chances of on-site pairing seem slim, we cannot rule out the possibilities of such pairings. In the event of such on-site pairing, the issue of coexistence of superconducting orders becomes complex.

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