Orbital selectivity and emergent superconducting state from quasi-degenerate $s$– and $d$–wave pairing channels in iron-based superconductors

Emilian M. Nica,¹ Rong Yu,² and Qimiao Si¹

¹Department of Physics and Astronomy, Rice University, Houston, Texas 77005
²Department of Physics, Renmin University of China, Beijing 100872, China

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A major puzzle about the nature of the iron-based superconductivity appears in the case of the alkaline iron selenides. Compared to the iron pnictides, these systems have only electron Fermi pockets (i.e., no hole Fermi pockets) but comparable superconducting transition temperatures. The challenge lies in reconciling the two basic experimental features of their superconducting state: a node-less gap and the existence of a resonance in the spin excitation spectrum. Here we propose a mechanism based on reconstructing two quasi-degenerate pairing states, one in an $s$-wave $A_{1g}$ channel that is fully gapped, and the other in a $d$-wave $B_{1g}$ channel whose pairing function changes sign across the electron Fermi pockets at the Brillouin-zone boundary. The resulting intermediate pairing state, which we call an orbital-selective $s \times \tau_3$ state, incorporates both of the above two properties. When the leading spin-singlet pairing is in the $d_{xz}, d_{yz}$ orbital subspace, this pairing state retains the $s$-wave form factor but has a $B_{1g}$ symmetry due to an internal $\tau_3$ structure in the orbital space. Within a five-orbital $t - J_1 - J_2$ model with orbital-selective exchange couplings, we show that the proposed pairing state is energetically competitive over a finite range of control parameters. We calculate the dynamical spin susceptibility in the orbital-selective $s \times \tau_3$ superconducting state and show that a spin resonance arises and has the characteristics of observed by inelastic neutron experiments in the alkaline iron selenides. More generally, the formation of the orbital-selective $s \times \tau_3$ state represents a novel means of relieving the quasi-degeneracy between $s$– and $d$–wave pairing states, which is a hitherto unsuspected alternative to the conventional route of linearly superposing the two into a time-reversal symmetry breaking $s + id$ state.

I. INTRODUCTION

Understanding the nature of the iron-based superconductivity remains a central challenge in condensed matter physics. The superconductivity grows out of a bad-metal normal state, with room-temperature resistivity that reaches the Mott-Ioffe-Regel limit [1, 2]. This observation has been interpreted in terms of electron correlations that are sufficiently strong to place the system in proximity to an electronic localization transition [3, 4]. In addition, the iron-based superconductivity typically occurs near an antiferromagnetic ground state [5]. The combination of these features have motivated a strong-coupling approach [6–8], in which short-range exchange interactions among quasi-local moments drive the formation of Cooper pairs. Minimal exchange couplings involve $J_1$, the interaction among the nearest-neighbor sites on the Fe-square lattice, and $J_2$, its next-nearest-neighbor counterpart. Inelastic neutron scattering experiments have demonstrated the importance of such interactions, both for the iron pnictides and iron chalcogenides [5]. The $J_2$ interaction promotes an $s$–wave $A_{1g}$ state, for which there is considerable evidence in the iron pnictides case [11]. In this scenario, the pairing wave function changes sign between the hole Fermi surfaces near the center of the Brillouin zone and the electron Fermi surfaces at the boundary of the Brillouin zone [9], a switch which is believed to be responsible for a resonance spin excitation at the wave vector $(\pi, 0)$ [5]. For the properties of the superconducting state, the distinction between the strong and weak coupling approaches arise subtly. For instance, in the strong coupling approach, the pairing order parameter is naturally defined in the orbital basis, such that the local Coulomb repulsion is minimized [10], ultimately leading to the orbital selectivity of the gap function [11, 12]. The latter, in turn, can cause the appearance of double resonances in the spin excitation spectrum [11] as has been experimentally observed [13, 14].

In spite of some theoretical successes, our understanding of the iron-based superconductivity remains quite limited. One way to make progress is to take advantage of the large materials basis and gain new insights from systems with different microscopic electronic behavior. In this context, a prominent puzzle has come from the "122" alkaline iron selenide compounds such as $K_2Fe_2Se_2$. These systems show electron Fermi pockets only, lacking the hole pockets that occur in the iron pnictides at the center of their 1-Fe Brillouin Zone (BZ) [13, 15, 16]. Yet, the superconducting transition temperatures ($T_c$) for the two classes of materials are comparable. What is striking is the apparently conflicting nature of the pairing function. ARPES experiments indicate a fully gapped quasiparticle dispersion [13, 15, 16], including the electron Fermi pockets at the center of the BZ [17, 18]. This is compatible with the usual $s$-wave $A_{1g}$ pairing state, but not with a $d$-wave $B_{1g}$ state. On the other hand, neutron scattering experiments [19, 20] observe a sharp resonance peak around the wavevector $(\pi, \pi/2)$. These observations are consistent with a sign change between the two Fermi pockets at the edge of the 1-Fe BZ, such as would occur in a $d$-wave $B_{1g}$ state, but not in the usual $s$-wave $A_{1g}$ case.

In this paper, we identify an intermediate pairing state that is reconstructed from the conventional $s$-wave $A_{1g}$ and $d$-wave $B_{1g}$ states in the parameter regime where the two are quasi-degenerate [6]. Orbital selectivity plays an essential role in the formation of this state. When the spin-singlet pairing is

* Corresponding author: en5@rice.edu
restricted to the \(d_{xz}, d_{yz}\) orbital subspace, the candidate pairing state belongs to the \(B_{1g}\) representation of the associated point group but has a form factor belonging to the \(A_{1g}\) representation. Specifically, the pairing function can be written as \(\Delta_0 \times g_{x^2-y^2}(k) \times \gamma_3\), where \(g_{x^2-y^2}(k) = \cos(k_x)\cos(k_y)\) is a \(s\)-wave form factor and \(\gamma_3\) is a Pauli matrix in the \(2 \times 2, d_{xz}, d_{yz}\) orbital subspace. Therefore, we’ll refer to this state as the orbital-selective \(s \times \gamma_3\) state. When the spin-singlet pairings in the remaining orbital sectors are considered, additional \(B_{1g}\) components are mixed in but the gap remains nodeless. The gap function also changes sign across the electron state as the orbital-selective and a summary of the results are presented in Section V. Some additional studies of the salient features of the simplified two-orbital case in the normal state of these systems have already been carried out, both in theory and experiment \([21,22]\). A particularly striking phenomenon is the orbital-selective Mott transition, where the orbital-dependency is developed to such degree as to allow the vanishing of the spectral weights for a subset of \(d\) orbitals. In our discussion below, we will invoke orbital selectivity at two levels. At the level of effective Hamiltonian, we will allow the short-range exchange interactions to be orbital dependent. In addition, at the level of the resulting phases, we will consider pairing functions that are orbitally selective \([11,12]\).

The remainder of the paper is organized as follows: Section II discusses the \(s_{x^2-y^2} \times \gamma_3, B_{1g}\) pairing at length for a simplified two-orbital \(d_{xz}, d_{yz}\) system and shows the nodeless resulting state and the sign-changing features in the band basis. Section III introduces the five-orbital \(t-J_1-J_2\) model with orbital-differentiated exchange couplings and comments on the numerical solution. In Section IV we show the results obtained from the calculation and highlight the survival of the essential features of the simplified two-orbital case in the more realistic five-orbital systems. Concluding remarks and a summary of the results are presented in Section V. Some supplementary material is relegated to the Appendix.

II. THE ORBITAL SELECTIVE \(s \times \gamma_3\) PAIRING IN A TWO-ORBITAL, \(d_{xz}, d_{yz}\) SYSTEM

We start by introducing the intermediate \(s_{x^2-y^2} \times \gamma_3, B_{1g}\) spin-singlet pairing state in a simplified two-orbital \(d_{xz}, d_{yz}\) case. Our aim here is to demonstrate that the quasiparticle excitations in this state are fully gapped and, at the same time, that the pairing wave function changes sign across the electron Fermi pockets near the \(M\) points at the boundary of the 1-Fe BZ. To be definite, we discuss the pairing state using a single-particle dispersion for such a two-orbital system \([26]\). Readers not interested in the details of our exposition of the two-orbital case can consult Figure 1, which gives a summary of the most important results of this section.

\[
\mathbf{H} = \sum_{\mathbf{k}} \psi^\dagger(\mathbf{k}) \left\{ \xi_+^\dagger(\mathbf{k}) \gamma_0 + \xi_-(\mathbf{k}) \gamma_3 + \xi_{xy}(\mathbf{k}) \gamma_1 \right\} \otimes \gamma_3 + \Delta_0 g_{x^2-y^2}(\mathbf{k}) \gamma_3 \otimes \gamma_1 \psi(\mathbf{k}),
\]

where \(\psi^\dagger(\mathbf{k}) = (c_{i\mathbf{k}\sigma}, c_{-\mathbf{k}\sigma}(i\gamma_2)_{\sigma\sigma})\) is a spinor in Nambu space, \(i, j\) are orbital indices, and \(\tau, \sigma\) and \(\gamma\) are Pauli matrices in the \(2 \times 2\) orbital, spin, and Nambu spaces respectively. The exact forms of \(\xi_+, \xi_-\), and \(\xi_{xy}\) functions and of the resulting bands are given in Appendix A. The form of the spinor is chosen to reproduce the antisymmetry of the spin-singlet
pairing matrix under exchange. We choose a real amplitude $\Delta_0$ for convenience.

The pairing changes sign under a $C_4$ rotation and belongs to a $B_{1g}$ representation of the associated point group. The minus sign comes entirely from the matrix structure since the transformation leaves the $s$-wave form factor $g_{xz^2-y^2}$ invariant.

In order to understand the appearance of a full gap in this $B_{1g}$ pairing we can exploit the analogy between the two-orbital system and $^3$He with spin-triplet pairing. As in Ref. [27] we can define an isospin quantum number for the $\xi$-matrix as 

$$H = \sum_k \psi_k^\dagger \left( \xi_+^\dagger(k) \tau_0 + \overline{B}_k \cdot \vec{\tau} \right) \otimes \gamma_3
+ \left( \overline{d}_k \cdot \vec{\tau} \right) \otimes \gamma_1 \right) \psi_k.
\tag{2}$$

where

$$\overline{B}(k) = (\xi_{xy}(k), 0, \xi_z^-(k))
\quad \overline{d}(k) = (0, 0, \Delta_0 g_{xz^2-y^2}(k)).
\tag{3}$$

As observed in Ref. [27] the $\overline{B}(k)$ factor is analogous to a $k$-dependent spin-orbit coupling for $^3$He. We mention some differences. For $^3$He, the spin-orbit coupling forces the spin and spatial degrees of freedom to lock, ensuring that the pairing transform under an element of the point group $g$ as [28]

$$g \overline{d}(k) = \overline{D}_G^+(g) \overline{d}(\overline{D}_G^-(g) \overline{k}).$$

The matrices $\overline{D}_G^+(g)$ and $\overline{D}_G^-(g)$ belong to irreducible representations of the point group even and odd under inversion respectively. In the Fe-based superconductors the transformation in Eq. [3] holds even when there is no isospin-orbit coupling $\overline{B}(k)$ because the spatial and orbital degrees of freedom are always locked. In addition, spin-singlet pairing does not force $\overline{d}(k)$ to be odd under space inversion.

To see the consequences of the non-trivial structure of the pairing in orbital space, we write the square of the Hamiltonian matrix:

$$H^2 = \sum_k \left[ \xi_+^\dagger(k) \tau_0 + \left( \overline{B}_k \cdot \vec{\tau} \right) \right] \otimes \gamma_0 + \left| \overline{d}(k) \right|^2 \gamma_0 \otimes \gamma_0
+ 2i \left( \overline{B}(k) \times \overline{d}(k) \right) \cdot \vec{\tau} \otimes i \gamma_2.
\tag{4}$$

The first two terms are the squares of the free particle Hamiltonian and of a pairing contribution with no structure in orbital space. The last term is a consequence of the non-commuting free particle and pairing parts of the Hamiltonian. When the commutator is zero this term vanishes while the other two terms reduce to a simple BCS-like matrix, where the anisotropy in the resulting dispersion is entirely determined by the symmetry of the form factor. For example, a $d_{x^2-y^2} \times \tau_0, B_{1g}$ pairing will generate nodes along the $k_x = k_y$ lines in the BZ whereas a $s_{z^2} \times \tau_0, A_{1g}$ produces nodes at $k_{x/y} = \pm \pi/2$ in the 1-Fe BZ. As is apparent from Eq. [4] the non-Abelian term effectively mixes two BCS-like states and can generate a fully gapped dispersion even when the pairing is of $B_{1g}$ type.

Since the Nambu matrices $\gamma_0$ and $i \gamma_2$ commute, $H^2$ in Eq. [4] can be trivially brought to block diagonal form. The quasiparticle dispersion is given by

$$E_{\pm}(k) = \sqrt{\xi_+^2(k) + \left| \overline{B}(k) \right|^2 + \left| \overline{d}(k) \right|^2 \pm \frac{4 \xi_+^2(k) \left| \overline{B}(k) \right|^2 + 4 \left| \overline{B}(k) \times \overline{d}(k) \right|^2}{\sqrt{\left( \xi_+^2(k) + \left| \overline{d}(k) \right|^2 \sin^2 \phi(k) \right)^{1/2} + \left| \overline{d}(k) \right|^2 (1 - \sin^2 \phi(k))}}
\tag{5}$$

$$\sin \phi(k) = \frac{\xi_{xy}(k)}{\sqrt{\xi_+^2(k) + \xi_{xy}^2(k)}}$$
\tag{6}

From Eq. [5] and general $\overline{d}(k)$ we see that the quasiparticle dispersion can vanish only when both terms in the square root vanish. The second of these goes to zero when either $\sin \phi(k) = 1$ or, trivially, when $\left| \overline{d}(k) \right| = 0$. When $\sin \phi(k) = 1$, the dispersion reduces to

$$E_{\pm}(k) = \sqrt{\xi_+^2(k) + \left| \overline{d}(k) \right|^2 \pm \left| \overline{B}(k) \right|},
\tag{7}$$

which can acquire accidental nodes for general $k$. On the Fermi surface however, we have $\xi_+^2(k) = \left| \overline{B}(k) \right|^2$ and the expression above is zero only when $\left| \overline{d}(k) \right| = 0$, that is,
along the lines given by the symmetry of the form factor. For our particular choice of $\hat{d}(k)$ (Eq. 3) corresponding to the $s_{x^{2}y^{2}} \times \tau_{3}, B_{1g}$ pairing, these are the $k_{x} = \pm \frac{\pi}{2}, k_{y} = \pm \frac{\pi}{2}$ lines. We conclude that while this type of pairing can generate accidental nodes, it guarantees zero energy states only when the Fermi surface intersects the nodes of the form factor. When the Fermi surface is away from these points, the dispersion will be generally gapped with an enhanced anisotropy relative to the commuting case.

The expression for the quasi-particle dispersion above can also be used to tentatively understand how a pairing of the $s_{x^{2}y^{2}} \times \tau_{3}$ type can become energetically competitive w.r.t. one of a pure $s_{x^{2}y^{2}} \times \tau_{0}, d_{x^{2}−y^{2}} \times \tau_{0}$ or even the combined $s + id$ type. In all these cases, the $|\hat{B}(k) \times \hat{d}(k)|^{2}$ vanishes or equivalently there is no inter-band pairing. The putative gain in energy can be accounted for by the additional anisotropy introduced by the non trivial matrix structure in the orbital space. Although this does not ensure that the $s_{x^{2}y^{2}} \times \tau_{3}$ pairing is always dominant since the minimization of the free-energy generally depends on the specifics of the dispersion and the pairing, the argument above sketches how such a combined state can in principle become leading.

We proceed to comment on another important property of the $s_{x^{2}y^{2}} \times \tau_{3}$ pairing function. In the band basis the pairing matrix is given by

$$\hat{\Delta}(k) = -\Delta_{0} g x^{2}y^{2}(k) \left(\frac{\xi_{-}(k)}{\sqrt{\xi_{-}^{2}(k) + \xi_{x^{2}y^{2}}^{2}(k)}} \otimes \alpha_{3} + \frac{\xi_{x^{2}y^{2}}(k)}{\sqrt{\xi_{-}^{2}(k) + \xi_{x^{2}y^{2}}^{2}(k)}} \otimes \alpha_{1}\right)$$

However, we find that the key features of the simplified system survive in the full five-orbital scenario.

III. ORBITALLY DIFFERENTIATED EXCHANGE AND PAIRING IN A 5-ORBITAL $t-J_{1}−J_{2}$ MODEL

We now turn to the question of how the $s_{x^{2}y^{2}} \times \tau_{3}, B_{1g}$ pairing state can become energetically competitive. We also partially address the issue of its relation to the more conventional $s$– and $d$–wave pairing channels. To make our discussion concrete, we turn to the five-orbital $t−J_{1}−J_{2}$ model.

The use of such a model is motivated by the bad metal nature of the normal state for the iron pnictides as probed by optical conductivity experiments [2] and by the the proximity to the insulating state in the case of the iron selenides. These properties suggest the placement of the two classes of materials in the vicinity of a Mott insulating transition [6].

We proceed to describe the effective $t−J_{1}−J_{2}$ model we used in our calculations. These were done for an effective 1-Fe unit cell or equivalently in an unfolded BZ [29]. To simplify our analysis, we consider the free-particle part for all $d$ orbitals but restrict the exchange couplings and hence the pairing interactions to $d_{xz}, d_{yz},$ and $d_{xy}$ orbitals only. Specifically, the Hamiltonian in the orbital basis is given by

$$H = -\sum_{i<j} (t_{ij}^{\alpha\beta} c_{i\alpha}^{\dagger} c_{j\beta} + H.C.) + \sum_{i,\alpha} (\epsilon_{i\alpha} - \mu) n_{i\alpha} + \sum_{<ij>,\alpha,\beta} J_{1}^{\alpha\beta} \left( S_{i\alpha} \cdot S_{j\beta} - \frac{1}{4} n_{i\alpha} n_{j\beta} \right) + $$

$$+ \sum_{<<ij>>,\alpha,\beta} J_{2}^{\alpha\beta} \left( S_{i\alpha} \cdot S_{j\beta} - \frac{1}{4} n_{i\alpha} n_{j\beta} \right)$$

$J_{2}^{xz/yz} \neq J_{2}^{xy}_{1,2}$

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where \( \alpha, \beta \in \{1, 2, 3, 4, 5\} \) are orbital indices representing all five \( d_{xz}, d_{yz}, d_{x^2-y^2}, d_{xy}, \) and \( d_{3z^2-r^2} \) orbitals, \( \epsilon_i \) are the on-site energies, and \( \mu \) is the chemical potential. The local moments can be written as \( S_{i\alpha} = \sum_{\alpha'} \frac{1}{2} C_{i\alpha}^\dagger \sigma_{\alpha\alpha'} C_{i\alpha'} \) in terms of the conduction electrons. We take only intra-orbital exchange (\( \alpha = \beta \)) and set \( J_{1(2)}^{x^2-y^2} = J_{1(2)}^{3z^2-r^2} = 0 \). We consider general exchange couplings which reflect the possible orbital selectivity by allowing \( J_{xz,xz} = J_{yz,yz} \neq J_{xy,xy} \) (Eq. 10).

The interactions in Eq. 9 can be decomposed into nearest-neighbor (NN) and next-nearest neighbor (NNN) singlet pairings. The double occupancy constraint can be incorporated in practice through a band renormalization by the doping factor \( \delta = \sum_{i,s} n_{i\alpha s} - 2 \). The pairing Hamiltonian can be solved numerically in a 1-Fe unit cell mean-field calculation by varying the exchange couplings. For more details on the method, we refer the reader to Refs. 6 and 11. Here we also define an exchange orbital anisotropy factor \( A_O = \frac{J_{xy,xy}}{J_{xz,xz}} = \frac{J_{yz,yz}}{J_{xz,xz}} \) and an orbital-independent NN-NNN exchange anisotropy factor \( A_L = \frac{J_{xy,xy}}{J_{xz,xz}} \) for all three non-zero intra-orbital exchange couplings for \( d_{xz}, d_{yz}, \) and \( d_{xy} \).

We also calculate the dynamical spin susceptibility in the superconducting state given by

\[
\chi(q, i\omega_n) = \sum_{\alpha\beta} \chi_{\alpha\beta}(q, i\omega_n),
\]

where

\[
\chi_{\alpha\beta}(q, i\omega_n) = \sum_{\gamma} \left[ I + J(q) \sum_{\delta\mu} \chi_{0,\delta\mu}(q, i\omega_n) \right]^{-1} \times \chi_{\alpha\gamma \beta}(q, i\omega_n),
\]

\[
\chi_{0,\alpha\beta}(q, i\omega_n) = \int_1^{1/T} d\tau e^{i\omega_n \tau} \left\langle T \left[ S_{\alpha}^-(\tau) S_{\beta}^+(0) \right] \right\rangle,
\]

and,

\[
J(q) = J_2^\frac{1}{2} (\cos q_x + \cos q_y) + J_2 \cos q_x \cos q_y.
\]

To explore the zero-temperature superconducting phases corresponding to different classes of Fe-based materials we consider the associated free-electron dispersion for \( K_\text{F}Fe_2\text{Se}_2 \), iron pnictides and single-layer FeSe. We subsequently tune the exchange couplings for various NN-NNN and orbital anisotropy ratios (\( A_L \) and \( A_O \)) and determine the real-space pairing functions.

### IV. ORBITAL SELECTIVITY AND THE ZERO TEMPERATURE SUPERCONDUCTING STATE WITH DOMINANT \( s \times \tau_3 \) PAIRING

We are now in position to discuss how the intermediate pairing state emerges in a range of parameters where the \( s^- \) and \( d^- \)–wave pairing channels are quasi-degenerate. Within the 5-orbital \( t - J_1 - J_2 \) model, we focus on the case with a kinetic part appropriate for \( K_\text{F}Fe_2\text{Se}_2 \) although similar behavior emerges in the iron pnictides and single-layer FeSe. All quantities are given in units of a half-bandwidth \( D/2 \), which already incorporates a doping-dependent renormalization of the kinetic energy.

The \( s_{x^2-y^2} \times \tau_3 \) pairing becomes dominant over a finite range of the tuning parameters (\( A_L \) and \( A_O \)). For small \( A_O \) and \( A_L \), the leading pairing occurs in the \( s_{x^2-y^2} \times \tau_0, A_{1g} \) (\( "s^\pm" \))
channel. In this regime the strongest contribution comes from the NNN exchange coupling in the $d_{xz}$, $d_{yz}$ sector. By increasing the $J_1 - J_2$ ratio $A_L > 1$ i.e. moving along the horizontal axis, the $d_{x^2-y^2} \times \tau_0, B_{1g}$ in the $d_{xz}, d_{yz}$ subspace favored by a large NN coupling eventually takes over. These two limiting phases are consistent with the results obtained in Ref. 11 where $A_O$ was set to unity for all values of $A_L$. For the intermediate values of the the $J_1 - J_2$ anisotropy factor $0.9 \leq A_L \leq 1.1$, near the regime where the above two pairing channels are quasi-degenerate, the intermediate $s_{x^2-y^2} \tau_0, B_{1g}$ pairing state emerges as the dominant channel. The phase diagram for the alkaline iron selenides is shown in Fig. 2(a). Note that the $s_{x^2-y^2} \tau_0$ phase also persist for a finite range of $A_O < 0.3$. Similar phase diagrams are obtained for the iron pnictides and single-layer FeSe shown in Figs. 2(b) and 7(Appendix) respectively. A typical dominant $s_{x^2-y^2} \tau_0, B_{1g}$ pairing case is shown in Fig. 5 in the Appendix for a number of subleading symmetry-allowed channels [8] for alkaline iron selenide dispersion with fixed $J_2 = 1.5$, $A_O = 0.3$ and varying $A_L$ (horizontal axis).

The Fermi surface and the sign of the band-diagonal pairing for the band generating the pockets around $(\pm \pi, 0) (\delta)$ and $(0, \pm \pi)$ for the alkaline iron selenides with $J_2 = 1.5, A_O = 0.3$ and $A_L = 0.9$ is shown in Fig. 3(a). The sign of the real pairing was obtained by projecting the full pairing matrix onto the band basis. The dominant contribution is from the $s_{x^2-y^2} \tau_3$ component but all sub-leading channels (see Fig. 6) were included. The arbitrary phase which results from the global $U(1)$ symmetry breaking is subtracted from all components ensuring that the resulting pairing is real. We see that the band-diagonal pairing does indeed change sign between the two pockets at the edge of the BZ zone. In Fig. 3(b) we show the gap at the Fermi surface as a function of winding angle $\theta$. The figure clearly illustrates the node-less dispersion as the gap is finite for all $\theta$.

The free-particle dispersion considered here does not produce any Fermi pockets close to $\Gamma$ in the 1-Fe BZ. This is in contrast to ARPES experiments on K$_x$Fe$_2$As$_2$ [30] which show a small electron pocket near $\Gamma$. Because this small electron pocket has very small spectral weight, it is to be expected that even if such a pocket were included, the dominant $s_{x^2-y^2} \tau_3$ pairing will still arise; moreover, the gap on this Fermi pocket will be node-less as discussed in the two-orbital case. To substantiate this, we consider the results for the iron pnictides class, which do have significant (albeit hole) Fermi pockets at the zone center yet exhibit a full gap. In Figs. 4(a), (b) we show the Fermi surface and the gaps as functions of winding angle $\theta$ for $A_O = 0.5$ and $A_L = 1.3$ corresponding to a dominant $s_{x^2-y^2} \tau_3$ pairing. The gap along $\beta$ is finite and exhibits an anisotropy consistent with the two orbital results in Eq 5. In the latter case, at winding angle $\theta = 0$, $\sin \phi = 0$ and the spectrum has a minimum/maximum gap for $E_{+/-}$. As $\theta$ is increased the $|\vec{B}(k) \times \vec{d}(k)|^2$ term increases reaching a maximum at $\theta = \pi/4$. Here the gap is maximum/minimum for $E_{+/-}$. This is consistent with the anisotropy in the gap shown in Fig. 4. We stress that the fully gapped dispersion is not the result of a sub-leading s-wave $A_{1g}$ channel. As in the alkaline iron selenide case, all $A_{1g}$ pairing functions are strongly suppressed ($O(10^{-3})$) at this point (See Fig. 6 in the Appendix).

FIG. 3. (a) The Fermi surface (solid line) and the real intra-band pairing for the band generating the $\delta$ pockets at the edge of the 1-Fe unit BZ for a dispersion typical of the alkaline iron selenides. Note the clear change in sign between pockets separated by the BZ diagonal. The dashed arrow indicates the $q = (\pi, \pi/2)$ wave-vector associated with the resonance in the spin spectrum found in experiment [5]. (b) The size of the gap along the $\delta$ pocket. Both figures are for $J_2 = 1.5$, $A_O = 0.3$, $A_L = 0.9$ with dominant $s_{x^2-y^2} \tau_3$ pairing.
FIG. 4. (a) Fermi surface for the iron pnictides which includes hole pockets with dominant $s_{x^2-y^2} \times \tau_3, B_{1g}$ close to $\Gamma$ for $J_2 = 1, A_L = 1.3, A_O = 0.5$. For the tight-binding parameters used please consult Ref. 6. (b) The gaps along the $\beta$ and $\delta$ pockets close to the center and edge of the 1-Fe BZ. A similar gap forms around the $\alpha$ pocket.

five-orbital $t - J_1 - J_2$ model has a behavior very similar to the two-orbital case and that it can be considered a viable candidate for the alkaline iron selenide superconductors.

In Fig. 5 we show the spin-excitation spectrum calculated for the alkaline iron selenides with dominant $s_{x^2-y^2} \times \tau_3, B_{1g}$ pairing at wave-vector $q = (\pi, \pi/2)$ for $J_2 = 1.5$. We note the complicated frequency behavior which can be traced to the anisotropy in the effective gap affecting both the coherence factors and the position of minimum in quasi-particle energy. We show the minimum and maximum p-h thresholds corresponding to twice the minimum and twice the maximum gaps. As suggested by Figs. 3(a) and (b), states connected by $q = (\pi, \pi/2)$ would correspond to a p-h threshold given roughly by the sum of the minimum and maximum gap $\approx 0.41$. A sharp feature appears below this threshold at $\omega \approx 0.36$, confirming the existence of the resonance for $q = (\pi, \pi/2)$ as found in experiments on the alkaline iron selenides [5].

V. CONCLUSION

We have shown that, through orbital selectivity, an intermediate pairing state emerges in the regime where the conventional $s-$ and $d-$wave pairing channels are quasi-degenerate. This superconducting state is energetically competitive, as illustrated by our calculations in a five-orbital $t - J_1 - J_2$ model with orbital-selective exchange couplings.

This intermediate pairing state inherits aspects of the properties of both the conventional $s-$ and $d-$wave pairing channels. As we have explicitly illustrated in the case of $d_{xz}, d_{yz}$ orbital subspace, this orbital-selective $s \times \tau_3, B_{1g}$ pairing state has the $s$-wave form factor but also has a $B_{1g}$ symmetry. Going beyond this two-orbital subspace, the contributions of the other orbitals mix into the pairing function. Nonetheless, the pairing state still incorporates some of the properties of both the $s-$ and $d-$wave pairing states.

For the iron-based superconductors, this intermediate state is of considerable phenomenological interest. In particular, it has the salient properties observed in the alkaline iron selenides. These properties include seemingly contradictory as-
pects. The single-particle excitations are fully gapped, as observed in ARPES experiments. At the same time, the pairing function changes sign across the electron Fermi surfaces at the BZ boundary, as indicated by the resonance peak near $(\pi, \pi/2)$ in the inelastic neutron scattering experiments.

More generally, a conventional means of relieving quasi-degenerate $s-$ and $d-$wave pairing states is to linearly superpose the two into an $s + id$ state. This state, breaking the time-reversal symmetry, would be stabilized at temperatures sufficiently below the superconducting transition temperature. The mechanism advanced here preserves the time-reversal symmetry, and represents a new means to relieve the quasi-degeneracy through the development of orbital selectivity.

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In Appendix A: Supplementary Material

The components of the dispersion part of the two-orbital Hamiltonian discussed in Sec. [I] are given by

\begin{align}
\xi_{k+} &= -(t_1 + t_2) \left( \cos k_x + \cos k_y \right) - 4t_3 \cos k_x \cos k_y, \\
\xi_{k-} &= -(t_1 - t_2) \left( \cos k_x - \cos k_y \right), \\
\xi_{kxy} &= -4t_4 \sin k_x \sin k_y,
\end{align}

where $t_1, t_2$ and $t_3$ are tight-binding parameters. The parameters of the two-orbital and five-orbital models are those given in Ref. [6] The free-band dispersion is given by

\begin{equation}
\xi_{\pm}(k) = \xi_+(k) \pm \sqrt{\xi_+^2(k) + \xi_{xy}^2(k)}. 
\end{equation}

In the single-band BCS case, the leading contribution to the dynamical spin susceptibility (see Eq. [11] for the multi-orbital case) depends [31, 32] on terms like

\begin{equation}
\chi_0(q, \omega) = \frac{1}{N} \sum_k \left[ \frac{1}{2} \left( 1 - \frac{\epsilon_{k+q} + \Delta_{k+q} \Delta_k}{E_{k+q} + E_{k}} \right) \frac{f(E_{k+q}) + f(E_k) - 1}{\omega - (E_{k+q} + E_k) + i0^+} \right].
\end{equation}

where $\epsilon$’s and $E$’s are the free particle and the BdG quasi-particle dispersions respectively. The existence of a sharp feature in the RPA spectrum below the particle-hole threshold (given roughly by twice the characteristic gap magnitude $2\Delta$) is related to the sign of the $\Delta_{k+q}$ term in the coherence factor in Eq. [A3]. Close to the Fermi surface, when the sign is positive, the coherence factor suppresses the real part of $\chi_0(q, \omega)$ and consequently, inhibits the appearance of a resonance. By contrast, when $\Delta_{k+q}$ and $\Delta_k$ have opposite signs, the resonance can form. For multi-band systems with non-trivial gap dependence, the situation is obviously more complicated. Nonetheless, the occurrence of the spin resonance is typically still connected with a sign change in the gap function.

[1] G.R. Stewart, Non-Fermi-liquid behavior in d- and f-electron metals, Rev. Mod. Phys. 73, 797 (2001).
[2] M. M. Qazilbash, J. J. Hamlin, R. E. Baumbach, Lijun Zhang, D. J. Singh, M. B. Maple, and D. N. Basov, Electronic correlations in the iron pnictides, Nat. Phys. 5, 647 (2009).
[3] Q. Si and E. Abrahams, Strong Correlations and Magnetic Frustration in the High Tc Iron Pnictides, Phys. Rev. Lett 101, 076401 (2008).
[4] Z. P. Yin, K. Haule, and G. Kotliar, Magnetism and charge dynamics in iron pnictides, Nat. Phys. 7, 294 (2011).
[5] P. Dai, Antiferromagnetic order and spin dynamics in iron-based superconductors, (arXiv:1503.02530v1) 1 (2015).
[6] R. Yu, P. Goswami, Q. Si, P. Nikolić, and J.-X. Zhu, Superconductivity at the border of electron localization and itinerancy, Nat. Commun. 4, 2783 (2013).
[7] K. Seo, B. A. Bernevig, and J. P. Hu, Pairing Symmetry in a Two-Orbital Exchange Coupling Model of Oxypnictides, Phys. Rev. Lett., 101, 206404 (2008).
[8] P. Goswami, P. Nikolic, and Q. Si, Superconductivity in multi-orbital $t-J_1-J_2$ model and its implications for iron pnictides, Europhys. Lett. 91, 37006 (2010).
[9] F. Wang and D.-H. Lee, The Electron-Pairing Mechanism of Iron-Based Superconductors, Science 332, 200 (2011).
[10] P. W. Anderson, Is There Glue in Cuprate Superconductors?, Science 316, 1705 (2007).
[11] R. Yu, J.-X. Zhu, and Q. Si, Orbital-selective superconductivity,
gap anisotropy, and spin resonance excitations in a multiorbital $t - J_1 - J_2$ model for iron pnictides, Phys. Rev. B 89, 024509 (2014).

[12] Z. P. Yin, K. Haule, and G. Kotliar, Spin dynamics and orbital-antiphase pairing symmetry in iron-based superconductors, Nat. Phys. 10, 845 (2014).

[13] C. Zhang, L. W. Harriger, Z. Yin, W. Lv, M. Wang, G. Tan, Y. Song, D.L. Abernathy, W. Tian, T. Egami, et al., Measurement of an Anisotropic Energy Gap for Underdoped Superconducting NaFeO$_{0.95}$Co$_{0.05}$As Using Inelastic Neutron Scattering, Phys. Rev. Lett. 111, 207002 (2013).

[14] C. Zhang, J. T. Park, X. Lu, R. Yu, Y. Li, W. Zhang, Y. Zhao, J. W. Lynn, Q. Si, and P. Dai, Neutron spin resonance as a probe of superconducting gap anisotropy in partially detwinned electron underdoped NaFeO$_{0.95}$Co$_{0.05}$As, Phys. Rev. B 91, 104520 (2015).

[15] D. Mou, S. Liu, X. Jia, J. He, Y. Peng, L. Zhao, L. Yu, G. Liu, S. He, X. Dong, et al., Distinct Fermi Surface Topology and Nodeless Superconducting Gap in a (Tl$_{0.58}$Rb$_{0.42}$)Fe$_{1.72}$Se$_2$ Superconductor, Phys. Rev. Lett. 106, 107001 (2011).

[16] X.-P. Wang, T. Qian, P. Richard, P. Zhang, J. Dong, H.-D. Wang, C.-H. Dong, M.-H. Fang and H. Ding, Strong nodeless pairing on separate electron Fermi surface sheets in (Tl, K)Fe$_{1.76}$Se$_2$ probed by ARPES, Europhys. Lett. 93, 57001 (2011).

[17] M. Xu, Q. Q. Ge, R. Peng, Z. R. Ye, Juan Jiang, F. Chen, X. P. Shen, B. P. Xie, Y. Zhang, A. F. Wang, et al., Evidence for an s-wave superconducting gap in K$_2$Fe$_{2-y}$Se$_2$ from angle-resolved photoemission, Phys. Rev. B 85, 220504 (2012).

[18] X.-P. Wang, P. Richard, X. Shi, A. Roekeghem, Y.-B. Huang, E. Razzoli, T. Qian, E. Rienks, S. Thirupathaiah, H.-D. Wang, et al., Observation of an isotropic superconducting gap at the Brillouin zone center of Tl$_{0.63}$K$_{0.37}$Fe$_{1.75}$Se$_2$, Europhys. Lett. 99, 67001 (2012).

[19] J. T. Park, G. Friemel, Yuan Li, J.-H. Kim, V. TSurkan, J. Deisenhofer, H.-A. Krug von Nidda, A. Loidl, A. Ivanov, B. Keimer, et al., Magnetic Resonant Mode in the Low-Energy Spin-Excitation Spectrum of Superconducting Rb$_2$Fe$_{4}Co$_4$S$_5$ Single Crystals, Phys. Rev. Lett. 107, 177005 (2011).

[20] G. Friemel, J. T. Park, T. A. Maier, V. TSurkan, Yuan Li, J. Deisenhofer, H.-A. Krug von Nidda, A. Loidl, A. Ivanov, B. Keimer, et al., Reciprocal-space structure and dispersion of the magnetic resonant mode in the superconducting phase of Rb$_2$Fe$_{2-y}$Se$_2$ single crystals, Phys. Rev. B 85, 140511(R) (2012).

[21] R.Yu and Q.Si, Mott transition in Multiorbital Models for Iron Pnictides, Phys. Rev. B 84, 235115 (2011).

[22] R. Yu, J.-X. Zhu, and Q. Si, Orbital-Selective Mott Phase in Multiorbital Models for Alkaline Iron Selenides K$_{1-x}$Fe$_{2-y}$Se$_2$ Phys. Rev. Lett. 110, 146402 (2013).

[23] L. de Medici, G. Giovannetti, and M. Capone, Selective Mott Physics as a Key to Iron Superconductors, Phys. Rev. Lett. 112, 177001 (2014).

[24] M. Yi, D. H. Lu, R. Yu, S. C. Riggs, J.-H. Chu, B. Lv, Z. K. Liu, M. Lu, Y.-T. Cui, M. Hashimoto, et al., Observation of Temperature-Induced Crossover to an Orbital-Selective Mott Phase in A$_2$Fe$_{2}$Se$_2$(A=K, Rb) Superconductors, Phys. Rev. Lett. 110, 067003 (2013).

[25] M. Yi et al., unpublished (2015).

[26] S. Raghu, Xiao-Liang Qi, Chao-Xing Liu, D. J. Scalapino, and Shou-Cheng Zhang, Minimal two-band model of the superconducting iron oxypnictides, Phys. Rev. B 77, 220503(R) (2008).
[27] T. Tzen Ong, P. Coleman, and J. Schmalian, *Entangled Orbital Triplet Pairs in Iron-Based Superconductors*, arXiv:1410.3554v1 (2014).

[28] M. Sigrist, K. Ueda, *Phenomenological theory of unconventional superconductivity*, Rev. Mod. Phys. 63, 239 (1991).

[29] E. M. Nica, R. Yu, and Q. Si, *Glide reflection symmetry, Brillouin zone folding and superconducting pairing for P4/nmm space group*, to be published (2015).

[30] Y. Zhang, L. X. Yang, M. Xu, Z. R. Ye, F. Chen, C. He, H. C. Xu, J. Jiang, B. P. Xie, J. J. Ying, *et al.*, *Nodeless superconducting gap in A3Fe2Se2(A=K,Cs) revealed by angle-resolved photoemission spectroscopy*, Nat. Mater. 10, 273 (2011).

[31] M. Eschrig, *The effect of collective spin-1 excitations on electronic spectra in high-Tc superconductors*, Adv. Phys. 55, 47 (2006).

[32] H. F. Fong, B. Keimer, P. W. Anderson, D. Reznik, F. Doan, and I. A. Aksay, *Phonon and Magnetic Neutron Scattering at 41 meV in YBa2Cu3O7*, Phys. Rev. Lett. 75, 316 (1995).