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Superconductivity in multi-orbital t - J_1 - J_2 model and its implications for iron pnictides

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Abstract – Motivated by the bad metal behavior of the iron pnictides, we study a multi-orbital t - J_1 - J_2 model and investigate possible singlet superconducting pairings. Magnetic frustration by itself leads to a large degeneracy in the pairing states. The kinetic energy breaks this into a quasi-degeneracy among a reduced set of pairing states. For small electron and hole Fermi pockets, an A_{1g} state dominates over the phase diagram but a B_{1g} state has close-by energy. In addition to the nodeless A_{1g} $s_{x^2-y^2}$ channel, the nodal A_{1g} $s_{x^2+y^2}$ and B_{1g} $d_{x^2-y^2}$ channels are also competitive in the magnetically frustrated $J_1 \sim J_2$ parameter regime. An $A_{1g} + iB_{1g}$ state, which breaks time-reversal symmetry, occurs at low temperatures in part of the phase diagram. Implications for the experiments in the iron pnictides are discussed.

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Introduction. – The discovery of high-temperature superconductivity in the iron pnictides [1–3] has spurred tremendous experimental and theoretical interest in these systems. While they are not Mott insulators, the undoped iron pnictides are nonetheless “bad metals”. This fact has motivated the placement of these systems in an intermediate coupling regime close to the boundary between Mott localization and itinerancy [4–6], where the Coulomb interactions bring about non-perturbative effects in the form of incipient lower and upper Hubbard bands. Accordingly, the low-energy Hamiltonian contains quasi-localized moments with J_1 - J_2 superexchange interactions [5–11], and it corresponds to an effective multi-band t - J_1 - J_2 model for the carrier-doped systems. Importantly, $J_1 \sim J_2 > J_1/2$ [5,7–9,12] so that the system not only has a $(\pi, 0)$ antiferromagnetic order, as seen experimentally [13], but also exhibits strong magnetic frustration. The incipient Mott picture is supported by the observations of both the Drude weight suppression [14–16] and the temperature-induced spectral-weight transfer [15,17,18]. In addition, the quasi-localized moments are supported by the inelastic neutron scattering experiments; ref. [19], for instance, observed zone-boundary spin waves and showed that J_1 is indeed comparable to J_2 . (By contrast, the Fermi surface in the magnetically ordered state

does not directly probe the strength of electron correlations [6].) Alternatively, perturbative treatments [20,21] of the Coulomb interactions have been used to study the magnetism of the iron pnictides. The weak-coupling approaches, mostly based on spin fluctuations, have been extensively used to address the superconductivity [21–26]. By contrast, strong-coupling studies of superconductivity have been more limited [27–30].

Experimentally, the pairing symmetry in the iron pnictides has remained inconclusive. The angle-resolved photoemission [31,32] (ARPES) and the Andreev spectroscopy [33] results suggest a nodeless gap. In contrast the nuclear magnetic resonance (NMR) [34] and some penetration depth [35] measurements suggest a nodal gap. The experimental results seem to vary among pnictide compounds. As an example, the P-doped BaFe_2As_2 appears to have nodal gaps [36,37] and this is in strong contrast with its K-doped counterpart.

In this letter we address the pairing in the pnictides from the incipient Mott approach, and treat the competing pairing channels on an equal footing. We are particularly motivated to consider the effect of the $J_1 \sim J_2$ magnetic frustration, and show that it leads to a quasi-degeneracy among several pairing states.

The Hamiltonian is given by

$$H = H_t + H_{J_1} + H_{J_2}. \quad (1)$$

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The kinetic part is $H_t = -\sum_{i<j,\alpha,\beta,s} t_{ij}^{\alpha\beta} c_{i\alpha s}^\dagger c_{j\beta s} + \text{h.c.} - \mu \sum_{i,\alpha} n_{i\alpha}$, where $c_{i\alpha s}^\dagger$ creates an electron at site i , with orbital α and spin projection s ; μ is the chemical potential and $t_{ij}^{\alpha\beta}$ the hopping matrix. The nearest-neighbor (n.n., $\langle ij \rangle$) and next-nearest-neighbor (n.n.n., $\langle\langle ij \rangle\rangle$) exchange interactions are, respectively, $H_{J_1} = \sum_{\langle ij \rangle, \alpha, \beta} J_1^{\alpha\beta} (\vec{S}_{i\alpha} \cdot \vec{S}_{j\beta} - \frac{1}{4} n_{i\alpha} n_{j\beta})$, and $H_{J_2} = \sum_{\langle\langle ij \rangle\rangle, \alpha, \beta} J_2^{\alpha\beta} (\vec{S}_{i\alpha} \cdot \vec{S}_{j\beta} - \frac{1}{4} n_{i\alpha} n_{j\beta})$. Here, $\vec{S}_{i\alpha} = \frac{1}{2} \sum_{s,s'} c_{i\alpha s}^\dagger \vec{\sigma}_{ss'} c_{i\alpha s'}$ and $n_{i\alpha} = \sum_s c_{i\alpha s}^\dagger c_{i\alpha s}$, with $\vec{\sigma}$ representing the Pauli matrices operating on the spin indices. The above Hamiltonian is augmented by the appropriate occupancy constraint for the fermions. Note that, while the nearest-neighbor interaction has been evidenced to be spatially anisotropic in the $(\pi, 0)$ collinear antiferromagnetic state [8,19], it is expected to be isotropic in the tetragonal paramagnetic phases and this is consistent with spin dynamical measurements [38,39].

Two-orbital model. – We will first consider a two-orbital model, retaining only the $d_{xz}(\alpha=1)$ and $d_{yz}(\alpha=2)$ orbitals, and later we consider a five-orbital model to better address the fermiology [21,26,40]. We further assume $J_i^{\alpha,\beta} = J_i \delta_{\alpha,\beta}$, and $J_i > 0$, and will subsequently address the role of inter-orbital exchange couplings.

Under the tetragonal point group symmetry transformations (D_{4h}), d_{xz} and d_{yz} orbitals transform, respectively, as x and y coordinates. The kinetic-energy part of the Hamiltonian is invariant under all point group symmetry operations (A_{1g}) and has the following form in the extended Brillouin zone: $H_0 = \sum_{\mathbf{k},s} \psi_{\mathbf{k}s}^\dagger [\xi_{\mathbf{k}+}\tau_0 + \xi_{\mathbf{k}-}\tau_z + \xi_{\mathbf{k}xy}\tau_x] \psi_{\mathbf{k}s}$, where $\mathbf{k} = (k_x, k_y)$ and $\psi_{\mathbf{k}s}^\dagger = (c_{\mathbf{k}1s}^\dagger, c_{\mathbf{k}2s}^\dagger)$. The identity and Pauli matrices (τ_0, τ_i) operate on the orbital indices, and $\xi_{\mathbf{k}+} = -(t_1 + t_2)(\cos k_x + \cos k_y) - 4t_3 \cos k_x \cos k_y - \mu$, $\xi_{\mathbf{k}-} = -(t_1 - t_2)(\cos k_x - \cos k_y)$, $\xi_{\mathbf{k}xy} = -4t_4 \sin k_x \sin k_y$ are, respectively, A_{1g} , B_{1g} , B_{2g} functions. The band dispersion relations $\mathcal{E}_{\mathbf{k}\pm} = \xi_{\mathbf{k}+} \pm \sqrt{\xi_{\mathbf{k}-}^2 + \xi_{\mathbf{k}xy}^2}$, give rise to two electron pockets at $\mathbf{k} = (\pi, 0)$ and $(0, \pi)$, and two hole pockets at $\mathbf{k} = (0, 0)$ and (π, π) . The carrier doping $\delta = |\sum_{\alpha} n_{i\alpha} - 2|$. Mostly we use the minimal tight-binding model of ref. [41], $t_1 = -t$, $t_2 = 1.3t$, $t_3 = t_4 = -0.85t$ obtained from a fitting of the LDA bands.

Magnetic frustration and degeneracy of pairing states. We start from the case with a vanishing kinetic energy, in order to highlight the connection between magnetic frustration and enhanced degeneracy of pairing states. We define the intra-orbital spin-singlet pairing operators $\Delta_{\mathbf{e},\alpha\alpha} = \langle c_{i\alpha\uparrow} c_{i+\mathbf{e}\alpha\downarrow} - c_{i\alpha\downarrow} c_{i+\mathbf{e}\alpha\uparrow} \rangle / 2$, where $\mathbf{e} = \hat{x}, \hat{y}, \hat{x} \pm \hat{y}$. Without the kinetic term, the problem decouples in the orbital basis and we can drop the orbital indices. When J_1 dominates, two degenerate pairing states $s_{x^2+y^2}$ and $d_{x^2-y^2}$, respectively defined by the pairing functions $g_{x^2 \pm y^2, \mathbf{k}} = \cos k_x \pm \cos k_y$, are naturally favored. In real space, they respectively correspond to $\Delta_x = \pm \Delta_y = \Delta_0$,

with $\Delta_{x+y} = \Delta_{x-y} = 0$. These $s_{x^2+y^2}$ and $d_{x^2-y^2}$ states are degenerate because the symmetry operation $c_{m\hat{x}+n\hat{y}} \rightarrow e^{i(2m+1)\pi/2} c_{m\hat{x}+n\hat{y}}$ transforms them into each other.

When J_2 dominates, the $s_{x^2y^2}$ and d_{xy} states, respectively defined by the pairing functions $g_{x^2y^2, \mathbf{k}} = \cos(k_x + k_y) + \cos(k_x - k_y)$ and $g_{xy, \mathbf{k}} = \cos(k_x - k_y) - \cos(k_x + k_y)$, are preferred, and they are degenerate. In real space, they correspond to $\Delta_{x+y} = \pm \Delta_{x-y} = \Delta_0$, with $\Delta_x = \Delta_y = 0$. The $s_{x^2y^2}$ and d_{xy} states transform into each other by the following symmetry operation: we break the square lattice into two interpenetrating sublattices; on the even sublattice ($m+n = \text{even}$), $c_{m\hat{x}+n\hat{y}} \rightarrow e^{i(m+n+1)\pi/2} c_{m\hat{x}+n\hat{y}}$, and on the odd sublattice, $c_{m\hat{x}+n\hat{y}} \rightarrow e^{i(m-n+1)\pi/2} c_{m\hat{x}+n\hat{y}}$.

As we tune the ratio J_2/J_1 , we expect a level crossing in the magnetically frustrated regime, $J_2 \sim J_1$. We can then anticipate that magnetic frustration promotes an enlarged degeneracy among the $s_{x^2y^2}$, $s_{x^2+y^2}$, d_{xy} , and $d_{x^2-y^2}$ pairing states.

The effect of the kinetic energy. When the kinetic term is incorporated, it lifts the exact degeneracies of the paired states discussed above. We study the full problem using a mean-field decoupling [42] of the two-band t - J_1 - J_2 model. To set the stage, we note that the D_{4h} point group symmetry operations allow the following four classes of pairing states for an orbitally diagonal J_1 - J_2 model [43]: i) A_{1g} : $[s_{x^2+y^2}^{A_{1g}} g_{x^2+y^2, \mathbf{k}} + s_{x^2y^2}^{A_{1g}} g_{x^2y^2, \mathbf{k}}] \tau_0 + d_{x^2-y^2}^{A_{1g}} g_{x^2-y^2, \mathbf{k}} \tau_z$; ii) B_{1g} : $d_{x^2-y^2}^{B_{1g}} g_{x^2-y^2, \mathbf{k}} \tau_0 + [s_{x^2+y^2}^{B_{1g}} g_{x^2+y^2, \mathbf{k}} + s_{x^2y^2}^{B_{1g}} g_{x^2y^2, \mathbf{k}}] \tau_z$; iii) A_{2g} : $d_{xy}^{A_{2g}} g_{xy, \mathbf{k}} \tau_z$; and iv) B_{2g} : $d_{xy}^{B_{2g}} g_{xy, \mathbf{k}} \tau_0$. Each pairing channel will have different symmetry depending on whether it is associated with τ_0 or τ_z in the orbital space; this distinction is denoted by the superscripts. The eight pairing amplitudes $s_{x^2+y^2}^{A_{1g}}$ etc. are linear combinations of eight intra-orbital pairing amplitudes $\Delta_{\mathbf{e},\alpha\alpha}$.

Mean-field theory. We decouple the exchange interactions in the pairing channel. In terms of $\Psi_{\mathbf{k}} = (\psi_{\mathbf{k}\uparrow}^\dagger, \psi_{-\mathbf{k}\downarrow})$, the Hamiltonian becomes

$$H_{mf} = \sum_{\mathbf{k}} \Psi_{\mathbf{k}}^\dagger \begin{bmatrix} \mathbf{h}_{\mathbf{k}} & \Delta_{\mathbf{k}} \\ \Delta_{\mathbf{k}}^* & -\mathbf{h}_{\mathbf{k}} \end{bmatrix} \Psi_{\mathbf{k}}, \quad (2)$$

where $\mathbf{h}_{\mathbf{k}} = \xi_{\mathbf{k}+}\tau_0 + \xi_{\mathbf{k}-}\tau_z + \xi_{\mathbf{k}xy}\tau_x$, and $\Delta_{\mathbf{k}} = \text{diag}[\Delta_{\mathbf{k},11}, \Delta_{\mathbf{k},22}]$ is the orbitally diagonal gap matrix, and $\Delta_{\mathbf{k},\alpha\alpha} = \sum_{\mathbf{e}} J_{\mathbf{e}} \Delta_{\mathbf{e},\alpha\alpha} \cos(\mathbf{k} \cdot \mathbf{e})$, with $J_{\mathbf{e}} = J_1$ for $\mathbf{e} = \hat{x}, \hat{y}$, and $J_{\mathbf{e}} = J_2$ for $\mathbf{e} = \hat{x} \pm \hat{y}$. Diagonalizing H_{mf} we obtain the quasi-particle dispersion spectra $E_{\mathbf{k},\pm}$. We determine the pairing gap matrix by minimizing the ground-state energy density

$$f = \sum_{\mathbf{e},\alpha} \frac{J_{\mathbf{e}}}{2} |\Delta_{\mathbf{e},\alpha\alpha}|^2 - \sum_{\mathbf{k},j=\pm} (E_{\mathbf{k},j} - \mathcal{E}_{\mathbf{k},j}), \quad (3)$$

with respect to *all* $\Delta_{\mathbf{e},\alpha\alpha}$. The primary effect of the constraints is to renormalize the kinetic energy via (both orbitally diagonal and off-diagonal) $t \rightarrow t\delta/2$, where t is the kinetic-energy scale. Our results, with an implicit treatment of the constraint through a band renormalization,

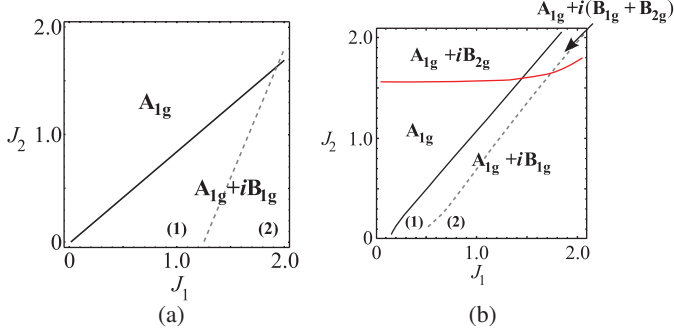


Fig. 1: (Color online) Zero temperature phase diagrams of (a) a two-orbital model and (b) a five-orbital model, both for electron doping $\delta = 0.14$. The onset of B_{1g} and B_{2g} phases are, respectively, marked by black and red solid lines. The dotted line characterizes a crossover between $s_{x^2+y^2}^{A_{1g}}$ (region (1)) and $s_{x^2+y^2}^{A_{1g}}$ (region (2)) as the dominant component in the A_{1g} pairing.

remain largely unchanged when the constraints are explicitly incorporated.

When the kinetic energy is absent, the $s_{x^2+y^2}$ and $d_{x^2-y^2}$ states are indeed degenerate, and each has a ground-state energy $\approx -0.17J_1$. Likewise, the energy of either $s_{x^2+y^2}$ or d_{xy} state is $\approx -0.17J_2$, and all four paired states become degenerate exactly at $J_1 = J_2$, as anticipated earlier.

We now turn to the results for the full problem in the presence of the kinetic terms. We show an illustrative zero-temperature phase diagram for $0 \leq J_1, J_2 \leq 2t$, in fig. 1(a) corresponding to an electron doping $\delta = 0.14$. A_{1g} pairing exists in the entire J_1 - J_2 plane. In a sizable portion of the phase diagram, the pairing is in the pure A_{1g} class. In this region $s_{x^2+y^2}^{A_{1g}}$ is the dominant pairing channel and coexists with the subdominant $d_{x^2-y^2}^{A_{1g}}$ channel. The onset of B_{1g} pairing state is marked by a solid line, which corresponds to a second-order phase transition. $d_{x^2-y^2}^{B_{1g}}$ and $s_{x^2+y^2}^{B_{1g}}$ are, respectively, the dominant and the subdominant components of the B_{1g} phase. In the large J_1 limit (to the right of the dotted line), $s_{x^2+y^2}^{A_{1g}}$ becomes the dominant component of the A_{1g} phase; the dotted line represents a crossover. The phase diagram for hole doping is identical, but the onset of B_{1g} pairing occurs for larger J_1 .

The competition among different symmetry classes, and the nature of the ground states are demonstrated in fig. 2, which plot the pairing amplitudes as a function of the coupling constants. The degeneracy between the $s_{x^2+y^2}$ and d_{xy} channels, occurs at very large J_2 limit and is not shown in fig. 2. For moderate values of J_1, J_2 , quasi-degeneracy among the pairing states occurs in the magnetically frustrated region corresponding to $J_2 \sim J_1$. In this region, fig. 2 shows that the weights of the $s_{x^2+y^2}^{A_{1g}}$ and $d_{x^2-y^2}^{B_{1g}}$ components are comparable, and those of $d_{x^2-y^2}^{A_{1g}}$ and $s_{x^2+y^2}^{B_{1g}}$ are close-by. This quasi-degeneracy also underlies the phase diagram shown in fig. 1(a). By

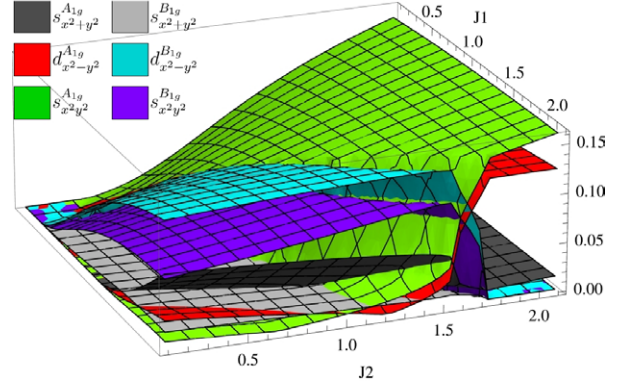


Fig. 2: (Color online) The amplitudes of different pairing gap components of a two-orbital model for electron doping $\delta = 0.14$. For $J_2 \gg J_1$ and $J_2 \ll J_1$, $s_{x^2+y^2}^{A_{1g}}$ (s_{\pm}), and $d_{x^2-y^2}^{B_{1g}}$ are, respectively, the dominant pairing channels.

contrast, for moderate values of J_2 and with $J_2 \gg J_1$, $s_{x^2+y^2}^{A_{1g}}$ dominates over $s_{x^2+y^2}^{B_{1g}}$, $d_{xy}^{A_{2g}}$, $d_{xy}^{B_{2g}}$ channels; likewise, for moderate values of J_1 and with $J_1 \gg J_2$, $d_{x^2-y^2}^{B_{1g}}$ dominates over $d_{x^2-y^2}^{A_{1g}}$, $s_{x^2+y^2}^{A_{1g}}$, $s_{x^2+y^2}^{B_{1g}}$ channels.

At the $T=0$ limit we study, the coexisting pairing channels will lock into a definite phase. Consider first the case of coexisting $s_{x^2+y^2}^{A_{1g}}$ and $d_{x^2-y^2}^{A_{1g}}$. We define $\Delta_{\mathbf{k}} = s_{x^2+y^2}^{A_{1g}} g_{x^2+y^2, \mathbf{k}} \tau_0 + d_{x^2-y^2}^{A_{1g}} g_{x^2-y^2, \mathbf{k}} \tau_z$, and use ϕ to denote the relative phase. Inserting this into eq. (3), we find that $\phi = \pi$ corresponds to the ground-state energy minimum, with $\partial f / \partial \phi = 0$ and $\partial^2 f / \partial \phi^2 > 0$ ($\phi = 0$ is a ground-state energy maximum). The A_{1g} gap is therefore real. Moreover, the relative minus sign associated with $\phi = \pi$ implies that the pairing function, in the band (as opposed to the orbital) basis, is $s_{x^2+y^2}^{A_{1g}} g_{x^2+y^2, \mathbf{k}} \tau_0 - d_{x^2-y^2}^{A_{1g}} g_{x^2-y^2, \mathbf{k}} (\xi_{\mathbf{k}-\tau_z} - \xi_{\mathbf{k}xy} \tau_x) (\xi_{\mathbf{k}-}^2 + \xi_{\mathbf{k}xy}^2)^{-1/2}$. Hence intra-band pairing function changes sign between the hole and electron pockets near $\mathbf{k} = (0, 0)$ and $\mathbf{k} = (\pi, 0), (0, \pi)$, respectively. A similar argument shows that the relative phase between $d_{x^2-y^2}^{B_{1g}}$ and $s_{x^2+y^2}^{B_{1g}}$ is π , and the gap changes sign between the two electron pockets near $\mathbf{k} = (\pi, 0), (0, \pi)$, respectively.

Consider next the case of coexisting $s_{x^2+y^2}^{A_{1g}}$ and $d_{x^2-y^2}^{B_{1g}}$. A similar analysis shows that, this time, $\phi = \pi/2$ corresponds to the ground-state energy minimum (while $\phi = 0, \pi$ represent energy maxima). The resulting $A_{1g} + iB_{1g}$ phase describes the state to the right of the solid line in fig. 1(a). This phase simultaneously breaks time-reversal and four-fold rotational symmetries, but preserves the combination of the two symmetries. Such a state also occurs in a phenomenological Landau-Ginzburg theory [44].

The role of fermiology can be clearly illustrated in the linearized gap approximation. For a set of small Fermi pockets at $(0, 0)$, $(\pi, 0)$ and $(0, \pi)$, compared to $g_{xy, \mathbf{k}}$, $g_{x^2+y^2, \mathbf{k}}$ has larger overlap with the pairing kernel. Thus, $s_{x^2+y^2}^{A_{1g}}$ and $s_{x^2+y^2}^{B_{1g}}$ gaps have higher T_c 's compared to $d_{xy}^{B_{2g}}$ and $d_{xy}^{A_{2g}}$ gaps; they become degenerate only in the

large J_2 limit. Similar reasoning shows that, unless a threshold value for J_1 is exceeded, $d_{x^2-y^2}^{A_{1g}}$ and $d_{x^2-y^2}^{B_{1g}}$ gaps have higher T_c 's compared to the $s_{x^2+y^2}^{A_{1g}}$ and $s_{x^2+y^2}^{B_{1g}}$ gaps. Related observations were made by Seo *et al.* [28]. If we consider a band structure that produces large pockets [27], $d_{xy}^{B_{2g}}$ replaces $s_{x^2+y^2}^{A_{1g}}$ as the dominant pairing state for $J_2 > J_1$, and we observe a competition between $d_{xy}^{B_{2g}}$ and $d_{x^2-y^2}^{B_{1g}}$ pairing states. Note that the magnetic oscillation and ARPES measurements suggest small sizes of the Fermi pockets for the iron pnictides, and this should make our A_{1g} and $A_{1g} + iB_{1g}$ phases more feasible.

Effects of inter-orbital exchange couplings. We stress that, while the detailed nature of the lattice symmetry and orbitals for the single-particle energy dispersion is important for a proper description of the Fermi surface, its counterpart for the exchange interactions is not obviously so. In the absence of a detailed knowledge about such structure in the exchange interactions, we have considered the simplest description and focused on the associated properties that are qualitative and robust. For instance, we have so far considered intra-orbital exchange interactions. Inclusion of inter-orbital super-exchange interactions does not change the phase diagram. Now the A_{1g} phase will have a small inter-orbital $d_{xy}^{A_{1g}}$ component and the B_{1g} phase will remain unchanged. Hund's coupling may lead to on-site triplet pairing, but this is prevented by the onsite Coulomb repulsion that is built in our model. Inter-site triplet pairing may arise if Hund's coupling is comparable to the Coulomb repulsion [29], but this is unlikely on general or *ab initio* grounds; it is also unlikely on empirical grounds since experimental evidence has so far been overwhelming for singlet pairing. Using a multi-orbital Hubbard model as their starting points, both the strong-coupling calculations of ref. [29] and the RPA calculations of ref. [21] find that a moderate J_H enhances repulsive inter-electron-pocket pair scattering and leads to stronger B_{1g} pairing. Thus, J_H can only enhance the $A_{1g} + iB_{1g}$ part of the phase diagram. We have preferred to consider the multiband t - J_1 - J_2 model, since J_1 and J_2 can be more readily connected with the magnetic frustration physics.

Five-orbital model. – To understand the robustness of our two-band results, against the inclusion of additional bands, and better address the fermiology we have considered a five-band model with the kinetic terms according to ref. [26]. To capture the important results within a simple model of interaction, we again choose a J_1 - J_2 model with $J_i^{\alpha\beta} = J_i \delta_{\alpha\beta}$. Now the general intra-orbital pairing matrix has the form $\Delta_{\mathbf{k}} = \sum_a \text{diag}[\Delta_{\mathbf{k},11}^a, \Delta_{\mathbf{k},22}^a, \Delta_{\mathbf{k},33}^a, \Delta_{\mathbf{k},44}^a, \Delta_{\mathbf{k},55}^a]$, where the index a corresponds to $s_{x^2+y^2}$, $d_{x^2-y^2}$, $s_{x^2+y^2}$ and d_{xy} symmetries. The results of minimizing the free energy with respect to all the twenty complex pairing amplitudes are given in an illustrative phase diagram, fig. 1(b), and in fig. 3, which shows the competition among the pairing

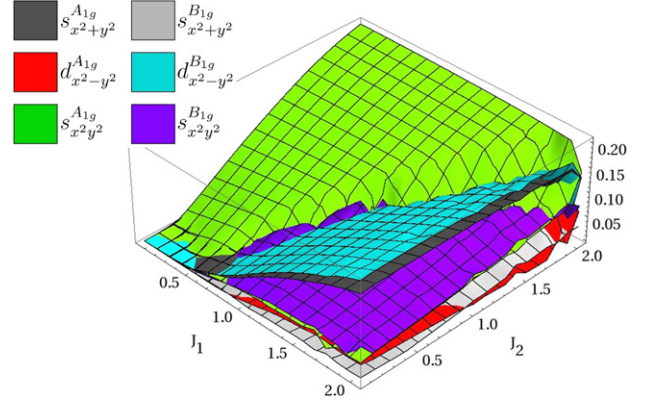


Fig. 3: (Color online) The pairing amplitudes for d_{xz} , d_{yz} orbitals, obtained from a five-orbital model for $\delta = 0.14$. For $J_2 \gg J_1$, the dominant pairing channel is $s_{x^2+y^2}^{A_{1g}}$ (s_{\pm}), and for $J_2 \ll J_1$, $d_{x^2-y^2}^{B_{1g}}$ and $s_{x^2+y^2}^{A_{1g}}$ pairing channels are dominant and nearly degenerate pairing channels. Compared to the two-orbital model, the $s_{x^2+y^2}^{A_{1g}}$ channel is more competitive and becomes significant for a relatively smaller value of J_1 .

amplitudes for xz and yz orbitals. We find that the competition between A_{1g} and B_{1g} pairings is a robust effect. In contrast to the two-band case, the $d_{x^2-y^2}^{A_{1g}}$ amplitude is reduced and the $s_{x^2+y^2}^{A_{1g}}$ amplitude is enhanced in the entire phase diagram. Indeed, for the magnetically frustrated $J_1 \sim J_2$ region, the nodal A_{1g} $s_{x^2+y^2}$ and B_{1g} $d_{x^2-y^2}$ states are competitive against the nodeless A_{1g} $s_{x^2+y^2}$ state. Compared to the two-band case, the B_{2g} pairing occurs for smaller J_2 , but it still occurs in the limit when J_2 is bigger than the kinetic-energy scale. The other three orbitals also demonstrate similar competition among $s_{x^2+y^2}$, $s_{x^2+y^2}$, $d_{x^2-y^2}$, and d_{xy} pairings.

Experimental implications of quasi-degenerate pairing channels. – Some of the weak-coupling studies [21,26] have also indicated a competition between various pairing states. However, the weak-coupling approaches are typically restricted to an instability analysis of the linearized gap equations. By contrast, the strong-coupling approach used here has the advantage of readily considering the non-linear gap equations. Our non-linear analysis is important in bringing out the connection between the quasi-degeneracy in the pairing channel and the $J_1 \sim J_2$ magnetic frustration. With only one requirement ($J_1 \sim J_2$), which is linked to magnetic frustration and has been supported by both theoretical considerations [5,7–9,12] and inelastic magnetic experiments [19,38], our result provides a parameter-insensitive mechanism for the near degeneracies of various pairing states. Moreover, our non-linear analysis is also essential in reaching the conclusion (cf. figs. 2 and 3) that, for $J_1 \sim J_2$, the pairing amplitudes for several competing nodeless and nodal pairing channels are comparable. This last result is particularly important for experiments in the iron pnictides. Indeed, our result

has anticipated the recent experimental finding [36,37] that pnictide superconductors with nodeless or nodal gaps have a comparable maximum T_c . Our $s_{x^2y^2}^{A_{1g}}$ (s_{\pm}), $s_{x^2+y^2}^{A_{1g}}$ states appear to be consistent with ARPES measurements that find full gap at hole pockets. However, in contrast to $s_{x^2y^2}^{A_{1g}}$, which is fully gapped on all the Fermi pockets as long as the pockets are not too large, the $s_{x^2+y^2}^{A_{1g}}$ state has nodes on the electron pockets. This may be the reason for seeing nodal behavior in P-doped 122 compounds in contrast to the fully gapped behavior in K-doped 122 compounds.

To summarize, we have shown that magnetic frustration effects lead to quasi-degeneracy among different pairing states. With the band structures appropriate for the iron pnictides, an extended A_{1g} state is the dominant pairing state, but this state contains both $s_{x^2y^2}$ and $s_{x^2+y^2}$ components. Moreover, a B_{1g} state has a close-by ground-state energy. The quasi-degeneracy makes it likely that the iron pnictides of different material families, or different dopings, have different superconducting states. Our detailed phase diagram contains a low-temperature phase with time-reversal symmetry breaking, which also can be tested by future experiments.

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