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Hund interaction, spin-orbit coupling and the mechanism of superconductivity in strongly hole-doped iron pnictides

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We present a novel mechanism of $s-$wave pairing in Fe-based superconductors. The mechanism involves holes near d_{xz}/d_{yz} pockets *only* and is applicable primarily to strongly hole doped materials. We argue that as long as the renormalized Hund's coupling J exceeds the renormalized inter-orbital Hubbard repulsion U', any finite spin-orbit coupling gives rise to s-wave superconductivity. This holds even at weak coupling and regardless of the strength of the intra-orbital Hubbard repulsion U. The transition temperature grows as the hole density decreases. The pairing gaps are four-fold symmetric, but anisotropic, with the possibility of eight accidental nodes along the larger pocket. The resulting state is consistent with the experiments on KFe_2As_2.

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Introduction. The pairing mechanism in iron-based superconductors (FeSCs) remains the subject of intense debates [1]. A common scenario is that superconductivity (SC) is mediated by anti-ferromagnetic spin fluctuations, which are enhanced by the presence Fermi pockets of both hole and electron type [1, 2]. This scenario yields an $s-$wave pairing amplitude with opposite sign on hole and electron pockets. Such an s^{+-} gap structure is consistent with experiments on moderately doped FeSCs, which contain hole and electron pockets.

However, SC is also observed in strongly doped FeSCs with only hole or only electron pockets [3, 4]. For these systems, it is not clear why spin fluctuations should be strong enough to overcome Coulomb repulsion.

In this paper we focus on the systems with only hole pockets, such as $K_xBa_{1-x}Fe_2As_2$. For KFe_2As_2, angle-resolve photoemission (ARPES) experiments show that only hole pockets are present [3, 4]. Yet, $T_c \approx 3K$ in KFe_2As_2 and increases as x decreases. The electronic structure of KFe_2As_2 consists of three hole pockets centered at Γ and hole "barrels" near $M = (\pi, \pi)$ in the Brillouin zone corresponding to a single Fe-As layer with two Fe atoms per primitive unit cell. The inner and the middle pockets at Γ are made predominantly out of d_{xz} and d_{yz} orbitals [2] with, potentially, some admixture of $d_{3z^2-r^2}$ orbital [4, 5], while the outer pocket is predominantly made out of d_{xy} orbital.

There is no consensus at the moment among both experimentalists and theorists about the *pairing* symmetry in KFe_2As_2. On the one hand, non-phase-sensitive measurements on KFe_2As_2, such as thermal conductivity and Raman scattering, were interpreted as evidence for a $d-$wave gap [6, 7]. On the other, laser ARPES reported full gap along the inner hole Fermi surface (FS), eight nodes along the middle FS, and negligible gap along the outer (d_{xy}) pocket [4]. This was interpreted as evidence of $s-$wave pairing [4, 9]. Specific heat data [8] on KFe_2As_2 were also interpreted in favor of $s-$wave with multiple gaps.

Existing theoretical proposals for superconductivity in KFe_2As_2 explore the idea that the origin of the pairing in this system is the same as in FeSCs with hole and electron pockets, i.e., that the pairing is promoted by magnetic fluctuations. This mechanism has been analyzed within RPA [10, 11] and within the renormalization group (RG) [12]. The outcome is that, depending on parameters, spin fluctuations either favor s^{+-} SC with the gap changing sign between the inner and the middle d_{xz}/d_{yz} pockets [10, 11], or $d-$wave SC with the gap predominantly residing on the outer d_{xy} pocket [12]

Each scenario has a potential to explain superconductivity in KFe_2As_2, but the key shortcoming of both is that $s-$wave and the $d-$wave attractions are very weak [11] because the mechanism is essentially of Kohn-Luttinger type [13]. Additionally, the $d-$wave pairing scenario yields the largest gap on the largest hole pocket, which is inconsistent with laser ARPES [4].

In this paper we propose a new mechanism for SC in KFe_2As_2 and other materials with only hole pockets. Consistent with laser ARPES[4], we assume that the pairing involves mainly fermions near the inner and the middle hole pockets (see Fig.1), and neglect the hole barrels near (π, π) and the outer hole pocket, where the observed pairing gap is much smaller. We focus on 2D physics and neglect the contribution from $d_{3z^2-r^2}$ orbital, inferred from the observed 3D variation of the middle hole pocket [4, 5]. The pairing in our theory arises from the combination of two factors: sizable Hund's electron-electron interaction J and sizable spin-orbit coupling (SOC) λ. Specifically, we argue that the system develops an $s-$wave SC as soon as the renormalized J exceeds the renormalized inter-orbital Hubbard repulsion U', *regardless* of the value of the intra-orbital Hubbard repulsion U. The effective dimensionless coupling constant in the $s-$wave pairing channel scales as $N_0(J-U')\left(\frac{\lambda}{\mu}\right)^2$, where N_0 is the density of states and μ is the chemical potential. That J is substantial has been discussed in

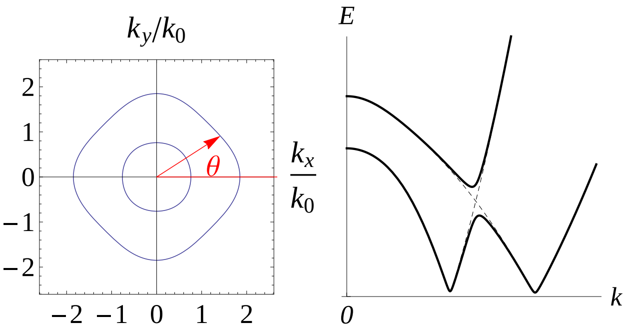

FIG. 1: Left panel: Illustrative Fermi surfaces (FS) for the d_{xz}/d_{yz} hole pockets, where $k_0 = \sqrt{2m\mu}$. In the SC state, the pairing amplitude on the outer Fermi surface is Δ_+ and on the inner Δ_-. Right panel: Schematic quasiparticle dispersion in the superconducting state (solid black lines). The gap away from the Fermi level is due to the A_{2g} pairing and is present already without SOC. Once SOC is included, the gaps on the FS appear. The dashed lines are approximations which capture the gaps on the FS only.

the context of "Hund metal" [14, 15]. At the bare (local) level, $U' > J$ [14, 16], but the ratio J/U' is energy dependent, and we assume that $J/U' > 1$ at low energies, relevant to the pairing. The magnitude of λ is also quite sizable in FeSCs. ARPES measurements (Ref.[17]) extracted $\lambda \sim 10 - 20$meV, comparable to μ.

Without SOC, the Cooper states at zero momentum can be classified according to their behavior separately under the crystal's point group operations and under spin SU(2) rotations. As such, the on-site Hubbard-Hund interaction with $U > U', J$ is repulsive in the s-wave (A_{1g}) and $d-$wave (B_{1g} and B_{2g}) spin singlet channels. The interaction in the A_{2g} spin-triplet channel, however, avoids U and is $\frac{1}{2}(U' - J)$, i.e., it is attractive when $J > U'$ [18]. By itself, an attraction in the A_{2g} channel does *not* necessarily lead to the Cooper instability because the pairing occurs between fermions from different bands and the pairing susceptibility is not logarithmically large at small temperature, T. Besides, A_{2g} pairing does not open gaps on the Fermi surfaces (see Fig.1). The situation changes when $\lambda \neq 0$ because SOC mixes the A_{1g} spin singlet and the A_{2g} spin triplet pairs [20]. The pairing susceptibility in A_{1g} channel diverges as $\log T$ at small T because the order parameter contains fermion pairs from the same band. We argue that $s-$wave superconductivity emerges as soon as $J > U'$. Remarkably, this conclusion is unaffected by the presence of a much stronger U despite the fact that the U determines the repulsion in the A_{1g} spin singlet channel.

The gaps on the two hole pockets are four-fold symmetric, but anisotropic. The solution of the self-consistency equations shows that the overall gap on the *larger* FS is smaller, in part, due to destructive interference between the A_{1g} and the A_{2g} components. For some range of parameters, the gap on this pocket has eight accidental nodes, as shown in the Fig.3. The relative magnitude of the A_{1g} and the A_{2g} components does not contain $\log T$, nevertheless, their ratio has a non-trivial temperature (T) dependence even at weak coupling. This may lead to a possibility that such accidental nodes appear only below some $T < T_c$.

Our results are summarized in Figs.2 and 3. We argue below that they are consistent with several experimental findings on $K_xBa_{1-x}Fe_2As_2$ for $x \approx 1$.

The model. We consider the itinerant model with two Γ-centered hole pockets made out of d_{xz} and d_{yz} orbitals (see Fig. 1). The effective Hamiltonian $\mathcal{H} = H_0 + H_{int}$ for the low-energy states near Γ can be obtained, quite generally, using the method of invariants [20, 21], without the need to assume a particular microscopic model. The non-interacting part of the Hamiltonian, describing d_{xz}/d_{yz} hole pockets, is

$$H_0 = \sum_{\mathbf{k}} \sum_{\alpha,\beta=\uparrow,\downarrow} \psi^\dagger_{\mathbf{k},\alpha} \left(h_{\mathbf{k}} \delta_{\alpha\beta} + h^{SO} s^z_{\alpha\beta} \right) \psi_{\mathbf{k},\beta}, \quad (1)$$

where the doublet $\psi^\dagger_{\mathbf{k},\sigma} = \left(d^\dagger_{yz,\sigma}(\mathbf{k}), -d^\dagger_{xz,\sigma}(\mathbf{k}) \right)$, s^z is the Pauli matrix, and

$$h_{\mathbf{k}} = \begin{pmatrix} \mu - \frac{\mathbf{k}^2}{2m} + b k_x k_y & c\left(k_x^2 - k_y^2\right) \\ c\left(k_x^2 - k_y^2\right) & \mu - \frac{\mathbf{k}^2}{2m} - b k_x k_y \end{pmatrix}, \quad (2)$$

$$h^{SO} = \lambda \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}. \quad (3)$$

The coefficients μ, m, b, c, and the SOC λ are material specific, but the forms of $h_{\mathbf{k}}$ and h^{SO} are universal.

The 4-fermion interaction Hamiltonian can also be written out in terms of the low energy doublet. Assuming spin SU(2) symmetry we can express H_{int} as

$$H_{int} = \sum_{j=0}^{3} \frac{g_j}{2} \int d^2\mathbf{r} :\psi^\dagger_\sigma(\mathbf{r})\tau_j\psi_\sigma(\mathbf{r})\psi^\dagger_{\sigma'}(\mathbf{r})\tau_j\psi_{\sigma'}(\mathbf{r}): \quad (4)$$

where :: implies normal ordering, the repeated spin indices σ, σ' are summed over, $\tau_0 = \mathbb{1}$ and the three Pauli matrices τ_j act on the two components of the doublet. The four couplings g_j can be parameterized in terms of effective Hubbard-Hund interactions U, U', J, J' as $g_0 = \frac{1}{2}(U + U')$, $g_1 = \frac{1}{2}(J + J')$, $g_2 = \frac{1}{2}(J - J')$, and $g_3 = \frac{1}{2}(U - U')$. We emphasize that g_i's include renormalizations from high energy modes and the effective U, U', J, and J' are not the same as the *bare* (local) Hubbard and Hund's interaction terms. We keep renormalized interaction local because relevant fermions are near hole pockets, and corresponding $(ak_F)^2$, which set the momentum dependence of the interactions, are small (a is interatomic spacing).

For $\lambda = 0$, the pairing can be decomposed into spin singlet A_{1g}, B_{1g}, and B_{2g} channels, as well as the spin triplet A_{2g}. The corresponding couplings are [20, 22] $g_{A_{1g}} = \tilde{g}_0 = (U + J')/2$, $g_{B_{1g}} = (U - J')/2$, $g_{B_{2g}} = (U' + J)/2$, and $g_{A_{2g}} = \tilde{g}_2 = \frac{1}{2}(g_0 - g_1 - g_2 - g_3) = (U' -$

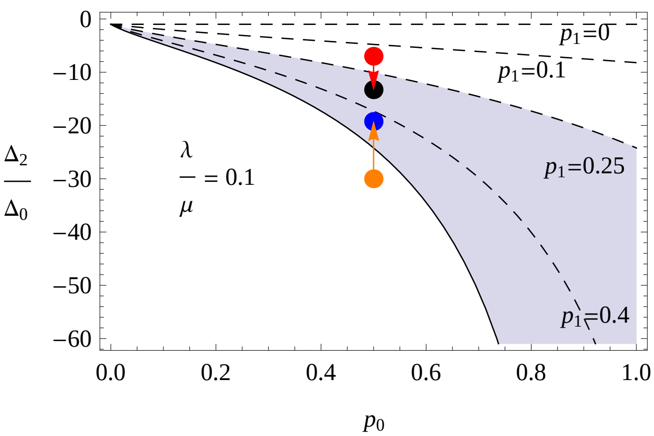

FIG. 2: The phase diagram at $T = 0$ calculated at a fixed ratio of the SOC λ to Fermi energy μ. Displayed are the boundaries of the nodal region, which depend on the ratio of A_{2g} (Δ_2) and A_{1g} (Δ_0) components of the pairing gap at $T = 0$. They also depend on p_0 and p_1, dimensionless parameters which enter into the angle dependence of the normal state band dispersion as in Eqs.(9) and (10). (p_0 is a measure of the off-diagonal orbital hopping, while p_1 is a measure of the anisotropy of the diagonal hopping). The pairing amplitudes on the larger and the smaller Fermi surfaces are $\Delta_+ = \Delta_0 + (\lambda/|\vec{B}_{\mathbf{k}}|)\Delta_2$ and $\Delta_- = \Delta_0 - (\lambda/|\vec{B}_{\mathbf{k}}|)\Delta_2$, respectively; $2|\vec{B}_{\mathbf{k}}|$ is the energy of the band splitting (9). Shaded area marks the appearance of the accidental nodes in Δ_+ for $p_1 = 0.25$. For a different value of p_1, the upper boundary of the shaded area shifts to the corresponding dashed line, while the lower boundary is p_1-independent. Below (above) the shaded region, the signs of Δ_+ and Δ_- are opposite (same) and the pairing state can be viewed as s^{+-} (s^{++}). Interestingly, numerical solutions of the self-consistency equations find that it is possible to start outside of the nodal region at T_c (red and orange circles) and end up inside of it at $T = 0$ (black and blue circles).

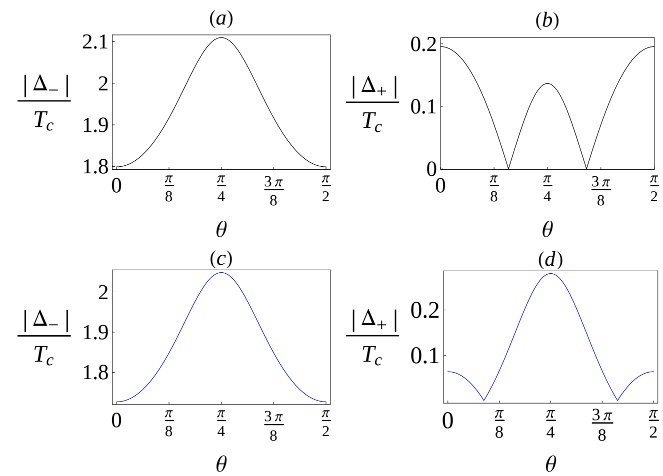

FIG. 3: Angle dependence of the gap at $T = 0$ on the inner (a) and the outer (b) hole Fermi surfaces (FS) for parameters corresponding to the (black) end point of the down (red) arrow in Fig.2. (c) and (d) show the same but for the parameters corresponding to the (blue) end point of the up (orange) arrow in Fig.2. In both cases, there are eight nodal points on the outer FS.

$J)/2$. The interactions in A_{1g}, B_{1g}, and B_{2g} channels are repulsive as the intra orbital Hubbard U is the largest local interaction. However the interaction in A_{2g} channel is attractive if $J > U'$. We assume this to hold. The A_{2g} order parameter is

$$\Delta_2 = \frac{1}{2}\tilde{g}_2\langle\psi^T_\alpha(\mathbf{r})\tau_2(is^z s^y)_{\alpha\beta}\psi_\beta(\mathbf{r})\rangle. \quad (5)$$

Because τ_2 is antisymmetric and $is^z s^y$ is symmetric, this order parameter is spin triplet. For $\lambda = 0$, Δ_2 in the band basis is composed entirely of fermions from different pockets. The susceptibility for such inter-pocket pairing does not contain the Cooper logarithm, and hence the attraction in A_{2g} channel alone does not give rise to Cooper pairing, at least at weak coupling. However, in the presence of the SOC, an arbitrarily weak A_{2g} attraction gives rise to a pairing instability, as we now show.

Role of SOC. For $\lambda \neq 0$, the A_{1g} and the A_{2g} channel in Eq.(5) mix[20]. Nevertheless, the $A-$channels and the $B-$channels remain decoupled. We focus on the A_{1g} channels because of the attraction in A_{2g}. Due to A_{2g}/A_{1g} mixing, the order parameter Δ_2 receives a contribution from fermions residing in the *same* band. The corresponding normal state pairing susceptibility is logarithmically large at small T. There is a caveat, however – the spin singlet A_{1g} pairing component is strongly repulsive. Our goal is to analyze whether it prevents pairing when $\tilde{g}_2 < 0$. To this end, we also introduce the conventional spin singlet A_{1g} order parameter,

$$\Delta_0 = \frac{1}{2}\tilde{g}_0\langle\psi^T_\alpha(\mathbf{r})\mathbb{1}(-is^y)_{\alpha\beta}\psi_\beta(\mathbf{r})\rangle, \quad (6)$$

and obtain the set of two coupled equations for Δ_2 and Δ_0 (Ref. [23]). At T_c, we have for $\tilde{g}_2 < 0$ and $\tilde{g}_0 > 0$

$$-\frac{\Delta_0}{\tilde{g}_0} = \sum_{\rho=\pm}\int\frac{d^2\mathbf{k}}{(2\pi)^2}\frac{\tanh\frac{\xi_\rho}{2T_c}}{2\xi_\rho}\left(\Delta_0 + \rho\Delta_2\frac{\lambda}{|\vec{B}_{\mathbf{k}}|}\right), \quad (7)$$

$$-\frac{\Delta_2}{\tilde{g}_2} = \sum_{\rho=\pm}\int\frac{d^2\mathbf{k}}{(2\pi)^2}\frac{1}{2\xi_\rho}\tanh\frac{\xi_\rho}{2T_c}\times \quad (8)$$
$$\times\left(\Delta_2\left(\frac{\lambda^2}{\vec{B}^2_{\mathbf{k}}} + \frac{\xi_\rho}{A_{\mathbf{k}}}\left(1 - \frac{\lambda^2}{\vec{B}^2_{\mathbf{k}}}\right)\right) + \rho\Delta_0\frac{\lambda}{|\vec{B}_{\mathbf{k}}|}\right),$$

where the normal state band dispersion has the form

$$\xi_\pm = A_{\mathbf{k}} \pm |\vec{B}_{\mathbf{k}}| = \mu - \frac{\mathbf{k}^2}{2m} \pm \sqrt{R_\theta\frac{\mathbf{k}^4}{4m^2} + \lambda^2}. \quad (9)$$

The angular anisotropy in momentum space enters via $0 < R_\theta < 1$, and is determined by the coefficients b and c in Eq.(2). We express it as

$$R_\theta = p_0\left(\frac{1}{2} + p_1 + \left(\frac{1}{2} - p_1\right)\cos 4\theta\right), \quad (10)$$

with $p_0 = 4m^2c^2$ and $p_1 = b^2/(8c^2)$. Without loss of generality, we may set $0 < p_0 < 1$ and $0 < p_1 < \frac{1}{2}$ (Ref. [24]). The Fermi surfaces shown in Fig.(1) correspond to $p_0 = 0.5$, $p_1 = 0.4$, and $\lambda/\mu = 0.1$. Eqs. (7-8) have the form

$$\begin{pmatrix} -\frac{1}{\tilde{g}_0} - \chi_{00}(T_c) & -\chi_{02}(T_c) \\ -\chi_{02}(T_c) & -\frac{1}{\tilde{g}_2} - \chi_{22}(T_c) \end{pmatrix} \begin{pmatrix} \Delta_0(T_c) \\ \Delta_2(T_c) \end{pmatrix} = 0. \tag{11}$$

Therefore, T_c is determined from requiring that the determinant vanishes

$$-\frac{1}{\tilde{g}_2} + \frac{\chi_{02}^2(T_c)}{\frac{1}{\tilde{g}_0} + \chi_{00}(T_c)} \ = \ \chi_{22}(T_c). \tag{12}$$

Brief inspection of (7-8) reveals that χ_{00} and χ_{22} scale as $\sim \ln \frac{1}{T}$. On the other hand, $\chi_{02}(T)$ remains finite due to an *exact cancellation* of two such logs. For $\mu \gg T_c$, we find

$$\chi_{02}(T_c) = \frac{m}{2\pi}\frac{\lambda}{\mu}\int_0^{2\pi}\frac{d\theta}{2\pi}\frac{\tanh^{-1}\sqrt{R_\theta + (1-R_\theta)\frac{\lambda^2}{\mu^2}}}{\sqrt{R_\theta + (1-R_\theta)\frac{\lambda^2}{\mu^2}}}, \tag{13}$$

where $\tanh^{-1} x = \frac{1}{2}\ln\frac{1+x}{1-x}$. As a result, T_c is finite regardless of how weak is the attractive coupling, $\tilde{g}_2 < 0$, and how strong is the repulsive coupling $\tilde{g}_0 > 0$. Moreover, $\chi_{02}(T_c)\lambda/\mu$ is positive. From the gap equations we then find that $\Delta_0(T_c) = -\mathcal{C}\Delta_2(T_c)\lambda/\mu$, where $\mathcal{C} > 0$. The gaps on the two pockets are

$$\Delta_\pm = \Delta_0 \pm \frac{\lambda}{|\vec{B}_{\mathbf{k}}|}\Delta_2, \tag{14}$$

where Δ_+ is on the larger and Δ_- is on on the smaller pocket. Analyzing the forms of these gaps, we find that (i) $|\Delta_+|$ is reduced relative to $|\Delta_-|$, (ii) the gaps are four-fold symmetric, but anisotropic, and (iii) for small $|\tilde{g}_2|$, Δ_0 is small compared to Δ_2, forcing opposite signs of Δ_+ and Δ_-, i.e. s^{+-} gap structure.

Below T_c. The mean field equations below T_c are non-linear in $\Delta_0(T)$ and $\Delta_2(T)$. We eliminate the couplings $\tilde{g}_0$ and $\tilde{g}_2$ by expressing Δ_0 and Δ_2 in units of T_c. Solving the non-linear set we obtain $\Delta_{0,2}(T)/T_c$ and the ratio $K(T) = \Delta_0(T)/\Delta_2(T)$ in terms of the same ratio at T_c. In a general case, when the cross term $\chi_{0,2}$ is non-logarithmic, $K(T)$ remains the same as at T_c, at least at weak coupling. In our case, the situation is different because a finite $\chi_{02}(T)$ is due to subtle cancellation of the logs, and leftover terms are T-dependent. In the limit of $K(T_c) \ll 1$ we found analytically $K(T = 0) = K(T_c)(1 + \mathcal{A})$, where $\mathcal{A} > 0$ (Ref. [23]). This also holds in the numerical solution of the mean-field equation, as indicated by the lower arrow in the Fig.2.

The numerical solutions of the gap equations are shown in the Fig. 3. We see that in some range of parameters, the gap on the larger hole pocket has eight accidental nodes. Interestingly, as shown in the Fig.2, we also found that over some range of parameters the nodes are absent at T_c, but appear at $T = 0$.

Comparison with experiments. Our results are consistent with several experimental findings on $K_xBa_{1-x}Fe_2As_2$ for $x \approx 1$. Namely, (i) a larger gap on the inner hole pocket at Γ, with no nodes, (ii) a smaller gap magnitude and the appearance of the accidental nodes on the larger d_{xz}/d_{yz} pocket (middle pocket at Γ), and (iii) angular correlation of the gap maxima on the two FSs are all consistent with the ARPES results [4]. The presence of the gap nodes is consistent with thermal conductivity and Raman scattering measurements [6, 7], and the near-absence of the gap on the d_{xy} pocket is consistent with ARPES [4] and specific heat measurements [8]. We also analyzed the temperature dependence of the the spin susceptibility $\chi(T)$ by adding a Zeeman coupling to $\mathcal{H}$. We found that $\chi(T)$ decreases below T_c for *any* orientation of the external magnetic field, even if Δ_0 is negligible compared to Δ_2. This result is non-trivial because for $\lambda = 0$ the pairing was in A_{2g} spin-triplet channel, and $\chi(T)$ was *not* suppressed below T_c when the magnetic field is perpendicular to the triplet $\mathbf{d}$-vector. The decrease of $\chi(T)$ for any orientation of the magnetic field is consistent with the Knight shift measurements in KFe_2As_2 (Ref. [25]). Finally, from Eq.(8) we readily see that the prefactor of the Cooper logarithm in $\chi_{22}(T_c)$ contains a factor of λ^2/μ^2. Therefore T_c *increases* as μ decreases, for fixed $\tilde{g}_{0,2}$ and fixed λ. The increase of T_c with decreasing x is consistent with the x dependence of T_c in $K_xBa_{1-x}Fe_2As_2$ at $x \leq 1$.

Conclusions. In this paper we presented a novel mechanism of $s-$wave pairing in FeSC, which involves fermions near d_{xz}/d_{yz} hole pockets. When the renormalized Hund's interaction J exceeds the renormalized inter-orbital Hubbard repulsion U', the interaction in A_{2g} channel is attractive. In the absence of SOC; this attraction would potentially give rise to spin-triplet superconductivity, but only when the attractive coupling exceeds a certain threshold. We argued that at a non-zero SOC, the same interaction gives an attraction in the s-wave channel, where the pairing condensate involves fermions from the same band and superconductivity emerges at an arbitrarily weak attraction. We demonstrated that T_c is only weakly affected by the large inter-orbital repulsion U in the A_{1g} channel, despite the fact that the SOC mixes the A_{2g} and the A_{1g} components. The gap functions are four-fold symmetric, but anisotropic, particularly on the larger FS, where over some range of parameters the gap has accidental nodes. Our results are consistent with ARPES and other experiments on strongly hole doped $K_xBa_{1-x}Fe_2As_2$.

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