Band renormalization and Fermi surface reconstruction in iron-based superconductors

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Abstract

Using the fluctuation exchange approximation and a three-orbital model, we study the band renormalization, Fermi surface reconstruction and the superconducting pairing symmetry in the newly-discovered iron-based superconductors. We find that the inter-orbital spin fluctuations lead to the strong anisotropic band renormalization and the renormalization is orbital dependent. As a result, the topology of Fermi surface displays distinct variation with doping from the electron type to the hole type, which is consistent with the recent experiments. This shows that the Coulomb interactions will have a strong effect on the band renormalization and the topology of the electron Fermi pocket. In addition, the pairing state mediated by the inter-orbital spin fluctuation is of an extended $s$-wave symmetry.

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I. INTRODUCTION

Recently, the discovery of superconductivity in the iron-based compounds has generated enormous interest, because these materials are the first non-copper superconductors with high superconducting (SC) critical temperature. These compounds share the same FeAs(or FeP) layers that are believed to be responsible for the superconductivity. Two classes of such compounds have been extensively investigated: (1) The LaOFeAs classes (denoted as FeAs-1111), space group $P_{4}/mmm$, with $T_c \approx 26$ K through electron doping with replacing $\text{O}^{2-}$ by $\text{F}^{-}$ and $T_c$ can be up to about 41 to 56 K by replacing lanthanum by other rare earth ions [1] and $T_c$ can be up to about 41 to 56 K by replacing lanthanum by other rare earth ions [2, 3, 4]. (2) The BaFe$_2$As$_2$ classes (denoted as FeAs-122), space group $I_{4}/mmm$, with $T_c \approx 38$ K through hole doping with substituting Ba$^{2+}$ for K$^+$ [5]. All parent compounds show a spin-density-wave (SDW) abnormality below a temperature $\sim 150$ K [6, 7, 8] and the superconductivity is associated with the suppression of the SDW. Most experiment measurements have shown that these superconductors open a full gap around both the hole and electron Fermi pockets [9, 10, 11, 12, 13, 18], though the NMR [14, 15] and transport [16, 17] experiments suggest the presence of gap nodes. At the same time, although the angle-resolved photoemission spectroscopy (ARPES) measurements of the band structure and Fermi surface (FS) in the undoped and electron doped samples [19, 21, 22] are qualitatively in agreement with the finding of the first-principle band calculation [23, 24], a strong anisotropic band renormalization is found. On the other hand, the ARPES data for the hole doped FeAs-122 reveal that the electron FS around $(\pi, \pi)$ consisting of disconnecting patches [18, 25], which exhibits a significant difference from the result obtained in the band structure calculation. Therefore, the understanding of the role played by the electron correlation and the origin of the different electron FS topology between the hole-doped and electron-doped system is of importance.

As the band structure calculations having shown, the FS and band structures of these compounds are qualitatively similar [23, 24, 26] and the Fe-3d orbitals represent the main contribution to the density of states, together with a contribution from As-p orbitals, within several eV of the Fermi level. In the FeAs layers, the Fe atoms form a square lattice and a Fe atom is coordinated by four As atoms in a tetrahedron. Due to the direct Fe-Fe bonds and the hybridization with the As-4p orbitals, the Fe-3d orbitals form a complex band structure. However, the main contribution to the bands near the Fermi level comes from the $d_{xz}$, $d_{yz}$
and the $d_{xy}$ orbitals (the direct Fe-Fe bonds along the $x$ and $y$ axes) of the Fe atoms \[26, 27, 28\]. In this paper, we employ a three-orbital (the $d_{xz}$, $d_{yz}$ and $d_{xy}$ orbitals) model \[29\] to investigate the band renormalization, FS reconstruction and superconducting gap symmetry in the iron-based compounds with the fluctuation exchange (FLEX) approximation. We find that a strong anisotropic band renormalization is resulted from the Coulomb interaction with the strongest effect occurring around the $\tilde{X} = (0, \pi)$ point, which is defined in the unfolded Brillouin zone (BZ), and this renormalization increases rapidly with the increase of the Hund’s coupling $J$ when $J > 0.18U$ ($U$ is the intra-orbital Coulomb interaction). Due to the band renormalization, the Fermi level for the undoped case is slightly below the flat band centered around the $\tilde{X}$ point which is the bottom of the band along the $\tilde{X}$ to $\tilde{M} = (\pi, \pi)$ direction. As a result, for the hole doped case, the Fermi level will situate below the flat band along the $\tilde{X}$ to $\tilde{M}$ direction, though it still crosses the renormalized band along the $\tilde{\Gamma}$ to $\tilde{X}$ direction. In this case, the FS around $\tilde{X}$ consists of disconnecting patches. However, in the electron-doped case, the Fermi level is lifted to be above the flat band and the circular-like FS is formed. This result provides a possible explanation for the different FS topology observed in the electron doped and hole doped materials. We also carry out the same calculation based on the two-orbital model \[30\], no similar FS reconstruction has been found. This difference is ascribed to be due to the orbital dependent renormalization. On the other hand, the most favored pairing state mediated by the inter-orbital spin fluctuations is found to be the extended $s$-wave with a sign change between the electron and hole Fermi pockets, which is consistent with the result obtained in the two-orbital model \[31, 32, 33\]. This indicates that the two models share the similar physics as far as the pairing symmetry is concerned, but exhibits difference in the band renormalization.

The paper is organized as following. In Sec.II, we present the three-orbital model and introduce the FLEX method. In Sec.III, the numerical results for the band renormalization is presented and discussed. We also give a brief discussion on the pairing symmetry in this section. In Sec.IV, we give a summary of the results.

### II. MODEL AND FLEX METHOD

The model Hamiltonian consists of two parts,

$$H = H_0 + H_{\text{int}},$$

\[1\]
where the bare Hamiltonian $H_0$ is given by the three-orbital model as introduced in Ref. [29].

In the unfolded(extended) BZ for the reduced unit cell (only one Fe atom in the unit cell as in Ref. [27]), it can be written as $H_0 = \sum_k \Psi_k^\dagger M_k \Psi_k$ with

$$M_k = \begin{pmatrix}
\varepsilon_{xz}(k + Q) & \varepsilon_{xz, yz}(k + Q) & \varepsilon_{xz, xy}(k) \\
\varepsilon_{xz, yz}(k + Q) & \varepsilon_{yz}(k + Q) & \varepsilon_{yz, xy}(k) \\
\varepsilon^*_{xz, xy}(k) & \varepsilon^*_{yz, xy}(k) & \varepsilon_{xy}(k)
\end{pmatrix}, \tag{2}
$$

and $\Psi_k = (c_{k+Q}^{xz}, c_{k+Q}^{yz}, c_{k}^{xy})^T$. Here the diagonal elements of $M_k$ denote the dispersion of Fe-3d orbitals $d_{xz}$, $d_{yz}$ and $d_{xy}$, while the others denote the hybridization among them.

Keeping up to the next nearest neighbor hopping terms, we have $\varepsilon_{xz}(k) = - \sum_k [2t_1 \cos k_x + 2t_2 \cos k_y + 4t_3 \cos k_x \cos k_y, \varepsilon_{yz}(k) = - \sum_k [2t_1 \cos k_y + 2t_2 \cos k_x + 4t_3 \cos k_x \cos k_y], \varepsilon_{xy}(k) = - \sum_k [2t_4 \cos k_x + \cos k_y] + 4t_5 \cos k_x \cos k_y], \varepsilon_{xz, yz}(k) = \varepsilon_{xz, xy}(k) = - \sum_k 4t_6 \sin k_x \sin k_y, \varepsilon_{xz, xy}(k) = \varepsilon^*_{xz, xy}(k) = - \sum_k 2i t_7 \sin k_x \sin k_y \varepsilon_{xy, yz}(k) = \varepsilon^*_{xy, yz}(k) = - \sum_k 2i t_7 \sin k_y \varepsilon_{xy, xy}(k) = \varepsilon^*_{xy, xy}(k)$,

In order to reproduce the FS and band structure feature, we set the parameters as $t_1 = -1.0 (\approx 0.4 \text{eV}), t_2 = 0.7, t_3 = -0.8, t_4 = -0.3, t_5 = 0.2, t_6 = 0.6, t_7 = -0.35$. As the three orbitals belong to the $t_{2g}$ manifold, we set the same on-site energy to the three orbitals. In Fig.1, we show the band structure and FS with $\mu = 1.15 (\text{electron density per site } n = 4.0)$ corresponding to the parent compound. We find that this three-orbital model can basically reproduce the main features of the FS and band structure obtained in the LDA calculation [23, 24].

The interaction between electrons is included in $H_{\text{int}}$ as following,

$$H_{\text{int}} = \frac{1}{2} U \sum_{i, l, \sigma \neq \sigma'} c_{i l \sigma}^\dagger c_{i l \sigma} c_{i l \sigma'}^\dagger c_{i l \sigma'} + \frac{1}{2} U' \sum_{i, l \neq l', \sigma, \sigma'} c_{i l \sigma}^\dagger c_{i l' \sigma'}^\dagger c_{i l' \sigma'} c_{i l \sigma} + \frac{1}{2} J \sum_{i, l \neq l', \sigma, \sigma'} c_{i l \sigma}^\dagger c_{i l' \sigma'} c_{i l' \sigma'} c_{i l \sigma} + \frac{1}{2} J' \sum_{i, l \neq l', \sigma \neq \sigma'} c_{i l \sigma}^\dagger c_{i l' \sigma'} c_{i l' \sigma'} c_{i l \sigma}, \tag{3}$$

where $U (U')$ is the intra-orbital(inter-orbital) Coulomb interaction, $J$ the Hund’s coupling and $J'$ the inter-orbital pair hopping.

We carry out the investigation using the FLEX approximation [34], in which the Green’s function and spin/charge fluctuations are determined self-consistently. For the three-orbital model, the Green’s function $\hat{G}$ and the self-energy $\hat{\Sigma}$ are expressed in a $3 \times 3$-matrix form,
FIG. 1: (color online) Band structure and FS of the three-orbital model. (a) The band structure in the folded BZ with $t_1 = -1.0, t_2 = 0.7, t_3 = -0.8, t_4 = -0.3, t_5 = 0.2, t_6 = 0.6, t_7 = 0.35$ and $\mu = 1.15$. (b) The FS in the unfolded BZ. The dashed lines denote the boundary of the folded BZ. The line with an arrow denotes the nesting vector between the hole and electron Fermi pockets. Panels (c) and (d) replot the hole and the electron Fermi pockets shown in Fig.(b), respectively, with the different colors representing the weight of the different orbitals.
while the susceptibility $\chi^0$ and the effective interaction $\hat{V}$ have a $9 \times 9$-matrix form. The Green’s function satisfies the Dyson equation \( \hat{G}(k)^{-1} = \hat{G}^0(k)^{-1} - \hat{\Sigma}(k) \), where the self-energy is given by \( \Sigma_{mn}(k) = \frac{T}{N} \sum_q \sum_{\mu \nu} V_{n \mu, m \nu}(q) G_{\mu \nu}(k - q) \) and the bare Green’s function reads \( \hat{G}^0(k) = (i\omega_n - \hat{M}_k + \mu)^{-1} \). The fluctuation exchange interaction is given by:

\[
V_{\mu m, \nu n}(q) = \frac{1}{2} [3\hat{U}^s\hat{\chi}^s(q)\hat{U}^s + \hat{U}^c\hat{\chi}^c(q)\hat{U}^c - \frac{1}{2}(\hat{U}^s + \hat{U}^c)\hat{\chi}^0(q)(\hat{U}^s + \hat{U}^c) + 3\hat{U}^s - \hat{U}^c]_{\mu m, \nu n}, \tag{4}
\]

with spin susceptibility $\hat{\chi}^s(q) = [\hat{I} - \hat{\chi}^0(q)\hat{U}^s]^{-1}\hat{\chi}^0(q)$ and charge susceptibility $\hat{\chi}^c(q) = [\hat{I} + \hat{\chi}^0(q)\hat{U}^c]^{-1}\hat{\chi}^0(q)$. The irreducible susceptibility is given by $\chi^0_{\mu m, \nu n}(q) = -\frac{T}{N} \sum_k \delta_{nk} G_{\mu \nu}(k + q) G_{\mu \nu}(k)$. In the above, $T$ is temperature, $k \equiv (\mathbf{k}, i\omega_n)$ with $\omega_n = \pi T(2n + 1)$, and $\hat{I}$ the identity matrix. The interaction matrix for the spin(charge) fluctuation $\hat{U}^s(\hat{U}^c)$ is given by:

For $i = j = k = l$, $U^s_{ij,kl} = U(U^c_{ij,kl} = U)$; For $i = j \neq k = l$, $U^s_{ij,kl} = J(U^c_{ij,kl} = 2U' - J)$; For $i = k, j = l$ and $i \neq j$, $U^s_{ij,kl} = U'(U^c_{ij,kl} = -U' + 2J)$; For $i = l, j = k$ and $i \neq j$, $U^s_{ij,kl} = J(U^c_{ij,kl} = J)$; For other cases, $U^s_{ij,kl} = 0(U^c_{ij,kl} = 0)$.

After obtaining the renormalized Green’s function $\hat{G}$, we can solve the ”Eliashberg” equation,

\[
\chi_{\mu n}(k) = -\frac{T}{N} \sum_q \sum_{\alpha \beta} \sum_{\mu \nu} V^{s,t}_{\alpha m, \beta n}(q) G_{\alpha \mu}(k - q) \times G_{\beta \nu}(q - k) \phi_{\mu \nu}(k - q), \tag{5}
\]

where the spin-singlet and spin-triplet pairing interactions $\hat{V}^s$ and $\hat{V}^t$ are given by,

\[
\hat{V}^s(q) = \frac{3}{2}\hat{U}^s\hat{\chi}^s(q)\hat{U}^s - \frac{1}{2}\hat{U}^c\hat{\chi}^c(q)\hat{U}^c + \frac{1}{2}(\hat{U}^s + \hat{U}^c), \tag{6}
\]

\[
\hat{V}^t(q) = -\frac{1}{2}\hat{U}^s\hat{\chi}^s(q)\hat{U}^s - \frac{1}{2}\hat{U}^c\hat{\chi}^c(q)\hat{U}^c + \frac{1}{2}(\hat{U}^s + \hat{U}^c). \tag{7}
\]

The most favorable SC pairing symmetry corresponds to the eigenvector $\phi_{\mu n}(k)$ with the largest eigenvalue $\lambda$.

The Dyson equation, the self-energy and the interaction matrix Eq.(4) form a closed set of equations and will be solved numerically on $64 \times 64 \mathbf{k}$ meshes with 1024 Matsubara frequencies. By symmetry, we set $J' = J$ and use the relation $U = U' + 2J$. In the following calculation, the intra-orbital Coulomb interaction $U = 3.0$(about 0.3 total bandwidth) is chosen, thus all interaction parameters are given by giving the Hund’s coupling $J$. 

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FIG. 2: (color online) Renormalization of the energy band for $J = 0.2U$, the red dotted (black solid) lines are the renormalized (bare) bands. The green, red and blue dashed lines indicate the Fermi levels for undoping, 10% electron doping and 20% hole doping, respectively. To show the renormalization more clearly, the energy bands presented here are plotted in the unfolded BZ.

III. RESULT AND DISCUSSION

A. Renormalization of band and Fermi surface

We show the renormalized bands for $J = 0.2U$ (correspondingly $U' = 0.6U$ according to the relation $U = U' + 2J$) together with the bare bands in Fig.2, in which the renormalized bands are calculated from the spectral function $A(k, \omega) = \frac{1}{\pi} \text{Im} G(k, \omega)$ with $G(k, \omega)$ the analytic continuation of the Matsubara Green’s function $G(k, i\omega_n)$ by the Padé approximation. The Fermi levels depicted in Fig.2 are determined by calculating the number of electrons via the renormalized Green’s function, and the undoped case is determined from the electron density per site $n = 4.0$. It is clearly seen that different bands exhibit different renormalization, and the strongest renormalization occurs around the $\tilde{X}$ point. Compared to the bare Fermi level, we find that the renormalized Fermi level is shifted up by $0.3(\approx 0.12\text{eV})$ for the
FIG. 3: (color online) (a) Renormalization factor of total bandwidth for different values of $J$. (b), (c) and (d) are the spin susceptibilities for $J = 0.2U$, $J = 0.05U$ and $J = 0.3U$ respectively.}

The undoped case. These features are consistent with the ARPES data [19, 20]. We define a total bandwidth renormalization factor as $W_B/W_R$, where $W_B(W_R)$ denotes the bandwidth of bare (renormalized) band. The renormalization factors for different values of $J$ are shown in Fig. 3(a). It increases from 1.4 to 2.3 when $J$ is increased to be around $0.5U$. In particular, a rapid rise is observed when $J$ is larger than $0.18U$. This shows that the Hund’s coupling plays an important role to enhance the renormalization effects.

For $U > U'$, the spin fluctuation will dominate over the charge fluctuation. In Fig. 3(b), we present the static spin susceptibility $\chi^s(\mathbf{q}, \omega = 0) = \sum_{\mu\nu} \chi^{s,\mu\nu}_\mu(\mathbf{q}, \omega = 0)$ for $J = 0.2U$. It shows four peaks around $(0, \pm\pi)$ and $(\pm\pi, 0)$ points, which is in agreement with the neutron scattering experiments [6]. This arises from the nesting between the hole and the electron pockets connected with the vectors $(0, \pm\pi)$ and $(\pm\pi, 0)$, as shown in Fig. 1(b). To show the orbital contribution to the FS, we replott the hole and the electron FS with different colors.
FIG. 4: (color online) Renormalized FS for 10% electron doping ((a) and (b)) and for 20% hole doping ((c) and (d)). (a) and (c) are the results shown in the unfolded BZ, while (b) and (d) in the folded BZ.

representing different weights of the three orbitals in Fig.1(c) and (d), respectively. For the nesting part of the FS, it is found that the $d_{yz}+d_{xy}$ orbitals contribute the main weight to the electron pockets and the $d_{xz}$ orbital mainly contributes to the hole pockets. This shows that the spin fluctuation is mainly due to the inter-orbital particle-hole excitations. As shown in Eq.(3), the Hund’s coupling favors the inter-orbital excitations, so the spin fluctuation around $(0, \pm \pi)$ and $(\pm \pi, 0)$ will be enhanced by the increase of $J$. This is evidenced from the results shown in Fig.2(c) and 2(d), where the spin susceptibilities for $J = 0.05U$ and $J = 0.3U$ are presented, respectively. For a small $J$ (0.05U), the $(0, \pm \pi)$ spin fluctuation disappears, while for a large $J$ ($J = 0.3U$) it is enhanced. Because the band renormalization is increased with the rise of $J$ as discussed above, it suggests that the strong renormalization around the $\tilde{X}$ point mainly comes from the coupling to the spin fluctuation around $(0, \pm \pi)$.

Inspecting the details of the renormalized bands around the $\tilde{X}$ point in Fig.2, one will
find that the energy band near the Fermi level is renormalized strongly along the $\Gamma - \tilde{X}$ direction, but less along the $\tilde{X} - \tilde{M}$ direction. Another feature is that the band crossing the Fermi level becomes flat around the $\tilde{X}$ point, and the flat portion situates at the bottom of the band along the $\Gamma - \tilde{X}$ direction. To identify the FS after renormalization, we calculate the distribution of the spectral weight $A(k, \omega)$ integrated over a narrow energy window $0.02(\approx 8\text{meV})$ around the Fermi level, a method used usually in the ARPES experiments. The results in the unfolded BZ are shown in Fig.4(a) for 10% electron doping and Fig.4(c) for 20% hole doping. To compare with experiments, their folded counterparts are shown in Fig.4(b) and Fig.4(d), respectively. In the undoped case, the Fermi level (the green dashed line) is just slightly below the flat band. Therefore, for the electron doped case, in which the Fermi level is shifted upwards as indicated by the red dashed line for the 10% electron doping, the Fermi level crosses the renormalized bands along both the $\Gamma - \tilde{X}$ and the $\tilde{X} - \tilde{M}$ directions. This gives rise to a large complete electron Fermi pocket around the $\tilde{X}$ point as shown in Fig.2(a) in the unfolded BZ and in Fig.2(b) in the folded one, which is similar to that predicted by the LDA calculation [23, 24, 26] and observed in the ARPES experiments [19, 21]. However, for the hole doped case, the Fermi level (the blue dashed line for 20% hole doping) is shifted below the flat band, so that it does not cross the energy band along the $\Gamma - \tilde{X}$ direction anymore. Consequently, the complete electron Fermi pocket in the bare case is broken and the spot-like portions are formed around the $\tilde{X}$ point, as clearly shown in Fig.4(c). After being folded, the electron FS shown in Fig.4(d) reproduces the experimental results in ARPES measurements [18, 25]. We note that due to the band renormalization the crossing between the two energy band along the $\tilde{X} - \tilde{M}$ directions is shifted up and approaches the Fermi level for 20% hole doping. This crossing gives rise to a large density of states. Therefore it adds an enhancement in the spectral weight around the spot-like portions and makes it be easily observed in experiments.

The anisotropic band renormalization along the $\Gamma - \tilde{X}$ and the $\tilde{X} - \tilde{M}$ direction can be traced to the different orbital weights composing the energy bands along these two directions. Specifically, the energy band near the $\tilde{X}$ point along the $\tilde{X} - \tilde{M}$ direction is composed of only the $d_{yz}$ orbital, while that along the $\Gamma - \tilde{X}$ direction is a mix of the $d_{xy}$ and $d_{yz}$ orbitals, as shown in Fig.1(c) and Fig.1(d) in which the different colors represent the weight of the respective orbitals. As noted above, the band renormalization is mainly due to the scattering off the inter-orbital spin fluctuations composed of the components $\chi_{xz, yz}, \chi_{xz, xy}$ and $\chi_{yz, xy}$.
We find that the magnitude of the components $\chi_{xz,xy}$ and $\chi_{yz,xy}$ is the same, while it is larger than that of the $\chi_{xz,yz}$. Therefore, the $d_{xy}$ orbital is renormalized most strongly by the spin fluctuation. This suggests that the anisotropic renormalization of the energy band near the $\tilde{X}$ point is orbital dependent.

We note that in the two-orbital model [30], the energy band near the $\tilde{X}$ point along both directions is composed of one orbital $d_{yz}$ as shown in Fig.5(a), so the similar band renormalization is expected. To show this, we have carried out the same calculation for the two-orbital model and the result is presented in Fig.5(b). Though the strong renormalization still occurs in one of the bands around the $\tilde{X}$ point, no strong anisotropic renormalization between the $\tilde{\Gamma} - \tilde{X}$ and the $\tilde{X} - \tilde{M}$ direction can be seen. Thus, no similar FS reconstruction as observed in the three-orbital model and in experiments [18, 25] can be obtained here.

**B. Symmetry of superconducting pairing**

With the static spin susceptibility, we will further investigate the pairing symmetry mediated by spin fluctuations. For $J = 0.2U$, which is the case with peaks around $(0, \pm \pi)$ and $(\pm \pi, 0)$ points in spin fluctuations, we find that the eigenvalue $\lambda$ has the maximum value.
FIG. 6: (color online) Pairing gap functions in the unfolded BZ for $U = 3.0$ with $T = 0.02$ for 10% electron doping and 20% hole doping. (a), (b), (c), (d) for $J = 0.2U$ and (e), (f) for $J = 0.05U$. (a) $\Delta_{hh}$ for electron doping. (b) $\Delta_{ee}$ for electron doping. (c) $\Delta_{hh}$ for hole doping. (d) $\Delta_{ee}$ for hole doping. (e) $\Delta_{hh}$ for electron doping. (f) $\Delta_{ee}$ for electron doping.

in the spin-singlet channel and it is nearly zero in the spin-triplet channel at temperature $T = 0.02$. We note that this is not the case considered in Ref. [29], where the spin-triplet state is expected with a larger $J$ (such as $J > U/3$, see also the analysis in Ref. [33]). The obtained gap functions of the hole band $\Delta_{hh}$ and the electron band $\Delta_{ee}$ for 10% electron doping and 20% hole doping are shown in Fig.3(a)-(d). It can be seen that the gap is basically an extended $s$-wave, which is nodeless around all the Fermi pockets and change sign between the hole pockets and the electron pockets. This result is consistent with the experiment measurements [9, 10, 11, 12, 13, 18] and the calculation based on the two-orbital model [31]. It is noted that the pairing symmetry is similar for both the electron doped and the hole doped systems, although their FS topology is different as discussed above.
Because the spin fluctuation is dominant over the charge fluctuation, the pairing interaction in the spin-singlet channel is positive (repulsive) [See Eq.(6)] and strongest around the wave vectors $Q$ at which the spin fluctuation has a largest intensity. For a repulsive pairing symmetry, the SC gap will satisfy the condition $\Delta(k)\Delta(k+Q) < 0$ to obtain the largest eigenvalue $\lambda$ of the ”Eliashberg” equation, as can be seen from Eq.(5). For $J > 0.1U$, the inter-band (inter-orbital) spin fluctuation is dominant and has peaks around $(\pm\pi, 0)$ and $(0, \pm\pi)$ which is the nesting wave vectors connecting the hole and the electron Fermi pockets. Thus, the gap will have an opposite sign between these two Fermi pockets. This gives rise to the extended $s$-wave. Because the SC pairing is mediated by the spin fluctuation around $(\pm\pi, 0)$ and $(0, \pm\pi)$, which is the same for the three-orbital and the two-orbital models (see Ref. [31]), the same pairing symmetry will be obtained based on these two models.

IV. CONCLUSION

In a summary, we have investigated the band renormalization, FS reconstruction and the symmetry of the superconducting gap in iron-based superconductors using a three-orbital model. A strong anisotropic band renormalization due to the scattering off the inter-orbital spin fluctuations is found. The band renormalization is shown to be orbital dependent. As a result, the electron Fermi pocket exhibits different topology between the electron doped and the hole doped cases, which provides a natural explanation for the recent ARPES experiments. In addition, we have found that the most favorable superconducting pairing symmetry mediated by the inter-band (inter-orbital) spin fluctuations is the extended $s$-wave.

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