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ORIGINAL PAPER

Three-orbital Model for Fe-Pnictides

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Abstract We formulate and study the three-orbital model for iron-based superconductors. Results for the band structure, Fermi surface, and the spin susceptibility in both normal and superconducting $s_{\pm}$ states are presented. We also discuss the pairing interaction and show that the dominant part of it should come from the intraorbital scattering.

Keywords Fe-based superconductors · Spin susceptibility · Low-energy model

One of the central problems in the field of the Fe-based superconductors (FeBS) is the microscopic nature of the superconducting pairing [1]. According to the density-functional studies (DFT) within LDA (local-density approximation), GGA (generalized gradient approximation), and ARPES (angle-resolved photo-emission spectroscopy), the states near the Fermi level in pncitides and chalcogenides originate mostly from Fe d-orbitals. The same orbitals form the Fermi surface (FS) that in the undoped and moderately doped systems consist of two hole and two electron sheets. Nesting between these two groups of sheets is the driving force for the spin-density wave (SDW) long-range magnetism in the undoped FeBS and the scattering with the wave vector $\mathbf{Q}$ connecting hole and electron pockets is the most probable candidate for superconducting pairing in the doped systems. In the spin-fluctuation studies [2–4], the leading instability is the extended s-wave gap, which changes sign between hole and electron sheets ($s_{\pm}$ state) [5]. Further, our discussion will be confined to the 1-Fe per unit cell Brillouin zone (BZ).

Neutron scattering is a powerful tool to measure dynamical spin susceptibility $\chi(\mathbf{q},\omega)$. It carries information about the order parameter symmetry and gap structure. For the local interactions (Hubbard and Hund's exchange), χ can be obtained in the random-phase approximation (RPA) from the bare electron-hole bubble $\chi_0(\mathbf{q},\omega)$ by summing up a series of ladder diagrams to give $\chi(\mathbf{q},\omega) = [I - U_s\chi_0(\mathbf{q},\omega)]^{-1}\chi_0(\mathbf{q},\omega)$, where U_s and I are interaction and unit matrices in orbital space, and all other quantities are matrices as well.

The fact that $\chi_0(\mathbf{q},\omega)$ describes particle-hole excitations has interesting consequences in the case of an unconventional superconducting state. Excitations are gapped below approximately $2\Delta_0$ with Δ_0 being the amplitude of the superconducting gap, and then $\mathrm{Im}\chi_0(\mathbf{q},\omega)$ becomes finite. Scattering between nearly nested hole and electron Fermi surfaces in FeBS produce a peak in the normal state magnetic susceptibility at or near $\mathbf{Q} = (\pi, 0)$. For the uniform s-wave gap, sign $\Delta_{\mathbf{k}} =$ sign $\Delta_{\mathbf{k}+\mathbf{Q}}$ and there is no resonance peak. For the $s_{\pm}$ order parameter as well as for an extended nonuniform s-wave symmetry, $\mathbf{Q}$ connects Fermi sheets with the different signs of gaps. The coherence factors entering χ_0 are then nonzero and the imaginary part of χ_0 possesses a discontinuous jump at $\Omega_c = \min(|\Delta_{\mathbf{k}}| + |\Delta_{\mathbf{k}+\mathbf{Q}}|)$. Due to the Kramers–Kronig relations, the real part exhibits a logarithmic singularity. For a range of interaction values entering matrix U_s, it results in the divergence of

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$\mathrm{Im}\chi(\mathbf{Q}, i\omega_m)$. Such an enhancement of the spin susceptibility at a frequency below Ω_c is called a "spin resonance" [6–8]. The existence of the spin resonance in FeBS was predicted theoretically [6, 7], and subsequently discovered experimentally with many reports of well-defined spin resonances in 1111, 122, and 11 systems [9–17].

Study of the spin-resonance starts with the model for the band structure. There are several low-energy models for pnictides already known. The simplest one is the two-orbital model [18] correctly postulating the dominant d_{xz}–d_{yz} contribution to the FS. It has many disadvantages including misplacement of the second hole pocket that should be around the Γ point, wrong Fermi velocities as compared to ARPES and DFT, and absence of d_{xy} orbital contribution, which is known to appear near or even at the Fermi level (both ARPES and DFT). The three-orbital model was developed sometime later [19–21]. It included d_{xy} in addition to d_{xz} and d_{yz} orbitals. As for the latter model, [19], the unexpected result was that the salient feature of FeBS, namely the peak in the magnetic susceptibility around the $(\pi, 0)$ point, was absent in this model [22]. Disappearance of the peak is somehow connected with matrix elements of the orbital-band transformation, but the exact origin is unclear.

Here, we present a simple three-orbital model for FeBS. It comes from the three t_{2g} d-orbitals. The xz and yz components are hybridized and form two electron-like FS pockets around $(\pi, 0)$ and $(0, \pi)$ points, and one hole-like pocket around the $\Gamma = (0, 0)$ point. The xy orbital is considered to be decoupled from them and form an outer hole pocket around the Γ point. The latter is based on the presence of the xy orbital near the Fermi level in the vicinity of the $(0, 0)$ point [23]. The one-electron part of the Hamiltonian is given by

$$H_0 = \sum_{\mathbf{k},\sigma,l,m} \varepsilon_{\mathbf{k}}^{lm} c_{\mathbf{k}l\sigma}^{\dagger} c_{\mathbf{k}m\sigma}, \tag{1}$$

where l and m are orbital indices, $c_{\mathbf{k}m\sigma}$ is the annihilation operator of a particle with momentum $\mathbf{k}$ and spin σ.

The matrix of the one-electron energies is

$$\hat{\varepsilon}_{\mathbf{k}} = \begin{pmatrix} \varepsilon_{1\mathbf{k}} - \mu & 0 & 0 \\ 0 & \varepsilon_{2\mathbf{k}} - \mu & \varepsilon_{4\mathbf{k}} \\ 0 & \varepsilon_{4\mathbf{k}} & \varepsilon_{3\mathbf{k}} - \mu \end{pmatrix}, \tag{2}$$

where

$$\begin{aligned} \varepsilon_{1\mathbf{k}} &= \epsilon_{xy} + 2t_{xy}(\cos k_x + \cos k_y) + 4t'_{xy} \cos k_x \cos k_y, \\ \varepsilon_{2\mathbf{k}} &= \epsilon_{yz} + 2t_x \cos k_x + 2t_y \cos k_y + 4t' \cos k_x \cos k_y \\ &\quad + 2t''(\cos 2k_x + \cos 2k_y), \\ \varepsilon_{3\mathbf{k}} &= \epsilon_{xz} + 2t_y \cos k_x + 2t_x \cos k_y + 4t' \cos k_x \cos k_y \\ &\quad + 2t''(\cos 2k_x + \cos 2k_y), \end{aligned}$$

$\varepsilon_{4\mathbf{k}} = 4t_{xzyz} \sin k_x/2 \sin k_y/2$.

To reproduce the topology of the FS in FeBS, we choose the following parameters (in eV): $\epsilon_{xy} = -0.70$, $\epsilon_{yz} = -0.34$, $\epsilon_{xz} = -0.34$, $t_{xy} = 0.18$, $t'_{xy} = 0.06$, $t_x = 0.26$, $t_y = -0.22$, $t' = 0.2$, $t'' = -0.07$, $t_{xzyz} = 0.38$.

To diagonalize (2), we use a unitary transformation with the matrix

$$\hat{U} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & u_{\mathbf{k}} & v_{\mathbf{k}} \\ 0 & -v_{\mathbf{k}} & u_{\mathbf{k}} \end{pmatrix}, \tag{3}$$

where $u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 = 1$, $u_{\mathbf{k}}^2 = \frac{1}{2}\left(1 + \frac{|g_{\mathbf{k}}|}{D_{\mathbf{k}}}\right)$ and $v_{\mathbf{k}}^2 = \frac{1}{2}\left(1 - \frac{|g_{\mathbf{k}}|}{D_{\mathbf{k}}}\right)$, $g_{\mathbf{k}} = (\varepsilon_{2\mathbf{k}} - \varepsilon_{3\mathbf{k}})^2$, $D_{\mathbf{k}} = g_{\mathbf{k}} + 4\varepsilon_{4\mathbf{k}}^2$. Applying this transformation, we find the energy dispersion as the following eigenvalues, $E_{1\mathbf{k}} = \varepsilon_{1\mathbf{k}}$, $E_{2,3\mathbf{k}} = \frac{1}{2}(\varepsilon_{2\mathbf{k}} + \varepsilon_{3\mathbf{k}} \pm \sqrt{D})$.

Number of electrons n on a filled d-orbital is 6 and for the three-orbital model we assume 2 orbitals to be completely filled, so for doping concentration x we have $n = 6-2-x = 4-x$.

In Fig. 1, we show the band dispersion and the Fermi surface for the undoped material, $x = 0$. FS is similar to those found in DFT calculations and five-orbital models [2, 3].

Physical susceptibility for Matsubara frequency ω_m is calculated as $\chi_0(\mathbf{q}, \omega_m) = \chi_0^{11}(\mathbf{q}, \omega_m) + \chi_0^{22}(\mathbf{q}, \omega_m) + \chi_0^{23}(\mathbf{q}, \omega_m) + \chi_0^{32}(\mathbf{q}, \omega_m) + \chi_0^{33}(\mathbf{q}, \omega_m)$, where intra and interband susceptibilities are

$$\chi_0^{11}(\mathbf{q}, \omega_m) = \frac{1}{2} \sum_{\mathbf{k}} \xi_{1\mathbf{k}+\mathbf{q}}^{1\mathbf{k}}, \tag{4}$$

$$\chi_0^{22}(\mathbf{q}, \omega_m) = \frac{1}{4} \sum_{\mathbf{k}} (1 + \gamma_{\mathbf{kq}}) \xi_{2\mathbf{k}+\mathbf{q}}^{2\mathbf{k}}, \tag{5}$$

$$\chi_0^{23}(\mathbf{q}, \omega_m) = \frac{1}{4} \sum_{\mathbf{k}} (1 - \gamma_{\mathbf{kq}}) \xi_{3\mathbf{k}+\mathbf{q}}^{2\mathbf{k}}, \tag{6}$$

$$\chi_0^{32}(\mathbf{q}, \omega_m) = \frac{1}{4} \sum_{\mathbf{k}} (1 - \gamma_{\mathbf{kq}}) \xi_{2\mathbf{k}+\mathbf{q}}^{3\mathbf{k}}, \tag{7}$$

$$\chi_0^{33}(\mathbf{q}, \omega_m) = \frac{1}{4} \sum_{\mathbf{k}} (1 + \gamma_{\mathbf{kq}}) \xi_{3\mathbf{k}+\mathbf{q}}^{3\mathbf{k}}. \tag{8}$$

Here

$$\xi_{\beta\mathbf{k}+\mathbf{q}}^{\alpha\mathbf{k}} = \frac{f(E_{\beta\mathbf{k}+\mathbf{q}}) - f(E_{\alpha\mathbf{k}})}{\omega_m + E_{\alpha\mathbf{k}} - E_{\beta\mathbf{k}+\mathbf{q}}}, \tag{9}$$

$$\gamma_{\mathbf{kq}} = \frac{g_{\mathbf{k}} g_{\mathbf{k}+\mathbf{q}} + 4\varepsilon_{4\mathbf{k}} \varepsilon_{4\mathbf{k}+\mathbf{q}}}{D_{\mathbf{k}} D_{\mathbf{k}+\mathbf{q}}}. \tag{10}$$

Calculated real part of the physical spin susceptibility at zero frequency is shown in Fig. 2. At zero doping, there is a peak at $(\pi, 0)$ point due to the nesting between hole and electron FSs. The large hump closer to the Γ point is due to

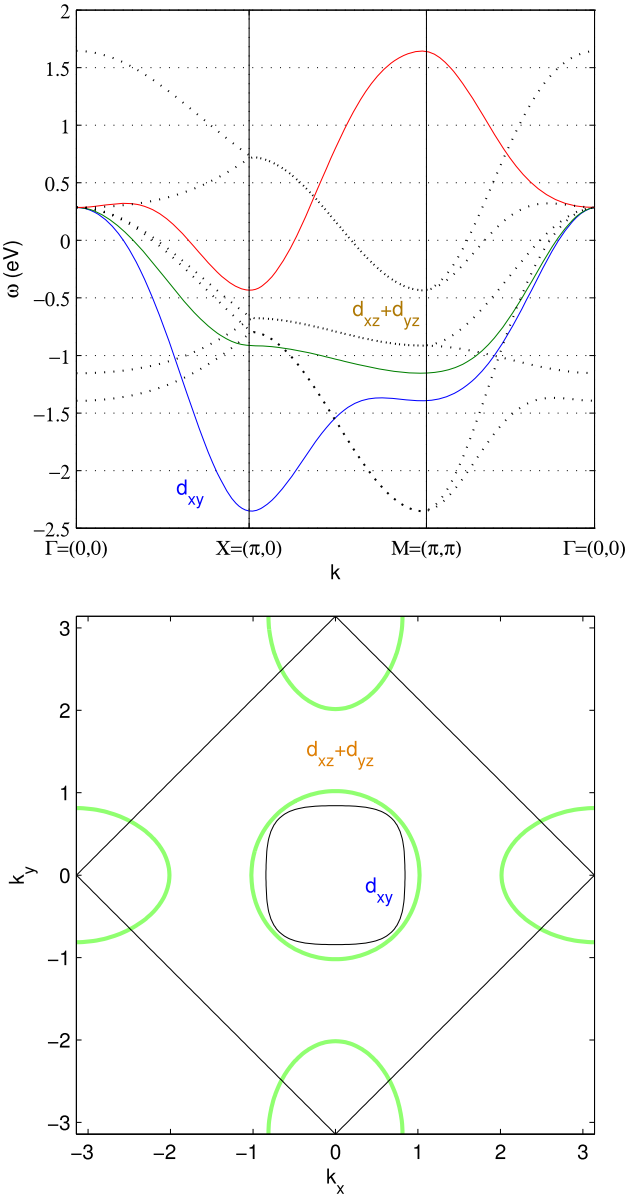

Fig. 1 Band dispersion (*top, solid curves*) and FS (*bottom*) for the three-orbital model in the 1-Fe BZ. Inner FS pocket around Γ point has a dxy orbital character, while other bands have a mixed $d_{xz} + d_{yz}$ character. *Black dotted curves* show bands in the 2-Fe BZ after the folding. Boundaries of the folded BZ are also shown in the FS plot as a *rotated square*

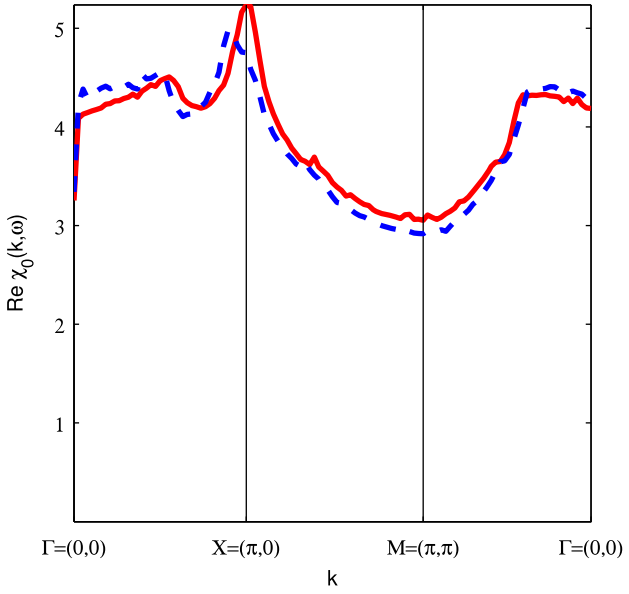

Fig. 2 $\mathrm{Re}\chi_0(\mathbf{k},\omega)$ for the undoped case $x = 0$ (*solid red curve*) and for the optimal doping $x = 0.12$ (*dashed blue curve*). (Color figure online)

the intraband scattering. At the optimal doping $x = 0.12$, the peak near the X-point becomes incommensurate and a bit suppressed compared to the $x = 0$ case because the system goes away from the perfect nesting.

Now we are going to discuss the superconducting pairing. Let us assume that annihilation operator $b_{\mathbf{k}\alpha\sigma}$ is defined in the band basis (band index α) where the Hamiltonian H_0 is diagonal, $H_0 = \sum_{\mathbf{k},\sigma,\alpha} E_{\mathbf{k},\alpha} b^\dagger_{\mathbf{k}\alpha\sigma} b_{\mathbf{k}\alpha\sigma}$. While the dominating pairing interaction may be interband (like spin-fluctuations [1]), the pairing itself is intraband only,

$$H_\Delta = \sum_{\mathbf{k},\alpha} \left(\Delta^*_{\mathbf{k}\alpha} b^\dagger_{\mathbf{k}\alpha\uparrow} b^\dagger_{-\mathbf{k}\alpha\downarrow} + \Delta_{\mathbf{k}\alpha} b_{\mathbf{k}\alpha\downarrow} b_{-\mathbf{k}\alpha\uparrow} \right). \tag{11}$$

If we apply the unitary transformation (3), we get a pairing term in the orbital basis,

$$H_\Delta = H_{\Delta 1} + H^\dagger_{\Delta 2,3} + H_{\Delta 2,3}, \tag{12}$$

$$H_{\Delta 1} = \sum_{\mathbf{k}} \left(\Delta^*_{\mathbf{k}1} a^\dagger_{\mathbf{k}1\uparrow} a^\dagger_{-\mathbf{k}1\downarrow} + \Delta_{\mathbf{k}1} a_{\mathbf{k}1\downarrow} a_{-\mathbf{k}1\uparrow} \right), \tag{13}$$

$$\begin{aligned} H_{\Delta 2,3} = \sum_{\mathbf{k}} \big[& \left(\Delta_{\mathbf{k}2} u^2_{\mathbf{k}} + \Delta_{\mathbf{k}3} v^2_{\mathbf{k}} \right) a_{\mathbf{k}2\downarrow} a_{-\mathbf{k}2\uparrow} \\ & + \left(\Delta_{\mathbf{k}2} v^2_{\mathbf{k}} + \Delta_{\mathbf{k}3} u^2_{\mathbf{k}} \right) a_{\mathbf{k}3\downarrow} a_{-\mathbf{k}3\uparrow} \\ & + u_{\mathbf{k}} v_{\mathbf{k}} (\Delta_{\mathbf{k}3} - \Delta_{\mathbf{k}2}) (a_{\mathbf{k}2\downarrow} a_{-\mathbf{k}3\uparrow} + a_{\mathbf{k}3\downarrow} a_{-\mathbf{k}2\uparrow}) \big]. \end{aligned} \tag{14}$$

One can clearly see that if $\Delta_{\mathbf{k}2} = \Delta_{\mathbf{k}3}$, then $H_{\Delta 2,3}$ will contain only intraorbital pairing terms,

$$H_{\Delta 2,3} = \sum_{\mathbf{k}} (\Delta_{\mathbf{k}2} a_{\mathbf{k}2\downarrow} a_{-\mathbf{k}2\uparrow} + \Delta_{\mathbf{k}2} a_{\mathbf{k}3\downarrow} a_{-\mathbf{k}3\uparrow}). \tag{15}$$

Therefore, if one considers only intraorbital pairing, it forces gaps on one of the hole FS pockets and on electron FS pockets to be the same. This is in qualitative agreement with ARPES data on $Ba_{1-x}K_xFe_2As_2$ [24, 25]. Spin-fluctuation theories also predict the pair interaction to be enhanced in the intraorbital channel [26].

We have calculated the frequency dependence of the spin susceptibility in both normal and superconducting states

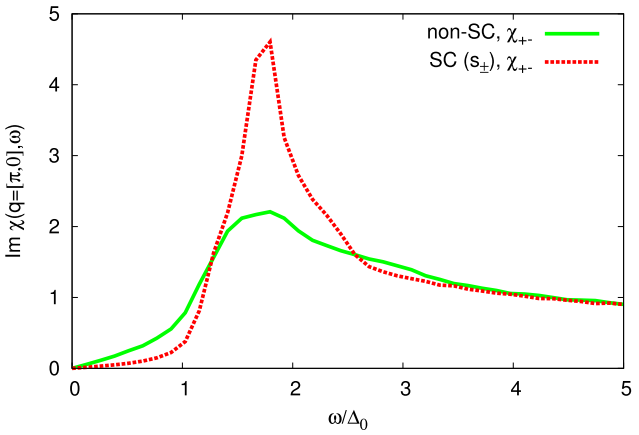

Fig. 3 $\mathrm{Im}\chi(\mathbf{Q},\omega)$, $\mathbf{Q}=(\pi,0)$, for $x=0$ in the normal state (*solid green curve*) and in the superconducting state with the $s_{\pm}$ order parameter symmetry (*dashed red curve*). (Color figure online)

with the $s_{\pm}$ gap symmetry; see Fig. 3. Multiorbital RPA (random phase approximation) was used [2] with the following interaction parameters (in eV) $U=0.9$, $U'=0.7$, $J=J'=0.1$, and the gap magnitude $\Delta_0=0.02$ eV. Spin-resonance appears in the $s_{\pm}$ state below the characteristic frequency of $2\Delta_0$. The resonance is similar to that found in the multiorbital models for FeBS [6, 8].

Summarizing, we presented the simple three-orbital model for FeBS allowing for exact analytical solution. It has FSs resembling the ones observed in ARPES and DFT studies, and the magnetic response similar to what is found in "realistic" multiorbital models. Analysis of the superconducting pairing and comparison to ARPES data on 122 systems leads to the conclusion that the dominant pairing interaction should be intraorbital.

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