Electronic states and pairing symmetry in the two-dimensional 16 band d-p model for iron-based superconductor

Yuki YANAGI[1]*, Youichi YAMAKAWA[1], and Yoshiaki ŌNO[1,2]

[1]*Department of Physics, Niigata University, Ikarashi, Niigata 950-2181, Japan*
[2]*Center for Transdisciplinary, Reserch, Niigata University, Ikarashi, Niigata 950-2181, Japan*

The electronic states of the FeAs plane in iron-based superconductors are investigated on the basis of the two-dimensional 16-band d-p model, where the tight-binding parameters are determined so as to fit the band structure obtained by the density functional calculation for LaFeAsO. The model includes the Coulomb interaction on a Fe site: the intra- and inter-orbital direct terms U and U', the exchange coupling J and the pair-transfer J'. Within the random phase approximation (RPA), we discuss the pairing symmetry of possible superconducting states including s-wave and d-wave pairing on the U'-J plane.

KEYWORDS: iron-based superconductors, 16-band d-p model, pairing symmetry, RPA

The newly discovered iron-based superconductors[1] $RFeAsO_{1-x}F_x$ (R=Rare Earth) with a transition temperature up to $T_c = 55$K[2] have attracted much attention. The mechanism of the superconductivity is one of the most significant issues. Several theoretical approaches have been done on simplified multi-orbital Hubbard models within weak coupling approaches.[3,4] The details of the band structure and the Fermi surface are crucial for determining the pairing symmetry. Therefore, we employ a realistic model which includes both the Fe 3d orbitals and the As 4p orbitals, so called d-p model.

We perform the density functional calculation for LaFeAsO with the generalized gradient approximation of Perdew, Burke and Ernzerhof[5] by using the WIEN2k package,[6] where the lattice parameters ($a = 4.03268$Å, $c = 8.74111$Å) and the internal coordinates ($z_{La} = 0.14134$, $z_{As} = 0.65166$) are experimentally determined.[7] Considering that there are two distinct Fe and As sites in the crystallographic unit cell, we then derive the two-dimensional 16-band d-p model,[8,9] where 3d orbitals ($d_{3z^2-r^2}$, $d_{x^2-y^2}$, d_{xy}, d_{yz}, d_{zx}) of two Fe atoms (Fe$_1$=A, Fe$_2$=B) and 4p orbitals (p_x, p_y, p_z) of two As atoms are explicitly included. We note that x, y axes are rotated by 45 degrees from the direction along Fe-Fe bonds. The model is given by the following Hamiltonian,

$$H = H_0 + H_{\rm int}, \tag{1}$$

$$\begin{aligned} H_0 &= \sum_{i,\ell,\sigma} \varepsilon^d_\ell d^\dagger_{i\ell\sigma} d_{i\ell\sigma} + \sum_{i,m,\sigma} \varepsilon^p_m p^\dagger_{im\sigma} p_{im\sigma} \\ &+ \sum_{i,j,\ell,\ell',\sigma} t^{dd}_{i,j,\ell,\ell'} d^\dagger_{i\ell\sigma} d_{j\ell'\sigma} \\ &+ \sum_{i,j,m,m',\sigma} t^{pp}_{i,j,m,m'} p^\dagger_{im\sigma} p_{jm'\sigma} \\ &+ \sum_{i,j,\ell,m,\sigma} t^{dp}_{i,j,\ell,m} d^\dagger_{i\ell\sigma} p_{jm\sigma} + h.c., \end{aligned} \tag{2}$$

where $d_{i\ell\sigma}$ is the annihilation operator for Fe-3d electrons with spin σ in the orbital ℓ at the site i and $p_{im\sigma}$ is the annihilation operator for As-4p electrons with spin σ in the orbital m at the site i. In eq. (2), the transfer integrals $t^{dd}_{i,j,\ell,\ell'}$, $t^{pp}_{i,j,m,m'}$, $t^{dp}_{i,j,\ell,m}$ and the atomic energies ε^d_ℓ, ε^p_m are determined so as to fit both the energy and the weights of orbitals for each band obtained from the tight-binding approximation (d-p model) to those from the density functional calculation. The doping x corresponds to the number of electrons per unit cell $n = 24 + 2x$ in the present model.

In eq. (1), $H_{\rm int}$ is the on-site Coulomb interaction in Fe-3d orbitals and includes the intra-orbital (inter-

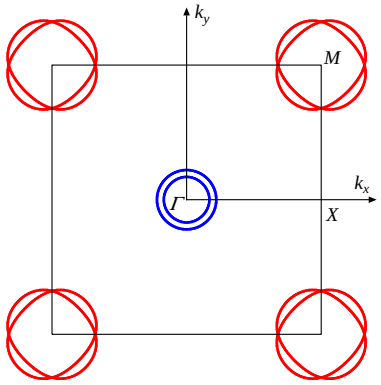

Fig. 1. Fermi surface obtained from the d-p model eq. (2) for $x = 0.1$

*E-mail address: yanagi@phys.sc.niigata-u.ac.jp

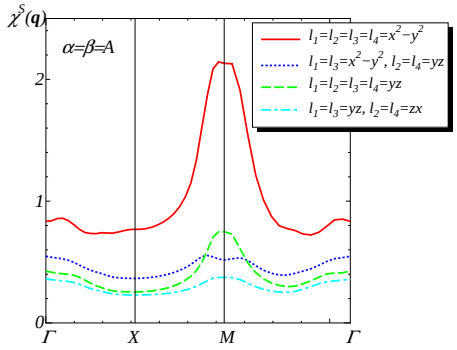

Fig. 2. Several components of the spin susceptibility obtained from the RPA $\chi^{s\ \alpha,\beta}_{\ell_1\ell_2,\ell_3\ell_4}(\mathbf{q})$ for $U = 1.5$eV, $U' = 1.0$eV, $J = J' = 0.25$eV, $T = 0.02$eV and $x = 0.1$.

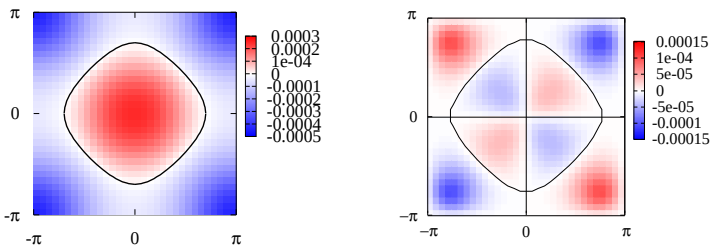

Fig. 3. The gap function $\Delta^{AA}_{x^2-y^2,x^2-y^2}(\mathbf{k})$ for extended s-wave (left) with $\lambda = 0.976$ and for d_{xy}-wave (right) with $\lambda = 0.836$ for the same parameters in Fig. 2. The solid line represents the node of the gap function.

orbital) Coulomb interaction U (U'), the Hund's rule coupling J and the pair-transfer interaction J'. In the weak coupling regime, the superconducting gap equation is given by

$$\lambda\Delta^{\alpha\beta}_{\ell\ell'}(\mathbf{k}) = \frac{1}{N}\sum_{\mathbf{k}'}\sum_{\ell_1\ell_2\ell_3\ell_4}\sum_{\alpha',\beta'}\sum_{\mu,\nu} \times \frac{f(\varepsilon_{-\mathbf{k}',\mu}) + f(\varepsilon_{\mathbf{k}',\nu}) - 1}{\varepsilon_{-\mathbf{k}',\mu} + \varepsilon_{\mathbf{k}',\nu}} V^{\alpha,\beta}_{\ell\ell_1,\ell_2\ell'}(\mathbf{k}-\mathbf{k}')\Delta^{\alpha'\beta'}_{\ell_3\ell_4}(\mathbf{k}') \times u^{\alpha'}_{\ell_3,\mu}(-\mathbf{k}')u^{\alpha}_{\ell_1,\mu}(-\mathbf{k}')^* u^{\beta'}_{\ell_4,\nu}(\mathbf{k}')u^{\beta}_{\ell_2,\nu}(\mathbf{k}')^* \quad (3)$$

where μ, ν (=1-16) are band indexes, α, β ($=A, B$) represent two Fe sites, $u^{\alpha}_{\ell,\mu}(\mathbf{k})$ is the eigenvector which diagonalizes H_0, $\varepsilon_{\mathbf{k},\mu}$ is the energy of band μ with wave vector $\mathbf{k}$, $f(\varepsilon)$ is the Fermi distribution function. Here, we approximate the effective pairing interaction $V^{\alpha,\beta}_{\ell_1\ell_2,\ell_3\ell_4}(\mathbf{q})$ within the RPA[10] and numerically solve the equation (3) to obtain the gap function $\Delta^{\alpha\beta}_{\ell\ell'}(\mathbf{k})$ with eigenvalue λ. At $T = T_c$, the largest eigenvalue λ becomes unity. We use 32×32 $\mathbf{k}$ points for numerical calculations.

Figure 1 shows the Fermi surface for the d-p model at $x = 0.1$, where we can see nearly circular hole pockets around the Γ point ($\mathbf{k} = (0, 0)$) and elliptical electron pockets around the M point ($\mathbf{k} = (\pi, \pi)$). The spin susceptibility $\chi^{s\ \alpha,\beta}_{\ell_1\ell_2,\ell_3\ell_4}(\mathbf{q})$ is given by 50×50 matrix and is calculated within the RPA as shown in Fig. 2. The peak around the Γ point is due to the effect of the nesting between the electron (hole) pockets, while the peak around the M point is due to that between the hole pockets and the electron pockets. We note that the x^2-y^2 component becomes dominant around the M point (see Fig. 2).

As the enhanced spin susceptibility contributes to the effective interaction within the RPA,[10] the gap function for the x^2-y^2 component $\Delta^{AA}_{x^2-y^2,x^2-y^2}(\mathbf{k})$ becomes dominant. The obtained gap functions with two largest eigenvalues λ are shown in Fig. 3. For $U = 1.5$eV, $U' = 1.0$eV, $J = J' = 0.25$eV, $T = 0.02$eV and $x = 0.1$, the gap function with the largest λ is extended s-wave symmetry and changes the sign between the hole pockets and the electron pockets, while that with second largest λ is d_{xy}-wave symmetry, as shown in Fig. 3. On the other hand, for $U = 1.68$eV, $U' = 1.4$eV, $J = J' = 0.14$eV, $T = 0.02$eV and $x = 0.1$, the gap function with largest λ is d_{xy}-wave ($\lambda = 0.978$), while that with second largest λ is extended s-wave ($\lambda = 0.967$). The detailed phase diagram of the pairing symmetry will be shown in the subsequent paper.[9]

In summary, we investigated the pairing symmetry of the two-dimensional 16-band d-p model by using the RPA. For a larger value of J/U', the most favorable pairing is extended s-wave symmetry whose order parameter changes its sign between the hole pockets and the electron pockets, while for a smaller value of J/U', it is d_{xy}-wave symmetry. According to the recent experiment of very weak T_c-suppression by Co-impurities,[11] we suppose that the d_{xy}-wave pairing is suppressed by pair breaking effect and the extended s-wave paring is realized in real materials.

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