Phase Diagram of the Two-dimensional 16-band *d-p* Model for Iron-based Superconductors

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Abstract

The electronic state of the Fe_2As_2 plane in iron-based superconductors is investigated on the basis of the two-dimensional 16-band *d-p* model. Using the random phase approximation for the on-site Coulomb interaction between Fe *d* electrons, we obtain the phase diagram including the magnetic ordered states and the superconductivity. It is found that the $s_{\pm}$-wave superconductivity, where the gap functions have different signs between the electron pockets and the hole pockets, is realized near the incommensurate magnetic ordered phase with $\mathbf{q} \sim (\pi, \pi)$. The absolute values of the gap functions on the Fermi surfaces are almost isotropic but largely depend on the energy bands.

Key words: iron-based superconductors, 16-band *d-p* model, pairing symmetry, gap function

Since the recent discovery of iron-based superconductors $LaFeAsO_{1-x}F_x$ with high transition temperatures [1], the symmetry of the superconducting gap and the pairing mechanism have been investigated intensively [2, 3]. In our previous works [4, 5], we investigated the electronic states of the Fe_2As_2 plane in iron-based superconductors on the basis of the two-dimensional 16-band *d-p* model, where the tight-binding parameters are determined so as to fit the density functional calculation for LaFeAsO. The model explicitly includes 3*d* orbitals (d_{3z^2-r2}, $d_{x^2-y^2}$, d_{xy}, d_{yz}, d_{zx}) of two Fe atoms (Fe^1=*A*, Fe^2=*B*) and 4*p* orbitals (p_x, p_y, p_z) of two As atoms and also includes the Coulomb interaction on a Fe site: the intra- and inter-orbital direct terms *U*

and U', the Hund's coupling J and the pair-transfer J'. Using the random phase approximation (RPA), we obtained the magnetic phase diagram including the stripe and the incommensurate order on the U'-J plane. We also solved the superconducting gap equation within the RPA and found that, for large J, the most favorable pairing symmetry is $s_{\pm}$-wave whose order parameter changes its sign between the hole pockets and the electron pockets, while it is d_{xy}-wave for small J.

The present paper is a straightforward extension of the previous works [4, 5] with some numerical improvements [6]. In addition, we discuss the structure of the gap function in more detail by obtaining that in the band representation instead of that in the orbital representation discussed in the previous papers [4, 5]. For simplicity, we change the parameters U' and J with fixing $U = U' + 2J$ and $J = J'$, and we set $T = 0.02$ eV and $x = 0.1$, where the doping level x corresponds to the electron number per unit cell $n = 24 + x$ in our 16-band model.

Fig. 1 (a) shows the phase diagram on the U'-J plane including the magnetic order and the superconductivity. The magnetic order is determined by the divergence of the spin susceptibility $\hat{\chi}^s(\mathbf{q})$ which has the 50×50 matrix form. The superconductivity is determined by $\lambda = 1$, where λ is the maximum eigenvalue of the linearized superconducting gap equation which can be regarded as an eigenvalue equation. It is found that the incommensurate magnetic order with $\mathbf{q} \sim (\pi, \pi)$ takes place at certain critical values of U' and J. The s-wave paring is realized near the magnetic ordered phase. We note that the d_{xy}-wave symmetry, which was observed for small J in the previous works [4, 5], is always second most favorable paring in the present work with the numerical improvements.

In the case with $U = U' + 2J$ and $J = J'$, the spin fluctuations always dominate over the orbital and charge fluctuations. Therefore, we focus on the spin susceptibility $\hat{\chi}^s(\mathbf{q})$. Fig. 1 (b) shows the $\mathbf{q}$-dependence of several components of the spin susceptibility $(\hat{\chi}^s(\mathbf{q}))^{\alpha,\beta}_{\ell_1\ell_2,\ell_3\ell_4}$ for $U' = 0.756$ eV and $J = 0.3$ eV with $\lambda \sim 1$, where α, β represent the two distinct Fe sites in the unit cell, ℓ_i represents the Fe $3d$ orbitals. The spin susceptibility $\hat{\chi}^s(\mathbf{q})$ has peaks around the Γ-point ($\mathbf{q} = (0, 0)$) and the M-point ($\mathbf{q} = (\pi, \pi)$). The peaks of $\hat{\chi}^s(\mathbf{q})$ around the Γ-point corresponding to the checkerboard-type antiferromagnetic fluctuations are due to effects of the nesting between the electron pockets near the M-point (see Fig. 2). The peaks of $\hat{\chi}^s(\mathbf{q})$ around the M-point corresponding to the stripe-type antiferromagnetic fluctuations are due to effects of the nesting between the hole pockets near the Γ-point

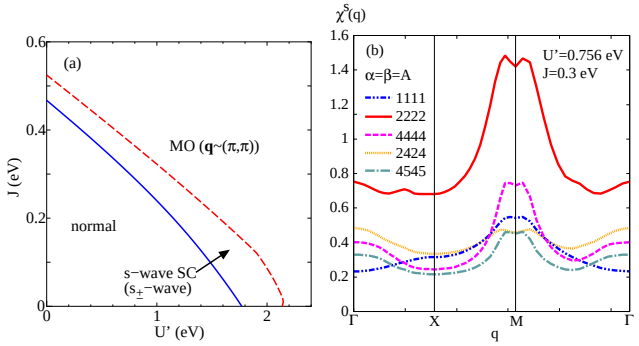

Figure 1: (a) The phase diagram on the U'-J plane at $x = 0.1$ and $T = 0.02$ eV. The solid and dashed lines represent the s-wave superconducting instability and the incommensurate magnetic instability with $\mathbf{q} \sim (\pi, \pi)$, respectively. (b) The several components of the spin susceptibility $\hat{\chi}^s(\mathbf{q})$ for $U' = 0.756$ eV and $J = 0.3$ eV at $x = 0.1$ and $T = 0.02$ eV. Note that we number the orbitals as follows: $d_{3z^2-r^2}(1), d_{x^2-y^2}(2), d_{xy}(3), d_{yz}(4), d_{zx}(5)$.

and the electron pockets near the M-point (see Fig. 2).

Fig. 2 shows the superconducting gap functions for the energy bands from 11th to 14th near the Fermi level together with the corresponding Fermi surfaces. The 11th and 12th bands construct the hole pockets near the Γ-point and the 13th and 14th bands construct the electron pockets near the M-point, respectively. We find that the gap functions have different signs between the electron pockets and the hole pockets without any nodes on the Fermi surfaces ($s_{\pm}$-wave symmetry) [2, 3]. The absolute values of the gap functions on the Fermi surfaces are almost isotropic but largely depend on the energy bands; those on the electron pockets of the 13th and 14th bands are twice or more larger than those on the hole pockets of the 11th and 12th bands. This is because the $d_{x^2-y^2}$ component, which has dominant contribution in $\hat{\chi}^s(\mathbf{q})$ as shown in Fig. 1 (b), for the 13th and 14th bands is larger than that for the 11th and 12th bands. We note that the 10th band (hole band) with the largest $d_{x^2-y^2}$ component has the largest absolute value of the gap function, although the Fermi level is just above the 10th band and does not cross it for $x = 0.1$.

In summary, we have investigated the electronic states and the superconductivity of the Fe_2As_2 plane in iron-based superconductors on the basis of the two-dimensional 16-band d-p model by using the RPA. It has been found that the most favorable paring is the $s_{\pm}$-wave and the second one is d_{xy}-wave

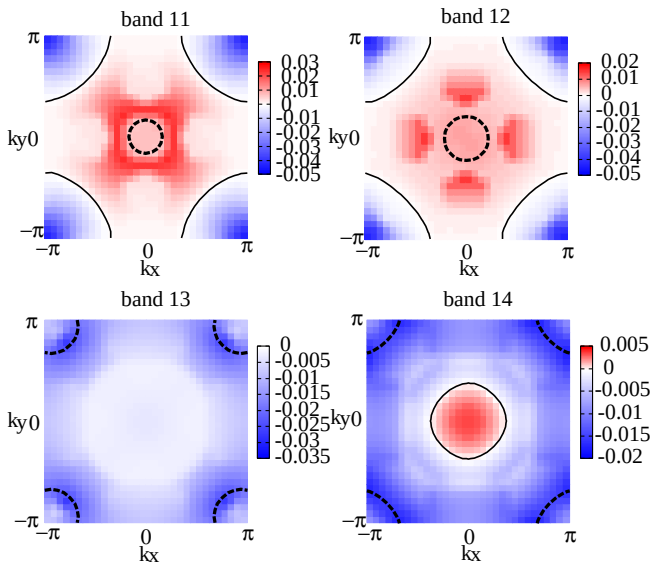

Figure 2: The gap function in the band representation for the bands from 11th to 14th near the Fermi level for $U' = 0.756$ eV and $J = 0.3$ eV at $x = 0.1$ and $T = 0.02$ eV. Solid and dashed lines represent the nodes of the gap function and the Fermi surfaces, respectively.

on the whole U'-J plane with keeping $U = U' + 2J$ and $J = J'$ at $x = 0.1$ and $T = 0.02$ eV. The absolute values of the gap functions on the electron pockets are twice or more larger than those on the hole pockets. The hole band with the largest gap function is just below the Fermi level for $x = 0.1$ but is expected to construct the inner hole pocket for $x < 0.1$ of electron doped compounds as well as for hole doped compounds.

The $s_{\pm}$-wave symmetry seems to be consistent with several experiments such as NMR relaxation rate, Knight shift, ARPES, magnetic penetration depth, although the sign of the gap function has not been directly observed. However, according to the recent theoretical studies of the nonmagnetic impurity effects [8], Anderson's theorem is violated for the $s_{\pm}$-wave superconductivity in contrast to the experimental results of weak T_c-suppression in the Fe substitution effect [9]. More recently, we have studied the 16-band d-p model in the wide parameter region away from the condition $U = U' + 2J$ [10] and have found that the the sign unchanged s-wave, which seems to be consistent with the weak T_c-suppression effects, takes place near the ferro orbital ordered phase. The explicit results will be shown in a subsequent

paper [10].

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