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Novel s-wave due to coexisting ferro- and antiferromagnetic fluctuations in iron pnictides

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Abstract. The five-orbital Hubbard model for iron pnictides is investigated by using the dynamical mean-field theory (DMFT) in conjunction with the Eliashberg equation in the strong correlation regime where the ferromagnetic (FM) and antiferromagnetic (AFM) fluctuations are simultaneously enhanced. When the intraorbital Coulomb interaction is a little smaller than the interorbital one, the FM fluctuation is largely enhanced due to the significant orbital dependence of the vertex correction and becomes comparable to the AFM fluctuation, in contrast to the result from the random phase approximation where the AFM fluctuation is exclusively enhanced due to the nesting between hole and electron Fermi surfaces (FSs). The enhanced FM fluctuation induces the large repulsive pairing interaction between inner and outer hole FSs while the AFM fluctuation does between the hole and electron FSs. The latter is partially counteracted by the attractive pairing interaction mediated by the antiferro-orbital fluctuation. The resulting pairing state is found to be a novel s-wave in which the gap function of the inner hole FS has the opposite sign to that of the outer hole and electron FSs.

1. Introduction

Since the discovery of iron pnictide 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. Two distinct s-wave pairings: the $s_{\pm}$-wave with sign change of the gap function between the hole and the electron Fermi surfaces (FSs) mediated by the antiferromagnetic (AFM) fluctuation[2, 3] and the s_{++}-wave without sign change mediated by the ferro-orbital (FO)[4] and/or the antiferro-orbital (AFO) fluctuations[5], were proposed. Recently, the spin-triplet p-wave pairing due to ferromagnetic (FM) fluctuation has been proposed in three-orbital Hubbard model for LiFeAs[6] where both FM and AFM fluctuations are observed[7]. More recently, another s-wave pairing with sign change between the two hole FSs (the hole-$s_{\pm}$-wave) mediated by coexisting AFM and AFO fluctuations has also been proposed in the five-orbital Hubbard model for LiFeAs[8]. Despite the numerous efforts, the pairing state and mechanism are still controversial.

In the present paper, we investigate the electronic state and the superconductivity in the five-orbital Hubbard model for iron pnictides especially focusing on the strong correlation regime where the FM and AFO fluctuations are simultaneously enhanced. As the electron correlation effect is known to be crucial for the magnetism, we employ the dynamical mean-field theory (DMFT)[9] which enables us to sufficiently take into account the local correlation effect. The DMFT has been extensively applied for the iron pnictides and has been found to describe well the strong correlation effects on the quasiparticle dispersion (FSs)[10] and the dynamical susceptibility[11]. Recently, we have investigated the five-orbital Hubbard model by using the DMFT in conjunction with the Eliashberg equation[12, 13] and have found that the s_{++}-pairing phase realized in the FO fluctuation-dominated case is largely expanded relative to


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the RPA result, while the $s_{\pm}$-pairing phase realized in the AFM fluctuation-dominated case is reduced. The present work is a straight forward extension of the previous work for the intermediate case between the two.

2. Model and Formulation

The five-orbital Hubbard model[3] is given by the following Hamiltonian

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

$$H_0 = \sum_{\boldsymbol{k}\ell\ell'\sigma} [\hat{H}_0(\boldsymbol{k})]_{\ell\ell'} d^{\dagger}_{\boldsymbol{k}\ell\sigma} d_{\boldsymbol{k}\ell'\sigma}, \tag{2}$$

$$\begin{aligned} H_{\rm int} = &\frac{1}{2}U \sum_i \sum_{\ell} \sum_{\sigma\neq\bar{\sigma}} d^{\dagger}_{i\ell\sigma} d^{\dagger}_{i\ell\bar{\sigma}} d_{i\ell\bar{\sigma}} d_{i\ell\sigma} + \frac{1}{2}U' \sum_i \sum_{\ell\neq\bar{\ell}} \sum_{\sigma,\sigma'} d^{\dagger}_{i\ell\sigma} d^{\dagger}_{i\bar{\ell}\sigma'} d_{i\bar{\ell}\sigma'} d_{i\ell\sigma} \\ &+ \frac{1}{2}J \sum_i \sum_{\ell\neq\bar{\ell}} \sum_{\sigma,\sigma'} d^{\dagger}_{i\ell\sigma} d^{\dagger}_{i\bar{\ell}\sigma'} d_{i\ell\sigma'} d_{i\bar{\ell}\sigma} + \frac{1}{2}J' \sum_i \sum_{\ell\neq\bar{\ell}} \sum_{\sigma\neq\bar{\sigma}} d^{\dagger}_{i\ell\sigma} d^{\dagger}_{i\ell\bar{\sigma}} d_{i\ell\bar{\sigma}} d_{i\bar{\ell}\sigma}, \end{aligned} \tag{3}$$

where $d_{i\ell\sigma}$ ($d_{\boldsymbol{k}\ell\sigma}$) is the annihilation operator for a Fe-3d electron at site i (wave vector $\boldsymbol{k}$) with spin σ in the orbital $\ell = xy, yz, zx, x^2-y^2, 3z^2-r^2$, and U and U' are the intra- and interorbital direct terms, J and J' are the Hund's coupling and the pair-transfer, respectively, and the matrix elements of the kinetic energy $[\hat{H}_0(\boldsymbol{k})]_{\ell\ell'}$ are explicitly given in Ref. [3]. In this paper, x, y axes (X, Y axes) are refer to the direction along the nearest (second nearest) Fe-Fe bonds.

On the basis of the DMFT[9], the model Eq. (2) is mapped onto an impurity five-orbital Anderson model embedded in an effective medium which is determined so as to satisfy the self-consistency condition:

$$\hat{G}(i\varepsilon_m) = \frac{1}{N}\sum_{\boldsymbol{k}} \hat{G}(\boldsymbol{k}, i\varepsilon_m) \tag{4}$$

with the Matsubara frequency $\varepsilon_m = (2m+1)\pi T$, where $\hat{G}(i\varepsilon_m)$ and $\hat{G}(\boldsymbol{k}, i\varepsilon_m)$ are the 5×5 matrix representations of the impurity Green's function and the lattice Green's function, respectively, which are explicitly given by

$$\hat{G}(i\varepsilon_m) = \left[\hat{\mathcal{G}}^{-1}(i\varepsilon_m) - \hat{\Sigma}(i\varepsilon_m)\right]^{-1}, \tag{5}$$

$$\hat{G}(\boldsymbol{k}, i\varepsilon_m) = \left[(i\varepsilon_m + \mu) - \hat{H}_0(\boldsymbol{k}) - \hat{\Sigma}(i\varepsilon_m)\right]^{-1}, \tag{6}$$

where $\hat{\Sigma}(i\varepsilon_m)$ is the 5×5 matrix representation of the impurity self-energy and $\hat{\mathcal{G}}(i\varepsilon_m)$ is that of the bare impurity Green's function describing the effective medium which is determined self-consistently. Within the DMFT, the spin (charge-orbital) susceptibility for the lattice model Eq. (2) is given in the 25×25 matrix representation as

$$\hat{\chi}_{s(c)}(q) = \left[1 - (+)\hat{\chi}_0(q)\hat{\Gamma}_{s(c)}(i\omega_n)\right]^{-1} \hat{\chi}_0(q) \tag{7}$$

with $\hat{\chi}_0(q) = -(T/N)\sum_k \hat{G}(k+q)\hat{G}(k)$, where $k = (\boldsymbol{k}, i\varepsilon_m)$, $q = (\boldsymbol{q}, i\omega_n)$ and $\omega_n = 2n\pi T$. In Eq. (7), $\hat{\Gamma}_{s(c)}(i\omega_n)$ is the local irreducible spin (charge-orbital) vertex in which only the external frequency (ω_n) dependence is considered as a simplified approximation[11, 12, 13] and is explicitly given by

$$\hat{\Gamma}_{s(c)}(i\omega_n) = -(+)\left[\hat{\chi}^{-1}_{s(c)}(i\omega_n) - \hat{\chi}^{-1}_0(i\omega_n)\right] \tag{8}$$

with $\hat{\chi}_0(i\omega_n) = -T\sum_{\varepsilon_m} \hat{G}(i\varepsilon_m + i\omega_n)\hat{G}(i\varepsilon_m)$, where $\hat{\chi}_{s(c)}(i\omega_n)$ is the local spin (charge-orbital) susceptibility. When the spin (charge) Stoner factor α_s (α_c), which is the largest eigenvalue of

$(-)\hat{\chi}_0(q)\hat{\Gamma}_{s(c)}(i\omega_n)$ in Eq. (7), for a wave vector $\boldsymbol{q}$ with $i\omega_n = 0$ reaches unity, the magnetic (charge-orbital) order with the corresponding $\boldsymbol{q}$ is realized.

To examine the superconductivity mediated by the magnetic and charge-orbital fluctuations which are enhanced towards the corresponding orders mentioned above, we write the effective pairing interaction for the spin-singlet state using the spin (charge-orbital) susceptibility and vertex given in Eqs. (7) and (8) obtained within the DMFT in the 25×25 matrix representation as[3, 4, 5, 12, 13]

$$\hat{V}(q) = \frac{3}{2}\hat{\Gamma}_s(i\omega_n)\hat{\chi}_s(q)\hat{\Gamma}_s(i\omega_n) - \frac{1}{2}\hat{\Gamma}_c(i\omega_n)\hat{\chi}_c(q)\hat{\Gamma}_c(i\omega_n) + \frac{1}{2}\left(\hat{\Gamma}_s^{(0)} + \hat{\Gamma}_c^{(0)}\right) \tag{9}$$

with the bare spin (charge-orbital) vertex: $[\Gamma^{(0)}_{s(c)}]_{\ell\ell\ell\ell} = U(U)$, $[\Gamma^{(0)}_{s(c)}]_{\ell\ell'\ell\ell'} = U'(-U' + 2J)$, $[\Gamma^{(0)}_{s(c)}]_{\ell\ell\ell'\ell'} = J(2U' - J)$ and $[\Gamma^{(0)}_{s(c)}]_{\ell\ell'\ell'\ell} = J'(J')$, where $\ell' \neq \ell$ and the other matrix elements are 0. Substituting the effective pairing interaction Eq. (9) and the lattice Green's function Eq. (6) into the linearized Eliashberg equation:

$$\lambda\Delta_{ll'}(k) = -\frac{T}{N}\sum_{k'}\sum_{l_1l_2l_3l_4} V_{ll_1,l_2l'}(k-k') \times G_{l_3l_1}(-k')\Delta_{l_3l_4}(k')G_{l_4l_2}(k'), \tag{10}$$

we obtain the gap function $\Delta_{ll'}(k)$ with the eigenvalue λ which becomes unity at the superconducting transition temperature $T = T_c$. In Eq. (10), the gap function $\Delta_{ll'}(k)$ includes the $1/d$ corrections yielding the $\boldsymbol{k}$ dependence of the gap function responsible for the anisotropic superconductivity which is not obtained within the zeroth order of $1/d$[9]. If we replace $\hat{\Gamma}_{s(c)}$ with $\hat{\Gamma}_s^{(0)}$ and neglect $\hat{\Sigma}$, Eq. (9) yields the RPA result of $\hat{V}(q)$[3, 4, 5]. Therefore, Eq. (10) with Eqs. (6) and (9) is a straightforward extension of the RPA result to include the vertex and the self-energy corrections within the DMFT without any double counting[12, 13]. In the actual calculations with the DMFT, we solve the effective five-orbital impurity Anderson model, where the Coulomb interaction at the impurity site is given by the same form as $\hat{H}_{\rm int}$ with a site i and the kinetic energy responsible for $\hat{\mathcal{G}}$ in Eq. (5) is determined so as to satisfy the self-consistency condition as possible, by using the exact diagonalization (ED) method for a finite-size cluster to obtain the local quantities such as $\hat{\Sigma}$ and $\hat{\chi}_{s(c)}$. Since the multi-orbital system requires rather CPU-time and memory consuming calculations, we employ the clusters with the site number $N_s = 4$ within a restricted Hilbert space[13]. All calculations are performed at $T = 0.02$eV for the electron number $n = 6.0$ corresponding to the non-doped case. We use 32×32 $\boldsymbol{k}$-point meshes and 1024 Matsubara frequencies in the numerical calculations with the fast Fourier transformation. Here and hereafter, we measure the energy in units of eV.

3. Results

In the previous papers[12, 13], we investigated the model Eq. (2) by using the formulation mentioned in Sec. 2 and found that the s_{++}-pairing phase due to the FO fluctuation realized in the case with $U < U'$ is largely expanded relative to the RPA result, while the $s_{\pm}$-pairing phase due to the AFM fluctuation realized in the case with $U > U'$ is reduced. In this paper, we concentrate our attention on the intermediate case with U being a little smaller than U' where both AFM and AFO fluctuations are expected to be enhanced.

Figs. 1 (a) and (b) show the $\boldsymbol{q}$-dependence of the spin susceptibility χ^s with $i\omega_n = 0$ for the $d_{X^2-Y^2}$ intraorbital component and the d_{ZX}-d_{XY} interorbital component, respectively, for the case with $U = 3.2$, $U' = 3.4$ and $J = J' = 0.27$. As shown in Fig. 1 (a), the AFM fluctuation with $\boldsymbol{q} = (\pi, 0)$ corresponding to the nesting vector between the hole and electron FSs is largely enhanced especially for $d_{X^2-Y^2}$ component which has the largest contribution to the density of states at the Fermi level. In addition to the AFM fluctuation, the FM fluctuation with $\boldsymbol{q} = (0, 0)$ is also enhanced for the d_{ZX}-d_{XY} interorbital component as shown in Fig. 1 (b). This is a striking contrast to the RPA result where the AFM fluctuation is exclusively enhanced, and then is nothing but a strong correlation effect. In fact, the

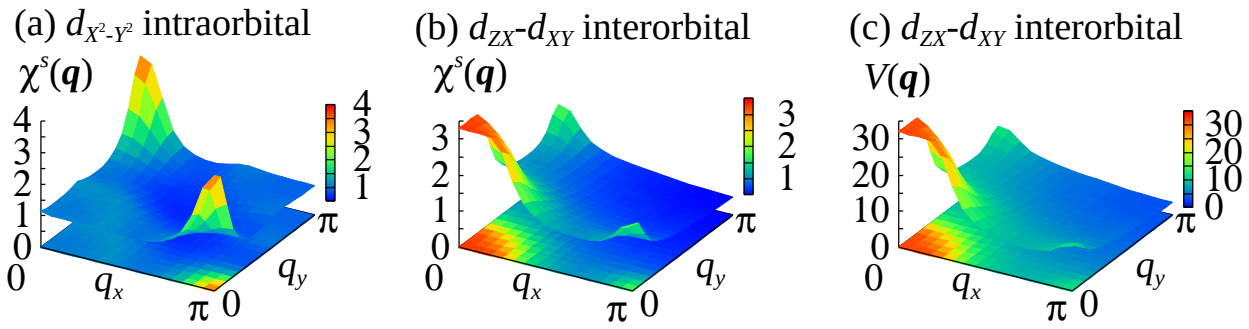

Figure 1. (Color online) The spin susceptibility χ^s with $i\omega_n = 0$ for the $d_{X^2-Y^2}$ intraorbital component (a) and the d_{ZX}-d_{XY} interorbital component (b), and the effective pairing interaction V with $i\omega_n = 0$ for the d_{ZX}-d_{XY} interorbital component as functions of the wave vector $\boldsymbol{q}$ for the case with $U = 3.2$, $U' = 3.4$ and $J = J' = 0.27$.

spin vertex $\hat{\Gamma}_s$ given in Eq. (8), which is not included in the RPA, shows significant orbital dependence with a maximum value for the component between d_{XY} and d_{ZX} (d_{YZ}) orbitals, and then yields the large enhancement of the FM fluctuation with the help of the nesting between the inner and outer hole FSs. In this case, the spin Stoner factor is $\alpha_s = 0.97$ for $\boldsymbol{q} = (\pi, 0)$ and $\alpha_s = 0.81$ for $\boldsymbol{q} = (0, 0)$, and then the AFM fluctuation dominates over the FM fluctuation (see also Figs. 1 (a) and (b)). However, with increasing U and U', the FM fluctuation is enhanced more steeply than the AFM fluctuation and then finally overcomes the AFM one for $U \sim U' \sim 5$ (not shown).

In Fig. 1 (c), the $\boldsymbol{q}$-dependence of the effective pairing interaction V with $i\omega_n = 0$ is plotted for the d_{ZX}-d_{XY} interorbital component for the same parameters in Figs. 1 (a) and (b). We find that the enhanced FM fluctuation yields the large repulsive V for $\boldsymbol{q} = (0, 0)$ (see Eq. (9)). The enhanced AFM fluctuation also yields the the large repulsive V for $\boldsymbol{q} = (\pi, 0)$ which is partially counteracted by the attractive V due to the AFO fluctuation which is also enhanced in the present case where the charge-orbital Stoner factor is $\alpha_c = 0.74$ for $\boldsymbol{q} = (\pi, 0)$.

In Figs. 2 (a)-(c), we show the $\boldsymbol{q}$-dependence of the gap function Δ with the lowest Matsubara frequency $i\varepsilon_m = i\pi T$ for the band 2 (with inner hole FS) (a), band 3 (with outer hole FS) (b) and band 4 (with electron FSs), respectively, for the same parameters in Fig. 1. We find that the pairing state is a novel s-wave in which Δ of the inner hole FS has the opposite sign to that of the outer hole and electron FSs. This is due to the cooperation between the FM and AFM fluctuations: the former favors the sign change of Δ between the inner and outer hole FSs and the latter dose between the hole and electron FSs. We note that the eigenvalue λ of the linearized Eliashberg equation (10) is $\lambda = 0.81$ for the present parameter but monotonically increases with increasing U and U' and finally reaches unity at $U \sim U' \sim 4.5$ where the pairing state is essentially unchanged from Figs. 2 (a)-(c) (not shown).

4. Summary

In summary, we have investigated the electronic state and the superconductivity in the five-orbital Hubbard model for iron pnictides by using the DMFT+Eliashberg approach especially focusing on the strong correlation regime where the FM and AFO fluctuations are simultaneously enhanced. Due to the significant orbital dependence of the vertex correction, the FM fluctuation is largely enhanced and becomes comparable to the AFM fluctuation in the strong correlation regime in contrast to the RPA result where the vertex correction is neglected and then the AFM fluctuation is exclusively enhanced. The resulting pairing state is a novel s-wave in which Δ of the inner hole FS has the opposite sign to that of the outer hole and electron FSs. Although the present case with U being a little smaller

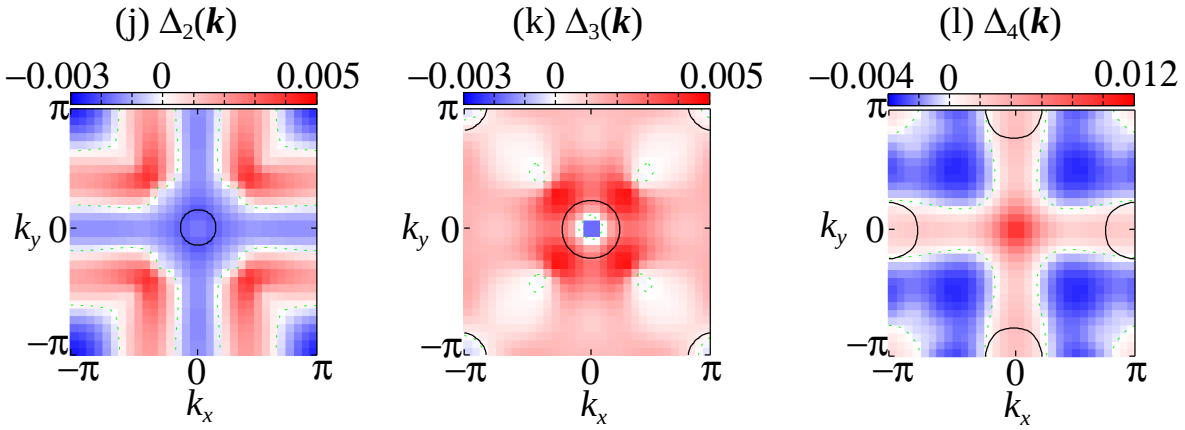

Figure 2. (Color online) The gap function Δ with the lowest Matsubara frequency $i\varepsilon_m = i\pi T$ together with the Fermi surfaces (solid lines) for the band 2 (inner hole FS) (a), band 3 (outer hole FS) (b) and band 4 (electron FSs) for the case with $U = 3.2$, $U' = 3.4$ and $J = J' = 0.27$.

than U' is not realistic, the same effects due to the vertex correction are expected to be realized for the realistic cases in the presence of the electron-phonon interaction[5, 14, 15] and/or the intersite Coulomb interaction[16, 17] and will be explicitly discussed in subsequent papers.

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