Dynamical mean-field study on the superconductivity mediated by spin and orbital fluctuations in the 5-orbital Hubbard model for iron pnictides

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We investigate the electronic state and the superconductivity in the 5-orbital Hubbard model for iron pnictides by using the dynamical mean-field theory together with the linearized Eliashberg equation. The renormalization factor exhibits a significant orbital dependence resulting in the band-dependence of the mass enhancement. The critical interactions towards the magnetic, orbital and superconducting instabilities are calculated and found to be suppressed as compared to the corresponding RPA results due to the correlation effects. Remarkably, the s_{++}-pairing phase due to the orbital fluctuation is expanded as compared to the RPA result, while the $s_{\pm}$-pairing phase due to the magnetic fluctuation is largely reduced.

KEYWORDS: dynamical mean-field approximation, iron-based superconductor, spin fluctuation, orbital fluctuation, Hubbard model, anisotropic superconductivity

1. Introduction

The phase diagrams of most iron-based superconductors show the tetragonal-orthorhombic structural transition and the stripe-type antiferromagnetic (AFM) transition [1,2]. Near the transitions, the AFM fluctuation is enhanced and shows a divergence towards the AFM transition [3], while the ferro-orbital (FO) fluctuation responsible for the softening of the elastic constant C_{66} [4,5] is enhanced and shows a divergence towards the structural transition. Correspondingly, two distinct s-wave pairings: the $s_{\pm}$-wave with sign change of the order parameter between the hole and the electron Fermi surfaces (FSs) mediated by the AFM fluctuation [6,7] and the s_{++}-wave without the sign change mediated by the FO fluctuation [8–10] and by the antiferro-orbital (AFO) fluctuation [11] which is also responsible for the softening of C_{66} through the two-orbiton process [12] were proposed. Despite the efforts of a number of investigations from both theoretical and experimental sides, the pairing state together with the mechanism of the superconductivity for the iron-based superconductors is still controversial.

As the details of the electronic band structure and the FS topology are crucial for the pairing states and the superconducting mechanisms, the theoretical studies have been done on the basis of the realistic multi-orbital models [7–12] where the tight-binding parameters are determined so as to reproduce the first-principles band structures which were found to agree with the experimental results from the angle-resolved photo-emission spectroscopy (ARPES) by reducing the band dispersion by a factor of 2 to 3 [13]. However, recent high-resolution ARPES measurements for $Ba_{0.6}K_{0.4}Fe_2As_2$ revealed significant band-dependence of the mass enhancement up to 9 in addition to the overall bandwidth renormalization by a factor 2. More recently, some evidences for an orbital-selective Mott transition, where the renormalization factor Z for d_{xy} orbital becomes zero while Z for the other orbitals are finite, were observed in $K_xFe_{2-y}Se_2$ [14] and KFe_2As_2 [15]. Therefore, it is important to investigate the superconductivity in the presence of the orbital dependent renormalization due to the strong correlation effect.

In the present paper, we investigate the 5-orbital Hubbard model [7] for iron pnictides by using the dynamical mean-field theory (DMFT) [16] which enables us to sufficiently describe the local correlation effects including the strong correlation regime where the orbital-selective Mott transition is observed [17]. To examine the superconductivity, we solve the Eliashberg equation in which the effective pairing interaction and the renormalized single-particle Green's function are calculated within the DMFT. In particular, we focus our attention on the local correlation effects on the possible pairing states, the magnetic fluctuation mediated $s_{\pm}$-wave and the orbital fluctuation mediated s_{++}-wave, beyond the random phase approximation (RPA) extensively developed in the previous works [7–11].

2. Model and formulation

The 5-orbital Hubbard model [7] is given by the Hamiltonian, $H = H_0 + H_{\rm int}$ with $H_0 = \sum_{\boldsymbol{k}\ell\ell'\sigma}[\hat{H}_0(\boldsymbol{k})]_{\ell\ell'} d^{\dagger}_{\boldsymbol{k}\ell\sigma} d_{\boldsymbol{k}\ell'\sigma}$ and

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

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 inter-orbital 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. [7]. In this paper, we set the x-y axes parallel to the nearest Fe-Fe bonds.

To solve the model, we use the DMFT [16] in which the lattice model is mapped onto an impurity Anderson model embedded in an effective medium which is determined so as to satisfy the self-consistency condition:

$$
\hat{G}(i\varepsilon_m) = \frac{1}{N}\sum_{\boldsymbol{k}} \hat{G}(\boldsymbol{k}, i\varepsilon_m) \tag{2}
$$

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 local (impurity) Green's function and the lattice Green's function, respectively, which are explicitly given by

$$
\hat{G}(i\varepsilon_m) = \left[\hat{\mathcal{G}}^{-1}(i\varepsilon_m) - \hat{\Sigma}(i\varepsilon_m)\right]^{-1}, \tag{3}
$$

$$
\hat{G}(\boldsymbol{k}, i\varepsilon_m) = \left[(i\varepsilon_m + \mu) - \hat{H}_0(\boldsymbol{k}) - \hat{\Sigma}(i\varepsilon_m)\right]^{-1}, \tag{4}
$$

where $\hat{\Sigma}(i\varepsilon_m)$ is the 5×5 matrix representation of the impurity (local) 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 is given in the 25×25 matrix representation as

$$
\hat{\chi}_{s(c)}(q) = \left[1 - (+)\hat{\chi}_0(q)\hat{\Gamma}_{s(c)}(i\omega_n)\right]^{-1} \hat{\chi}_0(q) \tag{5}
$$

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. (5), $\hat{\Gamma}_{s(c)}(i\omega_n)$ is the local irreducible spin (charge-orbital) vertex in which only the external frequency (ω_n) dependence is considered as a simplified approximation and is explicitly given by

$$\hat{\Gamma}_{s(c)}(i\omega_n) = -(+)\left[\hat{\chi}^{-1}_{s(c)}(i\omega_n) - \hat{\chi}_0^{-1}(i\omega_n)\right] \tag{6}$$

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 largest eigenvalue α_s (α_c) of $(-)\hat{\chi}_0(q)\hat{\Gamma}_{s(c)}(i\omega_n)$ in Eq. (5) for a wave vector $\boldsymbol{q}$ with $i\omega_n = 0$ reaches unity, the instability towards the magnetic (charge-orbital) order with the corresponding $\boldsymbol{q}$ takes place.

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. (5) and (6) obtained within the DMFT in the 25×25 matrix representation as [7–11]

$$\hat{V}(q) = \frac{3}{2}\hat{\Gamma}_s(i\omega_n)\hat{\chi}_s(q)\hat{\Gamma}_s(i\omega_n) - \frac{1}{2}\hat{\Gamma}_c(i\omega_n)\hat{\chi}_c(q)\hat{\Gamma}_c(i\omega_n) + \frac{1}{2}\left(\hat{\Gamma}^{(0)}_s + \hat{\Gamma}^{(0)}_c\right) \tag{7}$$

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. (7) and the lattice Green's function Eq. (4) into the linearized Eliashberg equation:

$$\lambda\Delta_{ll'}(k) = -\frac{T}{N}\sum_{k'}\sum_{l_1l_2l_3l_4} V_{ll_1,l_2l'}(k-k') \times G_{l_3l_1}(-k')\Delta_{l_3l_4}(k')G_{l_4l_2}(k'), \tag{8}$$

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. (8), 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 $1/d$ [16]. If we replace $\hat{\Gamma}_{s(c)}$ with $\hat{\Gamma}^{(0)}_s$ and neglect $\hat{\Sigma}$, Eq. (7) yields the RPA result of $\hat{V}(q)$ [7–11]. Therefore, Eq. (8) with Eqs. (4) and (7) is a straightforward extension of the RPA result to include the vertex and the self-energy corrections within the DMFT without any double counting.

In the actual calculations with the DMFT, we solve the effective impurity Anderson model, where the Coulomb interaction at the impurity site is given by the same form as Eq. (1) with a site i and the kinetic energies are determined so as to satisfy Eq. (2) 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 we need rather CPU-time and memory consuming calculations due to the large orbital number, we employ the clusters with the site number $N_s = 2$ in this paper. Even in the small system size with $N_s = 2$, one could obtain reliable results from the DMFT for the multi-band and multi-orbital models [18–21]. All calculations are performed at $T = 0.02$eV for the electron number $n = 6.0$ corresponding to the electron doping with $x = 0$. 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

It was found in the previous RPA study [8] that the $s_\pm$-pairing is mediated by the magnetic fluctuation near the AFM order for $U > U'$, while the s_{++}-pairing is mediated by the orbital fluctuation near the FO order for $U < U'$, where the superconductivity is investigated in the wide parameter space by treating U, U', J and J' as independent parameters apart from the condition satisfied in the

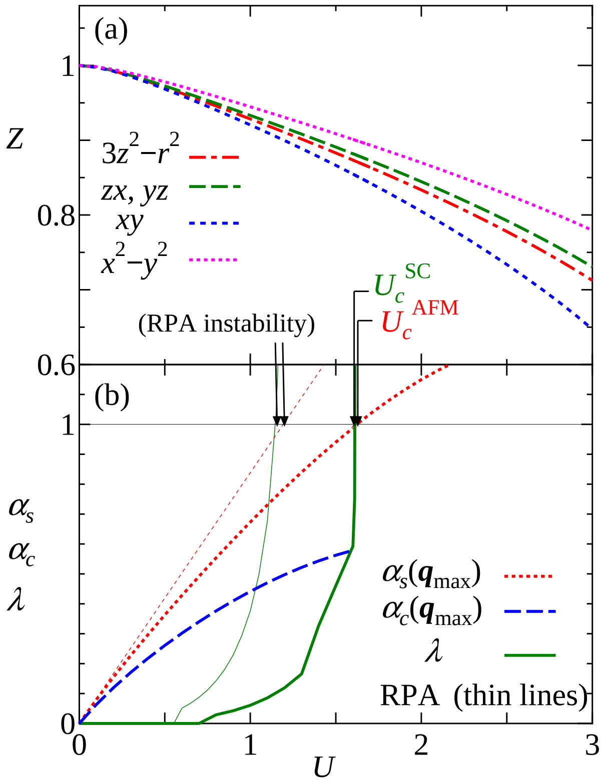

Fig. 1. (Color online) (a) The renormalization factor Z_ℓ with orbital $\ell = xy, yz, zx, x^2-y^2, 3z^2-r^2$, (b) the largest eigenvalues α_s, α_c, and λ which reach unity towards the magnetic, charge-orbital and superconducting instabilities, respectively, as functions of U with $U = U' + 2J$, $J/U = 0.1$ and $J = J'$ for $n = 6.0$ and $T = 0.02$. The RPA results are also plotted by thin lines in (b).

isolated atom: $U = U' + 2J$ and $J = J'$. Correspondingly, we consider the two specific cases with $U > U'$ and $U < U'$ to elucidate the correlation effects beyond the RPA on the magnetic and orbital orders and the superconductivity due to those fluctuations.

First, we consider the case with $U > U'$, where the magnetic fluctuation dominates over the orbital fluctuation, and show the several physical quantities as functions of U with $U = U' + 2J$, $J/U = 0.1$ and $J = J'$ for $n = 6.0$ and $T = 0.02$ in Fig. 1. Fig. 1 (a) shows the renormalization factor defined by: $Z_\ell = \left[1 - \frac{d\Sigma_\ell(i\varepsilon)}{d(i\varepsilon)}\Big|_{\varepsilon\to 0}\right]^{-1}$ with orbital $\ell = xy, yz, zx, x^2-y^2, 3z^2-r^2$. When U increases, all of Z_ℓ monotonically decrease with increasing the variance of Z_ℓ. We find that Z_{xy} is the smallest for all U and finally becomes zero at $U_c \sim 5$ while Z_ℓ for $\ell \neq xy$ are finite revealing the orbital-selective Mott transition (not shown), as recently obtained from the slave-spin mean-field approximation [14] and from the Gutzwiller slave-boson mean-field approximation [15]. Then, the correlation effect is most significant for d_{xy} orbital which has the largest spectral weight near the Fermi level. Fig. 1 (b) shows the U dependence of the largest eigenvalues α_s, α_c and λ which reach unity towards the magnetic, charge-orbital and superconducting instabilities, respectively. When U increases, both α_s and α_c increase with $\alpha_s > \alpha_c$ and α_s becomes unity at $U_c^{\rm AFM} \sim 1.62$ where the magnetic susceptibility with $\boldsymbol{q} \sim (\pi, 0)$ corresponding to the stripe-type AFM diverges. With increasing α_s, λ increases and finally reaches at $U_c^{\rm SC} \sim 1.61$ just below $U_c^{\rm AFM}$. From the analysis of the gap function $\Delta_{ll'}(k)$, the corresponding superconductivity is found to be the $s_\pm$ pairing mediated by the AFM fluctuation. We also plot the RPA results in Fig. 1 (b) and find that the superconducting phase with $U_c^{\rm SC} < U < U_c^{\rm AFM}$ from the DMFT is largely reduced as compared to that from the RPA

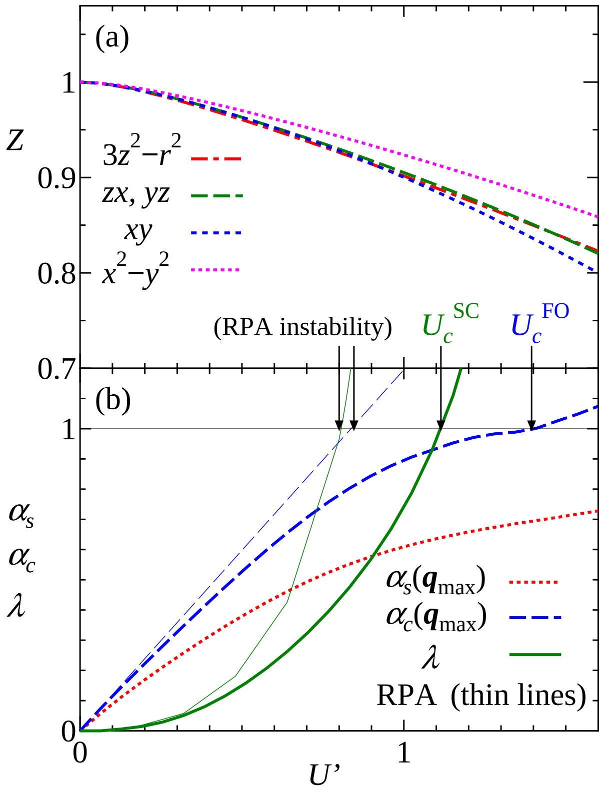

Fig. 2. (Color online) (a) The renormalization factor Z_ℓ with orbital $\ell = xy, yz, zx, x^2-y^2, 3z^2-r^2$, (b) the largest eigenvalues α_s, α_c, and λ which reach unity towards the magnetic, charge-orbital and superconducting instabilities, respectively, as functions of U' with $U = 0.25U' + 2J$, $J/U = 0.1$, $J = J'$ for $n = 6.0$ and $T = 0.02$. The RPA results are also plotted by thin lines in (b).

due to the local correlation effects beyond the RPA.

Next, we consider the case with $U < U'$, where the orbital fluctuation dominates over the magnetic fluctuation. Figs. 2 (a) and (b) show the renormalization factor Z_ℓ and the largest eigenvalues α_s, α_c and λ as functions of U' with $U = 0.25U'+2J$, $J/U = 0.1$, $J = J'$ for $n = 6.0$ and $T = 0.02$ in Fig. 2. When U' increases, Z_ℓ for all ℓ monotonically decrease with keeping the smallest value for $\ell = xy$ similarly to the case in Fig. 1 (a). When U' increases, both α_s and α_c increase with $\alpha_s < \alpha_c$ and α_c becomes unity at $U_c^{\mathrm{FO}} \sim 1.40$ where the orbital susceptibility with $\boldsymbol{q} \sim (0, 0)$ corresponding to the FO diverges. We note that, although the present result is different from the previous result in the 16-band d-p model [8] where the orbital susceptibility with $\boldsymbol{q} \sim (0, 0)$ corresponding to the FO diverges, the orbital susceptibilities for both $\boldsymbol{q} \sim (0, 0)$ and $(\pi, 0)$ are found to be enhanced at the same time in both cases with the present and previous models. With increasing α_c, λ increases and finally reaches at $U_c^{\mathrm{SC}} \sim 1.11$ where the gap function $\Delta_{ll'}(k)$ is found to be the s_{++}-pairing mediated by the AFO fluctuation. Remarkably, the DMFT result of the s_{++}-pairing phase with $U_c^{\mathrm{SC}} < U < U_c^{\mathrm{FO}}$ is expanded as compared to the RPA result due to the local correlation effects beyond the RPA, in contrast to the case with the $s_\pm$-pairing phase which is largely reduced as shown in Fig. 1 (b).

4. Summary

In summary, we have investigated the electronic state and the superconductivity in the 5-orbital Hubbard model for iron pnictides by using the DMFT+ED method together with the linearized Eliashberg equation. All of the critical interactions towards the magnetic, orbital and superconducting instabilities have been found to be suppressed as compared to the RPA results. Remarkably, the s_{++}-pairing phase due to the orbital fluctuation has been found to be expanded as compared to the RPA result, while the $s_{\pm}$-pairing phase due to the magnetic fluctuation is largely reduced. This is caused by the local correlation effects which enhance the local, i. e., the $\boldsymbol{q}$-independent magnetic (orbital) fluctuation resulting in the local component of the repulsive (attractive) pairing interaction responsible for the suppression (enhancement) of the $s_{\pm}$ (s_{++})-pairing.

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