Orbital Fluctuation Mediated Superconductivity in Iron Pnictides: Analysis of Five Orbital Hubbard-Holstein Model

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In iron pnictides, we find that the moderate electron-phonon interaction due to the Fe-ion oscillation can induce the critical d-orbital fluctuations, without being prohibited by the Coulomb interaction. These fluctuations give rise to the strong pairing interaction for the s-wave superconducting (SC) state without sign reversal (s±-wave state), which is consistent with experimentally observed robustness of superconductivity against impurities. When the magnetic fluctuations due to Coulomb interaction are also strong, the SC state shows a smooth crossover from the s-wave state with sign reversal (s±-wave state) to the s±-wave state as impurity concentration increases.

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The mechanism of high-\(T_c\) superconductivity in iron pnictides has been an important open problem. By considering the Coulomb interaction at Fe-ions, antiferromagnetic (AFM) fluctuation mediated fully-gapped sign-reversing s-wave state (s±-wave state) is also expected theoretically [1, 2]. Regardless of the beauty of the mechanism, there are several serious discrepancies for the s±-wave state. For example, although s±-wave state is expected to be very fragile against impurities due to the interband scattering [3], the superconducting (SC) state is remarkably robust against impurities [4] and \(\alpha\)-particle irradiation [5]. Moreover, clear “resonance-like” peak structure observed by neutron scattering measurements [6] is reproduced by considering the strong correlation effect via quasiparticle damping, without the necessity of sign reversal in the SC gap [7]. These facts indicate that a conventional s-wave state without sign reversal (s++-wave state) is also a possible candidate for iron pnictides.

Then, a natural question is whether the electron-phonon (e-ph) interaction is important or not. Although first principle study predicts small e-ph coupling constant \(\lambda \sim 0.21\) [8], several experiments indicate the significance of e-ph interaction. For example, the structural transition temperature \(T_S\) is higher than the Neel temperature in underdoped compounds, although the structural distortion is small. Also, prominent softening of shear modulus is observed towards \(T_S\) or \(T_c\) in Ba122 [9]. Raman spectroscopy [10] also indicates larger e-ph interaction.

Interestingly, there are several “high-\(T_c\)” compounds with nodal SC gap structure, like BaFe\(_2\)(As\(_{1-x}\)P\(z\))\(_2\) [11] and some 122 systems [12]. Although nodal s±-wave state can appear in the spin-fluctuation scenario due to the competition between the dominant \(Q = (\pi, 0)\) and subdominant fluctuations [1, 13], the \(T_c\) is predicted to be very low. Thus, it is a crucial challenge to explain the rich variety of the gap structure in high-\(T_c\) compounds.

In this letter, we introduce the five-orbital Hubbard-Holstein (HH) model for iron pnictides, considering the e-ph interaction by Fe-ion vibrations. We reveal that a relatively small e-ph interaction \((\lambda \lesssim 0.3)\) induces the large orbital fluctuations, which can realize the high-\(T_c\) s±-wave SC state. Moreover, the orbital fluctuations are accelerated by Coulomb interaction. In the presence of impurities, the s±-wave state dominates the s±-wave state for wide range of parameters.

First, we derive the e-ph iteration term, considering only Einstein-type Fe-Ion oscillations for simplicity. Here, we describe the d-orbitals in the XYZ-coordinate [1], which is rotated by \(\pi/4\) from the \(xyz\)-coordinate given by the Fe-site square lattice: We write \(Z^2, XZ, YZ, X^2-Y^2,\) and \(XY\) orbitals as 1, 2, 3, 4, and 5, respectively [1]. We calculate the e-ph matrix elements due to the Coulomb potential, by following Ref. [14]. The potential for a d-electron at \(r\) (with the origin at the center of Fe-ion) due to the surrounding As\(^{3-}\)-ion tetrahedron is \(U^R = 3e^2/\sum_{s=1}^4 |r + \mathbf{u} - \mathbf{R}_{s}^+|^{-1}\), where \(\mathbf{u}\) is the displacement vector of the Fe-ion, and \(\mathbf{R}_{s}^+\) is the location of surrounding As-ions; \(\sqrt{3}\mathbf{R}_{s}^+/R_{Fe-As} = (\pm \sqrt{2}, 0, 1)\) and \((0, \pm \sqrt{2}, -1)\) for Fe\(^1\), and \(\sqrt{3}\mathbf{R}_{s}^+/R_{Fe-As} = (\pm \sqrt{2}, 0, -1)\) and \((0, \pm \sqrt{2}, 1)\) for Fe\(^2\) in the unit cell with two Fe-sites. Note that \(u_X, Y\) and \(u_Z\) belong to \(E_g\) and \(B_{1g}\) phonons [10]. The linear term of \(U^R\), which gives the e-ph interaction, is obtained as \(V^R = u_A(2XZ\cdot u_X - 2YZ\cdot u_Y + (X^2 - Y^2)u_Z) + O(r^4)\), where \(A = 30e^2/\sqrt{3}R_{Fe-As}^4\). Then, its nonzero matrix elements are given as

\[
\begin{align*}
(2|V|4) &= \pm 2a^2\mu X/\gamma, \quad (3|V|4) = \pm 2a^2\mu Y/\gamma, \\
(2|V|2) &= \pm 2a^2\mu Z/\gamma, \quad (3|V|3) = \mp 2a^2\mu Z/\gamma,
\end{align*}
\]

where \(a\) is the radius of d-orbital. Here, we consider \(\langle i|V|j\rangle\) only for orbitals \(i, j = 2 \sim 4\) that compose the Fermi surfaces (FSs) in Fig. 1 (a) [1]. The obtained e-ph interaction does not couple to the charge density since \(\langle i|V|j\rangle\) is trace-less. Thus, the Thomas-Fermi screening for the coefficient \(A\) is absent. The local phonon Green function is \(D(\omega) = 2u_0^2\omega^2/(\omega^2 + \omega_0^2)\), which is given by the Fourier transformation of \(\langle T_{\mu}(\tau)u_\mu(0)\rangle (\mu = X, Y, Z) = \sqrt{\hbar/2M_{Fe-\omega_0})}\) is the position uncertainty.
of Fe-ions, $\omega_D$ is the phonon frequency, and $\omega_l = 2\pi lT$ is the boson Matsubara frequency. Then, for both Fe$^{(1)}$ and Fe$^{(2)}$, the phonon-mediated interaction is given by

$$
V_{24,42} = V_{24,43} = -(2A\alpha^2/\pi^2)D(\omega_l) \equiv -g(\omega_l),
$$

$$
V_{22,22} = V_{33,33} = -V_{22,23} = -g(\omega_l),
$$
as shown in Fig. 1 (b). Note that $V_{ll',mm'}$ is symmetric with respect to $l \leftrightarrow l'$, $m \leftrightarrow m'$, and $(ll') \leftrightarrow (mm')$. We obtain $g(0) \approx 0.4$ eV if we put $R_{Fe-As} \approx 2.4$ Å, $a \approx 0.77$ Å (Shannon crystal radius of Fe$^{2+}$), and $\omega_D \approx 0.018$ eV. We have neglected the $e$-ph coupling due to $d$-$p$ hybridization [14] considering the modest $d$-$p$ hybridization in iron pnictides [15]. Thus, we obtain the multiorbital HH model for iron pnictides by combining eq. (2) with the on-site Coulomb interaction; the intra- (inter-) orbital Coulomb $U$ ($U'$), Hund coupling $J$, and pair-hopping $J'$.

![Diagram](image1)

FIG. 1: (Color online) (a) FSs in the unfolded Brillouin zone. (b) Phonon-mediated electron-electron interaction. (c) A bubble diagram that indicates the critical orbital fluctuations between (2,4) orbitals. (d) A ladder-type diagram that is ignorable when $\omega_D \ll E_F$.

Now, we study the rich electronic properties realized in the multiorbital HH model [16]. The irreducible susceptibility in the five-orbital model is given by $\chi^{(l,l',mm',q)}(q) = -(T/N)\sum_k G^{0}_{l's}(k + q)G^{0}_{l'm'}(k)$, where $\tilde{G}^{0}(k) = [i\epsilon_n + \mu - \tilde{H}_k^{0}]^{-1}$ is the $d$-electron Green function in the orbital basis: $q = (q, \omega_l)$, $k = (k, \epsilon_n)$, and $\epsilon_n = (2n + 1)\pi T$ is the fermion Matsubara frequency. $\mu$ is the chemical potential, and $\tilde{H}_k^{0}$ is the kinetic term given in Ref. [1]. Then, the susceptibilities for spin and charge sectors in the random-phase-approximation (RPA) are given as [17]

$$
\chi^{(c)}(q) = \chi^{(c)}(0)[1 - \tilde{\Gamma}^{(c)}(q)^{-1}],
$$

where $G^{(c)}(q)$ shows one of bubble diagrams for (2,4)-channel due to the “negative exchange coupling $V_{24,42}$” that leads to a critical enhancement of $\chi^{(c)}(q)$ [18]. We neglect the ladder diagrams given by $\tilde{V}(\omega_l)$ in Fig. 1 (d) since $\omega_D \ll W_{band}$ [8, 10]. We put $\omega_D = 0.02$ eV, $U'/U = 0.69$, $J'/U = 0.16$ and $J = J'$, and fix the electron number $n = 6.1$ (10% electron doping); the density of states per spin is $N(0) = 0.66$ [eV$^{-1}$]. Numerical results are not sensitive to these parameters. We use $128^2 k$-meshes, and 512 Matsubara frequencies. Hereafter, the unit of energy is eV.

![Diagram](image2)

FIG. 2: (Color online) (a) Obtained $U'$-$g(0)$ phase diagram. (b) Obtained $\chi^{(c)}_{24,42}(q,0)$ and $\chi^{(c)}_{22,22}(q,0)$ for $\alpha_c = 0.97$.

Figure 2 (a) shows the obtained $U'$-$g(0)$ phase diagram. $\alpha_{s(c)}$ is the spin (charge) Stoner factor, given by the maximum eigenvalue of $\tilde{\Gamma}^{(c)}(q)^{-1}$. Then, the enhancement factor for $\chi^{(c)}(q)$ is $(1 - \alpha_{s(c)})^{-1}$, and $\alpha_{s(c)} = 1$ gives the spin (orbital) order boundary. Due to the nesting of the FSs, the AFM fluctuation with $Q \approx (\pi, 0)$ develops as $U$ increases, and $s_{\pm}$-wave state is realized for $\alpha_c \lesssim 1$ [1]. In contrast, we find that the orbital fluctuations develop as $g(0)$ increases. For $U = 1$, the critical value $g_{cr}(0)$ for $\alpha_c = 1$ is 0.4, and the critical $e$-ph coupling constant is $\lambda_{cr} \equiv g_{cr}(0)N(0) = 0.26$ [19]. Since the obtained $\lambda_{cr}$ is close to $\lambda$ given by the first principle study [8], strong orbital fluctuations are expected to occur in iron pnictides. At fixed $U$, $\lambda_{cr}$ decreases as $J'/U$ approaches zero.

Figure 2 (b) and (c) show the obtained $\chi^{(l,l',mm',q,0)}$ for $(l,l',mm') = (24,42)$ and $(22,22)$, respectively, for $U = 1.14$ and $\alpha_c = 0.97$ ($g(0) = 0.40$): Both of them are the most divergent channels for electron-doped cases. The enhancement of $(24,42)$-channel is induced by the multiple scattering by $V_{24,42}$. The largest broad peak around $q = (0,0)$ originates from the forward scat-
tering in the electron-pocket (FS3 or 4) composed of 2 ~ 4 orbitals. (FS1,2 are composed of only 2 and 3 orbitals.) These ferro-orbital fluctuations would induce the softening of shear modulus [9], and also reinforce the ferro-orbital-ordered state below \( T_S \) [20] that had been explained by different theoretical approaches [21]: The divergence of \( \chi_{24,42}^{(3,4)} \) pushes the 2,4 (3,4) orbitals away from the Fermi level, and the Fermi surfaces in the ordered state will be formed only by 3 (2) orbital, consistently with ref. [20]. The lower peak around \( Q = (\pi, 0) \) comes from the nesting between hole- and electron-pockets. Also, the enhancement of \((22,22)\)-channel for \( Q = (\pi, 0) \) is induced by the nesting via multiple scattering by \( V_{22,22} \) and \( V_{22,33} \). In contrast, the charge susceptibility \( \sum_{ll} \hat{\chi}_{l,m}^{(3,4)}(q, 0) \) is finite even if \( \alpha_c \to 1 \) since \( \chi_{22,33} \approx -\chi_{22,22}^{(3,4)}. \)

Now, we will show that large orbital fluctuations, which are not considered in the first principle study of \( T_c \) [8], can induce the \( s_{++} \)-wave state when \( g(0) > 0 \). We analyze the following linearized Eliashberg equation using the RPA [1], by taking both the spin and orbital fluctuations into account on the same footing:

\[
\lambda_E \Delta_{ll'}(k) = \frac{T}{N} \sum_{k', m} W_{lm_{1}m_{2}l_{2}}(k - k') \times G_{m_{1}m_{2}}(k') \Delta_{m_{2}m_{3}}(k') \times G_{m_{4}m_{3}}(-k'),
\]

where \( W(q) = \frac{-2}{3} \hat{\Gamma}^{\alpha} \chi_{\alpha}^{\alpha}(q) \hat{\Gamma}^{\alpha} + \frac{1}{3} \hat{\Gamma}^{\alpha} \chi_{\alpha}(q) \hat{\Gamma}^{\alpha} - \frac{1}{2} (\hat{\Gamma}^{\alpha} - \hat{\Gamma}^{\alpha}) \)

for singlet states. The eigenvalue \( \lambda_E \) increases as \( T \to 0 \), and it reaches unity at \( T = T_c \). In addition, we take the impurity effect into consideration since many iron pnictides show relatively large residual resistivity. Here, we assume the Fe site substitution, where the impurity potential \( I \) is diagonal in the \( d \)-orbital basis [3]. Then, the \( T \)-matrix in the normal state is given by \( T(\epsilon_n) = [T^{-1} - N^{-1} \sum_{k} \hat{G}(k, \epsilon_n)]^{-1} \) in the orbital basis [3]. Then, the normal self-energy is \( \Sigma_{ll'}^{n}(\epsilon_n) = n_{imp} \bar{T}(\epsilon_n) \), where \( n_{imp} \) is the impurity concentration. Also, the linearized anomalous self-energy is given by

\[
\Sigma_{ll'}^{\alpha}(\epsilon_n) = \frac{n_{imp}}{N} \sum_{k, m_{1}} T_{lm_{1}}(\epsilon_n) G_{m_{1}m_{2}}(k; \epsilon_n) \Delta_{m_{2}m_{3}}(k, \epsilon_n) \times G_{m_{4}m_{3}}(-k; -\epsilon_n) T_{l_{4}m_{4}}(-\epsilon_n).
\]

Then, the Eliashberg equation for \( n_{imp} \neq 0 \) is given by using the full Green function \( \bar{G}(k) = [\hat{\epsilon}_n + \mu - \hat{H}_0^0 - \hat{\Sigma}^{n}(\epsilon_n)]^{-1} \) in eqs. (4) and (5), and adding \( \Sigma_{ll'}^{\alpha}(\epsilon_n) \) to the right hand side of eq. (4). Hereafter, we solve the equation at relatively high temperature \( T = 0.02 \) since the number of \( k \)-meshes (128\(^2\)) is not enough for \( T < 0.02 \), due to the fact that \( k_F \) in iron pnictides is only 1/5 of that in cuprate superconductors.

Figure 3 shows the \( n_{imp} \)-dependence of \( \lambda_E \) at \( \alpha_c = 0.98 \), for \( U = 1.11, 1.14 \) and 1.18. Considering large \( \lambda_E \gg 0.8 \) at \( T = 0.02 \), relatively high-\( T_c \) (\( \lesssim 0.02 \)) is expected. For the smallest \( U \) (\( U = 1.11; \alpha_s = 0.85 \)), we find that nearly isotropic \( s_{++} \)-wave state is realized; the obtained \( \lambda_E \) is almost independent of \( n_{imp} \), indicating the absence of impurity effect on the \( s_{++} \)-wave state, as discussed in Refs. [3, 22]. For the largest \( U \) (\( U = 1.18; \alpha_s = 0.91 \), \( s_{+\pm} \)-wave state is realized at \( n_{imp} = 0 \); \( \lambda_E \) decreases slowly as \( n_{imp} \) increases from zero, whereas it saturates for \( n_{imp} \geq 0.05 \), indicating the smooth crossover from \( s_{+\pm} \) to \( s_{++} \)wave states due to the interband impurity scattering. For \( U = 1.14 \) (\( \alpha_s = 0.88 \)), the SC gap at \( n_{imp} = 0 \) is a hybrid of \( s_{++} \) and \( s_{\pm} \); only \( \Delta_{FS2} \) is different in sign.

The inset of Fig. 3 shows \( \lambda_E \) for \( s_{++} \)-wave state in the presence of impurities (\( n_{imp} = 0.15 \)): Since \( \lambda_E(\alpha_c = 0.98) = \lambda_E(\alpha_c = 0.90) \) is only \( 0.15 \) for each value of \( U \), we expect that relatively large \( T_c \) for \( s_{++} \)-wave state is realized even if orbital fluctuations are moderate. We stress that the obtained \( \lambda_E \) is almost constant for \( \omega_0 = 0.2 \sim 0.1 \), suggesting the absence of isotope effect in the \( s_{++} \)-wave state due to the strong retardation effect [14]. By the same reason, \( \lambda_E \) for the the \( s_{+\pm} \)-wave state is seldom changed if we put \( U = 3 \) in the Hartree-Fock term \( \frac{1}{2} (\hat{\Gamma}^{\alpha} - \hat{\Gamma}^{\alpha}) \) in \( W(q) \), indicating that the Morel-Anderson pseudo-potential almost saturates.

Here, we discuss the case \( U = 1.18 \) in detail: Figure 4 shows the SC gap on the FSs in the band-representation for (a) \( n_{imp} = 0 \), (b) 0.03, and (c) 0.08. They satisfy the condition \( N^{-1} \sum_{k, lm} (\Delta_{lm}(k))^2 = 1 \). The horizontal axis is the azimuth angle for the \( k \)-point with the origin at \( \Gamma \) (M) point for FS1,2 (FS4); \( \theta = 0 \) corresponds to the \( k_x \)-direction. In case (a), \( s_{+\pm} \)-state with strong imbalance, \( |\Delta_{FS1}|, |\Delta_{FS2}| \ll |\Delta_{FS4}| \), is realized, and \( \Delta_{FS4} \) takes the largest value at \( \theta = \pi/2 \), where the FS is mainly composed of orbital 4. In case (c), impurity-induced isotropic \( s_{+\pm} \)-state [23] with \( \Delta_{FS1} \sim \Delta_{FS2} \sim \Delta_{FS4} \) is realized, consistently with many ARPES measurements [24]. In case (b), \( \Delta_{FS} \) on FS1 is almost gapless. However, considering the \( k_x \)-dependence of the FSs, a (horizontal-
type) nodal structure is expected to appear on FS1,2. In real compounds with $T_c \sim 50$K, the $s_\pm \rightarrow s_{++}$ crossover should be induced by small residual resistivity $\rho_{\text{imp}} \sim 20 \, \mu\Omega \text{cm} \, (n_{\text{imp}} \sim 0.01 \, \text{for } I = 1)$, as estimated in Ref. [3].

![Fig. 4: (Color online) SC gap functions for $U = 1.18$ as functions of $\theta$ at (a) $n_{\text{imp}} = 0$, (b) 0.03, and (c) 0.08, respectively.](image)

We comment that at $n_{\text{imp}} = 0$, $s_\pm$-wave state is realized in the RPA even if $\alpha_s \lesssim \alpha_c$, due to factor 3 in front of $\frac{1}{2} \Gamma_{\text{f} \Gamma_{\text{f}}^*}(q) \Gamma_{\text{f} \Gamma_{\text{f}}}$ in $W(q)$. For the same reason, however, reduction in $\alpha_s$ (or increment of $U_{\text{ct}}$ for $\alpha_s = 1$) due to the “self-energy correction by $U^n$” is larger, which will be unfavorable for the $s_\pm$-wave state. Therefore, self-consistent calculation for the self-energy is required to discuss the value of $\alpha_s$, and the true pairing state.

Here, we discuss where in the $\alpha_s$-$\alpha_c$ phase diagram in Fig. 2 (a) real compounds are located. Considering the weak $T$-dependence of $1/T \gamma_T$ in electron-doped SC compounds [25], we expect that they belong to the area $\alpha_c \gg \alpha_s$. Then, $s_\pm$-wave SC state will be realized without (or very low density) impurities, like the case of $U = 1.11$ or 1.14 in Fig. 3. On the other hand, impurity-induced $s_\pm \rightarrow s_{++}$ crossover may be realized in BaFe$_2$(As$_{1-x}$P$_x$)$_2$ (undoped) or (Ba$_{1-x}$K$_x$)Fe$_2$As$_2$ (hole-doped) SC compounds, where AFM fluctuations are rather strong.

Finally, we discuss the non-Fermi-liquid-like transport phenomena in iron pnictides. For example, the resistivity might be irrelevant, antiferro-orbital and AFM fluctuations become stronger than the ferro-orbital ones. The $s$-wave superconductivity induced by orbital fluctuations has been discussed in Ref. [17] for $U' > U$; this condition can be realized by including the $A_{1g}$-phonon [28]. In the present model, however, $A_{1g}$-phonon is negligible since $g_{1g}(0)$ given by $A_{1g}$-phonon is much greater than $g_{1g}(0) \sim 0.4$ in Fig. 2 (a): The ferro-obtital fluctuations in Fig. 2 (b) originate from the negative exchange interaction caused by $E_g$-phonon, as shown in Fig. 1 (c).

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Note added in proof: After the acceptance of this work, we found that $g_{1g}(0) \sim 0.4$ in Fig. 2 (a) is reduced to half if all the $e$-ph matrix elements including 1,5 orbitals are taken into account. Results similar to Fig. 3 are obtained by using $g(0) \sim 0.2$, whereas (vertical-type) nodes appear on FS3,4 during the $s_{++} \rightarrow s_\pm$ crossover for $U = 1.18$.

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