Is Fermi-surface nesting the origin of superconductivity in iron pnictides?: A fluctuation-exchange-approximation study

Ryotaro Arita$^{1,2,3}$ and Hiroaki Ikeda$^4$

$^1$Department of Applied Physics, University of Tokyo, Tokyo 153-0044, Japan
$^2$JST, TRIP, Sanbancho, Chiyoda, Tokyo 102-0075, Japan
$^3$JST, CREST, Hongo, Tokyo 146-8566, Japan CREST
$^4$Department of Physics, Kyoto Univ, Kyoto 606-8502, Japan

(Received today)

We study whether Fermi-surface (FS) nesting can give rise to high-temperature superconductivity in iron pnictides. Starting with ab initio construction of an effective four-orbital model, we employ the fluctuation-exchange approximation to show that FS does not necessarily favor the stripe antiferromagnetic order observed in experiments, especially for realistic electronic correlations. If superconductivity in iron pnictides is magnetically mediated and has fully-gapped sign-reversing s-wave symmetry, our results suggest that the pairing interaction does not arise only from FS nesting and exchange interactions between local moments in the Fe 3d orbitals may play a crucial role.

KEYWORDS: iron-based superconductor, magnetism, unconventional superconductivity

The seminal discovery of superconductivity in LaFeAsO doped with fluorine$^1$ and subsequent updates of the record of the transition temperature ($T_c$) in related iron pnictides and iron chalcogenides$^2$ have attracted great interest in these compounds. Since there is close proximity of antiferromagnetic (AF) order and superconductivity in the phase diagram, the possibility of magneto-mediated superconductivity has been intensively studied.$^3$

When we consider the interplay between magnetism and superconductivity, one of the key issues to be clarified is, whether the magnetism should be understood in terms of localized spins or itinerant electrons. While there have been a variety of proposals and calculations for the so-called $J_1$-$J_2$ model based on the the strong coupling scenario,$^4$ it has also been claimed that the weak coupling approach should work better,$^5-11$ and the problem which picture describes the system more properly has been an issue of hot debates.$^3$

Among many studies based on the weak coupling scenario, recently, a detailed calculation by the random phase approximation (RPA) for a five-orbital model derived from ab initio calculation based on the local density approximation (LDA) has been performed. There, it has been discussed how changes in the crystal structure (i.e., the atomic configuration) affects superconductivity,$^6$ and it has been concluded that the weak coupling approach succeeds to explain the qualitative tendency of pairing instability in iron pnictides: when the pnictogen height is low (high) as in the case of LaFePO (LaFeAsO), low (high) $T_c$ nodal (nodeless) pairing is favored.$^{12}$

On the other hand, estimates of the interaction parameters by various ab initio methods suggest that iron pnictides are not weakly but moderately correlated.$^{13-15}$ Indeed, photoemission spectrum indicates that the mass enhancement due to the electron correlations is as large as $2 \sim 3$,$^{16}$ whose effect is neglected in RPA. Since Fermi-surface (FS) nesting plays a crucial role in the weak coupling approach, and the orbital/momentum dependence of the self-energy correction can seriously affect the nesting condition, it is of great interest to see whether the weak coupling approach based on FS nesting survives even if we consider the self-energy correction.

One of the standard ways to investigate the effect of the self-energy correction is to employ the dynamical mean field theory (DMFT).$^{17}$ While several DMFT calculations combined with LDA have been performed,$^{15,18-20}$ the recent calculation with realistic interaction parameters$^{20}$ for LaFeAsO has shown that the orbital-dependent DMFT correction lowers the level of $d_{x^2-y^2}$ at the Γ point in the Brillouin zone (hereafter, the local coordinate system centered at Fe is such that the $x$- and $y$-axis point towards neighboring As). As is discussed below, in such a situation, the nesting condition is expected to be worse, which suggests that the nesting scenario is not necessarily robust against the self-energy correction.

While the self energy in DMFT is momentum independent, the momentum dependence of the self energy is also crucial for FS nesting. The purpose of the present study is to investigate the effect of momentum-dependent self energy for realistic band structure and electronic correlations by means of the fluctuation-exchange approximation (FLEX).$^{21}$ Although FLEX can become problematic to address some high energy features (e.g., it fails to describe a Mott insulator), FLEX is generally expected to be reliable for description of low energy physics originating from FS nesting,$^{22}$ so that this tool is expected to work for the examination whether superconductivity in iron pnictides, which are moderately correlated, can indeed be understood in terms only of FS nesting.

Let us move on to the construction of the effective model which we employ in the following calculation. As for FLEX calculation for iron pnictides, while there have already been several studies for simplified models,$^9$ one of the present authors recently performed a calculation...
for a five-orbital model based on LDA. There, he set the intra-orbital Coulomb interaction $U$ and the Hund coupling $J$ to be 1.44 eV and 0.24 eV, which are relatively small compared to those estimated by an \textit{ab initio} method. In fact, it has been recognized that FLEX becomes problematic for the five-orbital model in the moderately correlated (realistic) regime since some uncontrolled treatment is needed to get a reasonable spectral function. Namely, we have to introduce an artificial level shift for $d_z$ to the original one-body Hamiltonian, otherwise the $d_z$ orbital makes a large FS around the $\Gamma$ point which is not consistent with the experiments.

The reason why we have to shift the level of $d_z$ can be understood as follows. Since the the $d_z^2$ orbital in the five-orbital model is localized and correlated\cite{13,14} (due to weak hybridization with As $4p$), the correlation already taken in LDA is expected to be large for $d_z$. Thus, while we have to introduce the so-called double counting (DC) term\cite{24} to combine LDA with FLEX, the DC term of $d_z$ should be larger than those of $d_{yz}$, $d_{xz}$ and $d_{x^2-y^2}$ (which make the FS in LDA). However, it is a non-trivial task to evaluate the orbital dependent DC term from first principles for the five-orbital model, especially when the system is moderately correlated.

In order to avoid this subtle problem and make our analysis on the validity of the nesting scenario be clearer, in the present study, we first construct an effective four-orbital model for $d_{xy}$, $d_{x^2-y^2}$, $d_{yz}$, and $d_{zz}$. As we can see in Fig. 1, since $d_z$ basically lies below the Fermi level, it is expected to be irrelevant for the physics of the FS nesting. In actual model construction, as was done in Ref.,\cite{5} we obtain the band structure of LaFeAsO with the Quantum-ESPRESSO package,\cite{25} and made maximally localized Wannier functions\cite{26} for the four orbitals to represent the Kohn-Sham Hamiltonian in terms of these orbitals.

In table I, we list the transfer integrals in the one-body part of the Hamiltonian. The onsite energies of $d_{yz}, d_{x^2-y^2}$, and $d_{xy}$ are 0.09, 0.28, and 0.11 eV with respect to the Fermi level. The spread of Wannier functions ($\sqrt{(r^2) - \langle r^2 \rangle}$) are 2.16, 2.55 and 2.11 Å, while in the five-orbital model,\cite{27} they are 2.05, 2.36, and 1.73 Å, respectively.

In Fig.1, we plot the band dispersion (in the unfolded Brillouin zone\cite{5} for the unit cell which contains only one Fe atom) of the four-orbital model, comparing with that of the five-orbital model.\cite{28} We can see that the FS is almost the same as that of the original five-orbital model. Thus we may expect that if the nesting scenario indeed captures the essential feature of the pairing mechanism, the four-orbital model should also be able to describe superconductivity in iron pnictides.

For the many-body part of the Hamiltonian, we consider the standard interactions that comprise the inter- and intra-orbital Coulomb interaction ($U$, $U'$) and the Hund coupling and the pair-hopping ($J$, $J'$). We assume that $U = U' + 2J$ and $J = J'$. Following the standard procedures of multi-orbital FLEX,\cite{8} we solve the linearized Eliashberg equation, and obtain the gap function along with the eigenvalue $\lambda$. $T_c$ corresponds to the temperature where $\lambda$ reaches unity. 32\times32\times4 three-dimensional $k$-point meshes and 1024 Matsubara frequencies are taken, while the temperature ($T$) is set to be 0.02 eV. Hereafter we denote the spin susceptibility, the gap function, and $\kappa_T$ for the former two) and $k_z = 0$ as $\chi_s(k_x, k_y)$, $\Delta(k_x, k_y)$, and $g(k_x, k_y)$, respectively.

First, we compare the four-orbital model and the five-orbital model by RPA. Both models have a peak in the spin susceptibility which corresponds to stripe AF instability, and the fully-gapped $s$-wave with sign reversing (the so-called $s_{+}$-wave) is most dominant for the undoped case (electron-filling $n$ is 4.0 for the four-orbital model and 6.0 for the five-orbital model). Interaction parameters are taken as $U = 1.2$, $U' = 0.9$, and $J = 0.15$ eV. In Fig. 2, we plot $\Delta$ of the the four(five)-orbital model, for the 1st (2nd) to 3rd (4th) bands from bottom to top in the band representation. We see that the gap functions of these two models are similar to each other in RPA.

Next let us move on to FLEX. In Fig. 3, we compare RPA and FLEX results of $g$ (which takes large values at FS, see also Fig. 1(c)) for $d_{x^2-y^2}$ in the orbital representation and $\chi_s$. Here we set $U = 1.2$, $U' = 0.9$ and $J = 0.15$ eV. Although we have a sharp peak in $\chi_s$ at $(k_x, k_y) = (\pi, 0)$ and $(0, \pi)$ in RPA, these peaks are severely suppressed in FLEX and a broad structure around $(\pi, \pi)$ becomes dominant. While the fully-gapped $s_{+}$-wave is dominant in both RPA and FLEX, $\lambda$ is much smaller in FLEX ($=0.18$) than in RPA ($=0.83$). These results suggest that, in order to have strong magnetic fluc-
tations and pairing instability from the nesting between small Fermi pockets, generally we need sufficiently large interactions.

In Fig. 4, we show the result of FLEX for $U = 1.8$, $U' = 1.2$ and $J = 0.3$. In contrast with Fig. 3(b), we have a sharp peak in $\chi_s$ (Fig. 4(a)). However, the position of the peak is located at $(\pi, \pi)$ which corresponds to the G-type AF instability. Here, rather than the fully-gapped $s_\pm$-wave pairing, the so-called gapless $s_\pm$-wave pairing (whose $|\Delta|$ becomes small on the Fermi surface) and a $d$-wave pairing are more favored ($\lambda$ is $\sim 0.34$ for these pairings, and see Fig. 4(c) in which $\Delta$ of these pairings for the third band in the band representation are plotted). For larger interaction parameters, the G-type AF instability is more and more enhanced and the gapful $s_\pm$-wave pairing never becomes dominant.

These results can be understood as follows. For undoped LaFeAsO, as we see in Fig. 1(b) and (c), there are four kinds of Fermi pockets: two hole pockets, $\alpha_1$ and $\alpha_2$, around $(0, 0)$ and electron pockets, $\beta_1$, $\beta_2$, around $(\pi, 0)$ and $(0, \pi)$ as well as a hole pocket $\gamma$ around $(\pi, \pi)$ (which disappears by $\sim 10\%$ doping of electrons). While $\alpha$ is made from $d_{xy}$ and $d_{xz}$, $\beta$ is made from $d_{yz}$, $d_{zx}$ and $d_{x^2-y^2}$, and $\gamma$ is made from $d_{x^2-y^2}$ (Fig. 1(c)). On top of the scattering channels which connect $\alpha$, $\beta$ or $\gamma$ and $\beta$ ($q_1$ and $q_2$ in Fig. 1(b)), there is also a channel between $d_{x^2-y^2}$ in $\gamma$ and $\beta_2$ ($q_3$ in Fig. 1(c)). As is discussed in Ref. 8 while $q_2$ is the key to induce the strong stripe AF fluctuations, in the absence of $\gamma$, $q_3$ suppresses the stripe AF fluctuations and the fully-gapped $s_\pm$-wave pairing. In fact, the low energy electronic structure in FLEX is quite similar to that in RPA: the spectral functions obtained by these approximations have similar size of structures in the Brillouin zone around $(\pi, 0)$, $(0, \pi)$, $(0, 0)$ and $(\pi, \pi)$ for low frequencies. However, the self-

---

### Table I. Hopping integrals $t(\Delta X, \Delta Y; \mu, \nu)$ in units of eV. $[\Delta X, \Delta Y]$ denotes the in-plane hopping vector (note that the X- and Y-axis point towards neighboring Fe atoms), and $(\mu, \nu)$ the orbitals. $\sigma_Y$, $I$, and $\sigma_d$ corresponds to $t(\Delta X, -\Delta Y; \mu, \nu)$, $t(-\Delta X, -\Delta Y; \mu, \nu)$, $t(\Delta X, \Delta Y; \mu, \nu)$, respectively, where $\pm$ and $\pm(\mu', \nu')$ in the row of $(\mu, \nu)$ mean that the corresponding hopping is equal to $\pm (\Delta X, \Delta Y; \mu, \nu)$ and $\pm (\Delta X, \Delta Y; \mu', \nu')$, respectively. This table, combined with the relation $t(\Delta X, \Delta Y; \mu, \nu) = t(-\Delta X, -\Delta Y; \nu, \mu)$, gives all the in-plane hoppings $\geq 0.02\text{eV}$ up to the fifth neighbors.

| $[\Delta X, \Delta Y]$ | $[1,0]$ | $[1,1]$ | $[2,0]$ | $[2,1]$ | $[2,2]$ | $\sigma_Y$ | $I$ | $\sigma_d$ |
|------------------------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|
| $(zx,xz)$              | $-0.22$          | $0.18$          | $-0.02$          | $+ (yz,yz)$      | $+$               | $+$               | $+ (yz,xy)$      | $-$               |
| $(zx,yz)$              | $0.12$           | $0.03$          | $-0.02$          | $+ (yz,yz)$      | $+$               | $+$               | $-$               | $-$               |
| $(zx,x^2-y^2)$         | $-0.29$          | $0.19$          | $0.06$           | $(zx,xz)$        | $+$               | $+$               | $+$               | $+$               |
| $(zx,xy)$              | $0.20$           | $0.03$          | $+ (yz,yz)$      | $-$               | $-$               | $-$               | $-$               | $-$               |
| $(yz,yz)$              | $-0.22$          | $0.30$          | $+ (zx,xz)$      | $+$               | $+$               | $+$               | $+$               | $+$               |
| $(yz,x^2-y^2)$         | $0.20$           | $0.03$          | $+ (yz,yz)$      | $-$               | $-$               | $-$               | $-$               | $-$               |
| $(yz,xy)$              | $-0.29$          | $0.19$          | $0.06$           | $(zx,xz)$        | $+$               | $+$               | $+$               | $+$               |
| $(x^2-y^2,x^2-y^2)$    | $0.15$           | $0.12$          | $-0.06$          | $- (yz,xy)$      | $-$               | $-$               | $+$               | $+$               |
| $(xy,xy)$              | $0.30$           | $-0.20$         | $0.02$           | $+ (yz,yz)$      | $+$               | $+$               | $+$               | $+$               |

Fig. 2. Gap functions for the four-orbital model (a) (the five-orbital model (b)) of LaFeAsO, for the 1st (2nd) to 3rd (4th) bands from bottom to top in the band representation with $n = 4.0$ (6.0). Solid lines represent the Fermi surface.

Fig. 3. RPA(a) and FLEX(b) results for the squared absolute value of the Green function for the $d_{x^2-y^2}$ orbital in the orbital representation (left) and spin susceptibility at the lowest Matsubara frequency (right) for the four-orbital model with $U = 1.2$, $U' = 0.9$, and $J = 0.15$ eV.
energy effect for $d_{x^2-r^2}$ around $(\pi, \pi)$ (where the LDA band dispersion is flat) is significantly large and severely suppresses $q_2$, which is dominant in RPA. While effects which have not been considered (such as spin-lattice coupling, off-site Coulomb interactions, etc.) may change the situation, the present study suggests that the nesting scenario is not necessarily robust against the momentum-dependent self-energy correction.

To summarize, we study whether FS nesting can be the origin of spin-fluctuation-mediated superconductivity in iron-pnictides by means of FLEX. Our result suggests that the nesting scenario has a serious dilemma: since all the FS pockets are small, we need sufficiently strong interactions to have large magnetic fluctuations from the pairing gap function of the $s_{\pm}$-wave pairing and the $d$-wave pairing at the lowest Matsubara frequency (c) are shown.

Acknowledgment

We would like to thank H. Aoki, P. Hansmann, M. Imada, G. Sangiovanni, A. Toschi for fruitful discussions and/or critical reading of the manuscript. This work is supported by a Grant-in-Aid for Scientific Research on Priority Areas “Super Clean Materials” under Grant No. 20029014 from MEXT, Japan. Numerical calculations were performed at the facilities of the Supercomputer center, ISSP, University of Tokyo.
Phys. Condensed Matter 9 (1997) 767

25) S. Baroni, A. Dal Corso, S. de Gironcoli and P. Giannozzi, http://www.pwscf.org/. Here we adopt the exchange correlation functional introduced by J. P. Perdew et al.[Phys. Rev. B 54 (1996) 16533], and the wave functions are expanded by plane waves up to a cutoff energy of 40 Ry. $10^3$ $k$-point meshes are used with the special points technique by H. J. Monkhorst and J. D. Pack [Phys. Rev. B 13 (1976) 5188].

26) N. Marzari and D. Vanderbilt, Phys. Rev. B 56 (1997) 12847; I. Souza, N. Marzari and D. Vanderbilt, Phys. Rev. B 65 (2002) 035109. In this study, we used the code developed by A. A. Mostofi, J. R. Yates, Y.-S. Lee, I. Souza, D. Vanderbilt and N. Marzari (http://www.wannier.org/) to construct the Wannier functions.

27) V. Vildosola L. Pourovskii, R. Arita, S. Biermann, A. Georges Phys. Rev. B., 78 (2008) 064518.

28) It should be noted that the band dispersion of the five-orbital model is exactly the same as that of ab-initio calculation.5,13