Possibility of Unconventional Pairing Due to Coulomb Interaction in Fe-Based Pnictide Superconductors: Perturbative Analysis of Multi-Band Hubbard Models

Takuji Nomura*

Synchrotron Radiation Research Center, Japan Atomic Energy Agency, Sayo, Hyogo 679-5148
(Received February 10, 2022)

Possibility of unconventional pairing due to Coulomb interaction in iron-pnictide superconductors is studied by applying a perturbative approach to realistic 2- and 5-band Hubbard models. The linearized Eliashberg equation is solved by expanding the effective pairing interaction perturbatively up to third order in the on-site Coulomb integrals. The numerical results for the 5-band model suggest that the eigenvalues of the Eliashberg equation are sufficiently large to explain the actual high $T_c$ for realistic values of Coulomb interaction and the most probable pairing state is spin-singlet $s$-wave without any nodes just on the Fermi surfaces, although the superconducting order parameter changes its sign between the small Fermi pockets. On the other hand the 2-band model is quite insufficient to explain the actual high $T_c$.

KEYWORDS: iron-pnictide superconductors, superconducting mechanism, pairing symmetry

Recent discovery of high-$T_c$ superconductivity in iron pnictides has generated highly intensive research activities in solid state physics. After the discovery of superconductivity in LaFeAsO$_x$F$_{1-x}$ system, it has become evident that transition temperature is raised above 40K by replacing La with other rare-earth elements (Ce, Pr, Nd, Sm, ...$^2$-$^6$) or by applying pressure.$^7$ Pairing mechanism and symmetry would be the most intriguing issues of this newly discovered superconductivity. In the present work, possibility of unconventional (i.e., not phonon-mediated) superconducting mechanism for Fe-pnictide superconductors is investigated theoretically. There are already several reasons why unconventional pairing may be realized in iron pnictides: (i) $T_c$ is high, compared with conventional (phonon-mediated) BCS superconductors, (ii) Fe3d states dominate the most part of the density of states near the Fermi level,$^8$-$^10$ and (iii) electron-phonon coupling is expected to be weak by first-principles calculations.$^9$

We introduce many-band Hubbard models for Fe3d-like orbitals and formulation. The Hamiltonian is given in the form $H = H_0 + H'$. $H_0$ is the non-interacting part:

$$H_0 = \sum_{i\ell j\ell'} \sum_{\sigma} c_{i\ell\sigma}^\dagger c_{j\ell'\sigma}$$

where $c_{i\ell\sigma}$ is the electron annihilation (creation) operator for Fe3d-like orbital $\ell$ with spin $\sigma$ at site $i$. The tight-binding parameters $t_{i\ell,j\ell'}$ are determined to reproduce a realistic electronic structure. $H'$ is the on-site Coulomb interaction part containing four kinds of Coulomb integrals: $U$ (intra-band repulsion), $U'$ (inter-band repulsion), $J$ (Hund’s coupling), $J'$ (inter-band pair-hopping). The same form of $H'$ was used for the Ru4d-like electrons of Sr$_2$RuO$_4$ in Ref. 12. Then the following linearized Eliashberg equation is solved numerically:

$$\lambda \cdot \Delta_{a',\sigma_1\sigma_2}(k) = -\frac{T}{N} \sum_{k',a',\sigma_3\sigma_4} V_{a\sigma_1\sigma_2,a'\sigma_3\sigma_4}(k,k') \times (G^{(0)}_{a'}(k') \Delta_{a',\sigma_3\sigma_4}(k'))$$

(1)

where $a$ and $a'$ are band indices, $G_{a'}^{(0)}(k)$ is the Green’s function for band $a$ (without self-energy corrections), $\sigma_i$’s are spin indices, $V_{a\sigma_1\sigma_2,a'\sigma_3\sigma_4}(k,k')$ is the effective pairing interaction, $\Delta_{a',\sigma_3\sigma_4}(k)$ is the anomalous self-energy on band $a$, and $\lambda$ is eigenvalue. The effective pairing interaction is evaluated by third order perturbation expansion in $H'$. The third order perturbation theory has been applied to many other unconventional superconductors, and suggests correctly pairing symmetries, e.g., singlet $d_{x^2-y^2}$-wave for cuprates and organic superconductors, triplet $p$-wave for Sr$_2$RuO$_4$, ... etc.$^{13}$ Transition point is determined by $\lambda = 1$. We take $32 \times 32$ $k$ points and 512 Matsubara frequencies for numerical calculations.

Firstly, we adopt two-dimensional 5-band tight-binding model proposed by Kuroki et al.$^{10}$ The electronic structure and the Fermi surface are given in Fig. 1 (in the unfolded representation, where each unit cell contains only one Fe atom). The Fermi surface consists of hole pockets around the $(0,0)$ and $(\pi,\pi)$ points and electron pockets around the $(\pi,0)$ and $(0,\pi)$ points. In the original folded representation, where each unit cell contains two Fe atoms, the $(0,0)$ and $(\pi,\pi)$ points are folded onto the $\Gamma$ point, while the $(\pi,0)$ and $(0,\pi)$ points onto the M point. The numerical results of eigenvalues are shown in Fig. 2(a). We see the most probable pairing symmetry is singlet $s$-wave and obtain sufficiently large eigenvalues to explain actual high $T_c$’s for realistic values of Coulomb integrals ($U = 1.2eV$, $U' = 0.9eV$, $J = J' = 0.15eV$). $T_c$ is evaluated to be about 100K. This is still higher than real values 20K-50K. If we include the self-energy corrections, then $T_c$ will be decreased somewhat due to the effect of quasi-particle damping. The $d_{x^2-y^2}$-electron component of anomalous Green’s function $F_{X^2-Y^2}(k,\omega_n)$ is shown in Fig. 2(b) ($X$ and $Y$ axes are those in the original folded representation, while $k = (k_x,k_y)$ is in the unfolded representation). The superconducting order parameter does not possess any nodes just on the Fermi surfaces, although
it changes its sign between the electron and hole pockets. In this sense the pairing symmetry is extended s-wave.

We proceed to another model, i.e., 2-band model only for the $d_{xz}$- and $d_{yz}$-like orbitals, proposed by Raghu et al.\textsuperscript{11)} (See Fig. 3(a)). The maximum eigenvalue is given by the triplet p-wave pairing state, but is too small to explain the actual $T_c$, as we see in Fig. 3(b). Thus we may conclude that the 2-band model is quite insufficient and the real multi-band situation is essential to describe the iron-pnictide high-$T_c$ superconductivity.

In conclusion, our perturbation theory suggests that the iron-pnictide superconductivity may be unconventional one induced by electron correlation effect, as other unconventional superconductivity. The most probable pairing symmetry is s-wave without any nodes on the Fermi surface. One of the important differences from other unconventional superconductors is that the order parameter will change its sign not on the Fermi surface but between the Fermi pockets. Possibility of triplet pairing is excluded.

The author would like to thank H. Ikeda, K. Kuroki, K. Nakamura, S. Onari and K. Yamada for valuable communications. Numerical work was performed at the Yukawa Institute Computer Facility of Kyoto University.

1) Y. Kamihara et al.: J. Am. Chem. Soc. \textbf{130} (2008) 3296.
2) G.F. Chen et al.: Phys. Rev. Lett. \textbf{100} (2008) 247002.
3) Z.A. Ren et al.; Mater. Res. Innovations \textbf{12} (2008) 105.
4) Z.A. Ren et al.: Europhys. Lett. \textbf{82} (2008) 57002.
5) X.H. Chen et al.: Nature \textbf{453} (2008) 761.
6) Z.A. Ren et al.: Chin. Phys. Lett. \textbf{25} (2008) 2215.
7) H. Takahashi et al.: Nature \textbf{453} (2008) 376.
8) D.J. Singh and M.H. Du: Phys. Rev. Lett. \textbf{100} (2008) 237003.
9) L. Boeri, O.V. Dolgov and A.A. Golubov: Phys. Rev. Lett. \textbf{101} (2008) 026403.
10) K. Kuroki et al.: Phys. Rev. Lett. \textbf{101} (2008) 087004.
11) S. Raghu et al.: Phys. Rev. B \textbf{77} (2008) 220503.
12) T. Nomura and K. Yamada: J. Phys. Soc. Jpn. \textbf{71} (2002) 1993.
13) Y. Yanase et al.: Phys. Reports \textbf{387} (2003) 1.