Resonant impurity scattering in the $\pm s$-wave state of the Fe-based superconductors

Yunkyu Bang
Department of Physics, Chonnam National University, Kwangju 500-757, and Asia Pacific Center for Theoretical Physics, Pohang 790-784, Korea

Han-Yong Choi
Department of Physics and Institute for Basic Science Research, SungKyunKwan University, Suwon 440-746, Korea
(Dated: February 15, 2009)

We study the impurity scattering on the $\pm s$-wave superconductor, with realistic parameters for the Fe-pnictide superconductors. Using the $\mathcal{T}$-matrix method, generalized for the two bands, we found that impurity scattering of the unitary limit forms off-centered bound states inside of the superconducting gap, which modifies, surprisingly, the density of states (DOS) of a fully opened gap to a V-shaped one as in the case of a d-wave superconductor. This behavior provides coherent explanations to the several conflicting experimental issues of the Fe-pnictide superconductors: the V-shaped DOS but with an isotropic gap observed in the photoemission and tunneling experiments; the power law behavior of the nuclear-spin-lattice relaxation rate $(1/T_1 \approx T^\alpha ; \alpha \approx 3)$, down to very low temperatures.

PACS numbers: 74.20,74.20-z,74.50

Introduction - The recent discovery of Fe-based superconducting (SC) compounds [1, 2], has greatly spurred the research activity of the superconductivity. With a discovery of new superconducting material, the most impelling question is to determine the SC gap symmetry. Identifying the pairing symmetry, the search for the possible pairing mechanisms can be more easily advanced. Various SC properties were already measured to determine the gap symmetry of these materials but there exist serious conflicts among data. Just list some of them, tunneling spectroscopy of Ref.[3], photoemission measurement of Ref.[4], and nuclear- spin-lattice relaxation rate measurements [5, 6] seem to indicate a d-wave type gap with lines of node. On the other hand, tunneling spectroscopy of Ref.[7], photoemission measurement of Ref.[8], specific heat [9], and the penetration depth measurements by several groups [10] all support a fully opened s-wave type gap.

On the theoretical side, it is almost agreed on that the pairing mechanism is non-phononic[11], and most probably of a magnetic origin [12, 13]. This conclusion is consistent with the overall phase diagram obtained by neutron scattering [12], where the SC phase starts to develop when the antiferromagnetic (AFM) order disappears, suggesting an universal mechanism for unconventional superconductivity of the compounds with d- and f-electron elements. For the Fe-based SC compounds, an AFM correlation induced interaction with the specific band structure - in particular, two topologically distinct hole and electron bands widely separated in the Brilluion Zone - favors to develop so-called $\pm s$-wave SC state, first proposed by Mazin et al.[14], and reconfirmed theoretically by several authors [15, 16, 17, 18].

Then the key question is : Is the $\pm s$-wave state consistent with all experiments? Up to now, the $\pm s$-wave state is the most natural candidate to understand the penetration depth behavior [10]. However, the nuclear-spin-lattice relaxation rate $1/T_1$ experiments by several groups [5, 6] all support a nodal gap SC state. Recently, several groups [19, 20], including the present authors [17], proposed that the unusual interband coherence factor, unique to the $\pm s$-gap state due to the opposite signs of the SC order parameter (OP) between the bands [21], can explain the absence of Hebel-Slichter peak as well as an approximate power law behavior of $1/T_1$, with a help of impurities. While this is an important observation, the calculations of these works [17, 19, 20] are not completely satisfactory to reproduce the $T^\alpha$ power law [22]. Also the works of Ref.[19] considered only the interband scattering process while the works of Ref.[17, 20] showed that both the interband and intraband processes have comparable contributions and hence both processes should be treated on equal footing. Therefore, it needs more quantitative and systematic studies to settle the issue; in particular, how robust and how low temperatures the power law behavior can extend to, and the nature of impurities.

In this paper, we employed the $\mathcal{T}$-matrix approximation, generalized to the $\pm s$-wave state of the two band model, to study the effects of impurities from weak (Born) to strong (unitary) scattering limit. The $\mathcal{T}$-matrix approximation has been successfully applied to the various unconventional superconductors such as heavy fermion [23] and high-temperature superconductors [24]. For example, it predicts a resonant bound state by unitary impurity scatterer inside the d-wave SC gap, which was crucial to explain the penetration depth of HTSC [24], $1/T_1$ experiments of Pu-115 superconductor [25], etc. The key principle of forming a resonance bound state in the d-wave gap is that the sign-changing d-wave SC OP guarantees the absence of the renormalization of the anomalous selfenergy due to impurity scattering. Therefore, we expect a similar mechanism to work with the sign-changing $\pm s$-wave superconductors. However, there are important differences: (1) the cancellation of the anomalous selfenergy would not be perfect unless the sizes of $s+$ and $s-$ gap and their corresponding DOSs $N_s(0)$ and $N_e(0)$ are exactly equal; (2) the DOS of the pure state is not linearly vanishing as in the d-wave
case but a fully gapped one. Considering these differences, it requires a quantitative and transparent investigation to understand the effects of impurity scattering on the $\pm s$-wave state.

**Formalism** - Recently we had proposed a minimal two band model with a phenomenological magnetic interaction for the Fe-based superconductors [17]. Assuming two SC order parameters, $\Delta_h$ and $\Delta_e$ on each band, the two coupled gap equations are written as

$$\Delta_h(k) = -\sum_{k'} [V_{hh}(k,k')\chi_h(k') + V_{he}(k,k')\chi_e(k')],$$

$$\Delta_e(k) = -\sum_{k'} [V_{eh}(k,k')\chi_h(k') + V_{ee}(k,k')\chi_e(k')].$$

where $V_{hh}(k,k')$ is the phenomenological pairing interaction originating from the AFM order. The above gap equations indeed provide the $\pm s$-wave state ($\Delta_h$ and $\Delta_e$ have the opposite signs) as the best solution [17]. The impurity effects enter through the pair susceptibility in the following way.

$$\chi_{h,e}(k) = T \sum_n N(0)_{h,e} \int_0^{\omega_{AFM}} d\omega \tilde{\Delta}_{h,e}(k) \frac{\tilde{\Delta}_{h,e}(k)}{\tilde{\omega}^2 + \tilde{\Delta}_{h,e}^2(k)}$$

where $N(0)_{h,e}$ are the DOS of the hole and electron bands, respectively, and $\omega_{AFM}$ is the cutoff energy of the pairing potential $V(q)$. $\tilde{\Delta}_{h,e}(k) = \Delta_h + \Sigma_h^{\uparrow}(\omega_h) + \Sigma_e^{\downarrow}(\omega_e)$ and $\tilde{\Delta}_{h,e} = \Delta_h + \Sigma_h^{\uparrow}(\omega_h) + \Sigma_e^{\downarrow}(\omega_e)$ (where $\omega_h = \pi T(2n + 1)$, and the impurity induced selfenergies are calculated with $\tau$-matrices as $\Sigma_{h,e}^{\uparrow}(\omega_h) = \Gamma \cdot \tau_{h,e}^{\uparrow}(\omega_h)$; $\Gamma = n_{imp}/\pi N_{tot}$ where $n_{imp}$ is the impurity concentration and $N_{tot} = N_h(0) + N_e(0)$ is the total DOS. The $\tau$-matrices $\tau_{h,e}^{\uparrow}$ are the Pauli matrices $\tau_{h,e}^{\uparrow}$ components in Nambu space. We can set $\tau^3 = 0$ assuming particle-hole symmetry and $\tau^2 = 0$ due to U(1) symmetry, respectively, without the loss of generality. Definitions of $\tau_{h,e}^{\uparrow}(\omega_h)$ are standard [23] in the literatures, but now need a generalization for the two bands as follows.

$$\tau_{a}^{\uparrow}(\omega_h) = \frac{G_{a}^{h}(\omega_h)}{D} \quad (i = 0, 1; \quad a = h, e),$$

$$D = c^2 + [G_{+}^{h} + G_{-}^{h}]^2 + [G_{+}^{e} + G_{-}^{e}]^2,$$  

$$G_{0}^{h}(\omega_h) = \frac{N_h}{N_{tot}} \left( \frac{\tilde{\omega}_{h}}{\tilde{\omega}^2 + \tilde{\Delta}_{h}^2(k)} \right),$$

$$G_{0}^{e}(\omega_h) = \frac{N_e}{N_{tot}} \left( \frac{\tilde{\omega}_{e}}{\tilde{\omega}^2 + \tilde{\Delta}_{e}^2(k)} \right),$$

where $c = \cot(\delta_0)$ is a convenient measure of scattering strength, with $c\rightarrow 0$ in the unitary limit and $c > 1$ in the Born limit scattering. (...) denotes the Fermi surface average. The above four $\tau$-matrices, $\tau_{a}^{\uparrow}$ are numerically solved together with the coupled gap equations Eq.(1) and Eq.(2), using realistic band parameters, resulted in the gap solutions such that $|\Delta_e|/|\Delta_h| \approx 2.5$ with $N_h(0)/N_e(0) \approx 2.6$ in the previous calculations [17]. Notice the substantial difference of the sizes of the gap for the hole and electron bands and the inverse relation between the gap ratios $N_h(0)/N_e(0)$ and $|\Delta_e|/|\Delta_h|$. This inverse relation between the gap sizes and the DOS sizes -- i.e., $|\Delta_h| < |\Delta_e|$ for $N_h(0) > N_e(0)$ and vice versa -- is a generic feature of the interband pairing model [23]. For most calculations in this paper, we used the above parameters.

In this paper, we are particularly interested in the effects of impurity scattering on the nuclear spin-lattice relaxation rate $1/T_1$ of the $\pm s$-wave state, which is calculated by

$$\frac{1}{T_1} \propto -T \int_0^\infty d\omega \frac{\hat{\omega}_{FD}(\omega)}{\omega} \sum_{a=h,e} \left\{ \frac{N_a^2(0)}{\langle Re \frac{\tilde{\omega}_a}{\omega^2 - \Delta_a^2(k)} \rangle_k^2} + \begin{cases} \langle Re \frac{\tilde{\omega}_a}{\omega^2 - \Delta_a^2(k)} \rangle_k^2 \quad N_a(0)N_e(0) \\ \langle Re \frac{\tilde{\omega}_a}{\omega^2 - \Delta_a^2(k)} \rangle_k^2 \end{cases} \right\}.$$
imperfection, when the other two intraband scattering processes (horizontal bars of the corresponding colors). (b) Impurity-induced selfenergies \( \Sigma_{\text{imp}}(\omega) = \int \mathcal{E} \, d\omega \) for comparison and other lines are offset for clarity (the zero baselines of the offset are marked by the narrow horizontal bars of the corresponding colors). (b) Impurity induced selfenergies \( \Sigma_{\text{imp}}(\omega) = \int \mathcal{E} \, d\omega \) with the same parameters as in (a). These curves are not offset.

**Results** - All energy scales are normalized by \( |\Delta_e| \) in this paper. Fig.1(a) shows the total DOS of two bands with different impurity concentrations \( \Gamma / \Delta_e = 0.0, 0.01, 0.04, 0.08 \) of the unitary scatterer (c=0), and Fig.1(b) shows the corresponding impurity induced selfenergy \( \text{Im} \Sigma_{\text{imp}}(\omega) = \text{Im} \Sigma_{\text{imp}}^0 + \text{Im} \Sigma_{\text{imp}}^1 \). Fig.1(a) shows how the fully opened gap of the pure state is filled with impurity states; the pattern of filling is very unusual and the \( \Gamma / \Delta_e = 0.04 \) case displays a perfect V-shape DOS down to zero energy as in a d-wave SC gap. The origin of this behavior is easily seen in Fig.1(b); the impurity bound state is never formed at zero energy but away from it (even in the unitary limit) because of the incomplete cancellation of \([G_{le}^1 + G_{le}^2]\), so the full gap around \( \omega = 0 \) is protected until this off-centered impurity band spills over to the zero energy with increasing the impurity concentration. When it touches the zero energy limit, the superconductor behaves gapless as in a pure d-wave superconductor, and this happens with the critical impurity concentration \( \Gamma_{\text{crit}} (= 0.04\Delta_e \) for our specific model parameters). Increasing the impurity concentration beyond \( \Gamma_{\text{crit}} \), the DOS still keeps the V-shape but now \( N_{\text{tot}}(\omega = 0) \) obtains a finite value (see the blue curve of \( \Gamma = 0.08\Delta_e \) case in Fig.1(a)).

This manner of evolution of the DOS with the impurity concentration results in the following consequences: (1) Beyond the critical impurity concentrations, direct measurements of the DOS at low temperature such as photoemission and tunneling spectroscopy would see a V-shape DOS, but at the same time would be extracting an isotropic gap [3, 8]; (2) Temperature dependence measurement such as \( 1/T_1(T) \) would see three different types of behavior. First, when \( \Gamma = \Gamma_{\text{crit}} \) (\( \Gamma = 0.04\Delta_e \) case in Fig.1(a)), the system sees the linear in \( \omega \) DOS for whole temperature region of \( 0 < T < T_c \). Second, when \( \Gamma > \Gamma_{\text{crit}} \) (\( \Gamma = 0.08\Delta_e \) case in Fig.1(a)), the linear in \( \omega \) DOS will prevail in the high temperature region, but at low temperatures the finite DOS of \( N_{\text{tot}}(\omega = 0) \) makes the system a gapless superconductor. Finally, when \( \Gamma < \Gamma_{\text{crit}} \) (\( \Gamma = 0.01\Delta_e \) case in Fig.1(a)), the system always behaves as a fully opened gap superconductor although the gap is weakened by impurities. This variation of DOS with the impurity concentration will be reflected in the behavior of \( 1/T_1(T) \) as will be shown below. In passing, note that \( \text{Im} \Sigma_{\text{tot}}^0(\omega) \) in Fig.1(b) shows two peaks on each side of the \( \omega \)-axis. Apparently, a smaller energy peak (\( \omega \sim 0.2\Delta_e \)) but with a larger spectral density due to the larger DOS of the hole band – is formed inside of the small gap \( \Delta_h \) and the larger energy peak (\( \omega \sim 0.7\Delta_e \)) is formed inside of the larger gap \( \Delta_e \).

Figure 2 shows the calculations of \( 1/T_1(T) \) with the variation of the impurity concentration using the same parameters as in Fig.1. It is clear that the puzzling \( T^3 \) behavior of \( 1/T_1 \) can be understood with the \( \pm s \)-wave; it has the same origin as in the d-wave gap, i.e., the linearly rising DOS. With \( \Gamma = \Gamma_{\text{crit}} = 0.04\Delta_e \), the \( T^3 \) behavior extends to the lowest possible temperatures as expected. With \( \Gamma > \Gamma_{\text{crit}} \), the \( T^3 \) behavior occurs only at high temperatures and at lower temperatures the system probes the finite DOS of \( N_{\text{tot}}(\omega = 0) \), hence displaying the \( T \)-linear behavior of \( 1/T_1 \). With \( \Gamma < \Gamma_{\text{crit}} \), the system should display a full gap behavior below \( T_c \), but somewhat weakened by impurities. As a consequence, \( 1/T_1 \) shows, in this case, a much weakened exponential drop for the extended temperature region below \( T_c \). This wide range of variation occurs with the impurity concentration \( 0 < \Gamma / \Delta_e < 0.08 \) and the reduction of \( T_c \) due to impurities is less than 10%; \( 8\Gamma_c / T_0^0 \) is proportional to \( (\Gamma / \Delta_e) / (\Delta_e / c^2 + 1) \). Finally, we emphasize that in order to capture this systematic evolution of \( 1/T_1 \) with impurity concentration, it is absolutely necessary to include both interband and intraband scattering process on equal footing.

Figure 3 shows an artificial case of the equal size \( \pm s \)-wave gap (\( |\Delta_e| = |\Delta_h| \) and \( N_h(0) = N_e(0) \)). Because of the perfect cancellation of \( |G_{le}^1 + G_{le}^2| \) term in the denominator of the \( T \)-matrices, any small amount of the impurity concentration
FIG. 2: (Color online) Calculated $1/T_1(T)$ for different impurity concentrations, $\Gamma/\Delta_c = 0.0, 0.01, 0.04, 0.08$ and with $2\Delta_h/\Delta_c = 3.0$. Experimental data is from Ref.[5]. The curves are offset for clarity.

immediately induces the bound state at zero energy as in the case of a d-wave superconductor. But this bound state spectral density is isolated inside of a full gap (see Fig.3(b)). Therefore, the superconductivity still remains as a full gap superconductor, until the bound state spectral density grows and touches the edge of the gap with increasing the impurity concentration. The inset of Fig.3(b) shows the imaginary part of the impurity selfenergy $\text{Im} \Sigma_{\text{tot}}(\omega)$, clearly showing the bound state centered at $\omega = 0$, which should be contrasted with the off-centered bound state for the unequal size gap case (see Fig.1(B)).

As a result, the SC state in this case shows an activated behavior for the high temperature region below $T_c$, and the impurity induced DOS only starts being sensed at very low temperatures. This behavior is well captured with $1/T_1(T)$ (Fig.3(A)). It shows that even the Hebel-Slichter peak around $T_c$ is not completely suppressed despite the perfect cancellation of $[G_h^2 + G_s^2]$, because at or near $T_c$ the impurity effect is only weakly sensed by the system. This result emphasizes that the assumption of the equal size gaps, as done in Ref.[19], results in a qualitatively different physics and it appears not consistent with experiments [3][4]. For comparison, we plot the experimental data by Kawasaki et al.[5] together with the theoretical result in Fig.3(a).

Conclusion - In conclusion, we studied the effect of impurities, in particular, of the strong scattering limit, on the $\pm s$-wave superconductor with a generalized $\sigma$-matrix method. The unique and generic feature of the $\pm s$-wave superconductor, i.e., the opposite signs of the gaps but with unequal sizes, results in a off-centered impurity bound states inside the gaps. With the variation of the impurity concentration, the DOS, $N_{\text{tot}}(\omega)$, evolves systematically from a fully gapped one to a V-shape one. We showed that several conflicting experimental issues such as photoemission, tunneling spectroscopy, and $1/T_1$ are coherently explained with the $\pm s$-wave SC state with the resonant impurity scattering.

Acknowledgement - This work was supported by the KOSEF through the Grants No. KRF-2007-521-C00081 (YB), No. KRF-2007-070-C00044 (YB,HYC), and Basic Research Program Grant No. R01-2006-000-11248-0 (HYC). We thank Guo-qing Zheng for useful discussions and sending us their experimental data.
To whom the correspondences should be addressed: ykbang@chonnam.ac.kr

[1] Y. Kamihara et al., J. Am. Chem. Soc., 128, 10012 (2006); Y. Kamihara et al., J. Am. Chem. Soc., 130, 3296 (2008).

[2] G. F. Chen et al., Phys. Rev. Lett. 100, 247002 (2008); G. F. Chen et al., Nature 453, 761 (2008).

[3] Y. Wang et al., arXiv:0806.1986 (unpublished); L. Shan et al., Europhys. Letters, 83, 57004 (2008).

[4] T. Sato et al., J. Phys. Soc. Jpn. 77, 063708 (2008).

[5] S. Kawasaki et al., Phys. Rev. B 78, 220506(R) (2008).

[6] Y. Kamihara et al., J. Am. Chem. Soc., 130, 3296 (2008).

[7] G. F. Chen et al., Phys. Rev. Lett. 100, 247002 (2008); G. F. Chen et al., Nature 453, 761 (2008).

[8] T. Y. Chen et al., Nature (London), 453, 1224 (2008).

[9] H. Ding et al., Europhys. Lett. 83, 47001 (2008); T. Kondo et al., Phys. Rev. Lett. 101, 147003 (2008); L. Wray et al., arXiv:0808.2185 (unpublished).

[10] L. Malone et al., arXiv:0806.3908 (unpublished); K. Hashimoto et al., Phys. Rev. Lett. 101, 087002 (2009); C. Martin et al., arXiv:0807.0876 (unpublished).

[11] L. Boeri, O. V. Dolgov, A. A. Golubov, Phys. Rev. Lett. 101, 026403 (2008).

[12] C. de la Cruz et L., Nature (London) 453, 899 (2008); J. Zhao ET AL., Nature Materials 7, 953 (2008).

[13] Y. Qiu et al., Phys. Rev. Lett. 101, 257002 (2008).

[14] I.I. Mazin, D.J. Singh, M.D. Johannes, M.H. Du, Phys. Rev. Lett. 101, 057003 (2008).

[15] K. Kuroki et al., Phys. Rev. Lett. 101, 087004 (2008).

[16] M.M. Korshunov and I. Eremin, Phys. Rev. B 78, 140509(R) (2008).

[17] Y. Bang and H.-Y. Choi, Phys. Rev. B, 78, 134523 (2008).

[18] F. Wang, H. Zhai, Y. Ran, A. Vishwanath, Dung-Hai Lee, Phys. Rev. Lett. 102, 047005 (2009).

[19] D. Parker, O.V. Dolgov, M.M. Korshunov, A.A. Golubov, I.I. Mazin , Phys. Rev. B 78, 134524 (2008); A.V. Chubukov, D.V. Efremov, I. Eremin, Phys. Rev. B 78, 134512 (2008).

[20] M. M. Parish, J. Hu, B. A. Bernevig, Phys. Rev. B 78, 144514 (2008).

[21] It is also possible to design a tunneling experiment to directly probe the $\pi$ phase difference between the $\pm s$-gaps as proposed in H.-Y. Choi and Y. Bang, arXiv:0807.4604 (unpublished).

[22] $T^3$ power law behavior extracted from experimental data of the Fe pnictide superconductors might be only an approximate definition unless its origin is due to the gap symmetry as in the d-wave SC. Our study shows, however, that it also arises from the V-shape DOS as in the d-wave case; therefore the $T^3$ power law of $1/T_1$ in the Fe pnictide superconductors has a rather firm ground.

[23] P. J. Hirschfeld, P. Wolfle, and D. Einzel, Phys. Rev. B 37, 83 (1988); A. V. Balatsky, I. Vekhter, and J.-X. Zhu, Rev. Mod. Phys. 78, 373 (2006) and see more references therein.

[24] L. S. Borkowski and P. J. Hirschfeld Phys. Rev. B 49, 15404 (1994).

[25] N. Curro, T. Caldwell, E.D.Bauer, L.A. Morales, M.J. Graf, Yunkyu Bang, A.V. Balatsky, J.D. Thompson, J.L.Sarrao, Nature 434, 622 (2005).

[26] HJ Vidberg and J.W. Serene, J. of Low Temp. Phys. 29, 179 (1977).

[27] D.J. Singh and M.-H. Du, Phys. Rev. Lett. 100, 237003 (2008) ; C. Cao, P. J. Hirschfeld, H.P. Cheng, Phys. Rev. B 77, 220506(R) (2008); E. Manousakis, Jun Ren, E. Kaxiras, arXiv:0806.3432 (unpublished).

[28] Although for most of cases, the approximate relation $N^h_e(0)\Delta_h^\ell \approx N^e_h(0)\Delta_e^\ell$ holds, this is not a rigorous identity. For more detail discussion, see Ref.[17].