Impurity effects on the ±s-wave state of the iron-based superconductors

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

Han-Yong Choi†
Department of Physics and Institute for Basic Science Research, SungKyunKwan University, Suwon 440-746, Republic of Korea

Hyekyung Won‡
Department of Physics, Hallym University, Chuncheon 200-702, Republic of Korea
(Received 16 September 2008; revised manuscript received 1 February 2009; published 27 February 2009)

We studied the impurity scattering on the $\pm s$-wave superconductor (SC), with realistic parameters for the Fe pnictide SCs. Using the $\mathcal{T}$-matrix method, generalized for the two bands, we found that the strong scattering limit of impurities forms an off-centered resonance state inside the superconducting (SC) gap, which modifies, surprisingly, the density of states (DOS) of a fully opened gap to a V-shaped DOS as if in the case of a d-wave SC. This behavior provides coherent explanations to the several conflicting experiments of the Fe-based SC: (1) the V-shaped DOS observed in photoemission and tunneling spectroscopy but with an isotropic gap; (2) the power-law behavior of the nuclear-spin-lattice relaxation rate ($1/T_1 \sim T^{\alpha}$ with $\alpha \sim 3$) down to very low temperatures. We also extended the same $\mathcal{T}$-matrix method to study the impurity suppression of the critical temperature T_c of the $\pm s$-wave pairing state. We found that both magnetic and nonmagnetic impurities suppress T_c with a rate that is practically indistinguishable from the standard d-wave case despite a possibly large difference of the positive and the negative s-wave order parameter magnitudes.

DOI: 10.1103/PhysRevB.79.054529 PACS number(s): 74.20.Mn, 74.20.Rp, 74.25.Nf

I. INTRODUCTION

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

On the theoretical side, it is almost agreed on that the pairing mechanism is nonphononic,[10] and most probably of a magnetic origin. This conclusion is consistent with the overall phase diagram obtained by neutron scattering,[11] where the SC phase starts to develop when the antiferromagentic (AFM) order disappears, suggesting a universal mechanism for the unconventional superconductivity of the compounds with d- and f-orbital 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 Brillouin zone—favors development of the so-called $\pm s$-wave SC state, proposed by Mazin *et al.*[12] (these authors use notation "$s_{\pm}$"), and reconfirmed theoretically by several authors.[13,14]

Then the key question is: Is the $\pm s$-wave state consistent with all experiments? Summarizing the current experimental situation: Tunneling measurements and their interpretations can be reconciled with both a d-wave type state and the $\pm s$-wave state. Photoemission spectroscopies may now be considered to be more consistent with the $\pm s$-wave state. The exponentially flat behavior of the low temperature penetration depth[9] can only be explained by the $\pm s$-wave state.[14] However, the nuclear-spin-lattice relaxation rate $1/T_1$ experiments[4,5] all report a power law of $\sim T^3$ behavior[15] and this T^3 power law is a well-known evidence of a nodal gap SC state.

To come to the rescue, several groups[16,17] including the present authors[14] recently pointed out that the unusual interband coherence factor, unique to the $\pm s$-wave state due to the π-phase difference[18] of the SC order parameter (OP) between the bands, can lead to an approximate power-law behavior of $1/T_1$ as well as the absence of Hebel-Slichter peak, with a help of impurities. While this is an important observation, the calculations of these works[14,16,17] are not completely satisfactory. First of all, the works of Ref. 16 considered only the interband scattering process while the works of Refs. 14 and 17 showed that both the interband and intraband processes have comparable contributions and hence both processes should be treated on equal footing. Second, the results of the works of Refs. 14 and 17, which correctly included both the interband and intraband processes, reproduced the T^3 behavior only for the limited temperature window. Therefore, it needs more quantitative and systematic studies to settle the issue.

In this paper, we study the impurity effects on the $\pm s$-wave state of the two band minimal model for the Fe pnictide SCs.[14] In particular, we would like to address the following questions: (1) how robust and how low temperatures the power law in $1/T_1$ can extend to? (2) the nature of impurities to explain experiments; the weak coupling or the strong coupling limits? Our key finding is that the strong coupling limit of impurity scattering introduces an off-centered resonance state inside the SC gap, which then modifies the fully gapped DOS of the $\pm s$-wave SC into a V-shaped DOS. With this evolution of DOS with impurities, several puzzling and conflicting experimental issues such as photoemission,[7] tunneling spectroscopy,[2] as well as the power law of $1/T_1$ (Refs. 4 and 5) are coherently explained. In particular, our finding shows that the T^3 power law of $1/T_1$ in the Fe pnictide SCs is not due to an accidental material property but has a rather firm physical ground.

We also studied the impurity suppression of the critical temperature T_c of the $\pm s$-wave state. We found that the T_c suppression rate is practically indistinguishable from the standard d-wave case despite a possibly large difference of the positive and negative s-wave OP magnitudes. However, when the difference of the gap size between the bands becomes very large, the s-wave nature of the order parameter renders the magnetic impurities a slightly stronger pair breaker than the nonmagnetic impurities. In the case of the d-wave state, there is no difference between the magnetic and nonmagnetic impurities for the T_c suppression.

II. FORMALISM

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. The $\mathcal{T}$-matrix approximation has been successfully applied to the various unconventional superconductors (SCs) such as heavy fermion and high-temperature SCs.[19] For example, it predicted a resonant bound state by unitary impurity scatterer inside the d-wave SC gap, which was crucial to explain the penetration depth, $1/T_1$, etc. of the high-T_c cuprates.[19] The key principle of forming a resonance bound sate in the d-wave gap is that the sign-changing d-wave SC OP guarantees the absence of the renormalization of the anomalous self-energy due to the impurity scattering. Therefore, we expect that a similar mechanism will work with the sign-changing $\pm s$-wave state. However, there are some differences: (1) the cancellation of the anomalous self-energy would not be perfect unless the sizes of $+s$ and $-s$ gaps and their corresponding DOSs $N_h(0)$ and $N_e(0)$ are exactly equal; (2) the DOS of the pure $\pm s$-wave state is not linearly vanishing as in the d-wave case but fully gapped and the impurity bound state is very sensitive to the fine details of the low energy DOS. Considering these differences, it requires quantitative and transparent investigations for the impurity effects on the $\pm s$-wave state.

Recently we had proposed a minimal two band model with a phenomenological magnetic interaction for the Fe-based SCs.[14] Assuming two SC OPs, Δ_h and Δ_e, on each band, the two coupled gap equations are written as

$$\Delta_h(k) = -\sum_{k'} [V_{hh}(k,k')\chi_h(k') + V_{he}(k,k')\chi_e(k')], \quad (1)$$

$$\Delta_e(k) = -\sum_{k'} [V_{eh}(k,k')\chi_h(k') + V_{ee}(k,k')\chi_e(k')], \quad (2)$$

where $V_{h,e}(k,k')$ is the phenomenological pairing interaction originating from the antiferromagnetic (AFM) correlation. The above gap equations permit two solutions: $\pm s$-wave state and double d-wave state. When the interband pairing interaction $V_{he}=V_{eh}$ are repulsive and dominant over the intraband interactions, the state where Δ_h and Δ_e have the relative phase of π, referred to as $\pm s$-wave pairing state, is the ground state. The pair susceptibility is given by

$$\chi_{h,e}(k) = T\sum_n N(0)_{h,e}\int_{-\omega_{\mathrm{AFM}}}^{\omega_{\mathrm{AFM}}} d\xi \frac{\tilde{\Delta}_{h,e}(k)}{\tilde{\omega}_n^2 + \xi^2 + \tilde{\Delta}_{h,e}^2(k)}, \quad (3)$$

where $N(0)_{h,e}$ are the DOS of the hole and electron bands, respectively, and ω_{AFM} is the cutoff energy of the pairing potential $V(q)$.

The impurity effects are included using the $\mathcal{T}$-matrix method as

$$\tilde{\omega}_n = \omega_n + \Sigma_h^0(\omega_n) + \Sigma_e^0(\omega_n), \quad (4)$$

$$\tilde{\Delta}_{h,e} = \Delta_{h,e} + \Sigma_h^1(\omega_n) + \Sigma_e^1(\omega_n), \quad (5)$$

$$\Sigma_{h,e}^{0,1}(\omega_n) = \Gamma \cdot \mathcal{T}_{h,e}^{0,1}(\omega_n), \quad \Gamma = \frac{n_{\mathrm{imp}}}{\pi N_{\mathrm{tot}}}, \quad (6)$$

where $\omega_n = T\pi(2n+1)$ is the Matsubara frequency, n_{imp} the impurity concentration, and $N_{\mathrm{tot}}=N_h(0)+N_e(0)$ is the total DOS. The $\mathcal{T}$ matrices $\mathcal{T}^{0,1}$ are the Pauli matrices $\tau^{0,1}$ components in the Nambu space. The impurity induced self-energies are calculated with the $\mathcal{T}$ matrix generalized to a two band superconductivity as

$$\mathcal{T}_a^i(\omega_n) = \frac{G_a^i(\omega_n)}{D} \quad (i=0,1;\ a=h,e), \quad (7)$$

$$D = c^2 + [G_h^0 + G_e^0]^2 + [G_h^1 + G_e^1]^2, \quad (8)$$

$$G_a^0(\omega_n) = \frac{N_a}{N_{\mathrm{tot}}}\left\langle \frac{\tilde{\omega}_n}{\sqrt{\tilde{\omega}_n^2 + \tilde{\Delta}_a^2(k)}} \right\rangle, \quad (9)$$

$$G_a^1(\omega_n) = \frac{N_a}{N_{\mathrm{tot}}}\left\langle \frac{\tilde{\Delta}_a}{\sqrt{\tilde{\omega}_n^2 + \tilde{\Delta}_a^2(k)}} \right\rangle, \quad (10)$$

where $c=\cot\delta_0$ is a convenient measure of scattering strength, with $c=0$ for the unitary limit and $c>1$ for the Born limit scattering. $\langle\ldots\rangle$ denotes the Fermi surface (FS) average. The above four $\mathcal{T}$ matrices, $\mathcal{T}_a^i$, are numerically solved together with the coupled gap Eqs. (1) and (2) in Matsubara frequencies. Then Pade-approximant method is used to obtain the real and imaginary part of self-energies $\Sigma_{h,e}^{0,1}(\omega+i\eta)$, with which various physical quantities can be straightforwardly calculated.

Note Eq. (8), which is the denominator of $\mathcal{T}$ matrices $\mathcal{T}_a^i$. The last term of it, $[G_h^1+G_e^1]$, would exactly vanish for a d-wave SC because of the FS average over the d-wave OP and that is the technical reason for the formation of the resonance bound state at zero energy when $c=0$. For the $\pm s$-wave case, a cancellation still occurs because G_h^1 and G_e^1 have opposite signs [see Eq. (10)]. However, this cancellation is never perfect unless $|\Delta_e|=|\Delta_h|$ and $N_h(0)=N_e(0)$. With an incomplete cancellation, the finite remnant acts as weakening impurity scattering strength (increasing the effective value of c). For the middle term $[G_h^0+G_e^0]$ of D, G_h^0, and G_e^0 always have the same sign, so that the normal scattering process is additive with number of bands.

With the typical band structure of the Fe-based pnictides,[20] $N_h(0)$ and $N_e(0)$ are not equal. Then the coupled gap Eqs. (1) and (2), using realistic band parameters, resulted in the gap solution such that $|\Delta_e|/|\Delta_h| \approx 2.5$ with $N_h(0)/N_e(0) \approx 2.6$ in the previous calculations of Ref. 14. Notice the substantial difference of the size of two gaps for the hole and electron bands and the inverse relation between two ratios $N_h(0)/N_e(0)$ and $|\Delta_h|/|\Delta_e|$ (Ref. 21). For most calculations in this paper, we used the above parameters but the physical results of this paper are independent of the specific choice of theses parameters.

III. NUCLEAR-SPIN-LATTICE RELAXATION RATE $1/T_1$

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

$$\frac{1}{T_1} \sim -T\int_0^\infty d\omega \frac{\partial f_{FD}(\omega)}{\partial \omega}\Bigg\{ \sum_{a=h,e} N_a^2(0) \times \left[\left\langle \mathrm{Re}\frac{\tilde{\omega}}{\sqrt{\tilde{\omega}^2-\tilde{\Delta}_a^2(k)}} \right\rangle_k^2 + \left\langle \mathrm{Re}\frac{\tilde{\Delta}_a(k)}{\sqrt{\tilde{\omega}^2-\tilde{\Delta}_a^2(k)}} \right\rangle_k^2 \right] + 2N_h(0)N_e(0) \times \left[\left\langle \mathrm{Re}\frac{\tilde{\omega}}{\sqrt{\tilde{\omega}^2-\tilde{\Delta}_h^2(k)}} \right\rangle_k \left\langle \mathrm{Re}\frac{\tilde{\omega}}{\sqrt{\tilde{\omega}^2-\tilde{\Delta}_e^2(k')}} \right\rangle_{k'} + \left\langle \mathrm{Re}\frac{\tilde{\Delta}_h(k)}{\sqrt{\tilde{\omega}^2-\tilde{\Delta}_h^2(k)}} \right\rangle_k \left\langle \mathrm{Re}\frac{\tilde{\Delta}_e(k')}{\sqrt{\tilde{\omega}^2-\tilde{\Delta}_e^2(k')}} \right\rangle_{k'} \right] \Bigg\}, \tag{11}$$

where $\tilde{\omega}$ and $\tilde{\Delta}_{h,e}(\omega)$ are the real frequency quantities obtained from $\tilde{\omega}_n$ and $\tilde{\Delta}_{h,e}(\omega_n)$ by analytic continuation $i\omega_n \to \omega + i\eta$. The Eq. (11) of $1/T_1$ consists of three scattering processes: two intraband scattering processes in the hole band and electron band, respectively, and one interband scattering process between the hole and electron bands. The unique feature of the $\pm s$-wave state is the interband scattering process. Having the opposite signs for Δ_h and Δ_e, this process [the last term in Eq. (11)] substantially cuts out the $1/T_1$ relaxation rate below T_c.[14,16,17] It is contrasted to the usual coherence peak contribution from the intraband scattering processes [the first two terms in Eq. (11)] as shown by recent papers.[14,17] We reemphasize that the correct theory should include both inter- and intraband processes on equal footing, and when we do that, we found that the interband process is not sufficiently strong to completely suppress the coherence peak from the two intraband process contributions and it is necessary to introduce impurities to kill the remained coherence peak.[14,17] For the temperature dependence of the gaps $\Delta_{h,e}(k,T)$, we use a phenomenological formula, $\Delta_{h,e}(k,T) = \Delta_{h,e}(k,T=0)\tanh(\beta\sqrt{T_c/T-1})$. By choosing the values of $\Delta_{h,e}^{\max}/T_c$, we can partially take into account of the effect of the strong coupling superconductivity. We fix $\beta = 1.74$ as usual, which is not a sensitive parameter for final results.

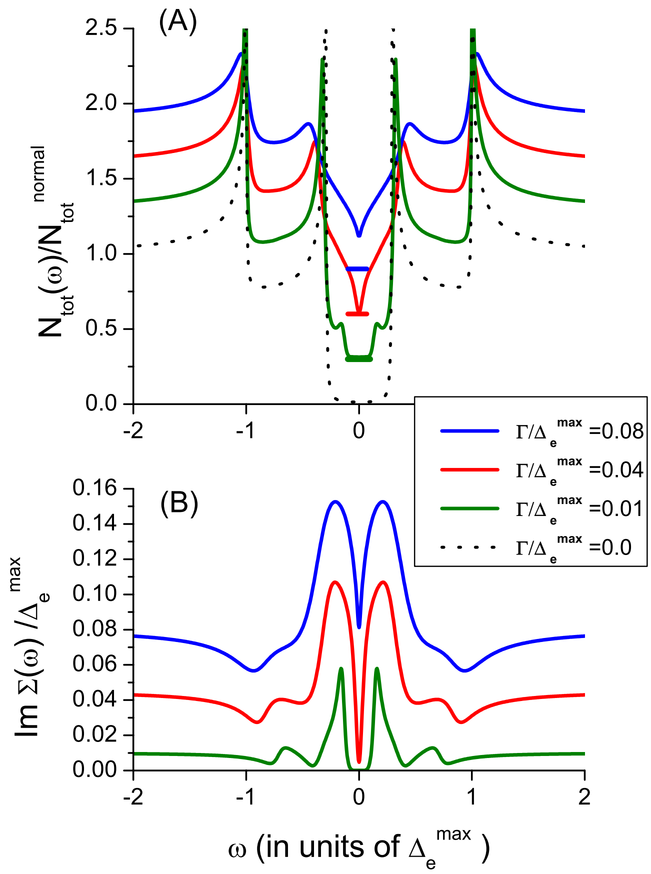

FIG. 1. (Color online) (a) Normalized DOS $N_{\mathrm{tot}}(\omega)$ for different impurity concentrations, $\Gamma/\Delta_e = 0.0$, 0.01, 0.04, and 0.08. Thin dotted line is of the pure state for comparison and other lines are offset for clarity (the zero baselines of the offset are marked by the narrow horizontal bars of the corresponding colors). (b) Impurity induced self-energies $\mathrm{Im}\,\Sigma_{\mathrm{tot}}^0(\omega) = \mathrm{Im}\,\Sigma_h^0 + \mathrm{Im}\,\Sigma_e^0$ with the same parameters as in (a). These curves are not offset.

Numerical results and discussions

All energy scales are normalized by $|\Delta_e|$ in this paper. Figure 1(a) shows the total DOS of two bands with different impurity concentrations $\Gamma/\Delta_e = 0.0$, 0.01, 0.04, and 0.08 of the unitary scatterer ($c=0$), and Fig. 1(b) shows the corresponding impurity induced self-energy $\mathrm{Im}\,\Sigma_{\mathrm{tot}}^0(\omega) = \mathrm{Im}\,\Sigma_h^0 + \mathrm{Im}\,\Sigma_e^0$. Figure 1(a) shows how the fully opened gap of the pure state is filled by impurity states; the pattern of filling is very unusual and the $\Gamma/\Delta_e = 0.04$ case displays a perfect V shape down to zero energy similar to a pure d-wave SC DOS. 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 because of the incomplete cancellation of

$[G_h^1+G_e^1]$, so that *the full gap around* $\omega=0$ is protected until this off-centered impurity band spills over to the zero energy with increasing impurity concentration. When it touches the zero energy limit, the $\pm s$-wave SC will thermodynamically behave like a pure d-wave SC, and this happens with the critical impurity concentration $\Gamma_{crit}/\Delta_e=0.04$ for our specific model parameters. Increasing impurity concentration beyond Γ_{crit}, the DOS still keeps the V shape but now $N_{tot}(\omega=0)$ obtains a finite value [see the $\Gamma=0.08\Delta_e$ case in Fig. 1(a)]. This manner of evolution of the DOS with impurity concentration results in the following consequences: (1) beyond the critical impurity concentrations, direct measurements of the DOS at low temperature such as photoemission[3,7] and tunneling spectroscopy[2] would see a V-shape DOS, but at the same time would extract isotropic gaps;[7] (2) temperature dependence measurement such as $1/T_1(T)$ would see three different types of behavior. First, when $\Gamma=\Gamma_{crit}$ ($\Gamma=0.04\Delta_e$ case), the system sees the linear in ω DOS for whole temperature region of $0<T<T_c$. Second, when $\Gamma>\Gamma_{crit}$ ($\Gamma=0.08\Delta_e$ case), the linear in ω DOS will prevail in the high-temperature region, but at low temperatures the finite DOS of $N_{tot}(\omega=0)$ makes the system as a gapless SC. Finally, when $\Gamma<\Gamma_{crit}$ ($\Gamma=0.01\Delta_e$ case), the system behaves always as a fully gapped SC although the gap is weakened by impurities. In passing, note that Im $\Sigma^0_{tot}(\omega)$ in Fig. 1(b) shows two peaks on each side of the ω axis. Apparently, a smaller energy peak ($\omega\sim 0.2\Delta_e$) with a larger spectral density is formed inside of the small gap Δ_h of the hole band which has a larger DOS and the larger energy peak ($\omega\sim 0.7\Delta_e$) is formed inside of the larger gap Δ_e of the electron band.

Figure 2 shows the calculations of $1/T_1(T)$ with the variation in the impurity concentration 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 state; it has the same origin as in the d-wave SC, i.e., the linearly rising DOS. With $\Gamma=\Gamma_{crit}=0.04\Delta_e$, the T^3 behavior extends to the lowest possible temperatures as expected. With $\Gamma>\Gamma_{crit}$, the T^3 behavior occurs only at high temperatures and at lower temperatures the system probes the finite DOS of $N_{tot}(\omega=0)$, hence displaying the T-linear behavior of $1/T_1$. With $\Gamma<\Gamma_{crit}$, $1/T_1$ displays a full gap behavior below T_c, but somewhat weakened by impurities. As a result a very much weakened exponential drop occurs for the extended temperature region below T_c. 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. Also this wide range of variation occurs with the impurity concentration $0<\Gamma/\Delta_e<0.08$ and the reduction in T_c, $\delta T_c/T_c^0$, due to impurities is proportional to $(\Gamma/\Delta_e)/[c^2+1]$, which is less than 10% reduction as will be discussed more in detail in Sec. IV.

With the results of Fig. 2, we need to carefully reexamine the experimental situation. Figure 2 shows that the experimental data of Kawasaki *et al.*[5] are best fit with $\Gamma_{crit}/\Delta_e=0.04$ down to the lowest temperature. However, most experimental data up to now are limited for the temperature range of $0.2-0.3T_c<T$ or even narrower range. Our calculations show that although the T^3 behavior over the whole temperature range below T_c occurs only with a critical concentration Γ_{crit}, if we limit the temperature range for

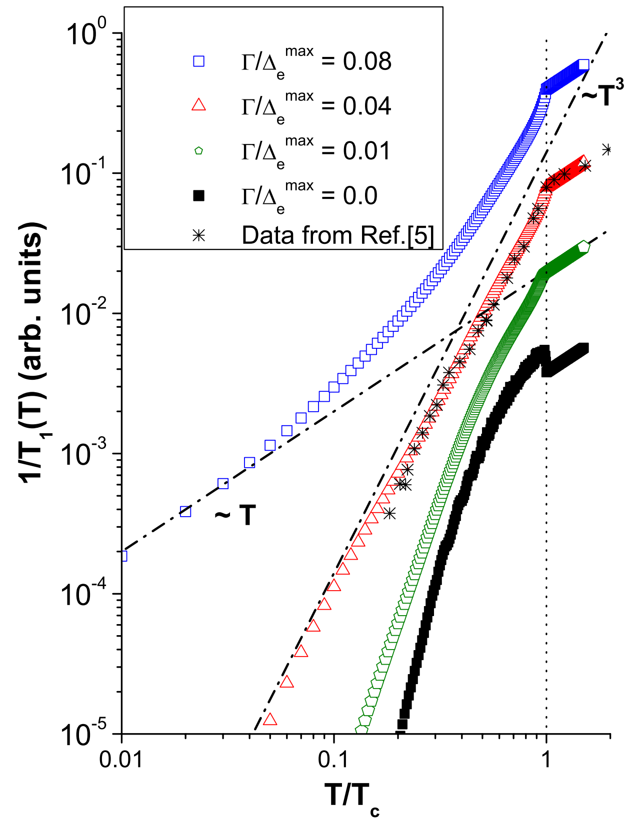

FIG. 2. (Color online) Calculated $1/T_1(T)$ for different impurity concentrations, $\Gamma/\Delta_e=0.0$, 0.01, 0.04, and 0.08 and with $2\Delta_h/T_c=3.0$. Experimental data are from Ref. 5. The curves are offset for clarity.

$0.2-0.3T_c<T$, there is a finite window of impurity concentration around Γ_{crit} where our calculated $1/T_1$ behaves as $\sim T^3$. As a stringent test for our theory, experiment should be done with cleaner samples to observe a hint of the presence of gap which will show a steeper decrease in $1/T_1$ than T^3 below T_c.

Figure 3 shows an artificial case of the equal size $\pm s$-wave case [$|\Delta_e|=|\Delta_h|$ and $N_h(0)=N_e(0)$]. Because of the perfect cancellation of $[G_h^1+G_e^1]=0$ in D, any small amount of the unitary ($c=0$) impurities immediately induces a bound state at zero energy as in the case of a d-wave SC. But this impurity bound state is isolated inside of the full gap [see Fig. 3(b)]. Therefore, the superconductivity behaves as a full gap SC until the spectral density of the impurity bound state grows and touches the edge of the gap with increasing impurity concentration. The inset of Fig. 3(b) also clearly shows this zero energy bound state in Im $\Sigma_{tot}(\omega)$. It should be contrasted with the off-centered bound state of the unequal size gap case in Fig. 1(b). As a result, the SC state in this case shows an activated behavior in the high-temperature region below T_c and then abruptly changes to the T-linear regime where impurity band starts being sensed at low temperatures. This behavior is well captured with $1/T_1(T)$ in Fig. 3(a). It shows that even the Hebel-Slichter peak around T_c is not completely suppressed despite the perfect cancellation of $[G_h^1+G_e^1]$, because at or near T_c the impurity effect is only weakly sensed by the system. This result

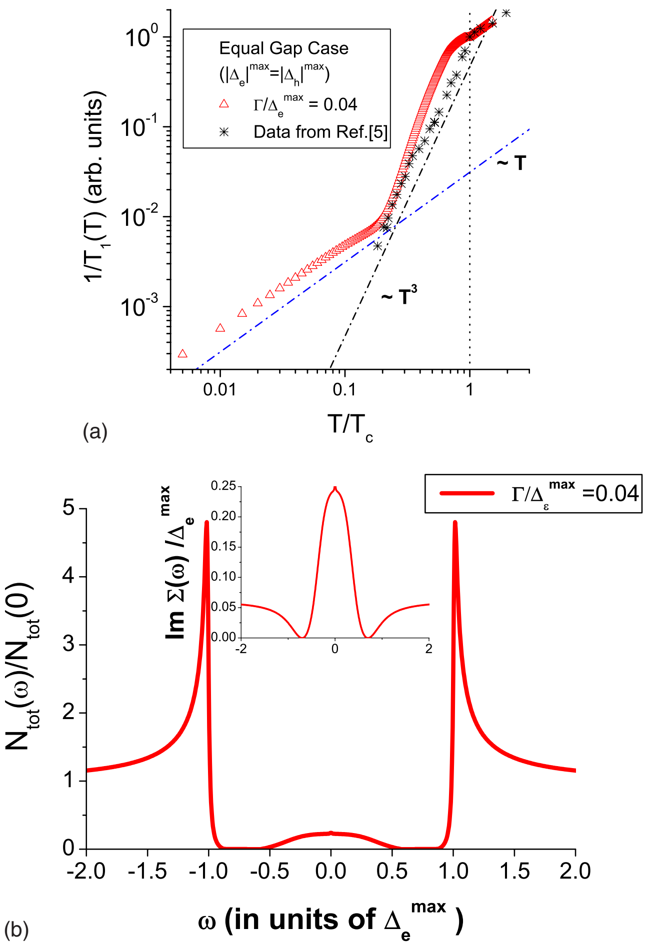

FIG. 3. (Color online) The case of the equal size $\pm s$-wave gap $[|\Delta_e|=|\Delta_h|$ and $N_h(0)=N_e(0)]$. (a) $1/T_1(T)$ with $2\Delta/T_c=3.0$. Experimental data are from Ref. 5. (b) Normalized DOS $N_{\rm tot}(\omega)$. Inset: Impurity induced self-energy Im $\Sigma^0_{\rm tot}(\omega)$.

emphasizes that the assumption of the equal size gaps, as done in Ref. 16, leads to a qualitatively different result and it appears not consistent with experiments of the Fe pnictide SCs. For comparison, we plot the experimental data by Kawasaki *et al.*[5] together with the theoretical results in Fig. 3(a).

IV. IMPURITY SUPPRESSION OF THE CRITICAL TEMPERATURE T_c

To determine T_c, we take $T\rightarrow T_c$ limit and linearize the gap Eqs. (1) and (2) with respect to the OPs $\Delta_{h,e}$. First, the impurity renormalized Matsubara frequency Eq. (4) and the OPs Eq. (5) are written as

$$\tilde{\omega}_n = \omega_n(1+\eta_\omega), \tag{12}$$

$$\tilde{\Delta}_{h,e} = \Delta_{h,e}(1+\delta_{h,e}), \tag{13}$$

with

$$\eta_\omega = \frac{\Gamma}{1+c^2}\frac{1}{|\omega_n|}, \tag{14}$$

$$\delta_{h,e} = \frac{\Gamma}{1+c^2}\frac{1}{|\tilde{\omega}_n|}\frac{[\tilde{N}_h\Delta_h+\tilde{N}_e\Delta_e]}{\Delta_{h,e}}, \tag{15}$$

where $\tilde{N}_a=N_a/N_{\rm tot}(a=h,e)$, and the pair susceptibility Eq. (3) is now simplified as

$$\chi_{h,e}(k) = \pi T\sum_n N(0)_{h,e}\frac{\Delta_{h,e}(k)(1+\delta_{h,e})}{|\omega_n(1+\eta_\omega)|}. \tag{16}$$

It is immediately clear that $\eta_\omega=\delta_a$ for a single band s-wave gap state and there is no renormalization of the pair susceptibility $\chi_a(k)$ with the impurity scattering. This is just the Anderson theorem of T_c for the s-wave SC. In our two band case, it is more complicated to draw any simple conclusion. In particular, the signs of δ_h and δ_e are opposite because of the opposite signs of $\Delta_{h,e}$.

Before we show the numerical results, we can analyze a simpler case. The main pairing process in the $\pm s$-wave pairing state is the interband interaction so that we keep only $V_{he}=V_{eh}$ interactions in the gap Eqs. (1) and (2), and use Eq. (16) for the pair susceptibilities. Then the coupled gap Eqs. (1) and (2) are reduced into one equation as

$$\Delta_h = \pi^2T^2\sum_n\sum_m \lambda^2_{\rm eff}\frac{(1+\delta_e)(1+\delta_h)}{|\omega_n(1+\eta_\omega)||\omega_m(1+\eta_\omega)|}\Delta_h, \tag{17}$$

where $\lambda_{\rm eff}=\sqrt{N_hN_eV_{he}V_{eh}}$ is the effective dimensionless coupling constant. This equation can be compared with the similarly reduced gap equation without impurities as

$$\Delta_h = \pi^2T^2\sum_n\sum_m \lambda^2_{\rm eff}\frac{1}{|\omega_n||\omega_m|}\Delta_h, \tag{18}$$

which yields the standard single band s-wave result with $T_c^0\approx 1.14\omega_D\exp(-1/\lambda_{\rm eff})$. Equation (17) would yield definitely smaller T_c than T_c^0 because δ_a is smaller in magnitude than η_ω. When both δ_a are set to zeros we obtain another reduced gap equation as

$$\Delta_h = \pi^2T^2\sum_n\sum_m \lambda^2_{\rm eff}\frac{1}{|\omega_n(1+\eta_\omega)||\omega_m(1+\eta_\omega)|}\Delta_h \tag{19}$$

which is just the case that we would obtain for a double d-wave gap state[14] where the anomalous self-energy corrections δ_a are absent because of the sign-changing OP with equal sizes. The result of Eq. (17) is not straightforward. If both δ_a are positive (their magnitudes are always smaller than η_ω), the T_c reduction would be simply in between the case of a s wave (no T_c suppression) and the case of a d wave. But in the $\pm s$-wave case, δ_h and δ_e will have always opposite signs and as a result the T_c reduction can be faster or slower than the d-wave case of Eq. (19). A simple rule is the following: in the leading approximation the reduction rate depends on the sign and the magnitude of the quantity $(\delta_h+\delta_e)$. If it is positive, the T_c reduction is slower than the d-wave case, and if it is negative, the T_c reduction is faster than the d-wave case.

We can utilize the relation $|\Delta_h|/|\Delta_e|=\sqrt{N_e/N_h}$ as $T\rightarrow T_c$ found in the minimal two band model in Ref. 14, and obtain

$$\delta_h \approx \sqrt{\tilde{N}_h}(\sqrt{\tilde{N}_h} - \sqrt{\tilde{N}_e}), \tag{20}$$

$$\delta_e \approx -\sqrt{\tilde{N}_e}(\sqrt{\tilde{N}_h} - \sqrt{\tilde{N}_e}). \tag{21}$$

From this we can find that $(\delta_h+\delta_e) \approx (\sqrt{\tilde{N}_h}-\sqrt{\tilde{N}_e})^2$ is always positive regardless whether $N_h > N_e$ or $N_h < N_e$. Therefore, the actual T_c reduction should be slower than the d-wave case. How much slower will be determined by the value of $(\delta_h+\delta_e)$. When this value is 0, the suppression rate is the same as a d-wave case, and when this value is 1, no suppression of T_c occurs. From the relation $(\delta_h+\delta_e) \approx (\sqrt{\tilde{N}_h}-\sqrt{\tilde{N}_e})^2$ we can guess that the mitigated rate of the T_c suppression would be rather close to the d-wave case because $(\delta_h+\delta_e) \approx 0$ for most cases unless we have unrealistically large difference of DOSs between N_h and N_e. Therefore, a practical rule is that the T_c suppression rate by nonmagnetic impurities in the $\pm s$-wave state should be quite similar to the d-wave case. In the following, we will show the numerical calculations of T_c obtained by directly solving the gap Eqs. (1) and (2) including the intraband interactions, which were neglected in the above analysis, and compare them with the above analytic predictions. We found that the simplified gap equation Eq. (17) provides excellent approximation.

A. Magnetic impurity

Let us now turn to the magnetic impurity scattering. For magnetic impurities, if we assume only an exchange coupling such as $\mathbf{S}\cdot\vec{\boldsymbol{\sigma}}$ (where $\mathbf{S}$ is the momentum of the impurity atom and $\vec{\boldsymbol{\sigma}}$ is the spin of the electrons), we can draw a simple result from the above analysis. Because the exchange coupling flips the spin part of the singlet wave function,[22] the result of the magnetic impurity scattering is to change the sign of Δ_a in the numerator of Eq. (15). The final result is to replace δ_a by $-\delta_a$ but to keep η_ω the same form in the reduced gap Eq. (17). Remember that, for the nonmagnetic impurity case, we had the relation

$$(1+\delta_e)(1+\delta_h) > 1. \tag{22}$$

The fact that this term is larger than 1 yields that the T_c suppression rate with nonmagnetic impurities of the $\pm s$-wave state is slower than the d-wave case. For the magnetic impurity scattering, we will have, as discussed above,

$$(1-\delta_e)(1-\delta_h) < 1. \tag{23}$$

It is then clear that the T_c suppression rate with magnetic impurities of the $\pm s$-wave state should be faster than the d-wave case. But with the realistic parameters for the Fe pnictides, both Eqs. (22) and (23) will have values very close to 1, and we can conclude that both magnetic and nonmagnetic impurities would cause a similar T_c suppression with the Fe pnictide SCs and the suppression rate is close to the one of a d-wave case.

B. Numerical results and discussions

With the typical band structure of the Fe pnictide SCs,[20] we obtained $N_h(0)/N_e(0) \approx 2.6$ in the previous calculations.[14]

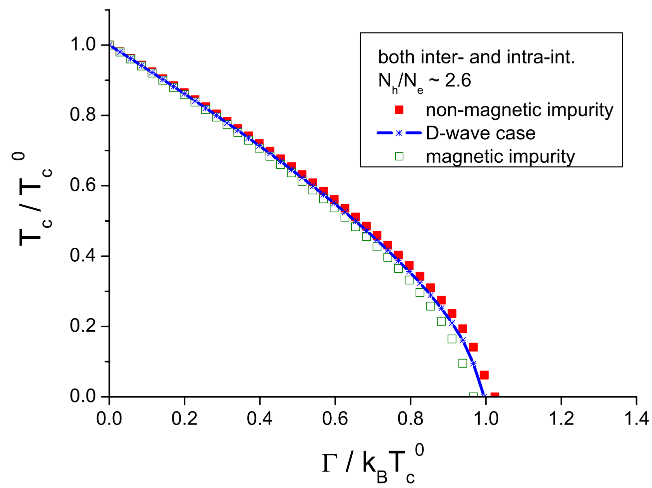

FIG. 4. (Color online) Normalized critical temperature T_c/T_c^0 vs normalized impurity scattering strength $\Gamma/k_B T_c^0$ $(c=0)$. The calculations are with the realistic bands $N_h/N_e \approx 2.6$ and with the full interactions V_{hh}, V_{ee}, V_{he}, and V_{eh}.

With this realistic band parameter and all interactions included, we numerically solved the coupled gap Eqs. (1) and (2). Figure 4 shows the calculation results of the normalized critical temperatures T_c/T_c^0 vs the normalized impurity scattering strength $\Gamma/k_B T_c^0$ with the unitary limit impurity scattering $(c=0)$. For a weaker coupling limit of impurity scattering, for example, with $c=1$ (Born limit), the suppression rate would become slower by a factor 2. As can be seen, there are almost no differences among all three cases: d-wave case, nonmagnetic impurity case, and magnetic impurity case. This is consistent with our analytic analysis because $(\delta_h+\delta_e) \approx 0.104 \ll 1$ in the case of Fig. 4. We normalize the impurity scattering strength Γ by T_c^0 instead of using the gap values $\Delta_{h,e}$ at $T=0$ for the convenience of comparison with future experiments. The fact that $\Gamma/k_B T_c^0 \sim 1$ when $T_c/T_c^0 \to 0$ is a pure coincidence of a parameter choice, which is clear in Fig. 6.

In Fig. 5, we artificially shut down the intraband interactions V_{hh} and V_{ee}; without the intraband repulsions T_c^0 itself increases by about 40%. But the normalized T_c/T_c^0 vs the impurity scattering strength $\Gamma/k_B T_c^0$ are indistinguishably similar to the case of Fig. 4. This result shows that the main results obtained from the analytic analysis from the simplified gap Eq. (17) will be excellent approximations for more realistic multiband model.

In Fig. 6, we used the artificially increased DOS ratio of $N_h/N_e=9$ which is of course a unrealistic ratio; this unrealistic parameter yields $(\delta_h+\delta_e) \approx 0.4$. The calculation results demonstrate that the suppression rate of T_c indeed follow the trend that we expected from the analytic investigation. It again reassures that in realistic case the T_c suppression of the $\pm s$-wave state by either magnetic or nonmagnetic impurities should be indistinguishably close to the case of the standard d-wave SC.

V. CONCLUSIONS

In this paper, we studied the impurity effects on the $\pm s$-wave pairing state based on the minimal two band model

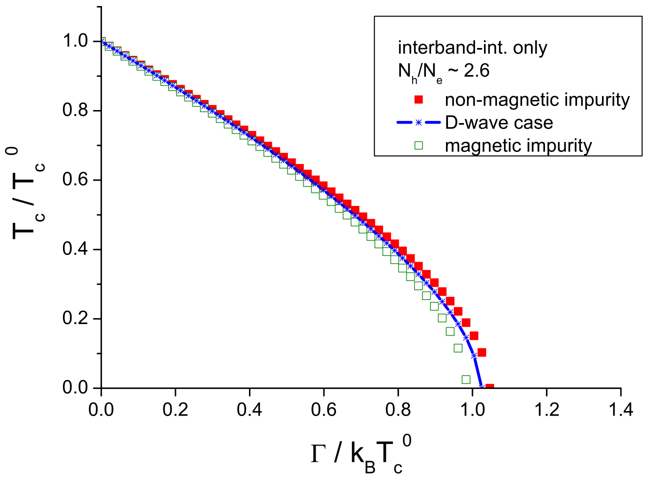

FIG. 5. (Color online) Normalized critical temperature T_c/T_c^0 vs normalized impurity scattering strength $\Gamma/k_BT_c^0$ $(c=0)$. The calculations are with the realistic bands $N_h/N_e \approx 2.6$ and with the interband interactions V_{he} and V_{eh} only.

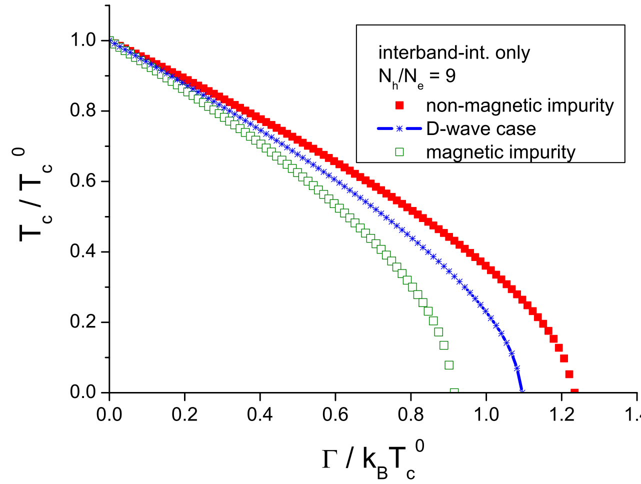

FIG. 6. (Color online) Normalized critical temperature T_c/T_c^0 vs normalized impurity scattering strength $\Gamma/k_BT_c^0$ $(c=0)$. The calculations are with the artificial bands $N_h/N_e=9.0$ and with the interband interactions V_{he} and V_{eh} only.

using a generalized $\mathcal{T}$-matrix method. In Sec. III, we calculated the nuclear-spin-lattice relaxation rate $1/T_1$ of the $\pm s$-wave state, in particular, in the strong coupling limit of impurity scattering $(c=0)$. The unique and generic feature of the $\pm s$-wave SC, namely, the opposite signs of the s-wave OPs with unequal sizes, results in the off-centered impurity bound states inside the gaps. With the variation in the impurity concentration, *the DOS* $N(\omega)$ *evolves systematically from a fully gapped one to the V-shape one*. With this evolution of DOS with impurities, several puzzling experimental issues such as photoemission,[7] tunneling spectroscopy,[2] and $1/T_1$ (Refs. 4 and 5) are coherently explained. These results demonstrate that the $\pm s$-wave SC state is the most consistent pairing state with current experimental data and the resonant impurity scattering of the strong coupling limit plays an important role to understand the SC properties of the Fe pnictide SCs.

In Sec. IV, extending the same $\mathcal{T}$-matrix method, we studied the effect of impurities on the T_c suppression of the $\pm s$-wave SC state. The main finding is that *despite a possibly large difference of the positive and negative s*-wave OP magnitudes, the T_c suppression rate is practically indistinguishable from the standard d-wave case. This is because the scattering process is a combined effect of the DOS multiplied with the OP magnitude. As a by-product, we find the subtle difference between the magnetic and the nonmagnetic impurities for the T_c suppression, which is, however, a quite small difference in magnitude in realistic case.

Finally, we would like to make a remark on the theoretical aspect of the current work. For the study of $1/T_1$ below T_c, it is crucial to capture the nonperturbative process of the impurity scattering in the SC state that can be treated by the $\mathcal{T}$-matrix method. This process leads to the formation of the off-centered resonant state of impurities, in particular, in the strong coupling limit. This noble impurity effect with the $\pm s$-wave state cannot be captured using a Born approximation. On the other hand, the T_c suppression by impurities does not involve the nonperturbative process because $\Delta_{h,e} \to 0$ as $T \to T_c$. Therefore, this problem could be treated with a Born approximation method if the impurity scattering is in weak coupling limit. Envisaging a strong coupling limit, we used the $\mathcal{T}$-matrix method to treat this problem. This method and its results can be easily extrapolated between the strong coupling limit and the weak coupling limit; these two limits of impurities make only a factor 2 difference for the T_c suppression rate.

ACKNOWLEDGMENTS

This work was supported by the KOSEF through Grants No. KRF-2007-521-C00081 (Y.B.), No. KRF-2007-070-C00044 (Y.B. and H.-Y.C.), and Basic Research Program Grant No. R01-2006-000-11248-0 (H.-Y.C.), and Hallym University Research Grant No. HRF-2007-030 (H.W.). We thank Guo-qing Zheng for useful discussions and sending us their experimental data.

*Author to whom correspondence should be addressed. ykbang@chonnam.ac.kr
†hychoi@skku.ac.kr
‡hkwon@hallym.ac.kr

[1] Y. Kamihara *et al.*, J. Am. Chem. Soc. **130**, 3296 (2008); G. F. Chen, Z. Li, D. Wu, G. Li, W. Z. Hu, J. Dong, P. Zheng, J. L. Luo, and N. L. Wang, Phys. Rev. Lett. **100**, 247002 (2008); X. H. Chen, T. Wu, G. Wu, R. Liu, H. Chen, and D. Fang, Nature (London) **453**, 761 (2008).
[2] Y. Wang, L. Shan, L. Fang, P. Cheng, C. Ren, and H. Wen,

Supercond. Sci. Technol. **22**, 015018 (2009); L. Shan, Y. Wang, X. Zhu, G. Mu, L. Fang, C. Ren, and H. Wen, Europhys. Lett. **83**, 57004 (2008).

[3] T. Sato, S. Souma, K. Nakayama, K. Terashima, K. Sugawara, T. Takahashi, Y. Kamihara, M. Hirano, and H. Hosono, J. Phys. Soc. Jpn. **77**, 063708 (2008).

[4] K. Matano, Z. A. Ren, X. L. Dong, L. L. Sun, Z. X. Zhao, and Guo-qing Zheng, Europhys. Lett. **83**, 57001 (2008); H.-J. Grafe, D. Paar, G. Lang, N. J. Curro, G. Behr, J. Werner, J. Hamann-Borrero, C. Hess, N. Leps, R. Klingeler, and B. Büchner, Phys. Rev. Lett. **101**, 047003 (2008); H. Mukuda, N. Terasaki, H. Kinouchi, M. Yashima, Y. Kitaoka, S. Suzuki, S. Miyasaka, S. Tajima, K. Miyazawa, P. Shirage, H. Kito, H. Eisaki, and A. Iyo, J. Phys. Soc. Jpn. **77**, 093704 (2008); Y. Nakai, K. Ishida, Y. Kamihara, M. Hirano, and H. Hosono, *ibid.* **77**, 073701 (2008).

[5] S. Kawasaki, K. Shimada, G. F. Chen, J. L. Luo, N. L. Wang, and Guo-qing Zheng, Phys. Rev. B **78**, 220506(R) (2008).

[6] T. Y. Chen, Z. Tesanovic, R. H. Liu, X. H. Chen, and C. L. Chien, Nature (London) **453**, 1224 (2008).

[7] H. Ding *et al.*, Europhys. Lett. **83**, 47001 (2008); T. Kondo *et al.*, Phys. Rev. Lett. **101**, 147003 (2008); L. Wray, D. Qian, D. Hsieh, Y. Xia, L. Li, J. G. Checkelsky, A. Pasupathy, K. K. Gomes, C. V. Parker, A. V. Fedorov, G. F. Chen, J. L. Luo, A. Yazdani, N. P. Ong, N. L. Wang, and M. Z. Hasan, Phys. Rev. B **78**, 184508 (2008).

[8] G. Mu, X. Zhu, L. Fang, L. Shan, C. Ren, and H. Wen, Chin. Phys. Lett. **25**, 2221 (2008).

[9] L. Malone, J. D. Fletcher, A. Serafin, A. Carrington, N. D. Zhigadlo, Z. Bukowski, S. Katrych, and J. Karpinski, arXiv:0806.3908 (unpublished); K. Hashimoto, T. Shibauchi, T. Kato, K. Ikada, R. Okazaki, H. Shishido, M. Ishikado, H. Kito, A. Iyo, H. Eisaki, S. Shamoto, and Y. Matsuda, Phys. Rev. Lett. **102**, 017002 (2009); C. Martin, R. T. Gordon, M. A. Tanatar, M. D. Vannette, M. E. Tillman, E. D. Mun, P. C. Canfield, V. G. Kogan, G. D. Samolyuk, J. Schmalian, and R. Prozorov, arXiv:0807.0876 (unpublished).

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

[11] C. de la Cruz, Q. Huang, J. W. Lynn, Jiying Li, W. Ratcliff II, J. L. Zarestky, H. A. Mook, G. F. Chen, J. L. Luo, N. L. Wang, and Pengcheng Dai, Nature (London) **453**, 899 (2008); J. Zhao, Q. Huang, C. de la Cruz, S. Li, J. W. Lynn, Y. Chen, M. A. Green, G. F. Chen, G. Li, Z. Li, J. L. Luo, N. L. Wang, and P. Dai, Nature Mater. **7**, 953 (2008).

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

[13] K. Kuroki, S. Onari, R. Arita, H. Usui, Y. Tanaka, H. Kontani, and H. Aoki, Phys. Rev. Lett. **101**, 087004 (2008); M. M. Korshunov and I. Eremin, Phys. Rev. B **78**, 140509(R) (2008); Fa Wang, Hui Zhai, Ying Ran, Ashvin Vishwanath, and Dung-Hai Lee, Phys. Rev. Lett. **102**, 047005 (2009); V. Cvetkovic and Z. Tesanovic, EPL **85**, 37002 (2009).

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

[15] This T^3 power-law behavior extracted from experimental data of the Fe pnictides SCs might be only an approximate definition unless its origin is due to the gap symmetry as in the d-wave SC. However, our study shows 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 pnictides SCs has a rather firm ground.

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

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

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

[19] P. J. Hirschfeld, P. Wölfle, 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.

[20] D. J. Singh and M.-H. Du, Phys. Rev. Lett. **100**, 237003 (2008); C. Cao, P. J. Hirschfeld, and H.-P. Cheng, Phys. Rev. B **77**, 220506(R) (2008); E. Manousakis, Jun Ren, and E. Kaxiras, *ibid.* **78**, 205112 (2008).

[21] The approximate relation $N_h(0)|\Delta_h| \approx N_e(0)|\Delta_e|$ here is not a rigorous identity. For more detailed discussions, see the appendix section in Ref. 14.

[22] A. A. Abrikosov and L. P. Gorkov, Sov. Phys. JETP **12**, 1243 (1961).