Impurity-induced in-gap state and $T_c$ in sign-reversing s-wave superconductors: analysis of iron oxypnictide superconductors

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Abstract. The sign-reversing fully gapped superconducting state, which is expected to be realized in oxypnictide superconductors, can be prominently affected by nonmagnetic impurities due to the interband scattering of Cooper pairs. We study this problem based on the isotropic two-band BCS model: in oxypnictide superconductors, the interband impurity scattering $I'$ is not equal to the intraband one $I$. In the Born scattering regime, the reduction in $T_c$ is sizeable and the impurity-induced density of states (DOS) is prominent if $I \sim I'$, due to the interband scattering. Although impurity-induced DOS can yield a power-law temperature dependence in $1/T_1$, it is inevitably accompanied by a sizeable suppression of $T_c$. In the unitary scattering regime, in contrast, the effect of impurities is very small for both $T_c$ and DOS except at $I = I'$. On comparing theory and experiments, we surmise that the degree of anisotropy in the $s_{\pm}$-wave gap function strongly depends on the compound.
1. Introduction

Recently, the mechanism of superconductivity in high-$T_c$ superconductors with FeAs layers [1]–[5] has been attracting considerable attention. The superconducting state is realized by introducing a carrier into the parent compound, which shows a spin density wave (SDW) state at $T_N \approx 130$ K [6, 7]. In the SDW state, the ordered magnetic moment is $\sim 0.3 \mu_B$ and the ordering vector is $\mathbf{Q} \approx (\pi, 0)$ [6], [8]–[10]. Nuclear magnetic resonance (NMR) studies have clearly shown that the singlet superconducting state is realized in iron oxypnictides [11]–[13]. A fully gapped superconducting state has been determined by penetration depth measurements [14], angle-resolved photoemission spectroscopy (ARPES) [15]–[18], specific heat measurements [19] and so on.

In the first-principles band calculations [20]–[22], the Fermi surfaces in iron oxypnictides are composed of two hole-like Fermi pockets around the $\Gamma = (0, 0)$ point and two electron-like Fermi pockets around the $M = (\pi, 0)$, $(0, \pi)$ points in the single Fe unit cell. The nesting between the hole and electron pockets is expected to give rise to a SDW state in undoped compounds. In doped compounds without SDW order, the antiferromagnetic (AF) fluctuations with $\mathbf{Q} \approx (\pi, 0)$ are expected to induce a fully gapped s-wave state with sign reversal, which is called the $s_{\pm}$-wave state [23]–[30]. Moreover, near the SDW boundary, the Hall coefficient and the Nernst signal show prominent anomalous behaviors [7, 12, 31], which are similar to those observed in high-$T_c$ cuprates and in CeMIn$_5$ ($M = $ Co, Rh or Ir) [32]. Theoretically, these anomalous transport phenomena indicate the existence of strong AF fluctuations [33]. At the same time, huge residual resistivity far beyond the s-wave unitary scattering is theoretically expected to appear near the SDW boundary [34].

To investigate the pairing symmetry of superconductivity, impurity effects on the superconducting state offer us decisive information. In iron oxypnictide superconductors, the impurity effect on $T_c$ due to Co, Ni, or Zn substitution for Fe sites seems to be very small [11, 12], [35]–[37]. This result clearly rules out the possibility of line-node superconductivity. One may also expect that the s-wave state with sign reversal is also eliminated, since the Cooper pair is destroyed by the interband scattering induced by impurities. However, we have recently shown that $T_c$ is almost unchanged by strong (unitary) impurities, since the interband impurity scattering potential $I'$ is different from the intraband one $I$ [38]. The reason for this unexpected result is that the effective interband scattering is renormalized to zero in the unitary limit except at $I = I'$ in the $T$-matrix approximation. Therefore, the experimental smallness of impurity
effects on $T_c$ in iron oxynitrides is well understood in terms of the $s_{\pm}$-wave state. On the other hand, $T_c$ will be prominently reduced by short-range weak (Born) impurities [38].

Recently, several authors found that an in-gap density of states (DOS) is induced by impurities in the $s_{\pm}$-wave state using the Born approximation for a general value of $x \equiv |I'/I|$ [39], or using the $T$-matrix approximation only for $x = 1$ [40, 41]. They also demonstrated that the relation $1/T_1 \propto T^3$ under $T_c$, which had been reported by several groups [13, 42–44] can be reproduced by the impurity-induced DOS. However, the assumed impurity parameters ($n_{\text{imp}}, I$ and $I'$) also yield a sizeable suppression in $T_c$ according to the analysis in [38]. Furthermore, the impurity-induced DOS should be sensitive to the value of $x$ in the unitary scattering regime, as suggested in [38]. Therefore, we have to study the impurity effects on the DOS and $T_c$ for general $x$, and compare their relationships in detail.

In this paper, we investigate the impurity-induced DOS and $T_c$ in the $s_{\pm}$-wave state using the $T$-matrix approximation for $n_{\text{imp}} \sim 0.01$. We stress that $x$ is not unity in iron oxynitrides since hole and electron pockets are not composed of the same d-orbitals. In the Born or intermediate scattering regime, a sizeable impurity-induced DOS appears for $x \gtrsim 0.7$, and therefore $1/T_1$ may deviate from a simple exponential behavior. Although impurity-induced DOS can yield a power-law temperature dependence in $1/T_1$ [39–41], we find that it is inevitably accompanied by a sizeable suppression of $T_c$. The anisotropy in the $s_{\pm}$-wave superconducting gap, which has been predicted theoretically [23, 25], might be responsible for the power-law temperature dependence of $1/T_1$ under $T_c$ as discussed in [45]. In contrast, unitary impurities affect both the superconducting DOS and $T_c$ only slightly, except at $I = I'$.

2. $T$-matrix approximation in the two-band BCS model

As studied in [29, 38, 39, 41], the $s_{\pm}$-wave state is realized in the two-band BCS model if we introduce the interband repulsive interaction, which represents the AF fluctuations due to the interband nesting in iron oxynitrides. In the present paper, we study the impurity effect using the $T$-matrix approximation for general $I'/I$. In the presence of mass enhancement due to the many-body effect, $m^*/m_0 > 1$, both the superconducting gap and the impurity effect (or impurity concentration $n_{\text{imp}}$) are renormalized by the factor $(m^*/m_0)^{-1}$. In the present analysis, we neglect the mass enhancement for simplicity.

In the Nambu representation, the two-band BCS model is given by [46, 47]

$$\hat{H}^0 = \sum_k \hat{c}^\dagger_k \hat{H}_k^0 \hat{c}_k,$$

where $\hat{c}^\dagger_k = (c_{k\uparrow}^\dagger, c_{k\downarrow}^\dagger, c_{k-1\uparrow}, c_{k-1\downarrow})$ and

$$\hat{H}_k^0 = \begin{pmatrix}
\epsilon_k^\alpha & 0 & \Delta_\alpha & 0 \\
0 & \epsilon_k^\beta & 0 & \Delta_\beta \\
\Delta_\alpha & 0 & -\epsilon_k^\alpha & 0 \\
0 & \Delta_\beta & 0 & -\epsilon_k^\beta
\end{pmatrix}.$$  

In equation (2), $\epsilon_k^\alpha$ and $\epsilon_k^\beta$ are the band dispersions measured from the Fermi level. Since we consider the isotropic $s_{\pm}$ superconducting state, only the DOSs for both bands at the Fermi level ($N_\alpha, N_\beta$) are taken into consideration in the present BCS study. $\Delta_\alpha$ and $\Delta_\beta$ in equation (2)
are the superconducting gaps. When only the interband repulsive interaction \((g_{\alpha\beta} = g_{\beta\alpha} > 0)\) is taken into consideration, the gap equation without impurities is given as [38, 40, 41]

\[
\Delta_{\alpha(\beta)} = -g_{\alpha\beta}N_{\beta(\alpha)}T \sum_n f_{\beta(\alpha)}(\epsilon_n)\theta(\epsilon_n - |\omega_c|),
\]

where \(\epsilon_n = \pi T (2n + 1)\) is the fermion Matsubara frequency and \(\omega_c\) is the cut-off energy. \(N_{\beta(\alpha)}\) is the DOS for the \(\beta(\alpha)\)-band at the Fermi energy in the normal state per spin. \(f_{\beta(\alpha)}(\epsilon)\) is the local anomalous Green function for the \(\beta(\alpha)\) band, which will be given later. Since \(f_{\beta(\alpha)} \propto \Delta_{\beta(\alpha)}\), the \(s_{\pm}\)-state \(\Delta_{\alpha} = -\Delta_{\beta}\) is realized for \(g_{\alpha\beta} > 0\) [38, 40, 41]. Moreover, \(|\Delta_{\alpha}/\Delta_{\beta}| \sim (N_{\beta}/N_{\alpha})^{1/2}\) since \(f_{\alpha}/f_{\beta} \sim \Delta_{\alpha}/\Delta_{\beta}\).

The Nambu matrix representation for the impurity potential is given as

\[
\hat{I} = \begin{pmatrix} I & I' \\ I' & I \end{pmatrix}
\]

\[
\begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}, \quad \begin{pmatrix} 0 & -I \\ -I' & -I \end{pmatrix}
\]

We can assume that \(I, I' \geq 0\) without losing generality. In the presence of impurities, the Green function in the Nambu representation is given by [47]

\[
\hat{G}_k(\tilde{\omega}) = (\hat{\omega} \hat{I} - \hat{H}_k^0 - \hat{\Sigma}(\tilde{\omega}))^{-1},
\]

where \(\tilde{\omega} \equiv \omega + i\delta (\delta = +0)\) and \(\hat{\Sigma}(\tilde{\omega})\) is the self-energy due to impurities.

Hereafter, we derive \(\hat{\Sigma}(\tilde{\omega})\) in the \(T\)-matrix approximation, which gives the exact result for \(n_{\text{imp}} \ll 1\) for any strength of \(I, I'\). The \(T\)-matrix in the Nambu representation is given by

\[
\hat{T}(\tilde{\omega}) = (\hat{I} \cdot \hat{g}(\tilde{\omega}))^{-1} \hat{I},
\]

where \(\hat{g}(\tilde{\omega}) \equiv \frac{1}{N} \sum_k \hat{G}_k(\tilde{\omega})\) is the local Green function, which is given by [47]

\[
\hat{g}(\tilde{\omega}) = \begin{pmatrix} g_{\alpha}(\tilde{\omega}) & 0 & f_{\alpha}(\tilde{\omega}) & 0 \\ 0 & g_{\beta}(\tilde{\omega}) & 0 & f_{\beta}(\tilde{\omega}) \\ f_{\alpha}(\tilde{\omega}) & 0 & g_{\alpha}(\tilde{\omega}) & 0 \\ 0 & f_{\beta}(\tilde{\omega}) & 0 & g_{\beta}(\tilde{\omega}) \end{pmatrix}
\]

In the above expression, \(g_i\) and \(f_i\) \((i = \alpha, \beta)\) are given by

\[
g_i(\tilde{\omega}) = -\pi N_i \frac{\tilde{\omega} Z_i(\tilde{\omega})}{\sqrt{-(\tilde{\omega} Z_i(\tilde{\omega}))^2 + (\Delta_i + \Sigma_i^a(\tilde{\omega}))^2}}.
\]

\[
f_i(\tilde{\omega}) = -\pi N_i \frac{\Delta_i + \Sigma_i^a(\tilde{\omega})}{\sqrt{-(\tilde{\omega} Z_i(\tilde{\omega}))^2 + (\Delta_i + \Sigma_i^a(\tilde{\omega}))^2}},
\]

\[
Z_i(\tilde{\omega}) = 1 - \frac{1}{2\tilde{\omega}} (\Sigma_i^a(\tilde{\omega}) - \Sigma_i^a(-\tilde{\omega})),
\]
where $\Sigma_\alpha^n$ and $\Sigma_\beta^n$ ($i = \alpha$ or $\beta$) are the normal and anomalous self-energies, respectively. In the $T$-matrix approximation, the self-energies are given, by using equation (6), as

$$
\Sigma_\alpha^n(\tilde{\omega}) = n_{\text{imp}} T_{11}(\tilde{\omega}),
\Sigma_\beta^n(\tilde{\omega}) = n_{\text{imp}} T_{22}(\tilde{\omega}),
$$

(11)

$$
\Sigma_\alpha^n(-\tilde{\omega}) = -n_{\text{imp}} T_{33}(\tilde{\omega}),
\Sigma_\beta^n(-\tilde{\omega}) = -n_{\text{imp}} T_{44}(\tilde{\omega}).
$$

(12)

$$
\Sigma_\alpha^n(\tilde{\omega}) = n_{\text{imp}} T_{13}(\tilde{\omega}),
\Sigma_\beta^n(\tilde{\omega}) = n_{\text{imp}} T_{24}(\tilde{\omega}).
$$

(13)

In the fully self-consistent $T$-matrix approximation, we have to solve equations (3) and (7)–(13) self-consistently. In this paper, however, we solve only equations (7)–(13) self-consistently, by neglecting the impurity effect on $\Delta_\alpha$ and $\Delta_\beta$ in equation (3). This approximation is justified when the reduction in $\Delta_\alpha(\beta)$ due to impurity pair-breaking is small.

3. Numerical results

Here, we discuss the impurity effect on the DOS and $T_c$ in the $s$±-wave superconducting state, based on the numerical results given by the $T$-matrix approximation.

3.1. The impurity effect on $T_c$

As derived in [38], the expression for the reduction of $T_c$ per impurity concentration based on the two-band BCS model is given as

$$
-\frac{\Delta T_c}{n_{\text{imp}}} = \frac{\pi^2}{8A} \left[ 3(N_\alpha + N_\beta) - 2\sqrt{N_\alpha N_\beta} \right] I^{\prime 2}
$$

(14)

For $n_{\text{imp}} \ll 1$, the transition temperature is given by $T_c = T_c^0 - (-\Delta T_c/n_{\text{imp}}) \cdot n_{\text{imp}}$, where $T_c^0$ is the transition temperature without impurities. In equation (14), $A = 1 + \pi^2 I^2(N_\alpha^2 + N_\beta^2) + 2N\alpha N_\beta \pi^2 I^2 + N_\beta^2 \pi^4 (I^2 - I^{\prime 2})^2$. In the case of $x = I'/I = 1$, the right-hand side of equation (14) is $[3(N_\alpha + N_\beta) - 2\sqrt{N_\alpha N_\beta}]/[8(N_\alpha + N_\beta)^2] + O(I^{-2})$ in the unitary regime. In the case of $x \neq 1$, in contrast, equation (14) is given by $x^2[3(N_\alpha + N_\beta) - 2\sqrt{N_\alpha N_\beta}]/[8\pi^2 N_\alpha^2 N_\beta^2 (1 - x^2) I^2] + O(I^{-4})$. Therefore, equation (14) approaches zero in the case of $x \neq 1$ in the unitary regime.

Figure 1(a) shows $-\Delta T_c/n_{\text{imp}}$ given in equation (14) in the case of $N_\alpha = N_\beta = 1$. In iron oxynitrides, the total DOS per Fe atom $(N_\alpha + N_\beta)$ is 1.31 eV$^{-1}$ per spin [20]. Then, $1/N = 1$ corresponds to 18 000 K. When $x = 1$, $-\Delta T_c/n_{\text{imp}}$ approaches $1/8 N \sim 2300$ K in the unitary regime ($IN \gg 1$). Therefore, the superconductivity in iron oxynitrides will vanish only at $n_{\text{imp}} \approx 8N \cdot T_c^0 = 0.01 - 0.02 (1 - 2\%)$. When $x \neq 1$, in high contrast, $-\Delta T_c/n_{\text{imp}}$ decreases and approaches zero as $I$ increases in the unitary regime, since the effective interband scattering is renormalized as $I_{\text{eff}} \sim I' \cdot (IN)^{-2} \ll I'$ [38].

According to first-principles calculations, $N_\beta/N_\alpha \geq 0.7$ in iron oxynitrides [48]. Here, we study the case of $N_\beta/N_\alpha = 0.5$ in order to clarify the the impurity effect on $T_c$ for the the particle–hole asymmetric case; $N_\beta/N_\alpha \neq 1$. Figure 1(b) shows $-\Delta T_c/n_{\text{imp}}$ for $N_\alpha = 1$ and $N_\beta = 0.5$. According to equation (14), $-\Delta T_c/n_{\text{imp}}$ for $x = 1$ and $I = \infty$ is $1/5.84 N_\alpha \sim 2400$ K, by taking into account the relation $N_\alpha + N_\beta = 1.31$ eV$^{-1}$ in iron oxynitrides. By comparing
\[ -\Delta T_c/n_{\text{imp}} \] as a function of \( I \) given by the \( T \)-matrix approximation in the case of (a) \( N_\alpha = N_\beta = 1 \) and (b) \( N_\alpha = 1, N_\beta = 0.5 \). In both figures, the unit of energy is \( 1/N_\alpha \), which corresponds to 18 000 K for (a) and 14 000 K for (b), since \( N_\alpha + N_\beta = 1.31 \text{ eV}^{-1} \) in iron oxypnictides. \( -\Delta T_c/n_{\text{imp}} \) for (a) \( N_\alpha = 1, N_\beta = 0.5 \) is \( 1/8N_\alpha \sim 2300 \text{ K} \) for (a) and \( 1/5.84N_\alpha \sim 2400 \text{ K} \) for (b). The superconducting DOSs for parameters denoted by filled diamonds are shown in figures 3 and 5.

Figure 2. Intraband and interband \( T \)-matrices in the normal state, \( T_{\alpha\alpha}^{I=0} \) and \( T_{\alpha\beta}^{I=0} \).

with the results for \( N_\alpha = N_\beta = 1 \) in figure 1(a), we find that \( -\Delta T_c/n_{\text{imp}} \) is insensitive to the value of \( N_\beta/N_\alpha \), under the condition that \( N_\alpha + N_\beta = \text{constant} \).

Previously, the impurity effect on \( T_c \) in the two-band BCS models has been studied by many authors in various contexts \([49]–[54]\)^4, and it was found that \( T_c \) is unchanged in the unitary limit \([50, 51]\). However, equation (14) for the \( s_\pm \)-state has not been derived. Here, we present a clear explanation of why the interband scattering (pair breaking) is absent in the unitary regime, which has not been discussed previously. Figure 2 shows the intraband and interband \( T \)-matrices in the normal state, \( T_{\alpha\alpha}^{I=0} \) and \( T_{\alpha\beta}^{I=0} \), in the case of \( I = 0 \) and \( N_\alpha = N_\beta = N \). Apparently, \( T_{\alpha\beta}^{I=0} \) approaches zero for \( I' \rightarrow \infty \). Next, we consider \( T_{\alpha\beta} \) for general \((I, I')\). If we construct \( T_{\alpha\beta} \) of \((T_{\alpha\alpha}^{I=0}, T_{\alpha\beta}^{I=0}, I)\), it contains at least one \( T_{\alpha\beta}^{I=0} \). For this reason, the interband \( T \)-matrix is expected to approach zero in the unitary regime. This expectation is correct unless \( x = 1 \), as shown in [38].

\[ T_{\alpha\beta} = \frac{I'}{\beta} \alpha \alpha \frac{I'}{\beta} \alpha \beta + \ldots = \frac{I'}{1 + (\pi I'N)^2} \rightarrow 0 \]

\[ T_{\alpha\alpha} = \frac{I'}{\alpha} \beta \alpha \beta \alpha \beta \alpha \beta + \ldots = \frac{i\pi (I')^2 N}{1 + (\pi I'N)^2} \rightarrow \frac{i}{\pi N} \]

The one-band BCS model in [49] corresponds to the present two-band \( s_\pm \) wave model with \( I = I' \) and \( N_\alpha \neq N_\beta \).

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3.2. Impurity effect on the DOS

In the $s_{\pm}$-wave superconducting state, impurity interband scattering not only reduces $T_c$ but also induces the in-gap state in the superconducting DOS [40, 49, 51, 55]. The DOS is given by the imaginary part of the local Green function, which is expressed in equation (8) as follows:

$$N(\omega) = -\frac{1}{\pi} \text{Im}\{g_\alpha(\tilde{\omega}) + g_\beta(\tilde{\omega})\}. \quad (15)$$

If $n_{\text{imp}} \ll 1$, the obtained DOS will be reliable for any $I$ and $I'$ in the present $T$-matrix approximation. The DOS in the superconducting state in the case of $N_\alpha = N_\beta = 1$ and $\Delta_\alpha = -\Delta_\beta = 0.005$ for $n_{\text{imp}} = 0.008$ is shown in figure 3. $|\Delta_{\alpha,\beta}| = 0.005$ corresponds to

![Figure 3](http://www.njp.org/)

**Figure 3.** Obtained DOS in the superconducting state for $N_\alpha = N_\beta = 1$ ($\sim 0.66 \text{eV}^{-1}$) and $\Delta_\alpha = -\Delta_\beta = 0.005$ ($\sim 100 \text{K}$), in the case of (a) $I = 0.25$, (b) $I = 0.5$, (c) $I = 2$ and (d) $I = 8$. Impurity concentration $n_{\text{imp}}$ is 0.008. The insets in (b)–(d) present the DOS for $n_{\text{imp}} = 0.001$. Note that $N(-\omega) = N(\omega)$.
90 K. Experimentally, in Ba$_{0.6}$K$_{0.4}$Fe$_2$As$_2$, $|\Delta| = 11–12$ meV for the $\alpha$ Fermi surface (hole-like) and for $\gamma$ and $\delta$ Fermi surfaces (electron-like), and $|\Delta| = 5.8$ meV for the $\beta$ Fermi surface (hole-like) [18]. As shown in figure 3(a), the superconducting gap is almost filled by the impurity-induced DOS when $I = I' = 0.25$ (the Born regime), which corresponds to $\sim 5000$ K. In this case, the nuclear relaxation ratio $1/T_1$ shows a power-law temperature dependence since the impurity-induced DOS is approximately linear in $\omega$, like in line-node superconductors.

Figure 4 shows $1/T_1$ below $T_c$ for $I = 0.25$, where $\sigma \equiv (\pi N I)^2/(1 + (\pi N I)^2) = 0.38$. We set $|\Delta_{\alpha(\beta)}| = 0.005 \sqrt{T - T_c}$ and $T_c = 0.002$. The method of calculation is explained in [40, 55]. For $x = 1.0$ and $0.9$, $1/T_1$ is inside of $T^2$ and $T^3$ lines for $T_c > T > 0.1 T_c$, consistent with the analysis by Parker et al for $\sigma = 0.4$ [40]. In these cases, however, reduction of $T_c$ due to impurities, which is given by $n_{\text{imp}} \times -\Delta T_c/n_{\text{imp}}$ in figure 1(a), reaches 13 K. The estimated reduction of $T_c$ would be underestimated since $-\Delta T_c/n_{\text{imp}}$ is an increase function of $n_{\text{imp}}$ for $T_c \lesssim T_c^0/2$ [41, 47]. In all the cases we have studied (figure 3(a)–(d)), power-law behavior in $1/T_1$ for $T \ll T_c$ due to the gapless superconducting state is always accompanied by a sizeable suppression of $T_c$, $-\Delta T_c \gtrsim 10$ K, for $|\Delta| = 90$ K. When $|\Delta| = 40$ K, the gapless superconducting state can be realized when $-\Delta T_c \sim 6$ K. Thus, it will be difficult to ascribe the experimental relation $1/T_1 \propto T^3$ below $T_c$ [42]–[44] in clean samples with high $T_c$ to the impurity effect.

In the intermediate ($I = 0.5$) or unitary ($I \geq 2$) regime, in figures 3(b)–(d), a large impurity-induced DOS appears at the zero energy in the case of $x = 1$, which is consistent with previous theoretical studies [40, 55]. In this case, however, $-\Delta T_c \sim 13$ K for $n_{\text{imp}} = 0.008$. If we put $x \leq 0.9$, in contrast, $-\Delta T_c$ in the unitary regime is prominently reduced as shown in figure 1. At the same time, the impurity-induced DOS quickly moves to the gap edge and disappears, as
Figure 5. Obtained DOS in the superconducting state for $N_A = 1, N_B = 0.5$ and $\Delta_\alpha = 0.005, \Delta_\beta = -0.0071$, in the case of (a) $I = 0.25$, (b) $I = 0.5$, (c) $I = 2$ and (d) $I = 8$. Impurity concentration $n_{\text{imp}}$ is 0.008. The insets show that the impurity-induced DOS is always located at a finite energy for $n_{\text{imp}} = 0.001$.

For $N_A = 1$ and $N_B = 0.5$, we put $\Delta_\alpha = 0.005$ and $\Delta_\beta = -0.0071$ by considering the relationship $|\Delta_\alpha/\Delta_\beta| \sim (N_\beta/N_\alpha)^{1/2}$ in the two-band BCS model with repulsive interband interaction, as explained in section 2. Figures 5(a) and (b) show the DOS in the superconducting state for $n_{\text{imp}} = 0.008$. When $I = I' = 0.25$, in figure 5(a), the impurity-induced DOS is reduced by changing $N_B$ from 1 to 0.5, compared with figure 3(a). As $x$ decreases from unity, the impurity-induced DOS moves to the gap edge. In the intermediate ($I = 0.5$) or unitary ($I \geq 2$) regime, the impurity-induced DOS covers the zero energy state in

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the case of \( x = 1 \) and \( n_{\text{imp}} = 0.008 \), as shown in figures 5(b)–(d). However, a finite gap appears around the Fermi level for \( x \lesssim 0.9 \). In the case of \( I = 8 \), in figure 5(d), the impurity-induced DOS is very large at \( x = 1 \), whereas it is strongly suppressed for \( x \lesssim 0.9 \). When the impurity concentration is very low (\( n_{\text{imp}} \sim 0.001 \)), the in-gap state deviates from \( \omega = 0 \) even if \( x = 1 \) as shown in the insets of figures 5(b)–(d), since \( f_\alpha + f_\beta \) given in equation (7) is nonzero in the case of \( N_\alpha \neq N_\beta \) [41].

4. Discussion

In the present paper, we have studied the effect of dilute impurity concentration on the \( s_\pm \)-wave superconducting state, which is expected to be realized in iron oxypnictide superconductors. There, nonmagnetic impurities can induce both the in-gap bound state and the reduction of \( T_c \). Based on the two-band BCS model, we have found that the zero-energy in-gap state emerges under the conditions that (i) \( x \equiv |I'|/I| = 1 \) and (ii) \( |I|N_\alpha, |I|N_\beta \gg 1 \). Deviating from these conditions, the in-gap state shifts to a finite energy, and disappears eventually.

Here, we discuss the case of unitary scattering: in iron oxypnictide superconductors, substitution of Fe by other elements (such as Co, Ni and Zn) will cause a unitary scattering potential. In this case, the impurity potential is diagonal with respect to the d-orbital [38]. The impurity potential has off-diagonal elements in the band-diagonal representation. As discussed in [38], \( x \sim \langle \sum_d O_{d,\alpha}(k)O_{d,\beta}(k') \rangle_{k\in\alpha,k'\in\beta}^{FS} \), where \( O_{d,\alpha}(k) = \langle d; k|\alpha; k \rangle \) represents the transformation matrix between the orbital representation (orbital d) and the band-diagonal representation (band \( \alpha \)). In iron oxypnictide superconductors, \( x \sim 0.5 \) since the hole-pockets are composed of \( d_{xz}, d_{yz} \) orbitals of Fe in the two-Fe unit cell, whereas half of the electron-pockets are composed of \( d_{x^2-y^2} \) orbitals [38]. Since the impurity effect is weak except when \( x = 1 \) in the unitary regime as shown in figures 3(d) and 5(d), substitution of Fe by other elements will affect the superconducting DOS and \( T_c \) only slightly.

We also discuss the case of Born scattering due to ‘in-plane’ weak random potential or disorder: as shown in figures 3(a) and (b), the impurity effect is rather insensitive to \( x \). Therefore, a broad impurity-induced in-gap state will emerge in the superconducting DOS, and a sizeable reduction in \( T_c \) occurs at the same time. Born impurity scattering will also be caused by ‘off-plane’ impurities like the substitution of As by other elements. In this case, the radius of impurity potential \( R \) for Fe sites will be about the unit cell length \( a \). Then, the impurity scattering (\( k \to k' \)) is restricted to \( |k - k'| \lesssim 1/R \sim 1/a \). Since \( |k - k'| \approx \pi/a \) in the interband scattering between electron-pockets and hole-pockets, \( I' \) should be rather smaller than \( I \). Therefore, the effect of off-plane impurities on the \( s_\pm \)-wave state will be small.

In summary, in iron oxypnictide superconductors, the Born or intermediate in-plane impurities cause prominent impurity effects since the \( s_\pm \)-wave state is violated by the interband scattering. Only 1\% Born impurities with \( x \gtrsim 0.5 \) induce not only plenty of in-gap DOS but also sizeable reduction of \( T_c \). For this reason, the relation \( 1/T_1 \propto T^3 \) below \( T_c \) observed in clean LaFeAsO\(_{1-x}\)F\(_x\) [42, 44] and in LaFeAsO\(_{0.7}\) [43] samples, which would be almost free from the impurity reduction in \( T_c \), cannot be explained by the present analysis based on the isotropic BCS model. Thus, anisotropy in the \( s_\pm \)-wave superconducting gap might be responsible for the relation \( 1/T_1 \propto T^3 \) [45]. Recently, rapid suppression of \( 1/T_1 \) (\( \propto T^d; d > 5 \)) below \( T_c \) has been observed in a clean LaFeAsO\(_{0.9}\)F\(_{0.1}\) sample with \( T_c = 28 \) K (= intrinsic \( T_c \)) [57]. This result is consistent with penetration depth measurements [14] and ARPES [15]–[18], and it is naturally explained by the present analysis. Theoretically, in a fully gapped s-wave superconductor, the
gap function becomes anisotropic due to magnetic fluctuations, in such a way that the two superconducting gap minima are connected by the nesting vector $\mathbf{Q}$. In iron oxypnictides, the degree of anisotropy in the $s_{\pm}$-wave gap function is rather sensitive to model parameters such as the nesting condition $|\mathbf{Q}|$. The wide variety of behaviors in $1/T_1$ would reflect the large sample dependence of the gap anisotropy in iron oxypnictide superconductors.

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