Effect of Impurities with Internal Structure on Multiband Superconductors
– Possible Enhancement of Transition Temperature –

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We study inelastic (dynamical) impurity scattering effects in two-band superconductors with the same \( (s_\pm, \text{wave}) \) or different \( (s_\pm, \text{wave}) \) sign order parameters. We focus on the enhancement of the superconducting transition temperature \( T_c \) by magnetic interband scattering with the interchange of crystal-field singlet ground and multiplet excited states. Either the \( s_\pm, \text{wave} \) or \( s_\pm, \text{wave} \) state is favored by the impurity-mediated pairing, which depends on the magnetic and nonmagnetic scattering strengths derived from the hybridization of the impurity states with the conduction bands. The details are examined for the singlet-triplet configuration that is suggestive of Pr impurities in the skutterudite superconductor \( \text{LaOs}_4\text{Sb}_12 \).

KEYWORDS: multiband superconductivity, \( s_\pm, \text{wave} \) superconductivity, \( s_\pm, \text{wave} \) superconductivity, heavy fermion, skutterudite, impurity, crystal field

1. Introduction

The study of impurity effects on multiband superconductivity is stimulated by the discovery of high-temperature (high \( T_c \)) superconductors with FeAs layers,¹–⁸ while it has been performed for another high-\( T_c \) superconductor, \( \text{MgB}_2 \).⁹–¹¹ One of the interesting points for the impurity problem is their anisotropic band property. In particular, much attention is paid to the \( s_\pm \)-wave pairing state characterized by sign reversal of order parameters with full gaps.¹²–¹⁶ For a depairing effect caused by impurity scattering, the \( s_\pm \)-wave state behaves like \( d \)-wave pairing rather than the conventional \( s \)-wave state.¹⁷ Multiband properties are also reported in the heavy-fermion superconductor \( \text{PrOs}_4\text{Sb}_12 \) whose higher \( T_c \) than \( \text{LaOs}_4\text{Sb}_12 \) implies a crucial role of the \( \text{Pr} f \)-electron states.¹⁸,¹⁹ Interband scattering due to impurities may be important in the multiband, the roles of which remain to be elucidated.

Recently, Senga and Kontani have studied the effects of intraband and interband nonmagnetic impurity scatterings in the \( s_\pm \)-wave state using a simple two-band BCS model.²⁰,²¹ They found that \( T_c \) is not markedly suppressed when the intraband and interband scattering strengths are not equal and are sufficiently strong. We also applied a similar model in a magnetic impurity case and solved a single-impurity problem.²² For the interband scattering in the \( s_\pm \)-wave state, the roles of magnetic impurities are equivalent to those of nonmagnetic impurities for the intraband scattering.²³ Very recently, it has been reported that \( T_c \) is not markedly suppressed so much by the interband magnetic scattering.²³ These results imply a possibility of \( T_c \) enhancement due to magnetic impurities having an internal structure. Such enhancement was argued by Fulde et al. for nonmagnetic impurities in single-band superconductors.²⁴ An attractive interaction stems from inelastic nonmagnetic scattering by impurities, which is analogous to the electron-phonon origin of BCS superconductors. \( T_c \) can be enhanced by doping such impurities with appropriate crystal-field level splitting, while it is suppressed by magnetic impurities.²⁴ This idea has recently been applied to a skutterudite superconductor \( \text{La}_{1-x}\text{Pr}_x\text{Os}_4\text{Sb}_12 \) to account for the \( T_c \) enhancement by \( \text{Pr} \) substitution for \( \text{La} \) in \( \text{LaOs}_4\text{Sb}_12 \).²⁵ Since only a single band is considered there, one always finds that magnetic impurities cause \( T_c \) suppression. However, this conventional understanding has to be reexamined for multiband superconductors. In the case of \( s_\pm \)-wave superconductivity, magnetic impurities for intraband scattering behave like nonmagnetic impurities for interband scattering, and vice versa. Accordingly, we can expect \( T_c \) to be enhanced by the inelastic (dynamical) magnetic scattering.

In this paper, we extend the theory of Fulde et al.²⁴ and show a case of magnetic impurities in the \( s_\pm \)-wave state in §2. Considering spin-dependent interband scattering, we examine a self-energy in the Born approximation to derive a gap equation for two bands. The increase in \( T_c \) is associated with the sign change of the superconducting order parameter via the inelastic impurity scattering. It is demonstrated for the \( s_\pm \)-wave state whose \( T_c \) is enhanced by the magnetic interband scattering due to the singlet-singlet configuration. In §3, we also show some typical examples of the corresponding interband scattering. There are various octupolar (combination of spin and orbital) scattering types that increase \( T_c \) accompanied by an interchange between two crystal-field singlet states. The same argument is applied to the singlet-multiplet configuration that can be realized for such \( f \)-electron impurities as rare-earth or actinide ions embedded in cubic or uniaxial anisotropic (tetragonal or hexagonal) crystals. For the singlet-doublet, we discuss the \( s_\pm \)-wave and \( s_{++} \)-wave combination via intraband scattering. The \( s_{++} \)-wave pairing is characterized by the same sign order parameters of the two bands. We show a possible crystal-field splitting for \( T_c \) enhancement, however, \( T_c \) is suppressed by the competition between mag-
netic and nonmagnetic scattering effects. For the singlet-triplet, we find a case in which the $s_{+}$ wave is favorable for the $T_c$ enhancement by magnetic interband scattering.

In this section, we present a formulation for $T_c$ enhancement by inelastic impurity scattering in multiband superconductors. First, we briefly review a work by Fulde et al. for single-band superconductors. Then, we extend it to a two-band system as a simple case of multiband and give an example to understand multiband effects on $T_c$.

2. Formulation for $T_c$ Enhancement

2.1 Inelastic impurity scattering and $T_c$ enhancement in single-band superconductors

Let us begin with the model Hamiltonian $H = H_C + H_I + H'$ that consists of conduction electron $H_C$, impurity $H_I$, and impurity scattering $H'$ terms. The first term is written as

$$H_C = \sum_{\sigma} \int d\mathbf{r} \psi_{\sigma}^\dagger(\mathbf{r}) \epsilon(-i\nabla)\psi_{\sigma}(\mathbf{r}) - \Delta \int d\mathbf{r} \left[ \psi_{\uparrow}^\dagger(\mathbf{r}) \psi_{\downarrow}^\dagger(\mathbf{r}) + \psi_{\downarrow}(\mathbf{r}) \psi_{\uparrow}(\mathbf{r}) \right].$$

(1)

Here, $\psi_{\sigma}(\mathbf{r})$ is a field operator of the conduction electron of the $\sigma(\uparrow, \downarrow)$ spin whose kinetic energy is expressed by the operator $\epsilon(-i\nabla) = -\nabla^2/2m_e - E_F$ measured from the Fermi energy $E_F$, where $m_e$ represents the electron mass and the Planck constant $\hbar$ is taken as unity. $\Delta$ is the $s$-wave superconducting order parameter that we assume to be a real value. The Hamiltonian $H_I$ for the impurity states is given by

$$H_I = \sum_{\mathbf{R}_i} \sum_{m} \delta_m a_{\gamma m}^\dagger a_{\gamma m},$$

(2)

Here, $\mathbf{R}_i$ represents the position of the $\gamma$th impurity. $a_{\gamma m}^\dagger$ and $a_{\gamma m}$ are the pseudo-fermion creation and annihilation operators, respectively, for the $m$th impurity energy level $\delta_m$ at the $\gamma$th impurity site. The interaction Hamiltonian at the impurities is defined by

$$H' = \sum_{\mathbf{R}_i} \sum_{m n} \sum_{\sigma} \int d\mathbf{r} a_{\gamma m}^\dagger a_{\gamma n} \delta(\mathbf{r} - \mathbf{R}_i) M_{m n} \psi_{\sigma}^\dagger(\mathbf{r}) \psi_{\sigma}(\mathbf{r}).$$

(3)

We consider here only nonmagnetic impurity scattering since magnetic impurity scattering cannot enhance $T_c$ in a single-band case. $M_{m n}$ is a matrix element that describes the scattering of conduction electrons accompanied by an interchange among the $m$th and $n$th energy levels.

We introduce the following $4 \times 4$ matrix form of the thermal Green’s function:

$$\hat{G}(\tau, \mathbf{r}, \mathbf{r}') = -(\tau \hat{\Psi}(\mathbf{r}, \tau) \Psi^\dagger(\mathbf{r}', 0)),$$

(4)

where $\Psi(\mathbf{r})$ and $\Psi^\dagger(\mathbf{r})$ are four-dimensional vectors defined as

$$\Psi(\mathbf{r}) = \begin{pmatrix} \psi_{\uparrow}(\mathbf{r}) \\ \psi_{\downarrow}(\mathbf{r}) \\ \psi_{\uparrow}(\mathbf{r}) \\ \psi_{\downarrow}(\mathbf{r}) \end{pmatrix},$$

(5)

with their Heisenberg representations

$$\Psi(\mathbf{r}, \tau) = e^{iH\tau} \Psi(\mathbf{r}) e^{-iH\tau}, \quad \Psi^\dagger(\mathbf{r}, \tau) = e^{iH\tau} \Psi^\dagger(\mathbf{r}) e^{-iH\tau}.$$

(6)

In the absence of impurity scattering, the unperturbed Green’s function is Fourier-transformed to

$$\hat{G}_0(\mathbf{w}_l, \mathbf{k}) = -\frac{\omega_l + \epsilon_k \rho_\alpha + \Delta \delta_\alpha \delta_\gamma}{\omega_l^2 + \epsilon_k^2 + \Delta^2},$$

(7)

where $\delta_\alpha$ and $\rho_\alpha$ ($\alpha$ is denoted by 1, 2, and 3 instead of $x$, $y$, and $z$, respectively, hereafter) are the Pauli matrices for the spin space and particle-hole space, respectively. Similarly, the matrix for impurity scattering is given by

$$\hat{\Psi}_m = M_{m n} \rho_\alpha.$$

(8)

Following Fulde et al., we study the $T_c$ enhancement on the basis of the second Born approximation. For the scattering matrix $\hat{U}_{m n}$ in eq. (8), Fig. 1 shows the self-energy given by

$$\Sigma(\mathbf{w}_l) = -n_{\text{imp}} T^2 \sum_{m n} \sum_{\mathbf{w}_1} \frac{1}{\omega_1 - \delta_m} \frac{1}{\omega_2 - \delta_n} \times \frac{1}{\Omega} \sum_k \hat{U}_{m n} \hat{G}_0(\mathbf{w}_l + \mathbf{w}_1 - \mathbf{w}_2, \mathbf{k}) \hat{U}_{n m}.$$

(9)

Here, $n_{\text{imp}}$ represents the impurity density. $1/(\mathbf{w}_1 - \delta_m)$ is an unperturbed Green’s function for the $m$th impurity energy level. $\omega_1$ and $\omega_2$ are Matsubara frequencies for fermions. $\Omega$ represents the system volume. The Boltzmann constant $k_B$ is taken as unity. The important point is that $\Delta$ in eq. (7) changes its sign with the $\hat{\Sigma}(\mathbf{w}_l)$.

In the presence of the impurities, the linearized gap equation is given by

$$\Delta \log \frac{T_c}{T(0)} = \pi T_c \sum_{\mathbf{w}_l} \frac{\Delta}{\mathbf{w}_l} \left[ \Sigma_{\Delta}(\mathbf{w}_l) - \Sigma_{\omega}(i\mathbf{w}_l) \right],$$

(10)

where $T_c$ ($T(0)$) is the transition temperature in the presence (absence) of impurities. $\Sigma_{\Delta}$ and $\Sigma_{\omega}$ are self-energies corresponding to the order parameter and Matsubara frequency components, respectively. In Green’s function, the renormalized frequency $\tilde{\omega}_l$ and the order parameter
Here, $\omega_i$ is given by
\[
\omega_i = \omega_l + i \Sigma_\omega (i \omega_l), \quad \Delta_l = \Delta [1 + \Sigma_\omega (i \omega_l)]. \tag{11}
\]
The self-energy in Fig. 1 leads to different signs of $\Sigma_\Delta$ in eq. (10) between time-reversal invariant scattering and non-time-reversal invariant scattering. The former (nonmagnetic scattering in a single band) contributes to $T_c$ enhancement. In a simple case of two energy levels ($\delta_2 > \delta_1$), after the lengthy calculation of the self-energy, we obtain each term on the right-hand side of eq. (10) as
\[
\pi T_c \sum_l \frac{1}{|\omega_l|} \Sigma_\Delta (i \omega_l) = -\frac{\pi}{8T_c \tau_{12}} f_\Delta (x),
\]
\[
f_\Delta (x) = -\frac{\tanh x}{x} + A(x) - \frac{1}{2} B(x), \tag{12}
\]
\[
\pi T_c \sum_l \frac{1}{|\omega_l|} \frac{\Sigma_\omega (i \omega_l)}{\omega_l} = -\frac{\pi}{8T_c \tau_{12}} f_\omega (x),
\]
\[
f_\omega (x) = 1 + \frac{\tanh^2 x}{x} - \frac{1}{2} B(x), \tag{13}
\]
with
\[
x = \frac{\delta_2 - \delta_1}{2T_c} > 0, \quad A(x) = S_1 (x) \tanh x, \quad B(x) = S_2 (x) \tanh x.
\]
\[
S_1 (x) = \frac{4x}{\pi^4} \text{Re} \sum_{n=0}^\infty \psi \left( 1 + n + \frac{x}{2\pi} \right) - \psi \left( 1 + \frac{x}{2\pi} \right),
\]
\[
S_2 (x) = \frac{8}{\pi^3} \text{Im} \sum_{n=0}^\infty \psi \left( 1 + n - \frac{x}{2\pi} \right) - \psi \left( 1 + \frac{x}{2\pi} \right).
\]
Here, $\tau_{12}$ represents the lifetime due to the impurity scattering. $N_0$ is the density of states at the Fermi energy. $\psi (x)$ is the digamma function. As a consequence, eq. (10) leads to a gap equation for the nonmagnetic scattering ($\tau_{12}$ is denoted by $\tau^0_{12}$),
\[
\frac{8T_c}{\pi} \tau^0_{12} \log \frac{T_c}{T_{c0}} = -f_\Delta (x) + f_\omega (x) \equiv f_0 (x) > 0, \tag{14}
\]
and to that for the magnetic scattering ($\tau_{12}$ is denoted by $\tau^0_{12}$),
\[
\frac{8T_c}{\pi} \tau^0_{12} \log \frac{T_c}{T_{c0}} = f_\Delta (x) + f_\omega (x) \equiv f_0 (x) < 0. \tag{15}
\]
These equations show that for any finite crystal-field splitting, $T_c$ is enhanced by nonmagnetic impurities in single-band s-wave superconductors, while it is suppressed by magnetic impurities.\(^{24}\) For the nonmagnetic scattering in eq. (14), we note that $T_c$ keeps $T_{c0}$ for $x = 0$ (elastic scattering) that gives $f_0 (0) = 0 [f_\Delta (0) = f_\omega (0) = -1]$, while $|f_\Delta (x)| > |f_\omega (x)| [f_\Delta (x) < 0, f_\omega (x) < 0]$ for $x > 0$ leads to $T_c > T_{c0}$. Once the two levels are split, the exchange scattering process gives rise to an attractive interaction for pairing, by analogy with the optical phonon effects in superconductivity.\(^{24}\)

We would like to mention a linear combination of eqs. (14) and (15), $[f_0 (x)/\tau^0_{12} + f_\omega (x)/\tau^0_{12}]$, which is derived from the singlet-multiplet configuration since both magnetic and nonmagnetic scatterings coexist. In this case, the weight of $f_\Delta (x)$ becomes smaller in the combined equation, so that $x$ has to be sufficiently large to satisfy the condition $|f_\Delta (x)| > |f_\omega (x)|$ for $T_c$ enhancement. The details will be examined for the singlet-doublet configuration in §3.2.

2.2 Extension to multiband superconductors

2.2.1 Bulk property

Before extending the above single-band case to a two-band one, we briefly review the earlier works by Shul et al.\(^{27}\) and Kondo\(^{28}\) for multiband superconductivity. The unique property of the multiband is described by the following model Hamiltonian:
\[
\mathcal{H}_{\text{bulk}} = \sum_{\mu = \pm} \sum_{\sigma = \uparrow, \downarrow} \sum_k \epsilon_{k\mu\sigma} c^\dagger_{k\mu\sigma} c_{k\mu\sigma} + \sum_{\mu, \mu' = \pm} \sum_{kk'} V_{\mu\mu'} c_{k\mu}^\dagger c_{-k\mu'} c_{-k'\mu'} c_{k'\mu'} \tag{16}
\]
Here, the first term represents the kinetic energy for the $\mu = \pm$ conduction band and $c^\dagger_{k\mu\sigma}$ ($c_{k\mu\sigma}$) is the creation (annihilation) operator. The second term represents the interaction between electrons with coupling constants $V_{\mu\mu'}$: $\mu = \mu'$ for the intraband and $\mu \neq \mu'$ for the interband. $T_c$ is determined by the following form of the linearized gap equation:
\[
\begin{pmatrix}
-V_{++} N_0 + & -V_{+-} N_0 + & 0 \\
-V_{-+} N_0 + & -V_{--} N_0 + & 0 \\
0 & 0 & \frac{1}{\log \left[2e^\gamma \omega_c / (\pi T_c) \right]} \begin{pmatrix}
\Delta_+ \\
\Delta_-
\end{pmatrix}
\end{pmatrix} \begin{pmatrix}
\Delta_+ \\
\Delta_-
\end{pmatrix} = 0. \tag{17}
\]
Here, $\Delta_\pm$ and $N_{0\pm}$ are the order parameters and density of states at the Fermi energy for the $\mu = \pm$ band, respectively. $\gamma (\simeq 0.577)$ is Euler’s constant and we have assumed the same cut-off energy $\omega_c (\gg T_c)$ for the two bands. $T_c$ corresponds to a positive eigenvalue of the $2 \times 2$ matrix on the left-hand side of eq. (17). The multiband superconductivity is characterized by whether the interband interaction is attractive or repulsive. To see this point clearly, let us consider a simple case of two identical bands, where $V_{++} = V_{--} < 0$, $V_{+-} = V_{-+}$, and
$N_{0+} = N_{0-} = N_0$. The solution of eq. (17) is obtained as

$$T_{cA} = \frac{2\gamma \omega_c}{\pi} \exp \left[ -\frac{1}{(|V_{+}| - |V_{-}|)N_0} \right],$$

$$T_{cB} = \frac{2\gamma \omega_c}{\pi} \exp \left[ -\frac{1}{(|V_{+}| + |V_{-}|)N_0} \right].$$

(18)

Here, $T_{cA}$ and $T_{cB}$ are the transition temperatures for

$$\Delta_A = \frac{\Delta_+ + \Delta_-}{2}, \quad \Delta_B = \frac{\Delta_+ - \Delta_-}{2},$$

(19)

respectively. When $V_{+-} < 0$, $T_{cA} > T_{cB}$ ($T_{cB} = 0$ if $|V_{+-}| > |V_{++}|$). This means that the higher $T_c$ is due to the attractive interband interaction for the order parameters with the same sign ($\Delta_+ \Delta_- > 0$). Conversely, when $V_{+-} > 0$, the higher $T_c$ is obtained for their opposite signs ($\Delta_+ \Delta_- < 0$). The former and latter are called the $s_{++}$-wave and $s_{\pm}$-wave states, respectively.

### 2.2.2 Impurity effect

Although electron-phonon and Coulomb interactions were taken into account as possible origins of the interband interaction before, we here propose inelastic (dynamical) impurity scattering as another origin that can give rise to $T_c$ enhancement in multiband superconductors even if it is due to magnetic impurities. For this purpose, we extend the work by Fulde et al. to a two-band case.

Then, we reexamine the gap equation in eq. (10) for a two-band $s$-wave superconducting state with order parameters, $\Delta_\mu$ for the $\mu$ band. In the absence of impurities, the superconducting transition temperatures are expressed as $T_{c\mu}$ for the $\mu = \pm$ bands, respectively. Here, the interband interaction is not taken into account for simplicity ($V_{+-} = 0$). Considering both magnetic and nonmagnetic scattering processes, we obtain the following linearized gap equation in the two-band case:

$$8T_c \log \left( \frac{T_{cA}}{T_{cB}} \right) \left( \frac{\Delta_+ \log \frac{T_{cA}}{T_{cB}}}{\Delta_- \log \frac{T_{cA}}{T_{cB}}} \right) = \sum_{\chi = 0, \pm} \frac{1}{\gamma} \left| \frac{T_{cA}}{T_{cB}} \right|^2 \left( f_{\Delta}(x)\hat{\lambda}_B^X + f_{\omega}(x)\hat{\lambda}_A^X \right) \left( \begin{array}{c} \Delta_+ \\ \Delta_- \end{array} \right),$$

(20)

where $T_c$ is the transition temperature in the presence of impurities. The energy difference $x$ between the impurity singlet ground and multiplet excited states is scaled by $2T_c$ [see eq. (13)]. The matrices $\hat{\lambda}_A^X$ and $\hat{\lambda}_B^X$ express the impurity intraband and interband scattering contributions to the self-energies, $\Sigma_{\Delta}(i\omega)$ and $\Sigma_{\omega}(i\omega)$, respectively:

$$\hat{\lambda}^X = \left( \begin{array}{cc} \hat{\lambda}^{X+}_{\Delta+} & \hat{\lambda}^{X+}_{\Delta-} \\ \hat{\lambda}^{X-}_{\Delta+} & \hat{\lambda}^{X-}_{\Delta-} \end{array} \right) (\xi = \Delta, \omega).$$

(21)

In the following study, it is convenient to use the order parameters given in eq. (19), where $\Delta_A$ and $\Delta_B$ are order parameters for the $s_{++}$-wave and $s_{\pm}$-wave states, respectively. By the unitary transformation

$$\hat{\Lambda}^X = U^{-1}\hat{\lambda}^X U, \quad U = \frac{1}{\sqrt{2}} \left( \begin{array}{cc} 1 & 1 \\ 1 & -1 \end{array} \right),$$

(22)

the linearized gap equation is rewritten as

$$\left[ \frac{1}{2} \log \left( \frac{T_{cA}}{T_{cB}} \right) \left( \begin{array}{cc} 0 & 1 \\ 1 & 0 \end{array} \right) + \hat{\Lambda}(x) \right] \left( \begin{array}{c} \Delta_A \\ \Delta_B \end{array} \right) = \frac{8T_c}{\pi} \log \left( \frac{T_c}{\sqrt{T_{cA}T_{cB}}} \right) \left( \begin{array}{c} \Delta_A \\ \Delta_B \end{array} \right).$$

(23)

$$\hat{\Lambda}(x) = \sum_{\chi = 0, \pm} \frac{1}{\gamma} \left| \frac{T_{cA}}{T_{cB}} \right|^2 \sum_{\xi = \pm} f_{\xi}(x)\hat{\lambda}_A^X \hat{\lambda}_B^X.$$

We can see that $T_c$, which is the superconducting transition temperature in the presence of impurities, plays a role as an eigenvalue of the matrix on the left-hand side in eq. (23). The largest eigenvalue corresponds to the highest $T_c$. When $T_{cA} = T_{cB}$ for simplicity, only $\hat{\Lambda}(x)$ is left on the left-hand side, and a positive eigenvalue of $\hat{\Lambda}$ leads to $T_c$ enhancement.

Next, we consider a case of two identical bands with interband interaction ($V_{+-} \neq 0$). In this case, the $T_c$ values are different for the $s_{++}$-wave and $s_{\pm}$-wave states, as given by eq. (18). In the absence of impurities, we introduce transition temperatures $T_{cA}$ and $T_{cB}$ for the $s_{++}$ and $s_{\pm}$-wave states, respectively. For $T_c$ in the presence of impurities, the gap equation is expressed as

$$\left[ \frac{1}{2} \log \left( \frac{T_{cA}}{T_{cB}} \right) \left( \begin{array}{cc} 0 & 1 \\ 1 & 0 \end{array} \right) + \hat{\Lambda}(x) \right] \left( \begin{array}{c} \Delta_A \\ \Delta_B \end{array} \right) = \frac{8T_c}{\pi} \log \left( \frac{T_c}{\sqrt{T_{cA}T_{cB}}} \right) \left( \begin{array}{c} \Delta_A \\ \Delta_B \end{array} \right).$$

(24)

Here, the contribution of the impurities is expressed by $\hat{\Lambda}(x)$ and it modifies the transition temperatures in the bulk.

In the following part of this paper, we consider only two identical bands without the interband scattering ($V_{+-} = 0$) to capture the essence of the $T_c$ enhancement caused by the inelastic scattering impurities, where $T_{cA} = T_{cB} = T_c$. We note that it is easy to extend the formulation to $T_{cA} \neq T_{cB}$ cases.

### 2.3 Example of magnetic interband scattering for $T_c$ enhancement in $s_{\pm}$-wave state

As mentioned above, $T_c$ is enhanced by inelastic nonmagnetic impurity scattering in single-band $s$-wave superconductors. In this subsection, we show that magnetic interband scattering can also cause $T_c$ enhancement in multiband cases. For this purpose, we focus on the roles of spin-dependent scattering in the $s_{\pm}$-wave state, which is suggested as one of possible superconducting states realized in Fe pnictide superconductors. As we will see, the interband scattering is important for $T_c$ enhancement, which is unique to the multiband and is never seen in the single-band case. In fact, neither intraband nor elastic impurity scattering can be neglected in real systems. These effects cause $T_c$ suppression. Whether $T_c$ is enhanced or not depends on how to balance the pairing and depairing effects caused by impurities.
Here, we extend the formulation given in §2.1 straightforwardly. The conduction electron part for the $\mu$ band is given by

$$\mathcal{H}_\mu = \sum_\sigma \int \mathrm{d} r \psi_{\mu\sigma}^\dagger (r) e(-i\nabla) \psi_{\mu\sigma}(r)$$

$$- \Delta_\mu \int \mathrm{d} r \left[ \psi_{\mu\uparrow}^\dagger (r) \psi_{\mu\downarrow}^\dagger (r) + \psi_{\mu\downarrow}^\dagger (r) \psi_{\mu\uparrow}^\dagger (r) \right]$$

$$+ \sum_\alpha \Delta_\mu \int \mathrm{d} r \left[ \hat{T}_\alpha \psi_{\mu\sigma}^\dagger (r) \psi_{\mu\sigma}(r) \right]$$

$$\left( \mu = +, - \right). \quad (25)$$

Here, $\psi_{\mu\sigma}(r)$ is a field operator of the conduction electron for the $\mu$ band. $\Delta_\mu$ is the $\mu$ band superconducting order parameter for the $s_\pm$-wave superconductivity, where $\Delta_\mu$ takes a real value. For spin-dependent intraband and interband scatterings at the impurities, the interaction Hamiltonian is defined by

$$\mathcal{H}' = \sum_{R_\gamma} \sum_{\mu\nu} \sum_{\rho\sigma} \sum_{\alpha} \int \mathrm{d} r a_{\mu\nu}^\dagger(r) a_{\rho\sigma}(r)$$

$$\times M_{\mu\nu\rho\sigma} \hat{\sigma}_\alpha \psi_{\mu\nu}(r) \psi_{\rho\sigma}(r),$$

where $\hat{\sigma}$ is the Pauli matrix with the three components $\hat{\sigma}_\alpha$ ($\alpha = 1, 2, 3$). As the corresponding spin exchange, $M_{\mu\nu\rho\sigma}$ is the scattering matrix element that depends on the band components as well.

We introduce the following $4 \times 4$ matrix form of the thermal Green’s function for the $\mu$ band:

$$\hat{G}_\mu(\tau, r, r') = -(T \Psi_\mu(\tau, r) \Psi_\mu^\dagger(r', 0)), \quad (27)$$

where $\Psi_\mu(\tau, r)$ and $\Psi_\mu^\dagger(\tau, r)$ are defined for each band as

$$\Psi_\mu(\tau, r) = \begin{pmatrix} \psi_{\mu\uparrow}(r) \\ \psi_{\mu\downarrow}(r) \\ \psi_{\mu\uparrow}(r) \\ \psi_{\mu\downarrow}(r) \end{pmatrix},$$

$$\Psi_\mu^\dagger(\tau, r) = \begin{pmatrix} \psi_{\mu\uparrow}^\dagger(r) & \psi_{\mu\downarrow}^\dagger(r) & \psi_{\mu\uparrow}^\dagger(r) & \psi_{\mu\downarrow}^\dagger(r) \end{pmatrix}. \quad (28)$$

Their Heisenberg representations $\Psi_\mu(\tau, r)$ and $\Psi_\mu^\dagger(\tau, r)$ are given in the same manner as eq. (6). After introducing the unperturbed Green's function

$$\hat{G}_\mu(\omega, k) = -\frac{i\omega + \epsilon_k \hat{\rho}_3 + \Delta_\mu \hat{\rho}_2 \hat{\sigma}_2}{\omega^2 + \epsilon_k^2 + \Delta_\mu^2}, \quad (29)$$

as in eq. (7), and combining the two-band forms, we use the following $8 \times 8$ matrix form of Green’s function:

$$\hat{G}_0(\omega, k) = \begin{pmatrix} \hat{G}_+(\omega, k) & 0 \\ 0 & \hat{G}_-(\omega, k) \end{pmatrix}. \quad (30)$$

In particular, for the $s_\pm$-wave state ($\Delta_+ = -\Delta_- = \Delta$), it is rewritten as

$$\hat{G}_0(\omega, k) = -\frac{i\omega + \epsilon_k \hat{\rho}_3 + \Delta \hat{\rho}_2 \hat{\sigma}_2}{\omega^2 + \epsilon_k^2 + \Delta^2}, \quad (31)$$

where $\hat{\sigma}_\alpha$ ($\alpha = 1, 2, 3$) is the Pauli matrix for the band space. Similarly, the matrix for impurity scattering is given by, for instance,

$$\hat{U} = \sum_{mn} \sum_{\alpha=x, y, z} \hat{U}_{mn}^\alpha,$$

$$\hat{U}_{mn}^x = M_{mn}^x \hat{\tau}_1 \hat{\rho}_3 \hat{\sigma}_1, \quad \hat{U}_{mn}^y = M_{mn}^y \hat{\tau}_1 \hat{\sigma}_2.$$
priate for $T_c$ enhancement by the interband scattering in the $s_\pm$-wave state. On the other hand, it must be pointed out that $T_c$ suppression is caused by elastic scattering due to the impurity singlet ground state or by intraband scattering [for instance, $\tilde{\tau}_1$ is replaced by unity in eq. (32)], which have been neglected here. The most important point is the internal structure of impurities that intensifies the interband magnetic scattering to overcome these pair-breaking effects.

3. Typical Impurity Interband Scattering for $T_c$ Enhancement

In $\S$ 2.3, we have discussed $T_c$ enhancement due to the spin-dependent interband scattering in $s_\pm$-wave states as one of the examples, where the details of such impurity scattering have been put aside. In this section, we study typical impurity scattering for a singlet-multiplet configuration that can give rise to $T_c$ enhancement in multiband superconductors. First, we show possible examples for the singlet-singlet and next apply the same argument to the singlet-multiplet case. In $\S$ 3.2, we take account of not only the interband impurity scattering effect but also the intraband impurity scattering effect neglected in the previous section.

3.1 Singlet-singlet configuration

In addition to the $\tilde{\tau}_1$ type in eq. (32) for the interband scattering, there is another type of magnetic scattering, $M_{mn} \hat{\sigma}_2$, due to an orbital moment (spin-independent scattering). Since it satisfies

$$\tilde{\tau}_2 (\hat{\tau}_3 \hat{\rho}_2 \hat{\sigma}_2) \tilde{\tau}_2 = -(\hat{\tau}_3 \hat{\rho}_2 \hat{\sigma}_2),$$

$T_c$ can be enhanced by the impurity scattering for the $s_\pm$ wave. Here, we consider realistic cases for $\tilde{U}_{mn}^z = M_{mn}^z \hat{\tau}_1 \hat{\rho}_3 \hat{\sigma}_3$ and $\hat{U}_{mn} = M_{mn} \hat{\tau}_2$. In practice, we check the possible symmetry of $M_{12}$ for the singlet-singlet configuration corresponding to each electron scattering type, assuming local orbital symmetries of band electrons at the impurity site. Although actual bands can include several orbital components, we represent each band by an orbital component that mainly contributes to the band construction.

First, let us begin with the spin-dependent case, $\tilde{U}_{mn}^z = M_{mn}^z \hat{\tau}_1 \hat{\rho}_3 \hat{\sigma}_3$. Within the subspace, $\psi_b = (\psi_{+\uparrow}, \psi_{+\downarrow}, \psi_{-\uparrow}, \psi_{-\downarrow})^t$, where $t$ denotes transposition, $\tilde{U}_{mn}^z$ is given as

$$\tilde{U}_{mn}^z = M_{mn}^z \hat{\tau}_1 \hat{\sigma}_3 = M_{mn}^z \left( \begin{array}{cccc} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{array} \right).$$

To identify the symmetry of electron scattering that depends on orbital components, we here assume the $yz$ and $xz$ orbital types for the $\mu = +$ and $\mu = -$ bands, respectively. The wave functions $\psi_{yz,\sigma}$ and $\psi_{xz,\sigma}$ at an impurity are connected to $j = 3/2$ angular momentum bases $\psi_{jz}$ (specifically, the $O_h T_g$ point-group bases) by the following unitary transformation as

$$\tilde{U}_{mn}^z \rightarrow M_{mn}^z \left( \begin{array}{cccc} 0 & 0 & i & 0 \\ 0 & 0 & 0 & 0 \\ -i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{array} \right)_{j=3/2 \text{ space}}.$$

This matrix expression corresponds to the $xyz$ type of tensor for $j = 3/2$. In the local scattering at the impurity, $M_{mn}^z$ has the same symmetry as $xyz$. In the cubic point group, $M_{mn}^z$ expresses $O_h \Gamma_2$ octupole coupling ($\Gamma_3$ for $D_{4h}$ point group). This coupling is realized in the $f^2$ configuration (doubly occupied $f$-electron state). For instance, it connects the $D_{4h}$ crystal-field ground state

$$|g\rangle = c_1(|4\rangle + | -4\rangle) + c_2|0\rangle,$$

with the first excited state

$$|e\rangle = \frac{1}{\sqrt{2}}(|2\rangle + | -2\rangle),$$

in the inelastic impurity scattering $\tilde{U}_{mn}^z$. Here, $|M\rangle (M = -4 \sim 4)$ is an eigenstate of $J_z$ for the $J = 4$ angular momentum state in the $f^2$ configuration. Within the two crystal-field states, the scattering matrix is expressed by

$$\left( \begin{array}{cc} M_{11}^f & M_{12}^f \\ M_{21}^f & M_{22}^f \end{array} \right) = |M_{12}^f| \left( \begin{array}{cc} 0 & -i \\ i & 0 \end{array} \right).$$

Next, we consider the spin-dependent case, $\tilde{U}_{mn} = M_{mn} \hat{\tau}_2$. In the subspace $\psi_b$, we obtain

$$\tilde{U}_{mn} = M_{mn} \left( \begin{array}{cccc} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & -i \\ i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{array} \right).$$

Assuming the $yz$ and $xz$ types for the two bands in this case as well, $\tilde{U}_{mn}$ is transformed to the $j = 3/2$ angular
momentum basis expression as
\[
\hat{U}_{mn} \rightarrow M_{mn} \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}_{j=3/2 \text{ space}},
\]
which expresses the combination of the \( z \) dipole and \( z(2z^2-3x^2-3y^2) \) octupole types of \( j = 3/2 \) electron scattering. For the inelastic impurity scattering, the matrix \( M_{mn} \) represents the dipole coupling between two low-lying singlet states, e.g., the ground state \(|g\rangle\) in eq. (43) and the excited state,
\[
|e\rangle = \frac{1}{\sqrt{2}}(|4\rangle - | -4\rangle),
\]
given as
\[
\begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} = |M_{12}| \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.
\]

Finally, we mention another pair of two-band types, \( (2z^2-x^2-y^2) \) and \( (x^2-y^2) \). Applying the above argument, we find that the \( \hat{t}_1\hat{\rho}_3\hat{S}_3 \) electron scattering is reduced to the \( z(x^2-y^2) \) octupole type, and the \( \hat{t}_2 \) type corresponds to the \( xyz \) octupole type expressed by eq. (42). In Appendix A, we give a different analysis for \( \hat{U}_{mn}^{(z)} \).

3.2 Singlet-doublet configuration

Here, we devote ourselves to extending the present theory of \( T_c \) enhancement to typical examples of impurities with internal degrees of freedom. Orbital degrees of freedom of conduction electrons give rise to magnetic and nonmagnetic exchange scatterings, both of which are considered here in the singlet-multiplet configuration. Whether \( T_c \) is enhanced or suppressed depends on the ratio of their scattering strengths that determines the signs of the two-band superconducting order parameters: they are the same (\( \Delta_+ \Delta_- > 0 \)) or different (\( \Delta_+ \Delta_- < 0 \)). For the \( T_c \) enhancement, the crystal-field ground state must be a singlet (a nonmagnetic doublet is also allowed). As mentioned for the \( s_{1/2} \)-wave state (\( \Delta_+ \Delta_- < 0 \)) in \( \S 2.3 \), \( T_c \) suppression is caused by elastic scattering due to the singlet, which is neglected here as well. First, we discuss a case of singlet-doublet configuration regarded as an \( S = 1 \) local pseudo-spin. This \( S = 1 \) spin is not a spin triplet but a spin and orbitally coupled state, as often studied for f-electron systems. The latter can be realized as an impurity low-lying state in a uniaxial (\( D_{4h} \) or \( D_{6h} \)) crystal field. In this framework, we tackle a more complicated case of singlet-triplet configuration discussed in the next subsection.

For spin and orbitally coupled impurity states, in general, local orbital exchange occurs as well as spin exchange during electron scattering by the impurity moment. In the case of an \( S^f = 1 \) pseudo-spin for an impurity, a spherical type of exchange interaction is expressed by coupling with, for instance, local \( S^c = 3/2 \) states, \( \psi^c = (\psi_{3/2} \psi_{1/2} \psi_{-1/2} \psi_{-3/2})^T \), formed by conduction electrons. This local interaction Hamiltonian is given by\(^{29} \)
\[
\hat{H}_{\text{loc}} = \psi^c \left( J_S \hat{S}^1 \hat{S}^c + J_Q \sum_{\eta=1}^5 Q^c_\eta Q^\eta \right) \psi^c + \frac{1}{3} \Delta_{\text{CF}} \left( 3 \left( S_z^c \right)^2 - 2 \right),
\]
where a potential (elastic) scattering term is neglected. The first and second terms represent dipolar and quadrupolar exchanges with the coupling constants, \( J_S \) and \( J_Q \), respectively. The quadrupole operators (\( Q^\eta \)) for an impurity; \( Q^c_\eta \) for an electron) are defined as
\[
\{Q_\eta, \eta = 1, \cdots, 5\} = \{S_xS_z + S_zS_x + S_xS_y + S_yS_z, S^2 - S^c - S_x^2 - S_y^2 \} / \sqrt{3}.
\]
The last term in eq. (50) introduces uniaxial (\( D_{4h} \) or \( D_{6h} \)) anisotropy to the impurity states, and \( \Delta_{\text{CF}} > 0 \) is taken to determine a singlet ground state here. For the \( S^c = 1 \) pseudo-spin, it is sufficient to consider the above dipoles and quadrupoles. We do not consider the anisotropy of each exchange coupling that usually exists in a realistic system, which does not affect the following argument.

On the other hand, we introduce some assumptions to electron states as follows. At impurity sites, partial waves of conduction electrons are represented by \( \psi \). This can be regarded as the \( O_h \) \( \Gamma_6 \) point-group basis in a cubic system. In general, actual conduction bands can include all four components of \( \psi \) point, and their mixing is expressed as
\[
\psi^c = \hat{V} \psi_b, \quad \psi^c = \begin{pmatrix} \psi_{3/2} \\ \psi_{1/2} \\ \psi_{-1/2} \\ \psi_{-3/2} \end{pmatrix}, \quad \psi_b = \begin{pmatrix} \psi_{+1/2} \\ \psi_{+3/2} \\ \psi_{-1/2} \\ \psi_{-3/2} \end{pmatrix},
\]
where each element in the transformation matrix \( \hat{V} \) is given by the overlap of local orbital and band wave functions such as \( \langle S^c_\mu | \mu \sigma \rangle \) (\( \mu = \pm; \sigma = \uparrow, \downarrow \)). To examine the orbital roles in the superconductivity, we consider here the simplest case in which two \( (\pm 3/2) \) of the orbital components enter the + band and the other two \( (\pm 1/2) \) enter the − band. In the above \( \hat{V} \), we assume that \( \langle 3/2 | \uparrow \rangle = \langle 1/2 | \downarrow \rangle = \langle -1/2 \downarrow \rangle = \langle -3/2 | + \rangle = V_0 \) and that the other matrix elements vanish:
\[
\hat{V} = V_0 \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{pmatrix}.
\]

Such a one to one correspondence clarifies the connection between the \( S^c = 3/2 \) pseudo-spin space and the \( SU(2) \) spin \( \otimes SU(2) \) band space, and the scattering matrices are expressed simply by eqs. (B-9) and (B-10). Although this simplification overestimates interband scattering compared with intraband scattering, it helps us examine what types of interband correlations are relevant to the relative signs of order parameters and how
intraband scattering modifies their relative amplitudes.

For the superconducting order parameters, we consider both the \( s_{++} \) wave (\( \Delta_+ = \Delta_- \)) and the \( s_{\pm} \) wave (\( \Delta_+ = -\Delta_- \)). Since we neglect any correlations between the two bands except for the impurity scattering, the local correlations directly affect the relative signs of order parameters together with their amplitudes. This is justified when the impurity effect is more relevant than any other interband correlation such as an interband Coulomb interaction. We respectively express the \( s_{++} \)-wave and \( s_{\pm} \)-wave states as

\[
\begin{align*}
\tilde{\Delta}_A &= \Delta_A \rho_2 \sigma_2 \quad \text{(} s_{++} \text{ wave)}, \\
\tilde{\Delta}_B &= \Delta_B \bar{\tau}_3 \rho_2 \sigma_2 \quad \text{(} s_{\pm} \text{ wave)},
\end{align*}
\]

with the order parameters \( \Delta_A \) and \( \Delta_B \), respectively. The matrix for the order parameter is given by their combination as

\[
\hat{\Delta} = \tilde{\Delta}_A + \tilde{\Delta}_B.
\]

The relevant impurity scatterings for the singlet-doublet configuration are described in Appendix B. First, we examine properties of the dipolar and quadrupolar scatterings separately. Let us start from the dipolar (magnetic) scattering case where \( J_S \neq 0 \) and \( J_Q = 0 \) in eq. (50). Applying \( \mathcal{H}' \) in eq. (B.7) to calculate the self-energy in Fig. 1, we obtain

\[
\Sigma(i\omega_l) = -\frac{n_{Imp}}{2} \sum_{n \neq n'} \sum_{\omega} \frac{1}{\omega_1 - \delta_n \omega_2 - \delta_{n'}} \left( \sqrt{2} \right)^2 \times \left( \frac{J_S}{2} \right)^2 \frac{1}{\Omega} \sum_k \left[ S^c_+ \tilde{G}_0 S^c_- + S^c_- \tilde{G}_0 S^c_+ \right],
\]

where \( \tilde{G}_0 \equiv \tilde{G}_0(i\omega_l + i\omega_1 - i\omega_2, k) \). \( \delta_1 \) (\( \delta_2 \)) corresponds to the energy level of the impurity singlet ground (doublet excited) state \( (n, n' = 1, 2) \) and \( \delta_2 - \delta_1 = \Delta_{CF} \). The factor \( \left( \sqrt{2} \right)^2 \) comes from the second-order process \( S_+ S_- \) or \( S_- S_+ \) between the singlet and doublet states. Then, we derive a gap equation. As in eq. (31), the Green’s function \( \tilde{G}_0 \) consists of three parts: \( i\omega_l, \epsilon_k \rho_3 \), and \( \tilde{\Delta} \). The \( \epsilon_k \rho_3 \) term disappears after the summation over \( k \). The other two parts are transformed by \( (S^c_+ \tilde{G}_0 S^c_- + S^c_- \tilde{G}_0 S^c_+) \).

For \( \Delta \),

\[
\begin{align*}
S^c_+ \Delta \tilde{S}^c_- + S^c_- \Delta \tilde{S}^c_+ &= (5\Delta_A - 2\Delta_B)\bar{\tau}_3 \rho_2 \sigma_2 + (\Delta_A - 2\Delta_B)\bar{\tau}_3 \rho_2 \sigma_2 \\
&= \Delta_A \bar{\tau}_3 \rho_2 \sigma_2 + \Delta_B \bar{\tau}_3 \rho_2 \sigma_2.
\end{align*}
\]

This means that the order parameters are transformed as

\[
\begin{pmatrix}
\Delta_A \\
\Delta_B
\end{pmatrix} = \hat{\Delta}_\Delta \begin{pmatrix}
\Delta_A \\
\Delta_B
\end{pmatrix}, \quad \hat{\Delta}^S = \begin{pmatrix}
5 & -2 \\
-2 & -1
\end{pmatrix}.
\]

Similarly, the \( i\omega_l \) part is

\[
S^c_+ i\omega_l S^c_- + S^c_- i\omega_l S^c_+ = i\omega_l(5 - 2\bar{\tau}_3).
\]

Since \( \bar{\tau}_3 \) is the Pauli matrix for the \( \pm \) band space, eq. (21)
is obtained as

\[
\hat{\lambda}^S = \begin{pmatrix}
3 & 0 \\
0 & 7
\end{pmatrix}, \quad \hat{\lambda}^\omega = \begin{pmatrix}
5 & -2 \\
-2 & 5
\end{pmatrix}.
\]

For \( X = S \) and \( \xi = \omega \). Then, eq. (22) yields

\[
\hat{\lambda}^S = \hat{U}^{-1} \hat{\lambda}^\omega \hat{U} = \begin{pmatrix}
3 & 0 \\
0 & -3
\end{pmatrix} + \begin{pmatrix}
2 & -2 \\
-2 & 2
\end{pmatrix}, \quad \hat{\lambda}^\omega = \begin{pmatrix}
3 & 0 \\
0 & 3
\end{pmatrix} + \begin{pmatrix}
2 & -2 \\
-2 & 2
\end{pmatrix}.
\]

If the intraband contribution, the second matrix on the right-hand side of each equation, is removed, the intraband contribution results in the \( T_c \) enhancement for the \( s_{\pm} \) state, as discussed in §2.3.

In the same manner, the above argument is applied to the quadrupolar (nonmagnetic) scattering case where \( J_S = 0 \) and \( J_Q \neq 0 \) in eq. (50). For the \( \Delta \) and \( i\omega_l \) parts in the self-energy,

\[
Q^c_+ \Delta Q^c_- + Q^c_- \Delta Q^c_+ = -12\Delta \bar{\tau}_3 \rho_2 \sigma_2 + 12\Delta \bar{\tau}_3 \rho_2 \sigma_2,
\]

\[
Q^c_+ i\omega_l Q^c_- + Q^c_- i\omega_l Q^c_+ = 12\omega_l,
\]

respectively, and we obtain

\[
\hat{\lambda}^Q = \begin{pmatrix}
-12 & 0 \\
0 & 12
\end{pmatrix}, \quad \hat{\lambda}^\omega = \begin{pmatrix}
12 & 0 \\
0 & 12
\end{pmatrix}.
\]

These lead to the \( T_c \) enhancement for the \( s_{++} \)-wave state.

Next, we see the more generic treatment combining both magnetic (\( S \)) and nonmagnetic (\( Q \)) scattering terms as

\[
\tilde{\eta}_{12} \hat{\Delta}(x) = \cos \zeta \left[ f_{\Delta}(x) \hat{\lambda}^S + f_{\omega}(x) \hat{\lambda}^\omega \right] + \sin \zeta \left[ f_{\Delta}(x) \hat{\lambda}^Q + f_{\omega}(x) \hat{\lambda}^\omega \right]
\]
in eq. (24), where

\[
\tilde{\tau}_{12} = \frac{f^S_{12} Q}{\sqrt{(f^S_{12})^2 + (\tilde{\tau}^Q_{12})^2}}, \quad \tan \zeta = \frac{J Q}{f^S} \equiv \kappa, \tag{68}
\]

and the lifetime \(\tilde{\tau}^Q_{12}\) is introduced for the magnetic (nonmagnetic) scattering. The highest eigenvalue of \(\tilde{\tau}_{12} \hat{\Lambda}\) determines the quantity of

\[
\frac{8T_c}{\pi} \tilde{\tau}_{12} \log \frac{T_c}{T_{c0}}, \tag{69}
\]

and its \(x\) dependence is shown in Fig. 3. The \(T_c\) enhancement is obtained for its positive value, which holds at \(x > 6.2\) for \(\kappa = 0\) and at \(x > 5.8\) for \(\kappa = 1.0\). In the presence of only nonmagnetic scattering for \(\kappa = \infty\), \(T_c\) is enhanced in the entire \(x > 0\) range. The \(T_c\) suppression, found for a small \(x\) or \(\kappa \approx 0.25\), is due to the competition between the magnetic and nonmagnetic exchange scatterings and to the depairing effect by the intraband scattering. Since \(f_0/f_s < 1\), the condition for a positive value of eq. (69) is given by

\[
(-5f_s + 12\kappa f_0)(3f_0 - 2f_s - 12\kappa f_s) - (2f_s)^2 < 0, \tag{70}
\]

the solution of which determines the minimum \(f_0/f_s\) as a function of \(x\):

\[
\left(\frac{f_0}{f_s}\right)_{\min} = \frac{1}{24\kappa} \left[(48\kappa^2 + 8\kappa + 5) \right. \\
- \sqrt{(48\kappa^2 + 8\kappa + 5)^2 - 96\kappa(10\kappa + 1)} \right]. \tag{71}
\]

The \(x\) dependence of \(f_0/f_s\) and the \(\kappa\) dependence of \((f_0/f_s)_{\min}\) are shown in Figs. 4 and 5, respectively. At both \(\kappa = 0.03\) and \(\kappa = 0.75\), for instance, eq. (71) takes almost the same value, \(\approx 0.51\), which gives the minimum \(x \approx 14.5\) for \(T_c\) enhancement, as shown in Fig. 3. The maximum at \(\kappa = 0.25\) in Fig. 5 indicates that there is no \(T_c\) enhancement for any finite crystal-field level splitting, implying that \(T_c\) is always suppressed by the competition between the magnetic and nonmagnetic scattering effects. We also find that \(\kappa\) determines the relative signs of the two order parameters: \(\Delta_+ \Delta_- < 0\) for \(\kappa < 0.25\) and \(\Delta_+ \Delta_- > 0\) for \(\kappa > 0.25\). The combination of \(\Delta_A\) (\(s_{++}\) wave) and \(\Delta_B\) (\(s_{+-}\) wave) is caused by the intraband scattering effect in the + band, due to the off-diagonal elements in \(\hat{\Lambda}(x)\), which leads to \(|\Delta_-| < |\Delta_+|\) in the vicinity of \(T_c\). At \(\kappa = 0.25\), \(\Delta_- = 0\) (\(\Delta_A = \Delta_B\)) means that only one band (+ band) is superconducting with \(T_c\) suppression.

The above argument is based on a rather artificial assumption about the local band character in eq. (53). More generic treatment of \(\hat{V}\) in eq. (52) provides us with various scattering effects on \(T_c\). This point is considered for the singlet-triplet configuration discussed below.

### 3.3 Singlet-triplet configuration

The singlet-triplet configuration is realized for a non-Kramers ion in an \(O_h\) crystal field environment like the Pr\(^{3+}\) or U\(^{4+}\) \(f^2\) low-lying states in heavy-fermion materials. For the strong spin-orbit coupling, the most relevant local \(f\)-electron states are described by the \(j = 5/2\) angular momentum. Then, we consider only the exchange coupling between the impurity states and the \(j = 5/2\) electrons hybridized with conduction bands. We assume here that the \(\Gamma_8\) and \(\Gamma_7\) partial waves (see Appendix C) are transferred independently to the + and - bands, respectively. In terms of eq. (C-6) for both \(\Gamma_8\) and \(\Gamma_7\), \(\psi_m = \langle \psi_{m1} \uparrow \psi_{m2} \downarrow \psi_{m3} \uparrow \psi_{m4} \downarrow \rangle\) is combined with \(\psi_b = \langle \psi_{+} \uparrow \psi_{+} \downarrow \psi_{-} \uparrow \psi_{-} \downarrow \rangle\) for the bands. This is expressed by \(\psi_m = \hat{V} \psi_b\):

\[
\hat{V} = \begin{pmatrix}
0 & v_+ u_{1+} & v_+ u_{1\downarrow} & 0 & 0 \\
v_+ u_{1+} & 0 & v_+ u_{1\downarrow} & 0 & 0 \\
v_+ u_{2+} & v_+ u_{2\downarrow} & 0 & 0 & 0 \\
v_+ u_{2\downarrow} & v_+ u_{2+} & 0 & 0 & 0 \\
0 & 0 & v_- & 0 & v_- \\
0 & 0 & 0 & v_- & 0
\end{pmatrix}. \tag{72}
\]

Here, \(v_\pm\) represents the hybridization amplitude of the \(f\)-orbitals and the \(\mu = \pm\) band, respectively, at the impurity sites:

\[
u_{i\uparrow} = \langle m_i \uparrow \uparrow \rangle, \quad v_{i\downarrow} = \langle m_i \uparrow \downarrow \downarrow \rangle, \\
u_{i\downarrow} = \langle m_i \downarrow \uparrow \rangle, \quad u_{i\uparrow} = \langle m_i \downarrow \downarrow \rangle. \tag{73}
\]
represent the impurity site overlaps of the wave functions \( \psi_{m',\sigma} \) (\( i = 1, 2 \)) and \( \psi_{+\sigma} \). We only simplify the connection between the \( m_3 \) orbital and the \( \Gamma \) band.

In Appendix C, the relevant impurity scatterings are described for the singlet-triplet configuration \( \Gamma_1 \oplus \Gamma_4 \) (\( \Gamma = \Gamma_4, \Gamma_5 \)). For \( H' \) in eq. (C-23), the self-energy in Fig. 1 is obtained as

\[
\hat{\Sigma}^\Gamma (i\omega_n) = -n_{\text{imp}} T^2 \sum_{\nu \neq \nu'} \sum_{n \neq n'} \sum_{\omega_{1\nu} + \omega_{2\nu} - \delta_n} \frac{1}{\omega_{1\nu} - \delta_n} \frac{1}{\omega_{2\nu} - \delta_n'} \times \sum_{X=\bar{X},Q} ^{c} \left( \frac{J^X_{\nu}}{\Omega} \right)^2 \sum_k \left\{ X^z_{\nu} \frac{\hat{G}_0 X^z_{\nu'}}{\Delta} + X^{-\nu}_{\nu} \frac{\hat{G}_0 X^{-\nu}_{\nu'}}{\Delta} \right\} \left[ \hat{G}_0 \equiv \hat{G}_0 (i\omega_n + \omega_1 - \omega_2, k) \right].
\]  

(74)

Here, \( \delta_1 \), \( \delta_2 \) corresponds to the energy level of the impurity singlet ground (triplet excited) state (\( n, n' = 1, 2 \)). For the gap equation in eq. (24), the transformation to \( \Delta \) in eq. (56),

\[
X^z_{\nu} \Delta X^z_{\nu'} + \frac{1}{2} (X^+_{\nu} \Delta X^+_{\nu'} + X^-_{\nu} \Delta X^-_{\nu'}),
\]  

(75)

leads to

\[
\hat{\Lambda}^\Delta = (-1) \hat{\Lambda}^Q = \frac{3}{8} \sum_{i=1}^{2} (u^*_{i\uparrow} v_{i\downarrow} - v_{i\uparrow}^* u_{i\downarrow}) \left( \begin{array}{cc} -1 & 0 \\ 0 & 1 \end{array} \right),
\]  

(76)

in both \( \Gamma = \Gamma_4 \) and \( \Gamma = \Gamma_5 \). For the derivation, we use \( u_{i\uparrow} v_{i\downarrow} = u_{i\downarrow}^* v_{i\uparrow}^* \) and \( v_{i\uparrow}^* u_{i\downarrow} = v_{i\downarrow} u_{i\uparrow} \) since the \( m_{i\uparrow} \) and \( m_{i\downarrow} \) local electrons are the time reversal partners. In the same manner, for both \( \Gamma_4 \) and \( \Gamma_5 \),

\[
X^z_{\nu} \Delta X^z_{\nu'} + \frac{1}{2} (X^+_{\nu} \Delta X^+_{\nu'} + X^-_{\nu} \Delta X^-_{\nu'}),
\]  

(77)

gives

\[
\hat{\Lambda}^S = \hat{\Lambda}^Q = \frac{3}{16} \sum_{i=1}^{2} \sum_{\sigma = \uparrow, \downarrow} \left( u_{i\sigma}^* u_{i\sigma} + v_{i\sigma}^* v_{i\sigma} \right) \left( \begin{array}{cc} 0 & 1 \\ 1 & 0 \end{array} \right).
\]  

(78)

Equation (76) implies the competition between the magnetic (S) and nonmagnetic (Q) scattering effects for \( T_c \) enhancement. Which has the higher \( T_c \), the \( s_+ \) wave or the \( s_- \) wave, depends on whether the sign of \( (u_{i\uparrow} v_{i\downarrow} - v_{i\uparrow}^* u_{i\downarrow}) \) is positive or negative, respectively. In realistic systems, both magnetic and nonmagnetic scatterings coexist. In the present case, we can calculate the coupling constants, \( J^S_{\nu} \) and \( J^Q_{\nu} \), based on the Anderson model including the \( j = 5/2 \) electron scattering due to a single impurity in the \( f^2 \) configuration, and obtain the ratio as \( [J^Q_{\nu}]/[J^S_{\nu}] = 1/3 \). This means that the magnetic interband scattering dominates the \( T_c \) enhancement for the singlet-triplet configuration. More detailed discussion is given below.

4. Pr Impurity Effect in LaOs\(_4\)Sb\(_{12}\) Superconductor

The \( Pr^{3+} f^2 \) configuration is a good candidate for raising \( T_c \) if \( Pr \) can be embedded in a multiband superconductor. In fact, for the skutterudite superconductor La\(_{1-x}\)Pr\(_x\)Os\(_4\)Sb\(_{12}\), the Pr singlet-triplet configuration may be relevant to \( T_c \) enhancement in LaOs\(_4\)Sb\(_{12}\). Here, we show an attempt to apply the above argument in this case. The most intriguing feature of the skutterudite compounds is that each rare-earth ion is located at the center of the pnictogen cage (Sb\(_{12}\)) having the \( a_{xy} \) and \( t_\text{u}(x, y, z) \) molecular orbitals. It is considered that the Pr \( f \)-electron states hybridize with the conduction bands via these orbitals. For a strong spin-orbit coupling, the \( a_{xy} \) electrons have the \( O_h \) \( \Gamma_7 \) symmetry and transfer directly to the \( m_3 \) electron state named in eq. (C-6). On the other hand, the \( t_\text{u} \) electrons with the \( O_h \) \( \Gamma_8 \) symmetry mix with both \( m_1 \) and \( m_2 \) states as

\[
|m_1, \uparrow\rangle \leftrightarrow \frac{1}{\sqrt{2}} ([x, \downarrow] - i[y, \downarrow]),
\]  

(79)

\[
|m_1, \downarrow\rangle \leftrightarrow -\frac{1}{\sqrt{2}} ([x, \uparrow] + i[y, \uparrow]),
\]  

(80)

\[
|m_2, \uparrow\rangle \leftrightarrow \frac{1}{\sqrt{3}} \left[ \sqrt{2} (x, \downarrow) - \frac{1}{\sqrt{2}} ([x, \downarrow] + i[y, \downarrow]) \right],
\]  

(81)

\[
|m_2, \downarrow\rangle \leftrightarrow \frac{1}{\sqrt{3}} \left[ \sqrt{2} (x, \downarrow) + \frac{1}{\sqrt{2}} ([x, \downarrow] - i[y, \downarrow]) \right].
\]  

(82)

We here consider two conduction bands, one of which is \( a_{xy} \)-dominant and the other is \( t_\text{u} \)-dominant. We assume that both are combined with each other through interband electron scattering. In the present case, the most relevant is the Pr impurity scattering due to the hybridization effect with the bands. Then, we can use the transformation in eq. (72) for mixing \( f \)-electron states with the \( t_\text{u} \)-dominant band (+ band) and the \( a_{xy} \)-dominant band (− band). Choosing the local \( t_\text{u}(x, y, z) \) component that mainly contributes to the + band and taking their onsite overlaps arbitrarily as

\[
\langle x|, \langle y|, \langle z| = \sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta,
\]  

(83)

we have

\[
u_{1\uparrow} = (1/\sqrt{2}) \sin \theta e^{i\phi}, \quad v_{1\uparrow} = -(-1/\sqrt{2}) \sin \theta e^{-i\phi};
\]  

\[
u_{2\uparrow} = u_{2\uparrow} = (\sqrt{2}/3) \cos \theta,
\]  

\[
u_{2\downarrow} = -(-1/\sqrt{6}) \sin \theta e^{-i\phi}, \quad v_{2\downarrow} = (1/\sqrt{6}) \sin \theta e^{i\phi}. \]  

(84)

Substituting them in eqs. (76) and (78), we obtain

\[
\hat{\Lambda}^S = (-1) \hat{\Lambda}^Q = \frac{1}{4} \left( \begin{array}{cc} -1 & 0 \\ 0 & 1 \end{array} \right),
\]  

(85)

\[
\hat{\Lambda}^Q = \frac{1}{4} \left( \begin{array}{cc} 1 & 0 \\ 0 & 1 \end{array} \right).
\]  

(86)

In the gap equation (24), we have

\[
\hat{\Lambda}(x) = \frac{1}{4\Gamma^S_{12}} \left( \begin{array}{cc} f_0(x) & 0 \\ 0 & -f_s(x) \end{array} \right) + \frac{1}{4\Gamma^Q_{12}} \left( \begin{array}{cc} -f_s(x) & 0 \\ 0 & f_0(x) \end{array} \right).
\]  

(87)
In the real system, we must consider the $T_h$ symmetry that combines the Pr $O_h$ $\Gamma_{4}$ and $\Gamma_{5}$ triplet states as \[\Gamma_{4}^{(2)}(\eta) = \sqrt{1 - d^2|\Gamma_{5}\eta|} + d|\Gamma_{4}\eta| \quad (\eta = +, 0, -), \tag{88}\]
where $d$ ($0 < d < 1/\sqrt{2}$) represents the deviation from the $O_h$ symmetry. In the above calculation of the self-energy, we usually have additional terms, namely,
\[
\left[ \chi_{c}^{G_{1}(3)} \Delta X_{c}^{G_{1}(3)} + \frac{1}{2} (X_{c}^{G_{1}(3)} \Delta X_{c}^{G_{1}(3)} + X_{c}^{G_{1}(3)} \Delta X_{c}^{G_{1}(3)}) \right] \\
+ (\Gamma_{4} \leftrightarrow \Gamma_{5}) \quad (X = s, q), \tag{89}\]

which vanish in this case. They also vanish when $\Delta$ is replaced with $i\omega$. If the $a_{u}$ band hybridizes with the $f$-orbitals more strongly than the $t_{u}$ band, which means $v_- > v_+$ here, the impurity interband scattering enhances $T_c$ for a finite crystal-field splitting $x = (\delta_{2} - \delta_{1})/(2T_{c})$, satisfying either $f_{0}/f_{<} > \tau_{12}^{Q}/\tau_{12}^{Q}$ or $f_{0}/f_{>} > \tau_{12}^{Q}/\tau_{12}^{Q}$. For the former, the $T_c$ enhancement is possible in the $s_{++}$-wave state, and a higher $T_c$ can be realized as the magnetic scattering becomes more dominant. In §3.3, we have mentioned that $|J_{Q}|/|J_{S}| = 1/3 (\tau_{12}^{Q}/\tau_{12}^{Q} = 1/9)$ is satisfied for $O_h$. It also holds for $T_{h}$, so that the gap equation chooses the $s_{++}$ wave for the $T_c$ enhancement. One may think that the quadrupolar scattering is the most relevant if $d$ is small in eq. (88), since the $\Gamma_{1}$-$\Gamma_{5}$ interchange dominates the exchange scattering. For the $\Gamma_{5}$ scattering type, however, the octupolar scattering cannot be neglected in the multiorbital exchange owing to the hybridization of $f$-electrons with the conduction bands. Thus, the magnetic scattering can contribute to the $T_c$ enhancement for the $\Gamma_{1}$-$\Gamma_{4}^{(2)}$ configuration in a multiband system. Our result indicates that the $s_{++}$-wave state is favorable for the La$_{1-x}$Pr$_{x}$Os$_{2}$Sb$_{12}$ superconductivity if the multiband picture is applicable and the Pr or Sb$_{12}$ site orbital symmetries reflect in the bands.

Finally, we mention the effect of inelastic scattering neglected in the above argument where $v_- > v_+$ is assumed for the hybridization amplitudes. If the $m_{1}$-$m_{2}$ scattering terms in eqs. (C-17) and (C-18) are considered in calculating the self-energy for the $\Gamma_{5}$ nonmagnetic scattering type, a correction term,
\[
C_{v} \frac{1}{\tau_{12}^{Q}} f_{0}(x) \left( \begin{array}{c} 1 \\ 1 \\ 1 \end{array} \right) \left( C_{v} \sim \frac{v_{2}^{2}}{v_{1}^{2}} \right), \tag{90}\]
is added on the right-hand side in eq. (87). It assists the $T_c$ enhancement, which resembles the effect of inelastic nonmagnetic scattering impurities in single-band $s$-wave superconductors.

5. Conclusion

We have studied inelastic (dynamical) impurity scattering effects on $T_c$ enhancement in the two-band superconducting states, $s_{++}$ wave and $s_{\pm}$ wave. The key is to check the sign change of the order parameters in the self-energy corresponding to the second order of the scattering process. We solve a gap equation, where both the $s_{++}$ wave and $s_{\pm}$ wave are combined by impurity scattering, and find out the possible atomic structure of the impurity that increases $T_c$. For the $T_c$ enhancement, the crystal-field ground state must be a singlet or a nonmagnetic doublet. If not, magnetic impurities will always cause $T_c$ suppression. For the $s_{\pm}$ wave, it is necessary for elastic (nonmagnetic) scattering to be relatively small. In the singlet-singlet configuration, we can easily determine what type of magnetic interband scattering contributes to pairing interaction. This simple analysis is very useful for determining a scattering type for the $T_c$ enhancement among multiorbital interaction terms when we consider such a complicated atomic structure as the $f^n$ configuration. Here, we have discussed the singlet-doublet and singlet-triplet configurations. We find that the $T_c$ of either the $s_{++}$-wave or $s_{\pm}$-wave state can be enhanced by the dynamical magnetic or nonmagnetic impurity interband scattering for a larger crystal-field splitting of impurity ground and excited states, while $T_c$ is suppressed if both scattering strengths are comparable. Whether $T_c$ is enhanced or not also depends on how the local electron states hybridize with the two bands. We show a case of $T_c$ enhancement in the $s_{++}$ wave by magnetic interband scattering due to the singlet-triplet configuration. This result may give useful information on a multiband picture of the La$_{1-x}$Pr$_{x}$Os$_{2}$Sb$_{12}$ superconductivity. In fact, the connection between the La-rich and Pr-rich superconductors is left to be clarified as well as the symmetry of the latter order parameter.\(^{15}\)

In the above argument, we have assumed weak scattering impurities. Strictly speaking, dynamical scattering effects should be investigated as a Kondo problem. It was shown theoretically in normal metallic cases that the impurity exchange scattering strength is renormalized to be weaker with the decrease in temperature since the crystal-field singlet competes with the Kondo-singlet formation.\(^{21-36,38}\) This holds even for a small crystal-field splitting of the singlet ground and excited multiplet states. Thus, our results shown here are valid for the $T_c$ enhancement due to the impurity scattering.

Throughout the paper, we focus on the hybridization between local orbitals and conduction electron states. For most of the $f$-electron systems, this may be more relevant than the admixture of orbitals formed by intersite electron hopping that we have neglected here. Our treatment is more practical since the latter contribution can be included effectively in the hybridization.

The possibility of the $s_{\pm}$-wave state has been the subject of debate for high-$T_c$ superconductors with FeAs layers. It is pointed out that the Fe $d$-orbitals contribute to the disconnected Fermi surfaces and the orbital degrees of freedom play an important role in pairing interaction.\(^{8}\) The interband Coulomb interactions may be relevant for the high $T_c$ of this multiband superconductivity,\(^{28,39,40}\) the roles of which are analogous to those of the local correlations in the $f$-electron systems we have considered here.

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Appendix A: Connection between the \( s_{\pm} \)-Wave
and Conventional \( s \)-Wave Superconductors

We attempt to apply the unitary transformation
\[
\begin{pmatrix}
\psi_{+,\sigma} \\
\psi_{-,\sigma}
\end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix}
\psi_{M\sigma} \\
\psi_{-M\sigma}
\end{pmatrix}
\] (A-1)
to the band basis, where \( M \) is a natural number. Using
this new basis set, \( \psi_M = (\psi_{M\uparrow} \psi_{M\downarrow} \psi_{-M\uparrow} \psi_{-M\downarrow})^T \),
\( \hat{U}_{mn}^z \) in eq. (40) is transformed as
\[
\hat{U}_{mn}^z \rightarrow -M_{mn}^z \begin{pmatrix} 1 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 \\
0 & 0 & -1 & 0 \\
0 & 0 & 0 & 1 \end{pmatrix}
\] (A-2)

If the number \( M \) is regarded as an orbital component,
this matrix indicates a quadrupole type of scattering. In
fact, \( \psi_{M=1} \) corresponds directly to \( \psi_{j=3/2} \) in \( \S 3.1 \).
In this case, the matrix in eq. (A-2) is expressed by \( (2j_z^2 - j_z^2 j_y^2) \).

On the other hand, for the conventional single-band \( s \)-wave
superconductivity, the pairing Hamiltonian is given by
\[
\mathcal{H}_\Delta = -\sum_k \Delta \left( c_{k+}^\dagger c_{-k}^\dagger + c_{-k} c_{k} \right)
\] (A-3)

After applying spherical expansion to the operators as
\[
c_{k\sigma} = \sum_{LM} i^{-L} (6\pi)^{1/2} \frac{1}{kr} Y_{LM}(\Omega_k) c_{kLM\sigma},
\] (A-4)
where \( R \) is the radius of the system, we rewrite the Hamiltonian (A-3) as
\[
\mathcal{H}_\Delta = -\sum_k \sum_{L,M \geq 0} \left(-1\right)^M \Delta
\times \left( c_{k+L+M}^\dagger c_{-k-L-M} + c_{-k-L-M} c_{k+L+M} \right)
\] (A-5)

This orbital component \( M \) can correspond to \( M \) in eq. (A-1) directly. The pairing interaction works between
the electrons with the different orbitals denoted by \( \pm M \).
Let us fix \( L \) and restrict the orbitals to a pair of \( \pm M \). If
\( \psi_{M\sigma} \) is transformed to \( \psi_{\mu\sigma} \) using eq. (A-1), eq. (A-5) is reduced to
\[
\mathcal{H}_\Delta = -\sum_{\mu = \pm} \sum_k \left(-1\right)^M \Delta \left( c_{k+\mu}^\dagger c_{k-\mu}^\dagger + c_{k-\mu} c_{k+\mu} \right)
\] (A-6)

It represents \( s_{\pm} \)-wave pairing in the two orbitals connected to the \( \mu \) bands.

Thus the spin-dependent interband scattering in eq. (40) in a two-band \( s_{\pm} \)-wave superconductor can be mapped to the quadrupole type of scattering in eq. (A-2) in a single-band \( s \)-wave superconductor. Both cases give
rise to the \( T_c \) enhancement if the electron scattering interchanges the impurity low-lying states with a finite crystal-field splitting.

Appendix B: Exchange Matrices for Singlet-
Doublet Configuration

At low temperatures, the most relevant terms in
eq. (50) are electron scatterings with interchange be-
tween the local ground and excited states given by
\[
J_S \left[ S_+^1 S_-^c + S_-^1 S_+^c \right] + J_Q \left[ Q_+^1 Q_-^c + Q_-^1 Q_+^c \right].
\] (B-1)

Using \( S_{\pm} = S_x \pm iS_y \) and \( Q_{\pm} = \pm iQ_1 + Q_2 \), it is rewritten as
\[
\frac{J_S}{2} \left[ S_+^1 S_-^c + S_-^1 S_+^c \right] + \frac{J_Q}{2} \left[ Q_+^1 Q_-^c + Q_-^1 Q_+^c \right].
\] (B-2)

By denoting \( S_+^1 = 0 \) (the impurity ground state) and
\( S_{\pm}^1 = 1, -1 \) (the impurity excited states) by \( |1\rangle, |2\rangle \), and
\( |3\rangle \), respectively, the \( (S_+^1)_{mn} \) and \( (Q_{\pm}^1)_{mn} \) \( (m,n = 1,2,3) \)
matrix expressions are given as
\[
S_+^1 = S_-^1 = \begin{pmatrix} 0 & 0 & \sqrt{2} \\
0 & 0 & 0 \\
\sqrt{2} & 0 & 0 \end{pmatrix}
\] (B-3)
\[
Q_+^1 = Q_-^1 = \begin{pmatrix} 0 & 0 & -\sqrt{2} \\
0 & 0 & 0 \\
\sqrt{2} & 0 & 0 \end{pmatrix}
\] (B-4)

For the \( S_+^c = 3/2 \) states, the operators \( S_+^c = S_-^c \) and
\( Q_+^c = Q_-^c \) are expressed by
\[
\psi^c S_+^c \psi^c = \psi^c \begin{pmatrix} 0 & \sqrt{3} & 0 \\
0 & 2 & 0 \\
0 & 0 & 0 \end{pmatrix} \psi^c,
\] (B-5)
\[
\psi^c Q_+^c \psi^c = \psi^c \begin{pmatrix} 0 & 2\sqrt{3} & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \end{pmatrix} \psi^c.
\] (B-6)

Following eq. (26), we examine the low-temperature physics using the impurity interaction Hamiltonian
\[
\mathcal{H}' = \sum_{X=S,Q} \sum_{R_\gamma} \sum_{mn} \int d\mathbf{r} a_\gamma^\dagger_{m,\alpha} \Psi^\dagger(r) \Psi(r).
\] (B-7)

Here, \( \Psi \) is an eight-dimensional vector for conduction electrons that is obtained by extending \( \Psi_b \) in eq. (52) to the particle-hole space as
\[
\Psi = \begin{pmatrix} \Psi_+ \\
\Psi_- \end{pmatrix}, \quad \Psi^\dagger = \begin{pmatrix} \Psi_+^\dagger \\
\Psi_-^\dagger \end{pmatrix}
\] (B-8)
where \( \Psi_\mu (\mu = +, -) \) is defined in eq. (28). Through \( \dot{V} \) in eq. (53) in this extended space (Pauli matrices \( \sigma \)
for spin, \( \rho \) for particle hole, and \( \tau \) for band), the above
electron scattering matrices are rewritten as
\[ S_+^\Gamma = \frac{\sqrt{3}}{2} \hat{\tau}_1 (\hat{\rho}_3 \hat{\sigma}_1 - i \hat{\sigma}_2) + \frac{1}{2} (1 - \hat{\tau}_3) (\hat{\rho}_3 \hat{\sigma}_1 + i \hat{\sigma}_2), \]
(B-9)
\[ Q_+^\Gamma = \sqrt{3} (i \hat{\tau}_2) (\hat{\sigma}_1 - i \hat{\rho}_3 \hat{\sigma}_2), \]
(B-10)
where \(|V_0|^2\) has been omitted. One can see that \(S_\pm^\Gamma\) consists of the interband scattering \(\tau_1\) and intraband scattering \((1 - \tau_3)\) terms. The former is comparable to \((U^z - iU^y)\) in eq. (32).

Appendix C: Exchange Matrices for Singlet-Triplet Configuration

On the basis of the \(J = 4\) total angular momentum, the \(O_8\) singlet and triplet states are given by\(^{33}\)
\[ |\Gamma_1\rangle = \frac{\sqrt{30}}{12} (|4\rangle + |-4\rangle) + \frac{\sqrt{21}}{6} |0\rangle, \]
(C-1)
\[
\begin{cases}
|\Gamma_4+\rangle = -\frac{1}{2} (|3\rangle - 3) - \frac{\sqrt{7}}{8} |1\rangle, \\
|\Gamma_40\rangle = \frac{1}{2} (|4\rangle - | -4\rangle), \\
|\Gamma_4-\rangle = \frac{1}{2} (|3\rangle + \frac{\sqrt{7}}{8} |1\rangle), \\
|\Gamma_5+\rangle = \frac{1}{2} (|3\rangle - \frac{\sqrt{7}}{8} |1\rangle), \\
|\Gamma_50\rangle = \frac{1}{2} (|2\rangle - | -2\rangle), \\
|\Gamma_5-\rangle = -\frac{1}{2} (|3\rangle + \frac{\sqrt{7}}{8} |1\rangle).
\end{cases}
\]
(C-2)
For the \(j = 5/2\) local electrons, they are classified into the \(O_8\) symmetric states as\(^{32}\)
\[
\begin{cases}
|\Gamma_{8/2}\rangle = -\frac{1}{2} (|3/2\rangle - \sqrt{5} |5/2\rangle), \\
|\Gamma_{8/1}\rangle = |1/2\rangle, \\
|\Gamma_{8,-1/2}\rangle = - |1/2\rangle, \\
|\Gamma_{8,-3/2}\rangle = \frac{1}{2} (|3/2\rangle + \sqrt{5} |5/2\rangle), \\
|\Gamma_{7,1/2}\rangle = \frac{1}{2} (|3/2\rangle - \frac{1}{2} |5/2\rangle), \\
|\Gamma_{7,-1/2}\rangle = \frac{1}{2} (|3/2\rangle - \frac{1}{2} |5/2\rangle).
\end{cases}
\]
(C-3)
In the following argument, we change their notations as
\[
\begin{align*}
\Gamma_{8,-3/2} & \rightarrow (m_1, \uparrow), \quad \Gamma_{8,3/2} \rightarrow (m_1, \downarrow), \\
\Gamma_{8,1/2} & \rightarrow (m_2, \uparrow), \quad \Gamma_{8,-1/2} \rightarrow (m_2, \downarrow); \\
\Gamma_{7,1/2} & \rightarrow (m_3, \uparrow), \quad \Gamma_{7,-1/2} \rightarrow (m_3, \downarrow).
\end{align*}
\]
(C-4)
In the same manner as that in eq. (B-3) for an impurity, the magnetic coupling between the \(\Gamma_1\) singlet ground (denoted by \([1]\)) and \(\Gamma = \Gamma_4, \Gamma_5\) triplet (+, 0 and – states denoted by \([2]\), \([3]\) and \([4]\), respectively) excited states is expressed by the following matrices:\(^{31}\)
\[
S_{+}^\Gamma = \begin{pmatrix} 0 & 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad C-8)
\]
For nonmagnetic coupling,
\[
Q_{+}^\Gamma = \begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad C-9)
\]
\[
Q_{+}^\Gamma = Q_{+}^\Gamma = \begin{pmatrix} 0 & 0 & 0 & -\sqrt{2} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \quad C-10)
\]
We note that the relative signs of the off-diagonal matrix elements are different between \(S_{+}^\Gamma\) (\(Q_{+}^\Gamma\)) for the pseudo-quartet and \(S_{+}^\Gamma\) (\(Q_{+}^\Gamma\)) for the \(S^\Gamma = 1\) pseudo-spin given in eq. (B-3) [in eq. (B-4)]. The singlet-triplet interchange processes are mediated by the corresponding \(\Gamma_8\) and \(\Gamma_7\) electron scatterings as follows:\(^{31}\)
\[
\psi_{m_3z_2}^{\Gamma} \psi_m = \frac{1}{2} (\psi_{m_1\uparrow}^{\Gamma} \psi_{m_3\uparrow} + \psi_{m_1\downarrow}^{\Gamma} \psi_{m_3\downarrow}) + H.c., \quad C-11)
\]
\[
\psi_{m_3z_2}^{\Gamma} \psi_m = \frac{1}{2} (\psi_{m_1\uparrow}^{\Gamma} \psi_{m_3\uparrow} + \psi_{m_1\downarrow}^{\Gamma} \psi_{m_3\downarrow}) \\
+ \frac{1}{2} (\psi_{m_2\uparrow}^{\Gamma} \psi_{m_3\uparrow} - \psi_{m_2\downarrow}^{\Gamma} \psi_{m_3\downarrow}) + H.c., \quad C-12)
\]
\[
\psi_{m_3z_2}^{\Gamma} \psi_m = \frac{1}{2} (\psi_{m_1\uparrow}^{\Gamma} \psi_{m_3\uparrow} + \psi_{m_1\downarrow}^{\Gamma} \psi_{m_3\downarrow}) + H.c., \quad C-13)
\]
\[
\psi_{m_3z_2}^{\Gamma} \psi_m = \frac{1}{2} (\psi_{m_1\uparrow}^{\Gamma} \psi_{m_3\uparrow} + \psi_{m_1\downarrow}^{\Gamma} \psi_{m_3\downarrow}) \\
+ \frac{1}{2} (\psi_{m_2\uparrow}^{\Gamma} \psi_{m_3\uparrow} - \psi_{m_2\downarrow}^{\Gamma} \psi_{m_3\downarrow}) + H.c., \quad C-14)
\]
\[
\psi_{m_3z_2}^{\Gamma} \psi_m = -\frac{1}{2} (\psi_{m_1\uparrow}^{\Gamma} \psi_{m_3\uparrow} + \psi_{m_1\downarrow}^{\Gamma} \psi_{m_3\downarrow}) + H.c., \quad C-15)
\]
\[
\psi_{m_3z_2}^{\Gamma} \psi_m = \frac{1}{2} (\psi_{m_1\uparrow}^{\Gamma} \psi_{m_3\uparrow} + \psi_{m_1\downarrow}^{\Gamma} \psi_{m_3\downarrow}) \\
+ \frac{1}{2} (\psi_{m_2\uparrow}^{\Gamma} \psi_{m_3\uparrow} - \psi_{m_2\downarrow}^{\Gamma} \psi_{m_3\downarrow}) + H.c., \quad C-16)
\]
\[
\psi_{m_3z_2}^{\Gamma} \psi_m = \frac{1}{2} (\psi_{m_1\uparrow}^{\Gamma} \psi_{m_3\uparrow} + \psi_{m_1\downarrow}^{\Gamma} \psi_{m_3\downarrow}) \\
+ 2 \sqrt{5} (\psi_{m_1\uparrow}^{\Gamma} \psi_{m_2\downarrow} - \psi_{m_1\downarrow}^{\Gamma} \psi_{m_2\uparrow}) \} + H.c., \quad C-17)
\]
\[
\psi_{m_3z_2}^{\Gamma} \psi_m = \frac{1}{2} (\psi_{m_1\uparrow}^{\Gamma} \psi_{m_3\uparrow} + \psi_{m_1\downarrow}^{\Gamma} \psi_{m_3\downarrow}) \\
+ \frac{1}{2} (\psi_{m_2\uparrow}^{\Gamma} \psi_{m_3\uparrow} + \psi_{m_2\downarrow}^{\Gamma} \psi_{m_3\downarrow}) \\
+ 4 \sqrt{5} (\psi_{m_1\uparrow}^{\Gamma} \psi_{m_2\downarrow} - \psi_{m_1\downarrow}^{\Gamma} \psi_{m_2\uparrow}) \}. \quad C-18)
\]
the transformation in eq. (72), the above multiorbital scattering operators are reduced to interband scattering operators. For the $Γ_4$ type,

$$ \psi_b^\dagger s^4 Γ_4 \psi_b = \psi_b^\dagger \frac{1}{2} \begin{pmatrix} 0 & 0 & u_{t+}^* & v_{t-}^* \\ 0 & 0 & u_{t-}^* & v_{t+}^* \\ u_{t+} & v_{t-} & 0 & 0 \\ v_{t+} & u_{t-} & 0 & 0 \end{pmatrix} \psi_b, $$  \hspace{1cm} (C-19)

$$ \psi_b^\dagger q^4 Γ_4 \psi_b = \psi_b^\dagger \frac{1}{2} \begin{pmatrix} 0 & 0 & \sqrt{3} u_{t+}^* & -u_{t-}^* \\ 0 & 0 & \sqrt{3} u_{t-}^* & -v_{t+}^* \\ u_{t+} & v_{t-} & 0 & 0 \\ -\sqrt{3} u_{t-} & -\sqrt{3 v_{t+}} & 0 & 0 \end{pmatrix} \psi_b, $$  \hspace{1cm} (C-20)

$$ \psi_b^\dagger q^4 Γ_4 \psi_b = \psi_b^\dagger \frac{1}{2} \begin{pmatrix} 0 & 0 & u_{t+}^* & v_{t-}^* \\ 0 & 0 & u_{t-}^* & v_{t+}^* \\ -u_{t+} & v_{t-} & 0 & 0 \\ -v_{t+} & u_{t-} & 0 & 0 \end{pmatrix} \psi_b, $$  \hspace{1cm} (C-21)

$$ \psi_b^\dagger q^4 Γ_4 \psi_b = \psi_b^\dagger \frac{1}{2} \begin{pmatrix} 0 & 0 & -\sqrt{3} u_{t+}^* & v_{t-}^* \\ 0 & 0 & -\sqrt{3} u_{t-}^* & v_{t+}^* \\ -u_{t+} & v_{t-} & 0 & 0 \\ -v_{t+} & u_{t-} & 0 & 0 \end{pmatrix} \psi_b, $$  \hspace{1cm} (C-22)

where $(v_+, v_-)$, which appears as the common factor in each matrix element, has been omitted. For the $Γ_5$ type, $s^4 Γ_5$ is obtained by switching the indices as $1 \leftrightarrow 2$ in the $s^4 Γ_4$ matrix, and $u^4 Γ_5$ by replacing $\sqrt{3} \rightarrow -\sqrt{3}$ in addition to switching $1 \leftrightarrow 2$ in the $s^4 Γ_4$ matrix; $q^4 Γ_5$ and $q^4 Γ_5$ are obtained from $q^4 Γ_5$ and $q^4 Γ_5$, respectively, in the same manner. We note that $s^4 Γ_5$ in eq. (C-19) is comparable to $\hat{U}_{mn}$ in eq. (40) if $u_{t+} = u_{t-} = u_{t+}^* = u_{t-}^*$ and $v_{t+} = v_{t-}$ are taken; $q^4 Γ_5$ in eq. (C-21) is comparable to $\hat{U}_{mn}$ in eq. (46) for $u_{t+} = u_{t-} = u_{t+}^* = u_{t-}^*$ and $v_{t+} = v_{t-} = 0$. These scatterings, whichever is magnetic or nonmagnetic, contribute to $T_c$ enhancement in the $s_+ \pm s_-$ wave state. As discussed in §3.3, whether $T_c$ is enhanced or suppressed by the interband scattering for the $s_+ \pm s_-$ wave and also for the $s_+ \pm s_-$ wave depends on the details of electron transfer, $u_{t\sigma}$ and $v_{i\sigma}$, between the $f$-orbitals and conduction bands at an impurity. As in eq. (B-7), we introduce the impurity interaction Hamiltonian for the singlet-triplet configuration for the $Γ = Γ_4, Γ_5$ scattering,

$$ \mathcal{H}_i = \sum_{X=S,Q} \sum_{R, \gamma} \sum_{m n} \int dr \rho_{\gamma m}^a \rho_{\gamma n}^a \delta(r - R_\gamma) \times \left[ \Psi^\dagger(r) J^X_X \left( X^\dagger_{\gamma m} X^\gamma_{\gamma n} \right) + \frac{1}{2} \left( X^\dagger_{\gamma m} X^{-\gamma}_{\gamma n} + X^\gamma_{\gamma m} X^{-\gamma}_{\gamma n} \right) \right] \Psi(r), $$  \hspace{1cm} (C-23)

where the band electron scattering operators

$$ S^{\Gamma} = s^{\Gamma}, \hspace{1cm} Q^{\Gamma} = q^{\Gamma}, $$  \hspace{1cm} (C-24)

are rewritten on the basis of the eight-dimensional vector $\Psi$ in eq. (B-8).