Effect of inelastic scattering on the
nuclear magnetic relaxation rate $1/T_1 T$ in
iron-based superconductors

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Abstract
We present a microscopic study of the nuclear magnetic relaxation rate $1/T_1$ based on the five-orbital model for iron-based superconductors. We mainly discuss the effect of the ‘inelastic’ quasi-particle damping rate $\gamma$ due to many-body interaction on the size of the coherence peak, for both $s^{++}$ and $s^\pm$-wave superconducting states. We focus on Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$, and systematically evaluate $\gamma$ in the normal state from the experimental resistivity, from optimally to overdoped compounds. Next, $\gamma$ in the superconducting state is calculated microscopically based on second-order perturbation theory. In optimally doped compounds ($T_c \sim 30$ K), it is revealed that the coherence peak on $1/T_1 T$ is completely suppressed due to large $\gamma$ for both $s^{++}$ and $s^\pm$-wave states. On the other hand, in heavily overdoped compounds with $T_c < 10$ K, the coherence peak could appear for both pairing states, since $\gamma$ at $T_c$ is quickly suppressed in proportion to $T_c^2$. By making careful comparison between theoretical and experimental results, we conclude that it is difficult to discriminate between $s^{++}$ and $s^\pm$-wave states from the present experimental results.

(Some figures may appear in colour only in the online journal)

1. Introduction
Since the discovery of superconductivity in LaFeAsO$_{1-x}$F$_x$ [1], the superconducting mechanism and paring symmetry had been discussed intensively. In many optimally doped compounds, the superconducting gap is fully gapped, as reported by penetration depth measurement [2] and angle-resolved photoemission spectroscopy (ARPES) [3, 4]. As for the superconducting mechanism, s-wave pairing with a sign change of the order parameter between the hole and electron Fermi pockets, the so called $s_{\pm}$-wave, mediated by the anti-ferromagnetic fluctuation had been proposed from the early stages as a possible pairing state in the iron pnictides [5–9]. It is supported by quasi-particle interference analysis by scanning tunneling microscopy/spectroscopy (STM/STS) measurement by Hanaguri et al [10]. However, the small $T_s$-suppression against nonmagnetic impurities is not consistent with the $s_{\pm}$-wave state [11–15].

On the other hand, an orbital fluctuation mediated s-wave superconducting state without sign reversal ($s^{++}$-wave state) had been investigated [16]. We have shown that strong ferro- and anti-ferro-orbital fluctuations develop due to the combination of Coulomb and e–ph interactions [17–21]. Consistently, a large softening of the shear modulus $C_{66}$ [22–24] and the renormalization of phonon velocity [25] are observed well above the orthorhombic structure transition temperature $T_s$. These phenomena strongly suggest the existence of strong ferro-orbital (charge quadrupole $O_{2z^2-r^2}$) fluctuations, considering the large strain–quadrupole coupling[19–21]. In addition, an experimental ‘resonance-like’ hump structure in the neutron inelastic scattering is well reproduced in terms of the $s^{++}$-wave state [26, 27].

The nuclear magnetic resonance (NMR) and the nuclear-quadrupole resonance (NQR) measurements are useful for the discussion of the pairing symmetry. The coherence effect of superconductivity, appearing as a Hebel–Slichter
peak (coherence peak) in the nuclear spin relaxation rate
(1/T₁), was one of the crucial experimental proofs of the
Bardeen–Cooper–Schrieffer (BCS) theory, characterized by
conventional s-wave Cooper pairs with an isotropic gap [28].
In the Fe-based superconductors, many experimental results of
1/T₁ have been published [29–35]. It was found that the
coherence peak in 1/T₁ is absent in many compounds,
such as electron-doped Ba(Fe₁₋ₓC₀ₓ)₂As₂ and hole-doped
Ba₁₋ₓKₓFe₂As₂.

The size of the coherence peak had attracted great
attention to distinguishing between s± and s²-wave states: in
a simple BCS theory, the peak size is larger in the s±-wave
state, while it is reduced in the s²-wave state. However, the
coherence peak is suppressed by the ‘inelastic’ quasi-particle
damping rate γ, which is prominent in moderately and
strongly correlated systems [36, 37]. For this reason, the
coherence peak is not observed even in several conventional
s-wave superconductors with Tc > 15 K, such as boron
carbide Y₁₁₂B₂C [38] and A-15 compounds V₃Si [39]. Thus,
inelastic scattering due to many-body effects has to be taken
into account for a quantitative analysis of 1/T₁.

The impurity effect (=‘elastic’ quasi-particle damping
effect) on Tc and 1/T₁ is also important in studying the
pairing symmetry. In the s±-wave state, both Tc and 1/T₁
are insensitive to impurities. In contrast, the s²-wave state
is easily suppressed by impurities like the d-wave state,
according to the study based on the five-orbital model [15].
The impurity-induced gapless state in the s²-wave state
would give strong influence on 1/T₁ for T ≪ Tc [7, 40, 41]. However, an impurity-induced gapless state is
realized only when Tc is strongly suppressed to be ∼3Tc/2
theoretically [42]. Thus, gapless behavior of 1/T₁ for T ≪ Tc
observed in some compounds cannot be explained by this
scenario.

Recently, the authors in [43] and [44] had shown that the
coherence peak in the s±-wave state disappears when
inelastic scattering γ at Tc is as large as the superconducting
gap at T = 0. However, quantitative estimations of γ and its
T and ω dependences are still lacking. Interestingly, a recent
NMR measurement reports a small coherence peak of 1/T₁
in the heavily overdoped LaFe₄AsO₁₋ₓFₓ, with low transition
temperature Tc ∼ 5 K [35]. Now, microscopic study of 1/T₁
by including an inelastic scattering effect is desired to discuss
the superconducting pairing state as s± or s±±.

In this paper, we investigate the effect of inelastic
scattering rate γ on the nuclear magnetic relaxation rate 1/T₁
for both s±± and s±-wave states. For a quantitative discussion
on the existence of the Hebel–Slichter coherence peak, we
employ the two-dimensional five-orbital model [5]. Here, γ
is the key parameter of the present study: at Tc, the value of γ
is carefully estimated from the experimental conductivity [27],
and its temperature and the frequency dependences below
Tc are obtained by the second-order perturbation theory. All
results shown below are obtained with band filling n = 6.1.

The contents of this paper are as follows: in section 2,
we explain how to calculate the nuclear magnetic relaxation
rate 1/T₁T and quasi-particle damping γ. The obtained
numerical results are explained in section 3. Finally, we make

\[ \gamma(T, \omega) = \text{constant} \]

a comparison between theoretical and experimental results in
section 4, and discuss the possible pairing symmetry.

2. Formulation

2.1. Green function

Now, we study the 10 × 10 Nambu BCS Hamiltonian \( \hat{H}_{10} \)
composed of the five-orbital tight-binding model [5] and the
band-diagonal SC gap [15]. The Hamiltonian is given by

\[ \hat{H}_{10}^0 = \sum_k \epsilon_k \hat{c}_k^\dagger \hat{c}_k, \]  

where \( \hat{c}_k^\dagger \) and \( \hat{c}_k \) are vectors,

\[ \epsilon_k = \{ \epsilon_{1,k,\uparrow}, \ldots, \epsilon_{5,k,\uparrow}, \epsilon_{1,k,\downarrow}, \ldots, \epsilon_{5,k,\downarrow} \}, \]

and \( \epsilon_{a,k,\sigma} (\epsilon_{a,k,\sigma}^\dagger) \) is a creation (annihilation) operator of an
electron for band \( \sigma \) with wavevector \( k \) and spin \( \sigma \). \( \hat{H}_{10}^0 \)
is the 10 × 10 Nambu BCS Hamiltonian given as

\[ \hat{H}_{10}^0 = \left( \hat{H}_k - \hat{\Delta}_k \right), \]

where \( \hat{H}_k \) and \( \hat{\Delta}_k \) are 5 × 5 matrices in the band-diagonal basis,

\[ \hat{H}_k = \begin{pmatrix} \epsilon_{1,k} & 0 \\ 0 & \epsilon_{5,k} \end{pmatrix}, \]

\[ \hat{\Delta}_k = \begin{pmatrix} \Delta_{1,k} & 0 \\ 0 & \Delta_{5,k} \end{pmatrix}, \]

where \( \epsilon_{a,k} \) and \( \Delta_{a,k} \) are a dispersion and a gap function of
quasi-particle for \( a \) and \( k \), respectively. Figure 1 shows the
Fermi surface (1 Fe atom/unit cell) for electron-doped iron
pnictides. Fermi surface $\alpha_1$ and $\alpha_2$ around the $\Gamma$ point are hole pockets and $\alpha_3$ and $\alpha_4$ are electron pockets. Hereafter, we approximate $\Delta_{\alpha,k}$ as follows:

$$
\Delta_{\alpha,k} \approx \Delta_0 \tanh \left( \frac{\pi}{2} \frac{T_c}{T} - 1 \right),
$$

(5)

where $\Delta_0$ is a superconducting gap at zero temperature and, in the present work, we assume that the superconducting gaps for each band are $k$-independent.

The $10 \times 10$ Green’s function $\hat{G}_k$ in the Nambu representation is given by [45]

$$
\hat{G}_k(i\omega_n) = \left( i\omega_n - \epsilon_{\alpha,k} - \underline{\Sigma}_k(i\omega_n) \right)^{-1},
$$

(6)

where $\omega_n = \pi T (2n + 1)$ is the fermion Matsubara frequency. The normal self-energy $\underline{\Sigma}_k(i\omega_n)$ represents the inelastic quasiparticle damping and mass enhancement due to many-body interactions. We neglect the impurity-induced self-energy since it does not change the density of states (DOS) in a simple s-wave state, equation (5) (Anderson theorem). When $\underline{\Sigma}_k(i\omega_n)$ has band-diagonal form, equation (6) also becomes a band-diagonal form, and the Green’s function for band $\alpha$ is given by a $2 \times 2$ matrix,

$$
\hat{G}_{\alpha,k}(i\omega_n) = \left( i\omega_n - \epsilon_{\alpha,k} - \Sigma_{\alpha,k}(i\omega_n) \right)^{-1},
$$

(7)

where $|\hat{G}_{\alpha,k}(i\omega_n)|^{-1}$ is the determinant of the inverse matrix of the Green’s function, and $G_{\alpha,k}$, $F_{\alpha,k}$ and $\Sigma_{\alpha,k}$ are the normal Green’s function, the anomalous Green’s function and the normal self-energy for band $\alpha$ with wavevector $k$, respectively. The local Green’s function $\hat{g}_\alpha$ is obtained by the $k$ summation;

$$
\hat{g}_\alpha(i\omega_n) = \frac{1}{N} \sum_k \hat{G}_{\alpha,k}(i\omega_n) = \int_{-\infty}^{\infty} d\epsilon N(\epsilon) \hat{G}_\alpha(\epsilon, i\omega_n),
$$

(8)

where $N(\epsilon)$ is the quasi-particle DOS. In this $\epsilon$ integral, the dominant contribution comes from the explicit $\epsilon$ term of the denominator $|\hat{G}_{\alpha,k}(i\omega_n)|^{-1}$. By neglecting the $\epsilon$ dependence of $N(\epsilon)$ and applying the infinite dimensional approximation for $\Sigma_{\alpha}(\epsilon, i\omega_n)$ (see the following section 2.3), we obtain

$$
\hat{g}_\alpha(i\omega_n) \approx \frac{-\pi N(0)}{\sqrt{\omega_0(i\omega_n)^2 + \Delta_0^2}} \left( \begin{array}{cc} \omega_0(i\omega_n) & \Delta_0 \\ \Delta_0 & \omega_0(i\omega_n) \end{array} \right) \left( \begin{array}{c} \Delta_0 \\ \omega_0(i\omega_n) \end{array} \right) = \left( \begin{array}{cc} g_{\alpha}(i\omega_n) & f_{\alpha}(i\omega_n) \\ f_{\alpha}(i\omega_n) & g_{\alpha}(i\omega_n) \end{array} \right),
$$

(9)

From the five-orbital model, the total DOS per spin is $N(0) = 0.66$ eV$^{-1}$ at Fermi level. Then, analytic continuation ($i\omega_n \rightarrow \omega = \omega + i\delta$) yields the retarded Green’s function as follows,

$$
g_{\alpha}^R(\omega) = -\frac{\pi N(0) \omega_{\alpha}^R(\omega)}{\sqrt{-\omega_{\alpha}^R(\omega)^2 + \Delta_0^2}},
$$

$$
f_{\alpha}^R(\omega) = -\frac{\pi N(0) \Delta_0}{\sqrt{-\omega_{\alpha}^R(\omega)^2 + \Delta_0^2}},
$$

(10)

where $\omega_{\alpha}^R(\omega)$ is defined as

$$
\omega_{\alpha}^R(\omega) = \omega - i \text{Im} \Sigma_{\alpha}^R(\omega)
$$

(11)

and

$$
\gamma^* = \frac{m^*}{m} \gamma.
$$

(12)

The mass enhancement factor $m^*/m$ is given by

$$
\frac{m^*}{m} = 1 - \lim_{\omega \to 0} \frac{\partial \text{Re} \Sigma_{\alpha}^R(\omega)}{\partial \omega},
$$

(13)

which is reported as 1–3 for iron pnictides, called 1111 and 222 systems, from various experiments such as de Haas–van Alphen measurements [46–48], optical spectral weight [49], and Seebeck effect with specific heat [50]. The mass enhancement factor has a relatively large value in the optimally doped systems and gradually decreases with carrier doping.

2.2. Nuclear magnetic relaxation rate

The nuclear magnetic relaxation rate $1/T_1$ in the superconducting state is given by the standard formula:

$$
\frac{1}{T_1} \propto \frac{1}{N} \sum_{\alpha, q} \lim_{\omega \to 0} \text{Im} \chi_{\alpha}^R(q, \omega),
$$

(14)

where $\chi_{\alpha}^R(q, \omega)$ is the superconducting spin susceptibility and given by

$$
\text{Im} \chi_{\alpha}^R(q, \omega) = \frac{1}{2\pi N} \sum_{\beta, k} \int_{-\infty}^{\infty} d\omega' \left( \tanh \frac{\omega + \omega'}{2T} - \tanh \frac{\omega'}{2T} \right) \times \left( \text{Im} C_{\beta, k+q, \omega}^{R}(\omega + \omega') \text{Im} C_{\alpha, k}^{R}(\omega') + \text{Im} F_{\beta, k+q, \omega}^{R}(\omega + \omega') \text{Im} F_{\alpha, k}^{R}(\omega') \right).
$$

(15)

In equation (14), the limitedime becomes a differential of the hyperbolic tangent and each summation of $\alpha$, $\beta$, $k$ and $q$ can be calculated independently. Then, $1/T_1$ becomes

$$
\frac{1}{T_1} \propto \int_{-\infty}^{\infty} d\omega \frac{\text{Im} \chi_{\alpha}^R(\omega)^2 + \text{Im} F_{\alpha, k}^{R}(\omega)^2}{4\pi T \cosh^2(\omega/2T)} = \int_{-\infty}^{\infty} d\omega X(\omega),
$$

(16)
with
\[ g^R(\omega) = \sum_a g^R_a(\omega), \quad f^R(\omega) = \sum_a f^R_a(\omega), \]  
(17)
where the integrand of \( \omega \) was defined as \( \chi(\omega) \).

### 2.3. Second-order perturbation theory

A quasi-particle excitation is well defined if the damping rate \( \gamma \) is small compared to the energy scale. In this case, the quasi-particle damping rate \( \gamma \) can generally be computed from the imaginary part of the self-energy [51].

\[ \text{Im} \Sigma^R_k(\omega) = -\gamma_k(\omega). \]  
(18)

By using the second-order perturbation theory, we derive the microscopic model of \( \gamma \) and analyze the NMR experimental result. We calculate the electron-electron scattering based on the single band Hubbard model for simplicity. From the second-order perturbation theory, the self-energy \( \Sigma_k \) due to the electron-electron scattering is given by

\[ \Sigma_k(i\omega_n) = (V^2_{\text{eff}} T/N) \sum_{k,x} G^R_{k} (i\omega_n) \chi^{0 \rightarrow 0}_{k-k'} (i\omega_n - i\omega_n'), \]  
(19)
where \( V_{\text{eff}} \) is the effective electron-electron interaction enhanced by spin and orbital fluctuations. Its value can be estimated from the observed conductivity in section 2.4. The imaginary part of the retarded self-energy, which is obtained by the analytic continuation, is given by

\[ \text{Im} \Sigma^R_k(\omega) = \frac{V^2_{\text{eff}}}{2\pi N} \sum_k \int_{-\infty}^{\infty} \text{d} \omega' \left( \tanh \frac{\omega'}{2T} + \coth \frac{\omega - \omega'}{2T} \right) \times \text{Im} G^R_{k} (\omega') \text{Im} \chi^{0 \rightarrow 0}_{k-k'} (\omega - \omega'), \]  
(20)
where the superscript ‘0’ on the Green function and susceptibility means the absence of self-energy correction.

In the infinite dimensional approximation, then each summation of wavevectors can be taken independently and we obtain the quasi-particle damping rate due to the electron-electron scattering as

\[ \gamma(\omega) = \frac{1}{N} \sum_k \gamma_k(\omega) = -\frac{1}{N} \sum_k \text{Im} \Sigma_k(\omega) \]
\[ = -\frac{V^2_{\text{eff}}}{2\pi} \int_{-\infty}^{\infty} \text{d} \omega' \left( \tanh \frac{\omega'}{2T} + \coth \frac{\omega - \omega'}{2T} \right) \times \text{Im} G^R_{k} (\omega') \text{Im} \chi^{0 \rightarrow 0}_{k-k'} (\omega - \omega'), \]  
(21)
with bare susceptibility,

\[ \text{Im} \chi^{0 \rightarrow 0}_{k-k'} (\omega - \omega') = \frac{1}{2\pi} \int_{-\infty}^{\infty} \text{d} \omega' \left( \tanh \frac{\omega + \omega'}{2T} - \tanh \frac{\omega'}{2T} \right) \times \text{Im} G^R_{k} (\omega + \omega') \text{Im} G^R_{k} (\omega') \]
\[ + \text{Im} G^R_{k} (\omega + \omega') \text{Im} G^R_{k} (\omega'). \]  
(22)

To see the role of coherence factor, we rewrite the imaginary part of the Green’s functions with \( \text{Im} G^R_{k} (\omega) = -\frac{\pi}{2}\delta(\omega - E_k) \) and \( \text{Im} G^R_{k} (\omega) = -\frac{\pi}{2}\delta(\omega - E_k) - \delta(\omega + E_k) \) where \( E_k = \sqrt{\epsilon_k^2 + \Delta^2} \). By neglecting the energy dependence of the DOS near the Fermi level, we obtain another notation of the self-energy as

\[ \text{Im} \Sigma^R_k(\omega) = \frac{\pi V^2_{\text{eff}}}{8N^2} \sum_{k'} \sum_{\epsilon} \frac{\cosh \frac{\omega}{2T}}{\cosh \frac{E_k - \epsilon - \Delta^2}{2T} \cosh \frac{E_k + \epsilon + \Delta^2}{2T}} \times \left[ \delta(\omega - |E_k - \epsilon - \Delta^2|) \times \frac{\Delta_k - \Delta^2}{\Delta_{k' + \Delta^2}} \right]. \]  
(23)
For \( T \ll T_c \), the first term with the coherence factor \( (1 + \Delta^2/|E'|) \) gives the dominant contribution for the s++-wave state. At \( T = 0 \), because of the thermal factor, the self-energy becomes

\[ \text{Im} \Sigma^R_k(\omega) \approx -\frac{\pi V^2_{\text{eff}}}{8N^2} \sum_{k'} \sum_{\epsilon} \left( 1 - \frac{\Delta_k - \Delta^2}{\Delta_{k' + \Delta^2}} \right) \times \delta(|\omega| - |E_k' + \epsilon - \Delta^2|) \]  
(24)
It is clear from the delta function that it equals 0 for \( \omega < 3\Delta_{\text{min}} \).

Experimental studies on the iron pnictides, such as ARPES [52], point-contact tunneling [53], NQR [31] and specific heat [54] have demonstrated that there are at least two different superconducting gaps, small gap \( \Delta_S \) and large gap \( \Delta_L \). Multi-gap superconductivity has been seen in a number of systems, including MgB\(_2\), which is an s-wave superconductor with a \( T_c \) of 39 K [55, 56]. Based on these experiments, we set the small and large superconducting gaps as

\[ \Delta^0_{\text{as}} = \Delta^0_{\text{as}} = \Delta_S, \quad \Delta^0_{\text{as}} = \Delta^0_{\text{as}} = \pm \Delta_L, \]  
(25)
Hereafter, we employ these values as \( 2\Delta_L/T_c = 5 \) and \( 2\Delta_L/T_S = 3 \), which are approximately satisfied in various Co-doped 122 systems according to the specific heat measurements [57].

Figure 2(a) shows the temperature dependence of \( \tilde{\gamma} \equiv \gamma / V^2_{\text{eff}} \tilde{T}^2 \) on the s++-wave superconducting state at various frequencies. The \( T \) dependence of \( \tilde{\gamma} \) is small in the normal state \( (T > T_c) \), but \( \tilde{\gamma} \) rapidly decreases with decreasing \( T \) in the superconducting state \( (T < T_c) \). Figure 2(b) shows the \( \omega \)-dependence of \( \tilde{\gamma} \). Two vertical dotted lines show the small and large superconducting gaps at zero temperature \( \Delta_S \) and \( \Delta_L \), respectively. In the normal state, \( \tilde{\gamma} \) is large due to the strong correlation. However, \( \tilde{\gamma} \) is strongly suppressed in the superconducting state since the inelastic damping \( \tilde{\gamma} \) is
reduced as the superconducting gap opens. It is satisfied that $\gamma(\omega)\big|_{T=0} = 0$ for $\omega < 3\Delta_S = \Delta_L$.

Figures 3(a) and (b) show the $T$ and $\omega$ dependences of $\tilde{\gamma}$ on the $s_{\pm}$-wave superconducting state, respectively. As is the case in $s_{++}$, $\tilde{\gamma}$ is strongly suppressed for $T < T_c$. The obtained quasi-particle damping for the $s_{\pm}$-wave state is similar to the $s_{++}$-wave state.

2.4. Quasi-particle damping

In this section, we estimate the absolute value of the inelastic damping rate $\gamma(0)$ in the normal state, which thus yields the effective interaction $V_{\text{eff}}$, from the experimentally observed resistivity. From the Nakano–Kubo formula, the conductivity is given by

$$\sigma = \frac{e^2}{4\pi c} \sum_\alpha \int_{FS_\alpha} dk \frac{|v_{\alpha,k}|}{2\gamma(0)},$$

(26)

where $\gamma(0)$ is the ‘unrenormalized’ damping at zero energy, and $v_{\alpha,k}$ is the Fermi velocity at $k$ on the $\alpha$ th Fermi surface. Here, we neglect the current vertex correction since it is not important for the diagonal conductivity [58]. $\gamma(0)$ is derived from the theoretical relation between $\rho(T)$ and $\gamma(0)$ [27],

$$\rho(T) - \rho(0) \approx \begin{cases} 0.0020\gamma(0) \ [\mu\Omega \text{cm}] & \text{for } c = 6 \ \text{Å} \\ 0.0028\gamma(0) \ [\mu\Omega \text{cm}] & \text{for } c = 8 \ \text{Å} \end{cases}.$$

(27)

The interlayer spacing $c \approx 6$ Å and $c \approx 8$ Å correspond to the 122 and 1111 systems, respectively. On the other hand, we solve equation (21) as a normal state ($\text{Im} f_{0,R}(\omega) = 0$) and the inelastic damping rate $\gamma(0)$ is represented as

$$\gamma(0)|_{T=T_c} = \frac{\pi^3}{2} V_{\text{eff}}^2 N(0)^3 T_c^2.$$

(28)
Then, the effective interaction $V_{\text{eff}}$ is derived by comparing equation (27) with (28).

In Table 1, we show $T_c$ and other parameters of Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$ for various doping rate $x$. The resistivity due to inelastic scattering, $\rho(T) - \rho(0)$, is estimated by fitting the experimental data below 150 K [59] with

$$\rho(T) = \rho(0) + aT^n,$$

where $\rho(0)$, $a$, and $n$ are free parameters. The obtained $\gamma = 69$ K for the optimally doped compound ($x = 0.08$) is larger than the transition temperature $T_c = 24$ K. On the other hand, $\gamma$ decreases rapidly with carrier doping, and $\gamma = 7.5$ K becomes smaller than $T_c = 11$ K for the overdoped compound ($x = 0.14$). The estimated effective interaction $V_{\text{eff}}$ is 17.7 eV for the optimally doped system, and 12.2 eV for the overdoped system. $V_{\text{eff}}$ is large as compared with the bare on-site Coulomb interaction $U = 2\sim3$ eV for 3d electrons on a Fe atom [60] because of the spin and charge Stoner enhancement that give large spin and orbital fluctuations.

### 3. Results

In Figures 4 and 5, we show the numerical results for the $T$ dependence of the nuclear spin relaxation rate for optimally and overdoping states, respectively. According to Table 1, the effective potential $V_{\text{eff}} = 17.7$ eV for optimally doped systems and $12.7$ eV for overdoped systems. The mass enhancement factors are $m^*/m = 2\sim3$ for optimally doped systems and $m^*/m = 1\sim2$ for overdoped systems [46–50]. Figures 4(a) and (b) show $1/T_1T$ in the $s_{++}$ and $s_{\pm}$-wave states for optimally doping with $T_c = 0.0025$ eV and $V_{\text{eff}} = 17.7$ eV. Solid and dashed lines represent $m^*/m = 2$ and $m^*/m = 3$, respectively. In this case, the Hebel–Slichter coherence peak is suppressed even in both the $s_{++}$ and $s_{\pm}$-wave states due to the strong inelastic quasi-particle damping $\gamma^*(0)/T_c = 1.0\sim1.5T_c$.

Figures 5(a) and (b) show $1/T_1T$ for overdoped systems ($T_c = 0.0010$ eV and $V_{\text{eff}} = 12.7$ eV) in $s_{++}$ and $s_{\pm}$-wave states, respectively. The coherence peak increases for smaller $V_{\text{eff}}$ since $\gamma$ is proportional to $V_{\text{eff}}^2$. Since the coherence peak is suppressed by $\gamma^* = (m^*/m)^2\gamma$, it is better restored by larger $m^*/m$. A small coherence peak is recognized in the overdoped $s_{++}$-wave state for $m^*/m = 2$. The insets of figure 5 show $1/T_1T$ for $T_c = 0.0005$ eV and $V_{\text{eff}} = 12.7$ eV. Since $\gamma$ decreases in proportion to $T_c^2$, a small coherence peak appears in both $s_{++}$ and $s_{\pm}$-wave states. These results indicate that the Hebel–Slichter coherence peak on $1/T_1T$ might be observed for a sample with $T_c \sim 5$ K, as reported in [35].

We discuss the Hebel–Slichter peak in both $s_{++}$ and $s_{\pm}$-wave states. We show the $\omega$ dependences of $X(\omega)$ (defined in equation (16)), $N^p(\omega)$ and $N^p(\omega)$ for overdoped systems ($T_c = 0.0005$ eV, $V_{\text{eff}} = 12.7$ eV and $m^*/m = 2$) in Figures 6(a), (b), and (c), respectively. The integral of $X(\omega) = \pi(N^p(\omega)^2 + N^p(\omega)^2)(-\frac{\partial f}{\partial \omega})(\omega = m^*/m)$ yields $1/T_1T$. Two peaks in $X(\omega)$ at $T_c = 0.97T_c$ correspond to two superconducting gaps $\Delta_s$ and $\pm\Delta_t$. These peaks yield the Hebel–Slichter peak in the inset of figure 5. For the $s_{\pm}$-wave state, the sign of $N^p$ reverses at

### Table 1. $T_c$ and other parameters of Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$ for various doping rate $x$ [59]. $\gamma(0)$ is estimated by fitting the experimental data and $V_{\text{eff}}$ is obtained by $\gamma(0)$ and $N(0) = 0.66$ eV$^{-1}$. We note that we obtain $n = 1.0$ and $a = 0.035$ $\mu\Omega$cm$^{-1}$ for $x = 0.08$ according to the measurement by Sefat et al [61]. In this case, we obtain $V_{\text{eff}} = 19.9$ eV. In this table, the units of $a$ and $\gamma$ are $\mu\Omega$cm and $\mu\Omega$cm$^{-1}$, respectively.

| $x$ | 0.08 | 0.12 | 0.14 | 0.20 |
|-----|------|------|------|------|
| $T_c$ (K) | 24 | 17 | 11 | — |
| $\rho(0)$ ($T_c$) | 73 | 65 | 65 | 57 |
| $\rho(T_c) - \rho(0)$ | 11.9 | 4.6 | 1.3 | — |
| $\gamma$ | 0.495 | 0.153 | 0.045 | 0.0011 |
| $n$ | 1.0 | 1.2 | 1.4 | 2.0 |
| $\gamma(0)/T_c$ | 0.0059 | 0.0023 | 0.00065 | — |
| $\gamma(0)/T_c$ | 0.0059 | 0.0023 | 0.00065 | — |
| $V_{\text{eff}}$ | 17.7 | 15.5 | 12.7 | 4.3 |

Figure 4. The normalized nuclear relaxation rate $(1/T_1T)/(1/T_1T)_{|\gamma=0}$ for the optimal doping state ($T_c = 0.0025$ eV and $V_{\text{eff}} = 17.7$ eV) in the (a) $s_{++}$ and (b) $s_{\pm}$-wave states as a function of reduced temperature $T/T_c$. Solid and dashed lines represent $m^*/m = 2$ and $m^*/m = 3$, respectively.
To summarize, we investigate the nuclear magnetic relaxation.

**4. Summary and discussion**

To summarize, we investigate the nuclear magnetic relaxation rate $1/T_1 T$ for both $s_{++}$ and $s_{\pm}$-wave states based on the five-orbital model. The inelastic quasi-particle damping rate $\gamma$ at $T_c$ is estimated from the experimental results of the resistivity, and $T$ and $\omega$ dependences of $\gamma$ are calculated using the second-order perturbation theory.

Using parameters for optimally doped systems, the Hebel–Slichter coherence peak on $1/T_1 T$ is suppressed due to the strong $\gamma^*(0)|_{T_c} \sim T_c$ even in the $s_{++}$-wave state for $T \geq 10$ K. This result is consistent with previous strong coupling theories [36, 37]. On the other hand, the relation $\gamma^*(0)|_{T_c} \ll T_c$ is expected in heavily overdoped systems with $T_c \sim 5$ K; in this case, a coherence peak may appear for both pairing states. Note that the tiny coherence peak in figure 5(b) in the $s_{\pm}$-wave state grows comparable to that in figure 5(a) in the $s_{++}$-wave state by halving the value of $\gamma^*(0)$. Thus, the condition for the appearance of a coherence peak is similar for both $s_{++}$ and $s_{\pm}$-wave states, so it is difficult to discriminate between these pairing states from the present NMR experimental data.

In [43, 44], the authors measured $1/T_1$ and discussed the effect of $\gamma$ on the coherence peak. They assumed the functional form $\gamma(\omega) = \gamma(0)|_{T=0} \exp[A(T/T_c - 1)]$ ($\omega$ dependence was neglected), chose parameters $A = 5$ and $\gamma^*(0)|_{T_c} = 3T_c$, and found that the coherence peak disappears even in the $s_{++}$-wave state. The large damping $\gamma(0)|_{T_c} = 3T_c$ is comparable to our estimation (1.0–1.5T_c) for optimum doping systems, so their analysis is consistent with the present study.

In this paper, we discussed only Co-doped Ba122 systems, since reliable resistivity data in single crystals are available. The coherence peak is also absent in LiFeAs ($c = 6.36$ Å, $T_c = 17$ K) [62]. In this compound, the resistivity is fitted as $\rho(T) = \rho(0) + aT^2$ and $a = 0.022 \, \mu\Omega\text{cm} \, \text{K}^{-2}$ in [63]. Then, the obtained effective potential is $V_{\text{eff}} = 15.9$ meV, which is comparable to the value of optimally doped Ba(Fe, Co)\textsubscript{2}As\textsubscript{2} (17.5 meV). Therefore, if we assume the gap structure given by ARPES measurements ($\Delta_L \sim \Delta_S \sim 3$ meV) [64, 65] the coherence peak disappears even for the $s_{++}$-wave state. However, since the sizes of each hole-pocket in LiFeAs [64, 65] are different from that in Ba(Fe, Co)\textsubscript{2}As\textsubscript{2}, more realistic tight-binding model for LiFeAs would be required for a quantitative analysis.

In LaFeAsO\textsubscript{1−x}F\textsubscript{x}, we cannot estimate $\gamma$ quantitatively because of the lack of resistivity data in single crystals. For a qualitative analysis, however, we can roughly estimate the single crystal resistivity of LaFeAsO\textsubscript{1−x}F\textsubscript{x} from the polycrystal resistivity in [66] by multiplying the factor 1/3, as discussed in [11]. Using this method, we can fit them by using $\rho(T) = \rho(0) + aT^2$ and obtain $\gamma(0)|_{T_c} = 0.0023$ eV and $V_{\text{eff}} \sim 10.2$ eV for LaFeAsO\textsubscript{0.89}F\textsubscript{0.11} ($T_c = 26$ K). Using these parameters, the Hebel–Slichter coherence peaks for optimally doped La1111 systems are also suppressed in both $s_{++}$ and $s_{\pm}$-wave states.

In both LiFeAs and La1111, conventional Fermi liquid resistivity ($\rho \propto T^2$) is observed. This fact would be consistent with the small spin fluctuations in these compounds. However, $\gamma$ at $T_c$ is large enough to suppress the coherence peak. Thus, both compounds are strongly correlated Fermi liquids due to relatively local fluctuations. In Sm1111 and Nd1111 ($T_c > 50$ K), $T$-linear-type behavior of resistivity is observed, indicating the enhancement of fluctuations as the $\text{As}_4$ tetrahedron approaches a regular tetrahedron [18].

Figure 5. The normalized nuclear relaxation rate $(1/T_1 T)/(1/T_1 T_f)^{1/2}$ for the overdoped state ($T_c = 0.0010$ eV and $V_{\text{eff}} = 12.7$ eV) in the (a) $s_{++}$ and (b) $s_{\pm}$-wave states as a function of reduced temperature $T/T_c$. Solid and dashed lines represent $m^*/m = 1$ and $m^*/m = 2$, respectively. $1/T_1 T$ for $T_c = 0.0005$ eV and $V_{\text{eff}} = 12.7$ eV are shown in the insets.
We stress that the inelastic scattering $\gamma$ also plays important roles in the neutron scattering spectrum: In neutron magnetic scattering measurements, a broad ‘resonance-like’ peak structure is observed in many FeAs superconductors below $T_c$; this fact had been frequently ascribed to the resonance due to the gap sign change. However, the ‘resonance condition’ is not surely confirmed since it is difficult to determine the gap size accurately. The resonance condition in FeAs superconductor is $\omega_{\text{res}} < \Delta_L + \Delta_S$, where $\omega_{\text{res}}$ denotes the peak energy of neutron scattering. In the following, we write down the experimental values of $\omega_{\text{res}}$, $\Delta_L$ and $\Delta_S$.

(A) BaFe$_{1.85}$Co$_{0.15}$As$_2$: $\omega_{\text{res}} = 10$ meV by neutron [67]
* Specific heat [54]:
  $\Delta_L = 5$ meV, $\Delta_S = 2$ meV: $\Delta_L + \Delta_S = 7$ meV.
* Penetration depth [68]:
  $\Delta_L = 6.1$ meV, $\Delta_S = 2.3$ meV: $\Delta_L + \Delta_S = 8.4$ meV.
* ARPES [69]:
  $\Delta_L = 6.6$ meV, $\Delta_S = 5$ meV: $\Delta_L + \Delta_S = 11.6$ meV.
(B) FeTe$_{0.6}$Se$_{0.4}$: $\omega_{\text{res}} = 7$ meV by neutron [70].
* ARPES [71]:
  $\Delta_L = 4.2$ meV, $\Delta_S = 2.5$ meV: $\Delta_L + \Delta_S = 6.7$ meV.

In case (A), the resonance condition $\omega_{\text{res}} < \Delta_L + \Delta_S$ is satisfied only by ARPES data. In case (B), although ARPES tends to report a larger gap size in FeAs superconductors, the resonance condition is still unclear.

Theoretically, we have revealed that a broad hump structure at $\omega \sim \Delta_L + \Delta_S$ can appear even in the $s_{\pm}$-wave state, not due to the resonance but due to strong suppression of the inelastic quasi-particle scattering rate $\gamma(\omega)$ for $|\omega| < 3\Delta$ ('dissipation-less mechanism' [26, 27]). Thus, both the absence of the coherence peak in $1/T_1$ as well as the hump structure in the neutron scattering spectrum are explained by the same many-body effect—inelastic quasi-particle scattering—using a similar inelastic scattering rate $\gamma(0)$ as evaluated from the resistivity.

Finally, we comment that large inelastic scattering $\gamma$ at $T_c$ in Fe-based superconductors also works as the depairing effect. In the random-phase-approximation (RPA), in which the depairing effect due to inelastic scattering is neglected, the obtained $T_c$ is about 200 K [5, 16]. However, in the fluctuation-exchange (FLEX) approximation, the obtained $T_c$ is strongly suppressed (below 50 K) due to the depairing effect (self-energy correction) [17].

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