Nuclear spin-lattice relaxation rate in noncentrosymmetric superconductor $Y_2C_3$

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Abstract

For a noncentrosymmetric superconductor such as $Y_2C_3$, we consider a parity-mixing model composed of spin-singlet $s$-wave and spin-triplet $f$-wave pairing components. The $d$-vector in $f$-wave state is chosen to be parallel to the Dreselhaus asymmetric spin-orbit coupling vector. It is found that, the quasiparticle excitation spectrum exhibits distinct nodal structure as a consequence of parity-mixing. Our calculation predict anomalous noninteger power laws for low-temperature nuclear spin-lattice relaxation rate $T_1^{-1}$. We demonstrate particularly that such a model can qualitatively account for the existing experimental results of the temperature dependence of $T_1^{-1}$ in $Y_2C_3$.

Keywords: Noncentrosymmetric superconductor $Y_2C_3$, Pairing symmetry, Nuclear spin-lattice relaxation rate

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1. Introduction

The physics of unconventional superconductivity in materials without inversion symmetry has become a subject of growing interest since the noncentrosymmetric (NCS) heavy Fermion superconductor CePt$_3$Si was found in 2004. In these materials the superconducting phase develops in a low-symmetry environment with a missing inversion center. This broken symmetry generates
an antisymmetric spin-orbit (SO) coupling and prevent the usual even/odd classification of Cooper pairs according to orbital parity, allowing a mixed-parity superconducting state \[4, 5\]. This mixture of the pairing channels with different parities may result in unusual temperature and field dependence of experimentally observed superconducting properties \[1, 2\].

For CePt\(_3\)Si, in particular, where the Rashba-type \[6\] SO coupling vector \(\gamma_k \propto (\hat{k}_y, -\hat{k}_x, 0)\) is generated, various low-energy thermodynamical and transport properties have been extensively investigated from both the experimental and theoretical sides. The NMR relaxation rate \[7\] \(T_1^{-1}\), thermal conductivity \[8\], and London penetration depth \[9\] indicate power law behavior at lowest temperatures, suggesting the presence of nodal lines in the quasiparticle excitation spectrum. Besides, the upper critical magnetic field \(H_{c2}\) is surprisingly large \[3, 10\], and no change in the Knight shift across the transition temperature \(T_c\) \[11\] has been observed. These characteristics are attributed to a spin triplet superconducting order parameter. Theoretically, Frigeri \textit{et al.} have proposed an \((s+p)\)-wave model \[12\] where the \(d\)-vector of \(p\)-wave state is chosen to be parallel to the SO coupling vector \((d_k \propto g_k)\). The gap function of this \((s+p)\)-wave model has the natural form for a system without inversion symmetry, and exhibits line nodes when the \(p\)-wave pair potential is larger than that of \(s\)-wave one. It should be noted that a nonzero \(s\)-wave pair potential is necessary to get expected line nodes. Hayashi \textit{et al.} \[13\] have demonstrated that the presence of line nodes in this \((s+p)\)-wave model may account for the experimentally observed low-temperature features of the nuclear spin-lattice relaxation rate \(T_1^{-1}\) in CePt\(_3\)Si on a qualitative level.

The cubic Pu\(_2\)C\(_3\)-type sesquicarbide compound Y\(_2\)C\(_3\) is a NCS superconductor known for its relatively high superconducting transition temperature \[14\] \((T_c \sim 18K)\). Different from the CePt\(_3\)Si case, the Dresselhaus \[15\] SO coupling vector \(\gamma_k \propto (\hat{k}_x(\hat{k}_y^2 - \hat{k}_z^2), \hat{k}_y(\hat{k}_x^2 - \hat{k}_z^2), \hat{k}_z(\hat{k}_x^2 - \hat{k}_y^2))\) is relevant to Y\(_2\)C\(_3\).

Even many years after its discovery, the nature and symmetry of the superconducting gap function in Y\(_2\)C\(_3\) appears to be full of contradiction. While the specific heat measurement \[16\] and tunneling experiment \[17\] are interpreted as
a fully gapped isotropic $s$-wave state, the nuclear spin-lattice relaxation rate $T_1^{-1}$ and muon spin rotation (μSR) measurements on $\text{Y}_2\text{C}_3$ are qualitatively fitted with a nodeless two-gap model similar to $\text{MgB}_2$. On the other hand, Chen et al. [20] have measured the magnetic penetration depth as a function of temperature and found a weak linear dependence at very low temperatures. They also reanalysed the NMR data reported in Ref. [18] and claimed that, where $T_1^{-1} \sim T^3$ at $T < 3K$, as a matter of fact. Such behavior seems to support the existence of line nodes rather than a fully opened gap in the superconducting state of $\text{Y}_2\text{C}_3$. In addition, the upper critical magnetic field $H_{c2}$ is found to be compatible with the paramagnetic limiting field [10, 20], and the Knight shift in NMR [18] is decreased to approximately 2/3 of its normal-state value. These features are again incompatible with the single gap or two-gap $s$-wave pictures. It is expected that line nodes (or point nodes of second-order) would be generated due to parity-mixing, similar to the case of CePt$_3$Si mentioned above. In order to shed light on these controversy, further experimental and theoretical studies on the superconducting properties of $\text{Y}_2\text{C}_3$ are required.

In this work, we theoretically investigate the nuclear spin-lattice relaxation rate $T_1^{-1}$ on the basis of $(s+f)$-wave model, where the $d$-vector in $f$-wave state is chosen to be parallel to the Dresselhaus-type asymmetric SO coupling vector. We analyse various possible nodal structures which can be generated by the effect of parity-mixing. In particular, the temperature dependence of the nuclear spin-lattice relaxation rate $T_1^{-1}$ is calculated and compared with the experimental result obtained in Ref. [18] for $\text{Y}_2\text{C}_3$.

2. Model Hamiltonian

Our starting point is the following mean-field $(s+f)$-wave pairing Hamiltonian

$$H = H_0 + H_{\text{int}}.$$  \hspace{1cm} (1)
The Hamiltonian $H_0$ describes the noninteracting conduction electrons in a NCS crystal,

$$H_0 = \sum_k \sum_{\alpha,\beta} (\epsilon_k \sigma_0 + \gamma_0 \gamma_k \cdot \sigma \alpha \beta c_{k\alpha}^\dagger c_{k\beta},$$  \(2\)

where $c_{k\alpha}^\dagger$ ($c_{k\alpha}$) creates (annihilates) an electron with wave vector $\mathbf{k}$ and spin $\alpha$, $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ denotes the vector of Pauli matrices, $\sigma_0$ is the $2 \times 2$ unit matrix, $\epsilon_k$ is the parabolic bare band dispersion measured relative to the chemical potential restricted to $|\epsilon_k| < \omega_c$, with $\omega_c$ being the usual cutoff energy. Furthermore, $\gamma_k = (\hat{k}_x (\hat{k}_y^2 - \hat{k}_y^2), \hat{k}_y (\hat{k}_x^2 - \hat{k}_x^2), \hat{k}_z (\hat{k}_x^2 - \hat{k}_x^2))$, with $\hat{k}_x = \sin \theta_k \cos \phi_k$, $\hat{k}_y = \sin \theta_k \sin \phi_k$, and $\hat{k}_z = \cos \theta_k$, is the asymmetric ($\gamma_k = -\gamma_{-k}$) Dresselhaus SO coupling vector considered to be relevant for Y$_2$C$_3$ and La$_2$C$_3$. The strength of SO coupling is denoted by $\gamma_0$.

The second term in Eq. (1) represents the pairing interaction:

$$H_{\text{int}} = \frac{1}{2} \sum_k \sum_{\alpha,\beta} [\Delta_{k,\alpha\beta} c_{k\alpha}^\dagger c_{-k\beta} + \Delta_{k,\alpha\beta}^\dagger c_{-k\alpha} c_{k\beta}] + \Delta_{k,\alpha\beta} F_{k,\alpha\beta}^\dagger,$$

with the anomalous averages $F_{k,\alpha\beta} = \langle c_{k\alpha} c_{-k\beta} \rangle$, and the gap function defined by [21]

$$\Delta_{k,\alpha\beta} = -\sum_{k',\lambda,\mu} V_{\alpha\beta,\lambda\mu}(k, k') F_{k',\lambda\mu}^\dagger,$$

where $V_{\alpha\beta,\lambda\mu}(k, k')$ is the pairing potential. In this work, we will adopt $V_{\alpha\beta,\lambda\mu}(k, k')$ as the phenomenological one [22]:

$$V_{\alpha\beta,\lambda\mu}(k, k') = -\frac{V_s}{2} \langle i \sigma_y \rangle_{\alpha\beta} \langle i \sigma_y \rangle_{\lambda\mu} + \frac{V_f}{2} \langle i \sigma_y \rangle_{\alpha\beta} \langle \gamma_k \cdot \sigma \rangle_{\lambda\mu} + \frac{V_m}{2} \langle \gamma_{k'} \cdot \sigma \rangle_{\alpha\beta} \langle i \sigma_y \rangle_{\lambda\mu} + \langle (i \sigma_y)_{\alpha\beta} \langle \gamma_{k'} \cdot \sigma \rangle_{\lambda\mu},$$

where the first two terms represent the interaction in the s-wave pairing channel and in the spin-triplet f-wave pairing channel, respectively, and the last term describes the scattering between the two channels. In the following, we will...
chose the interaction parameters $V_s$, $V_f$, and $V_m$ to be positive, and take for simplicity $V_m = \sqrt{V_s V_f}$ which yields $\Delta_s(T)/\Delta_f(T) = \text{const.}$ \cite{22}.

Owing to the lack of inversion symmetry, the superconducting gap function Eq. \cite{23} generally contains an admixture of even-parity spin-singlet and odd-parity spin-triplet pairing states,

$$\Delta_{k, \alpha \beta} = [\psi_k i \sigma_y + d_k \cdot \sigma i \sigma_y]_{\alpha \beta}, \quad (5)$$

where $\psi_k = \psi_{-k}$ and $d_k = -d_{-k}$ represent the spin-singlet and spin-triplet components, respectively. The direction of the $d_k$ (the $d$-vector) is assumed to be parallel to $\gamma_k$, as for this choice the antisymmetric SO interaction is not destructive for spin-triplet pairing\cite{12}. Hence, we parametrize the $d$-vector as $d_k = \Delta_f \gamma_k$. For the spin-singlet component we assume $s$-wave pairing $\psi_k = \Delta_s$, and choose the amplitudes $\Delta_s$ and $\Delta_f$ to be real and positive.

Using the vector operator $\Psi_k = (c_k \uparrow, c_{-k} \uparrow, c_{-k} \downarrow, c_k \downarrow)^t$, where $(\cdots)^t$ stands for the transposing operation, we can write the Hamiltonian in a more compact form:

$$H = \frac{1}{2} \sum_k \Psi_k^\dagger \hat{H}_k \Psi_k + \sum_k \epsilon_k + \frac{1}{2} \sum_k \sum_{\alpha, \beta} \Delta_{k, \alpha \beta} F_{k, \beta \alpha}^\dagger, \quad (6)$$

where

$$\hat{H}_k = \begin{pmatrix} \hat{M}_k & \hat{\Delta}_k \\ \hat{\Delta}_k^\dagger & -\hat{M}_{-k}^\ast \end{pmatrix}, \quad (7)$$

with

$$\hat{M}_k = \epsilon_k \sigma_0 + \gamma_0 \gamma_k \cdot \sigma, \quad \hat{\Delta}_k = (\Delta_s + \Delta_f \gamma_k \cdot \sigma)(i \sigma_y). \quad (8)$$
3. Nodal structures

The Bogoliubov-de Gennes quasiparticle excitation spectrum \( E(k) \) can be obtained readily by diagonalizing the matrix \( \hat{H}_k \) above. One can find four solutions, namely, \( E^e_\pm(k) \) and \( E^h_\pm(k) \), with \( E^h_\pm(k) = -E^e_\mp(k) \). We have

\[
E^e_\pm(k) = \sqrt{(\epsilon_k \pm \gamma_0 |\gamma_k|)^2 + (\Delta_s \pm \Delta_f |\gamma_k|)^2} \equiv E^k_\pm,
\]

(9)
corresponding to two sheets of Fermi surfaces with the energy gaps given by \( \Delta_{k+} = \Delta_s + \Delta_f |\gamma_k| \) and \( \Delta_{k-} = \Delta_s - \Delta_f |\gamma_k| \), respectively. Zeros of \( E^k_\pm \) determine the nodal structure of the superconducting state in momentum space. Here let us assume a sufficiently large value of the cutoff energy \( \omega_c (\omega_c \gg \gamma_0, \Delta_s, \Delta_f) \).

It is apparent that the upper branch \( E^{e}_+ \) is positive definite. Therefore, here we focus on the zeros of the lower branch \( E^{e}_- \).

The amplitude of the Dresselhaus SO coupling \( |\gamma_k| \) (see Fig. 1) becomes zero at 14 points (such as the south and north poles), possesses 24 saddle points at \( (\theta_k = \arctan 2\sqrt{2}, \phi_k = \arccos \sqrt{2}/4) \), etc. with \( |\gamma_k| = 2\sqrt{2}/9 \), and attains its maximum value 0.5 at 12 points \( (\theta_k = \pi/2, \phi_k = \pi/4) \), etc. on the Fermi surface. Therefore, one encounters different nodal topology depending on the ratio \( \kappa \equiv \Delta_s/\Delta_f \). When \( \kappa = 0 \) \((\kappa = 0.5)\), \( E^k_\pm \) shows 14 (12) nodal points of first-order (second-order), while exhibits line nodes for \( 0 < \kappa < 0.5 \) as displayed in Fig. 2. For \( \kappa > 0.5 \), however, we always have \( \Delta_{k-} \neq 0 \), and thus the quasiparticle excitation spectrum is gapped.
4. Nuclear magnetic relaxation rate

Let us consider the temperature dependence of the nuclear magnetic relaxation rate \( T_1^{-1} \) defined as

\[
\frac{1}{T_1 T} \propto \sum_q \Im \left[ \chi_{-+}(q, i\omega_n \to \omega + i0^+) \right] \left| \omega \right| \left| \omega \to 0 \right.,
\]

where \( \Im \) denotes the imaginary part. The dynamical susceptibility in imaginary time is given by

\[
\chi_{-+}(q, i\omega_n) = \int_0^{1/T} d\tau \sum_{kk'} T_{c} \left\langle \hat{T} c_{k'}^{\dagger} c_{k}\left( \tau \right) c_{k'}^{\dagger}(0)c_k(0) \right\rangle e^{i\omega_n \tau},
\]

where \( T \) denotes the time-ordering operator, \( \omega_n = (2n + 1)\pi T \) is the Matsubara frequency, and \( c_k(\tau) = e^{iH\tau} c_k e^{-iH\tau} \). We obtain an explicit expression for \( T_1^{-1} \) as

\[
\frac{1}{T_1 T} \propto \sum_{k,q} \sum_{\ell,\pm} \alpha(E_k^\ell - E_q^\ell) \left( 1 + \frac{\epsilon_{\ell,k} \epsilon_{\ell,q} + \Delta_{\ell,k} \Delta_{\ell,q}}{E_k^\ell E_q^\ell} \right),
\]

where \( \epsilon_{\pm,k} = \epsilon_k \pm \gamma_0 |\gamma_k| \). The temperature dependence of \( \Delta_s \) and \( \Delta_f \) are determined by the self-consistent gap equations:

\[
\Delta_s = \sum_{k,\ell} \frac{\tanh(E_k^\ell / 2T)}{4E_k^\ell} \Delta_{\ell,k}( V_s + \ell V_m |\gamma_k| ),
\]

\[
\Delta_f = \sum_{k,\ell} \frac{\tanh(E_k^\ell / 2T)}{4E_k^\ell} \Delta_{\ell,k}( V_m + \ell V_f |\gamma_k| ).
\]

It turns out that for given values of \( V_s, V_f, \) and \( \omega_c, 1/T_1 T \) depends on the \( \Delta_s \) and \( \Delta_f \) only through the ratio \( \kappa \), and is independent of the strength of SO coupling \( \gamma_0 \), similar to the case of Ref. 13. It is interesting to see how the low-temperature power law behaviour for the nuclear spin-lattice relaxation rate \( 1/T_1 T \propto T^n \) is changed with the ratio \( \kappa \). Plotted in Fig. 3 is the exponent of temperature, \( n \), as a function of \( \kappa \) at \( T = 0.04T_c \) calculated numerically according to \( n = d\ln(1/T_1 T)/d\ln T \). As we see, the exponent \( n \) attains its maximum \( n = 4 \) at \( \kappa = 0 \) (point node of first-order), decreases oscillatorily
Figure 2: Evolution of nodal structure with the parameter $\kappa$ ($0 \leq \kappa \leq 0.5$). At $\kappa = 0$ ($\kappa = 0.5$), $E^k$ shows 14 (12) nodal points of first-order (second-order), while exhibits line nodes for $0 < \kappa < 0.5$.

Figure 3: The exponent of temperature as a function of $\kappa$, calculated numerically according to $n = d\ln(1/T\gamma T)/d\ln T$. 

$\gamma$.
with increasing $\kappa$, and end with $n \approx 2.2$ at $\kappa = 0.5$. It is worth noting that, the exponent $n$ is not necessarily to be an integer here, similar to the cases in Ref. [23]. For $\kappa > 0.5$, however, the gap is open and $1/T_1T$ decays exponentially in nature. We present in Fig. 4 the temperature dependence of $1/T_1T$ obtained experimentally [18] by Harada et al. for $Y_2C_3$, together with the calculated results for $\kappa=0.47$, 0.50, and 0.53 for comparison. Shown in the inset of Fig. 4 is the detailed temperate dependence of $\Delta_s$ and $\Delta_f$ obtained by solving the gap equations Eq. (12) for $\kappa=0.53$. As can be seen form Fig. 4 there is a fair agreement between our simple theory and experimental results. However, further experimental measurements at low temperatures $T/T_c < 0.15$ are needed to obtain a decisive information about the pairing symmetry and to test the prediction of our theory.

5. Summary

In summary, we have calculated the temperature dependence of the nuclear magnetic relaxation rate $1/T_1T$ in the Dresselhaus-type noncentrosymmetric superconductor $Y_2C_3$. We have considered the $(s+f)$-wave parity-mixing model where the $d$-vector is chosen to be parallel to the Dresselhaus SO coupling vector. It is found that various types of nodal structures can be generated due to the effect of parity-mixing, depending on the value of $\kappa$. We also find that, for $\kappa \sim 0.5$, the $(s+f)$-wave model can explain the experimental results fairly well over a wide range of temperatures. However, accurate measurements of $1/T_1T$ at lower temperatures would be crucial to the further clarification of pairing symmetry and gap structure in $Y_2C_3$.

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Figure 4: Comparison of the experimental data in Ref. [18] with the calculated temperature dependence of $1/T_1 T$ for $\kappa = 0.47$, 0.5, and 0.53. Inset shows the temperature dependence of $\Delta_s$ and $\Delta_f$ at $\kappa = 0.53$. 
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