Possibility of the chiral \(d\)-wave state in the hexagonal pnictide superconductor \(\text{SrPtAs}\)

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We discuss the type of pairing in the hexagonal pnictide superconductor \(\text{SrPtAs}\) with taking into account its multiband structure. The topological chiral \(d\)-wave state with time-reversal-symmetry breaking has been anticipated from the spontaneous magnetization observed by the muon-spin-relaxation experiment. We point out in this paper that the recent experimental reports on the nuclear-spin-lattice relaxation rate \(T_{1}^{-1}\) and superfluid density \(n_{s}(T)\), which seemingly support the conventional \(s\)-wave pairing, are also consistent with the chiral \(d\)-wave state. The compatibility of the gap and multiband structures is crucial in this argument.

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Introduction. The first hexagonal pnictide superconductor \(\text{SrPtAs}\) \((T_{c} = 2.4K)\) has been paid attention, since the muon-spin-relaxation \((\mu SR)\) experiment\(^{4}\) observes the internal magnetization below \(T_{c}\). The result suggests the spontaneous time-reversal symmetry (TRS) breaking in the superconducting state. From the group theoretical consideration\(^{3}\) and functional renormalization group (FRG) analysis\(^{5}\) the most probable pairing symmetry is the topological chiral \(d\)-wave \((d_{x^{2}−y^{2}} \pm id_{xy})\) state with TRS breaking. This state has non-zero Chern number\(^{2}\) and supports the surface bound states with chiral energy spectrum\(^{2,3} \). Especially in \(\text{SrPtAs}\), it is expected that the chiral surface state causes spontaneous spin current and spin polarization\(^{2}\) of which is the staggered anti-symmetric spin-orbit coupling (SOC) coming from the hexagonal bi-layer structure of the crystal with local lack of inversion symmetry\(^{2}\).

We may explain intuitively the stability of the chiral \(d\)-wave pairing in \(\text{SrPtAs}\). The hexagonal structure of the crystal plays a role for supporting the chiral \(d\)-wave state, since there is the two-dimensional (2D) irreducible representation with \(d_{x^{2}−y^{2}}\) and \(d_{xy}\) wave functions in the crystal symmetry, and then the chiral \(d\)-wave pairing is easily obtained as the mixing of these two basis with relative phase \(\pm \pi/2\). Moreover, the band structure also assists the condensation energy gain, since quasi-2D bands with fully-gapped quasiparticle excitations dominate significantly compared to a minor three-dimensional (3D) band with point-nodal excitation\(^{5,10,11}\).

On the other hand, there are still some controversies on the chiral \(d\)-wave pairing. The nuclear spin-lattice relaxation rate \(T_{1}^{-1}\) measured by the nuclear quadrupole resonance shows the Hebel-Slichter (HS) peak near \(T_{c}\) and exponential decay in the low temperature region\(^{12}\). It has also been found from the magnetic-penetration-depth measurement that superfluid density \(n_{s}(T)\) exhibits the Arrhenius-type behavior (i.e., approaches to \(n_{s}(0)\) exponentially) at low temperature\(^{13}\). The conventional \(s\)-wave pairing without any nodal excitation is naively expected from these experimental results.

We address this issue in this paper and show based on the multiband quasiclassical formalism\(^{14,15}\) that observed \(T_{1}^{-1}\) and \(n_{s}(T)\) are consistent with the chiral \(d\)-wave pairing as well as the \(s\)-one. The point is that the density of states (DOS) and root mean square of the Fermi velocity in the 3D band with nodal excitation are less dominant\(^{10,11}\) and the power-law behavior in the low temperature region is smeared out. It should also be emphasized that the HS peak is not only from the coherence effect solely exists for the conventional \(s\)-wave state, but also from the full gap structure of the quasiparticle excitation\(^{15}\). Thus, an unconventional state without any nodes such as the chiral \(d\)-wave state in major quasi-2D bands is able to have a large HS peak.

Normal and pairing states. There are two distinct honeycomb-shaped \(\text{PTAs}\) layers \((l=1,2)\) in the unit cell of \(\text{SrPtAs}\). Although the entire crystal is inversion-symmetric, each layer does not contain the inversion center in itself, and the system is therefore staggered non-centrosymmetric.\(^{16}\) The band structure calculation reveals that the Pt 5\(d\) orbital is dominant in the conduction bands and there are six Fermi surfaces with spin degeneracy, five of which are quasi-2D and the other 3D.\(^{10,11}\) Including Pt nearest-neighbor hopping within the plane, as well as nearest- and next-nearest-neighbor hopping between the planes, and also the staggered anti-symmetric SOC, one finds the one-body effective tight-binding Hamiltonian at low energy\(^{10,11}\):

\[
H_{0} = \sum_{k\beta\sigma} \left( a_{k1\sigma}^{(\beta)} \right)^{\dagger} \begin{pmatrix} \epsilon_{k}^{(3)} & \epsilon_{k}^{(2)} \lambda_{k}\sigma & \epsilon_{k}^{(3)} \\ \epsilon_{k}^{(2)}} & \epsilon_{k}^{(3)} & \epsilon_{k}^{(3)} - \alpha^{(2)} \lambda_{k}\sigma \\ \epsilon_{k}^{(2)} & \epsilon_{k}^{(3)} - \alpha^{(2)} \lambda_{k}\sigma \end{pmatrix} \begin{pmatrix} a_{k1\sigma}^{(\beta)} \\ a_{k2\sigma}^{(\beta)} \end{pmatrix} \]

where \(\beta(=1,2,3)\) indicates the unsplit band, \(\epsilon_{k}^{(\beta)}(a_{k\beta})\) is the creation (annihilation) operator of an electron with the wave vector \(k\) and spin \(\sigma = \pm 1\) in the \(l\)-th layer of the unit cell, \(\epsilon_{k}^{(2)} = t_{0}^{(2)} \sum_{c} \cos(k_{c})+t_{1}^{(2)} \cos(k_{c}), \epsilon_{k}^{(3)} = t_{0}^{(3)} \cos(k_{c})/2[1 + \exp(-ik_{c}) \cdot T_{1} + \exp(ik_{c}) \cdot T_{2}],\) and \(\lambda_{k}\) is the net \(l\)-th layer charge density. The conventional \(s\)-wave pairing without any nodal excitation is naively expected from these experimental results.
FIG. 1. The cross section of Fermi surfaces at (a) $k_z = 0$ and
(b) $k_z = \pi/c$. Each Fermi surface is labeled by the set of
parameters $\beta = 1, 2, 3$ and $\gamma = \pm$ (see also Eq. (2)).

We may introduce phenomenologically the quasiparticle
damping (the smearing factor of the quasiparticle DOS) $\eta$ via the analytic continuation to obtain the
retarded and advanced Green’s functions

$$
\begin{align*}
\tilde{g}^{R,A}_{\gamma}(\epsilon, \mathbf{k}_F^{\beta\gamma}) &= \tilde{g}^{\gamma}_{\gamma}(i\epsilon - \epsilon \pm i\eta, \mathbf{k}_F^{\beta\gamma}), \\
\tilde{g}^{R,A}_{\gamma}(\epsilon, \mathbf{k}_F^{\beta\gamma}) &= \tilde{g}^{\gamma}_{\gamma}(i\epsilon - \epsilon \pm i\eta, \mathbf{k}_F^{\beta\gamma}), \\
\tilde{g}^{R,A}_{\gamma}(\epsilon, \mathbf{k}_F^{\beta\gamma}) &= \tilde{g}^{\gamma}_{\gamma}(i\epsilon - \epsilon \pm i\eta, \mathbf{k}_F^{\beta\gamma}), \\
\tilde{g}^{R,A}_{\gamma}(\epsilon, \mathbf{k}_F^{\beta\gamma}) &= \tilde{g}^{\gamma}_{\gamma}(i\epsilon - \epsilon \pm i\eta, \mathbf{k}_F^{\beta\gamma}).
\end{align*}
$$

For simplicity, we neglect the band dependence of $\eta$. We therefore have two fitting parameters, $\Delta_0/k_BT_c$ and $\eta$, in the following calculations.

The nuclear-spin-lattice relaxation rate $T_1^{-1}(T)$. The

relaxation rate is

$$
\frac{T_1(T_c)}{T_1(T)} = T \int_{-\infty}^{\infty} d\epsilon \left( N_s(\epsilon)^2 + M_s(\epsilon)^2 \right) \left( -\frac{\partial f(\epsilon)}{\partial \epsilon} \right)
$$

where $f(\epsilon)$ is the Fermi-Dirac distribution function, and $N_s(\epsilon)$ and $M_s(\epsilon)$ denote DOS and anomalous DOS of the

Bogoliubov quasiparticle normalized by the entire DOS at the Fermi level in the normal state $N(0)$. For the multi-band spin-singlet superconductor,\textsuperscript{14}

$$
\begin{align*}
N_s^2(\epsilon) &= (a_{\sigma\sigma}(\epsilon, k)) f(a_{\sigma\sigma}(\epsilon, k)) F, \\
M_s^2(\epsilon) &= -a_{\sigma\sigma}^2(\epsilon, k) f(a_{\sigma\sigma}^2(\epsilon, k)) F,
\end{align*}
$$

and

$$
\langle a_{\sigma\sigma}(\epsilon, k) \rangle_F = \frac{1}{N(0)} \sum_{\beta\gamma} \int \frac{d\Omega_{\mathbf{k}_F^{\beta\gamma}}}{(2\pi)^3} h_v^{\beta\gamma}(\epsilon, \mathbf{k}_F^{\beta\gamma})
$$

is the Fermi surface average.

The results for both $s$-wave and chiral $d$-wave states are shown in Fig. \textsuperscript{2} with experimental data.\textsuperscript{12} The fitting parameters are chosen as $\Delta_0/k_BT_c = 1.765$ for both states, and $\eta = 0.14(0.008)k_BT_c$ for the $s$-wave (chiral $d$-wave) state. We clearly see that both pairing states agree well with experimental data showing the HS peak just below $T_c$ and exponential decay at low temperature.

It is known that $M_s(\epsilon)$ from the coherence effect appears only for the $s$-wave state and contributes to the HS peak significantly.\textsuperscript{12} We should note, however, that the quasiparticle excitations of quasi-2D bands in the chiral $d$-wave state is fully gapped and $N_s(\epsilon)$ also gives rise to
We emphasize that the estimations for $\eta$ by the nodal excitation is negligible. These facts are crucial results are insensitive to the choice of the quasiparticle band ("3"-th band) is less dominant. The gap amplitude

\[ \bar{n}_s(T) = \sum_{\gamma} \bar{n}_s^{\gamma}(T), \]

\[ \bar{n}_s^{\gamma}(T) = \sum_{\gamma} \sum_{x,y,z} \int \frac{d\Omega_{k_F}}{(2\pi)^3|\mathbf{w}_{14}|} \left( \psi_{k_F}^{\beta \gamma} \right)^2 \left( 1 - Y_{k_F} \right), \]

\[ Y_k(T) = 1 - \pi k_B T \sum_{n=-\infty}^{\infty} \frac{\left| \Delta_k \right|^2}{(\epsilon_n^2 + \left| \Delta_k \right|^2)^{2/3}}, \]

is Yosida function. The parameter is taken as $\Delta_0/k_B T_c = 1.5$ for both states. We have also checked that the results are insensitive to the choice of the quasiparticle density $n_s(T)$. Superfluid density normalized by its zero-temperature value $n_s(0)$ is

| $\phi_{k_F}^{d s}$ of s-wave | "1 ±"-th | "2 ±"-th | "3 + (H)'"-th | "3 + (H)'"-th | "3 - (H)'"-th | "3 - (H)'"-th |
|---------------------------|-----------|----------|--------------|--------------|--------------|--------------|
| $\phi_{k_F}^{d s}$ of chiral d-wave | (δ$k_x + iδk_y$)$^2$ | (δ$k_x + iδk_y$)$^2$ | δ$p_x - iδp_y$ | δ$p_x - iδp_y$ | δ$q_x - iδq_y$ | δ$q_x - iδq_y$ |

The abbreviations "3"-th and "3"-th mean the disconnected Fermi pockets of "3"-th band enclosing $H$ and $H'$ points, respectively. Note that all the Fermi surfaces are quasi-2D, except for the 3D "3"-th one. Here, $k = k/|k|$, and δ$k = k_F^{\beta \gamma} - k_0$, δ$p = k_F^{\beta \gamma} - p_0$, δ$q = k_F^{\beta \gamma} - q_0$, and δ$q' = k_F^{\beta \gamma} - q_0'$ refer to the deviations from the centers of the long-wavelength expansions, and $k_0 = (0, 0, k_{F z})$, $p_0 = (2\pi/\sqrt{3}, 2\pi/3, k_{F z})$, $q_0 = (2\pi/\sqrt{3}, 2\pi/3, \pi/c)$, and $q_0' = (0, 4\pi/3, \pi/c)$ the centers of the expansions. We emphasize that δ$k$, δ$p$, and δ$q'$ lies in the 2D plane, whereas δ$q$ and δ$q'$ point in 3D directions. Thus, $\phi_{k_F}^{d s}$ for the chiral d-wave state has point nodes in the $k_y$-direction, while the others have no nodes.

FIG. 2. Temperature dependence of $T_1^{-1}$. Green dots are the experimental results. Red squares and blue triangles show the estimations for s-wave and chiral d-wave states. Used fitting parameters are $\Delta_0/k_B T_c = 1.765$ for both states, and $\eta = 0.14(0.008) k_B T_c$ for the s-wave (chiral d-wave) state.

FIG. 3. The contribution from the "3βγ"-th band to the normalized quasiparticle DOS $\bar{N}_s(\epsilon)$ in the chiral d-wave state, which is expressed as $\bar{N}_s^{\beta \gamma}(\epsilon) = \int a_1^{\beta \gamma}(\epsilon, k_F^{\beta \gamma})d\Omega_{k_F}/\left(\left(2\pi\right)^3 N(0) \mathbf{w}_{14}\right)$. The gap amplitude at $T = 0.5T_c$ is used in this estimation. We see that the 3D band ("3"-th band) is less dominant.

the HS peak. Moreover, the quasiparticle DOS of the 3D band is less dominant in this system (see Fig. 3), and then the power-law behavior at low temperature caused by the nodal excitation is negligible. These facts are crucial for the compatibility of the chiral d-wave state with experiment data.

We therefore cannot distinguish s- and chiral d-wave states from $T_1^{-1}$. It should be emphasized that we need to reduce $\eta$ for the chiral d-wave state to compensate the absence of the contribution from $\bar{N}_s(\epsilon)$. Namely, the reduction of $\eta$ causes the significant difference of $\bar{N}_s(\epsilon)$ for s- and chiral d-wave states (see Fig. 3). The observation of $\bar{N}_s(\epsilon)$ would be relevant for the distinction of two pairing states using, for instance, the scanning tunneling microscopy/spectroscopy (STM/STS) even in the (0001) surface without the chiral mode.

Superfluid density $n_s(T)$. Superfluid density normalized by its zero-temperature value $n_s(0)$ is

$\bar{n}_s(T) = \sum_{\beta \gamma} \bar{n}_s^{\beta \gamma}(T),$

$\bar{n}_s^{\beta \gamma}(T) = \sum_{\gamma} \sum_{x,y,z} \int \frac{d\Omega_{k_F}}{(2\pi)^3|\mathbf{w}_{14}|} \left( \psi_{k_F}^{\beta \gamma} \right)^2 \left( 1 - Y_{k_F} \right),$

where

$Y_k(T) = 1 - \pi k_B T \sum_{n=-\infty}^{\infty} \frac{\left| \Delta_k \right|^2}{(\epsilon_n^2 + \left| \Delta_k \right|^2)^{2/3}}.
FIG. 4. Dashed red and blue lines are the normalized DOS of quasiparticles $\bar{N}_s(\epsilon)$ in $s$- and chiral $d$-wave states with the gap amplitude at $T = 0.5T_c$. The smearing factor $\eta = 0.14(0.008)k_B T_c$, and the peaks are reduced (enhanced) in the $s$-wave (chiral $d$-wave) state. The point-nodal excitation of the chiral $d$-wave state from the less dominant 3D band causes feeble “V-shaped” behavior around $\epsilon = 0$ and tiny peaks at $\epsilon \approx \pm 2.3 k_B T_c$ in the blue line.

in the estimations of $T^{-1}_{1-}$.

We clearly see from Fig. 5 that the results of both states fit very well to experimental data, namely, both exhibit the thermal-activation-type behavior at low temperature. $\bar{n}_{s}(T)$ in Eq. 10 shows the contribution from each band and the result for the chiral $d$-wave state is plotted in Fig. 6. The contribution from the 3D band with power-law behavior is negligibly small, since $\bar{n}_{s}(T)$ depends strongly on root mean square of the Fermi velocity, and its value for the 3D band is minor (see Table. I in Ref. 11).

Summary. We have shown based on the multiband quasiclassical formalism that observed $T^{-1}_{1-}$ and $n_s(T)$ in the superconducting phase of SrPtAs are consistent with the chiral $d$-wave pairing as well as the $s$-wave one. In other words, the chiral $d$-wave state cannot be ruled out from these experiments. The measurement of quasiparticle DOS, which could be done by STM/STS, is relevant for the distinction of $s$- and chiral $d$-wave states (see Fig. 4).

We comment on the $f$-wave pairing suggested as the other possibility. The quasiparticle excitation of this state is fully gapped in two bands (“3±”-th) around the Brillouin zone corners, whereas has line nodes in four quasi-2D bands (“1±”-th and “2±”-th) around the zone center. We have checked that $T^{-1}_{1}$ for the $f$-wave state using the smallest $\eta = 0.0025k_B T_c$ fits well with observed data thanks to the large DOS of fully-gapped “3+”-th band. However, $n_s(T)$, dominant contribution for which comes from four line-nodal “1±”-th and “2±”-th bands with large root mean square of the Fermi velocity (see Table. I in Ref. 11), shows an evident power-law behavior at low temperature and contradicts strongly with the experiment. The results are summarized in Appendix. Besides, it would be hard to explain the spontaneous magnetization from the $f$-wave state as well as the $s$-wave one. The chiral $d$-wave state is thus the only one, which is consistent with all the experiments that have been done so far.

We should also mention that only poly-crystal samples have ever been used. The experiments with single crystals are highly desired.

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FIG. 5. Temperature dependence of normalized superfluid density $\bar{n}_s(T)$. Green dots denote experimental data. Dashed red and blue lines show the estimations for $s$-wave and chiral $d$-wave states. Used fitting parameters are $\Delta_0/k_B T_c = 1.5$ for both states, and $\eta = 0.14(0.008)k_B T_c$ for the $s$-wave (chiral $d$-wave) state. We note additionally that the results are insensitive to the choice of $\eta$.

FIG. 6. $\bar{n}_{s}(T)$ of the chiral $d$-wave state. We see that the contribution from the 3D band (“3+”-th band) with power-law behavior is negligibly small.
TABLE II. The list of $\phi_{k_F}$ for the $f$-wave state. Here, $\hat{k} = k/|k|, \delta k = k^{\gamma}_{\parallel} - k_0$, and $k_0 = (0,0,k^{\gamma}_{\parallel})$.

| $\phi_{k_F}$ of f-wave | $^1$ $\pm \beta$-th | $^2$ $\pm \gamma$-th | $^3 + (H')$-th | $^3 + (H')$-th | $^3 - (H')$-th | $^3 - (H')$-th |
|------------------------|---------------------|---------------------|-----------------|-----------------|-----------------|-----------------|
| $n$                   | $(3\delta k^2_{x} - \delta k^2_{\gamma})\delta k_y$ | $(3\delta k^2_{x} - \delta k^2_{\gamma})\delta k_y$ | 1               | -1              | 1               | -1              |

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Appendix: $T_1^{-1}$ and $n_s(T)$ for the $f$-wave state

We comment on the $f$-wave state suggested as the other possibility of the pairing symmetry in the hexagonal pnictide superconductor $\text{SrPtAs}_2$. The quasiparticle excitation of this state is fully gapped in two bands ($^3 \pm \gamma$)-th around the Brillouin zone corners, whereas has line nodes in four quasi-2D bands ($^1 \pm \beta$-th and $^2 \pm \gamma$-th) around the zone center. The function $\phi_{k_F}$ for the $f$-wave state is listed in Table II in this Appendix.

We show, in Fig. 7, $T_1^{-1}$ for the $f$-wave state using the parameters $\Delta_0/k_BT_c = 1.765$ and $\eta = 0.0025kB_Tc$. We see the result fits well with observed data thanks to the large DOS of fully-gapped $^3 \pm \gamma$-th band. However, $n_s(T)$ in Fig. 8 shows an evident power-law behavior at low temperature and contradicts strongly with the experiment. The power-law behavior comes from the fact that line-nodal $^1 \pm \beta$-th and $^2 \pm \gamma$-th bands with large root mean square of the Fermi velocity (see Table. I in Ref. 11) gives the dominant contribution to $n_s(T)$.

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16 We have taken different values of the fitting parameter $\Delta_0/k_B T_c$ for $T_1^{-1}$ and $n_s(T)$. It seems to be natural, since different samples are used in these experiments.[12,13]

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