Possible pairing symmetries in the ordered honeycomb network superconductor BaPtSb

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Abstract. We investigate the pairing symmetry of the ordered honeycomb network superconductor BaPtSb, which has a crystal structure without inversion center. There is a preliminary \(\mu\)SR report which implies the broken time-reversal symmetry in the superconducting state. In this paper, we classify the pairing symmetry and examine the pairing instability. Among the unconventional states with time-reversal symmetry breaking, we find that the state with a gap structure compatible with Fermi surfaces is the spin-triplet chiral \(p\)-wave state.

1. Introduction

The series of superconductors with ordered honeycomb network structure has been found, since the discovery of the superconductivity in SrPtAs [1]. In this paper we focus on the recently discovered one BaPtSb with inversion-symmetry breaking (\(T_c = 1.6\,\text{K}\), the point group; D\(_{3h}\)) [2, 3]. The first principle calculation reveals that the anti-symmetric spin-orbit coupling works significantly and causes band splitting [4]. The preliminary result of the muon spin relaxation (\(\mu\)SR) experiment implies a spontaneous field below \(T_c\) and the superconducting state may break the time-reversal symmetry [5].

In this paper, we classify the pairing symmetry using group theoretical approach and examine the pairing instability. Among the states with broken time-reversal symmetry, we find that the preferable one compatible with Fermi surface structures is the spin-triplet chiral \(p\)-wave state with \(S_z = 0\). This pairing is renowned as a topological state and supports the chiral surface state at the sample boundary.

2. Tight-binding model

The detail of the band structure of BaPtSb has been reported [4]. The result reveals that Pt 5d and Sb 5p orbitals are dominant in the low energy region. We have basically three Fermi surfaces with spin-orbit splitting. Two of them are cylindrical around the \(\Gamma\) point, and the other one is spherical around \(K\) and \(K'\) points. We should emphasize that the anti-symmetric spin orbit coupling coming from the broken inversion symmetry plays an important role.

We construct the tight-binding model for the low energy excitations, which would be relevant for the superconductivity. For simplicity, we take three Pt 5d orbitals into account and all the
hopping are diagonal with respect to the orbital degrees of freedom. The Hamiltonian is

\[ H_0 = \sum_{\mathbf{k} \sigma} \epsilon^{(b)}_{\mathbf{k} \sigma} c^\dagger_{\mathbf{k} \sigma} c_{\mathbf{k} \sigma}, \] (1)

\[ \xi^{(b)}_{\mathbf{k} \sigma} = \epsilon^{(b)}_{\mathbf{k}} + \sigma \alpha^{(b)}_{\lambda_{\mathbf{k}}}, \]
\[ \xi^{(b)}_{\mathbf{k}} = t^{(b)} \epsilon_{\mathbf{k} \mathbf{1}} + (t_{z1}^{(b)} + t_{z2}^{(b)} \epsilon_{\mathbf{k} \mathbf{1}} + t_{z3}^{(b)} \epsilon_{\mathbf{k} \mathbf{2}} + t_{z4}^{(b)} \epsilon_{\mathbf{k} \mathbf{3}}) \cos k_z c - \mu^{(b)}, \]
\[ \lambda_{\mathbf{k}} = \sum_{n=1}^{3} \sin \mathbf{k} \cdot \mathbf{T}_n, \epsilon_{\mathbf{k} \mathbf{1}} = \sum_{n=1}^{3} \cos \mathbf{k} \cdot \mathbf{T}_n, \epsilon_{\mathbf{k} \mathbf{2}} = \sum_{n=1}^{3} \cos \mathbf{k} \cdot \mathbf{T}^\prime_n, \epsilon_{\mathbf{k} \mathbf{3}} = \sum_{n=1}^{3} \cos \mathbf{k} \cdot 2 \mathbf{T}_n, \]

where \( b, \mathbf{k}, \sigma \) show the band, momentum, and \( z \)-component of spin, respectively. The in-plane nearest neighbor bond vectors are \( \mathbf{T}_1 = (0,a,0), \mathbf{T}_2 = (-\sqrt{3}/2,-a/2,0) \), and \( \mathbf{T}_3 = (\sqrt{3}/2,-a/2,0) \). We have also \( \mathbf{T}_1' = \mathbf{T}_1 - \mathbf{T}_2, \mathbf{T}_2' = \mathbf{T}_2 - \mathbf{T}_3, \) and \( \mathbf{T}_3' = \mathbf{T}_3 - \mathbf{T}_1 \). This model consists of the in-plane nearest neighbor hopping \( t^{(b)} \), and out-of-plane \( l \)-th nearest hoppings \( t_{z l}^{(b)} (l = 1,2,3,4) \). We also have the anti-symmetric spin-orbit coupling \( \alpha^{(b)} \) with \( \lambda_{\mathbf{k}} = -\lambda_{-\mathbf{k}} \) coming from the broken inversion symmetry. In this system, the symmetry breaking occurs in the in-plane direction and the spin-orbit coupling is diagonal with respect to \( \sigma \). The spectrum satisfies \( \xi^{(b)}_{\mathbf{k} \mathbf{1}} = \xi_{-\mathbf{k} \mathbf{1}} \) and the spin-singlet pairing or the spin-triplet pairing with \( S_z = 0 \) (i.e. \( S_z \) conserving states) are stabilized as we will see later.

We fit this model to the result of \textit{ab initio} calculation \cite{4}. The fitting parameters and Fermi surfaces are shown in Table 1 and Figure 1.

**Table 1.** The fitting parameters in the tight-binding model Eq. (1).

|          | \( t^{(b)} \) | \( t_{z1}^{(b)} \) | \( t_{z2}^{(b)} \) | \( t_{z3}^{(b)} \) | \( t_{z4}^{(b)} \) | \( \mu^{(b)} \) | \( \alpha^{(b)} \) |
|----------|----------------|-----------------|-----------------|----------------|----------------|-------------|-------------|
| Band 1 \( (b = 1) \) | 0.85           | -0.09           | -0.01           | 0.01           | 1.7            | 0.3         |
| Band 2 \( (b = 2) \) | 0.1            | -0.25           | -0.25           | 0.2            | 0.4            | 0.25        |
| Band 3 \( (b = 3) \) | -0.65          | 0.9             | -0.3            | 0.05           | 0.01           | 1.9         | 0.07        |

**Figure 1.** Fermi surfaces obtained from the tight-binding model Eq. (1) with parameters listed in Table 1. See also the result of \textit{ab initio} calculation \cite{4}.
3. Pairing instability

Using the point group $D_{3h}$, we find a basis of gap matrices in an irreducible representation $\Gamma$

$$\Delta^\Gamma_k = \Delta_s \psi^\Gamma_k + \Delta_i d^\Gamma_k \cdot \sigma$$

(2)

where $\psi^\Gamma_k$ and $d^\Gamma_k$ are the basis functions for spin-singlet and triplet channels normalized in the Brillouin zone, and $m = 1, \ldots, N$ in $N$-dimensional irreducible representation. The details of this classification would be discussed elsewhere.

We then argue the pairing instability. Although it may occur due to the inversion-symmetry breaking in principle, the mixing between spin-singlet and triplet channels is not expected to be large and neglected hereafter. The linearized gap equations are

$$\frac{1}{g_k(m(b))} = \sum n \frac{|\psi^\Gamma_k|^2}{2\xi^{(b)}_k} \tanh \frac{\xi^{(b)}_k}{2k_BT_c},$$

(3)

$$\frac{1}{g_i(m(b))} = \sum n \frac{|d^\Gamma_k|^2}{2\xi^{(b)}_k} \tanh \frac{\xi^{(b)}_k}{2k_BT_c}.$$  

(4)

We fix $T_c$ and estimate the integral in the r.h.s., and compare the obtained coupling constants in the l.h.s. of the equations. A basis would be more favorable if the obtained coupling constant is smaller. The most stable basis for each pairing range for each band is listed in Table 2. We note that spin-singlet states or triplet states with $\tilde{\sigma} = 0$ (the $d$ || $\hat{z}$) are stabilized strongly by the spin-orbit coupling $\sigma \alpha(\beta) \lambda_k$, which causes the band splitting with keeping the relation $\xi_k = \xi_{-k}$. We also see that the $E_2$ representation is favored in several cases. The locations of the peaks of these basis functions are well overlapped with that of Fermi surfaces, and thus the condensation energies are enhanced (see Figure 2).

| pairing range                  | Band 1                     | Band 2     | Band 3     |
|-------------------------------|-----------------------------|------------|------------|
| on-site                       | $\psi^{A1} = 1$             | $\psi^{A1} = 1$ | $\psi^{A1} = 1$ |
| in-plane nearest              | $\psi^{A1} = \epsilon_k$   | $d^{E2,1}_k = \tilde{\epsilon}_k$ | $d^{E2,1}_k = \tilde{\epsilon}_k$ |
| in-plane 2nd nearest          | $d^{E2,1}_k = \tilde{\epsilon}_k$ | $d^{E2,1}_k = \tilde{o}_k \hat{z}$ | $d^{E2,1}_k = \tilde{o}_k \hat{z}$ |
| out-of-plane nearest          | $\psi^{A1} = \cos k_z c$   | $\psi^{A1} = \cos k_z c$ | $\psi^{A1} = \cos k_z c$ |
| out-of-plane 2nd nearest      | $\tilde{\epsilon}_k$      | $d^{E2,1}_k = \tilde{\epsilon}_k$ | $\psi^{A1} = \tilde{\epsilon}_k$ |

The pairing states in the $E_2$ representation is

$$d_k = \eta_1 d^{E2,1}_k + \eta_2 d^{E2,2}_k,$$

(5)

where $\eta = (\eta_1, \eta_2)$ is the two-dimensional order parameter, and we mainly have two possible pairing states: the chiral $p$-wave state and the nematic one [6] (see Table 3). Both states are topological but only the chiral $p$-wave state breaks the time-reversal symmetry. The chiral state is fully gapped, whereas the nematic one has line nodes. Thus, the chiral state would be more favorable at least in the weak coupling regime.
Figure 2. The contour plots of the amplitudes of stable $E_2$ bases listed in Table 2; (a) in-plane nearest basis $|o_k^+ \hat{z}|$, (b) in-plane 2nd nearest basis $|\bar{o}_k^+ \hat{z}|$, and (c) out-of-plane 2nd nearest basis $|\tilde{o}_k^+ \hat{z}|$ at $k_z = 0$. We see that the peaks in (a) and (c) ((b)) are on the Fermi surfaces of Band 2 (Band 1 and 3).

Table 3. Possible pairing symmetries in the $E_2$ representation.

| pairing       | $(\eta_1, \eta_2)$ | small $k$ exp. of Eq. (5) | TRS     | topological surface state |
|---------------|---------------------|---------------------------|---------|--------------------------|
| chiral $p$-wave nematic | $(1, 0), (0, 1)$     | $k_x \pm ik_y$            | broken chiral | flat band         |
|                | $(1, 1), (1, -1)$   | $k_x, k_y$                | unbroken | flat band             |

4. Summary
We discuss the pairing states favored by the Fermi surface structures in BaPtSb using the linearized gap equations. The candidate with broken time-reversal symmetry is the chiral $p$-wave state with non-trivial topology. In other words, the Fermi surface structures favor the chiral $p$-wave state more than any other states with broken time-reversal symmetry, such as the chiral $d$-wave $(d_{x^2-y^2} \pm id_{xy}$wave) state included in $E_1$ and $E_2$ representations. The chiral $d$-wave state could be stabilized if there were a cylindrical Fermi surface in the proximity of the saddle points [7, 8, 9, 10].

We need further discussion for the comprehensive understanding of the superconducting state in this material. The polar Kerr effect measurement would be a relevant probe to examine the time-reversal symmetry breaking [11]. More information about the normal state properties and electronic correlation effects would be necessary to reveal the pairing mechanism that works in this system.

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