Anisotropic superconductivity in PrOs$_4$Sb$_{12}$

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Abstract. Recently two anisotropic superconducting gap functions have been observed in the skutterudite PrOs$_4$Sb$_{12}$. These order parameters are spin-triplet. There are at least 2 distinct phases in a magnetic field, bearing some resemblance to superfluid $^3$He. Here we present an analysis of the thermodynamic properties in these two superconducting states within the weak-coupling BCS theory.

PACS. 74.20.Fg BCS theory and its development

1 Introduction

Superconductivity in the body-centered cubic heavy-fermion (HF) skutterudite PrOs$_4$Sb$_{12}$ was discovered in 2002 by Bauer et al[1,2,3]. Since then many experimental and theoretical studies of this compound have been reported. This compound possesses several interesting and unusual characteristics: two distinct phases (the A phase and B phase) in a magnetic field, nodal superconductivity with point nodes, and triplet pairing with chiral symmetry breaking [6,7,8]. The phase diagram is still controversial. In Fig. 1 recent measurements by Measson et al [9] are shown.

It was recently observed that the magnetothermal conductivity data [7] in this compound are consistent with anisotropic superconductivity using the gap functions

$$\Delta_A(k) = d e^{\pm i\phi} \frac{3}{2}(1 - \hat{k}_x^4 - \hat{k}_y^4 - \hat{k}_z^4).$$

(1)

Here $e^{\pm i\phi}$ is one of $e^{i\phi_1} = (\hat{k}_y + i\hat{k}_z)/\sqrt{\hat{k}_y^2 + \hat{k}_z^2}, e^{i\phi_2} = (\hat{k}_y + i\hat{k}_z)/\sqrt{\hat{k}_y^2 + \hat{k}_z^2}, e^{i\phi_3} = (\hat{k}_y + i\hat{k}_z)/\sqrt{\hat{k}_y^2 + \hat{k}_z^2}$. The factor of $3/2$ ensures proper normalization of the angular dependence of the order parameter. In Eq.(2) the nodal direction is chosen to be parallel to (001).

We note that the proposed order parameter (2) lies outside of the usual classification scheme [11], in which order parameters correspond to a single irreducible representation of the rotation group. However, this hybrid order parameter appears to be necessary to reproduce the observed B-phase gap structure. A similar situation has been observed in the borocarbide superconductors [12].

The cubic symmetry of PrOs$_4$Sb$_{12}$ suggests order parameters which are invariant under the $T_h$ cubic tetrahedral symmetry group applicable to this crystal [10], as well as reflections (containing the origin) about the planes of the crystal parallel to the cube faces [13]. As suggested in [10], one possible invariant is $\hat{k}_x^2\hat{k}_y^2 + \hat{k}_y^2\hat{k}_z^2 + \hat{k}_z^2\hat{k}_x^2$. This belongs to the $A_1$ representation of $T_h$ [10].

This combination can be recast as $1 - \hat{k}_x^4 - \hat{k}_y^4 - \hat{k}_z^4$, thus forming the basis of the proposed order parameter of the A phase. Furthermore, in weak-coupling BCS theory the quasiparticle density of states and the thermodynamics depend only on $|f|^2$, the magnitude of the angle-dependent part of the order parameter. For this reason, an order parameter which breaks chiral symmetry still retains the essential features of the cubic symmetry, and is in fact necessitated by the triplet pairing observed in this compound [6,7,8].

Triplet pairing requires that the orbital wavefunction be antisymmetric under particle interchange. The phase factor proposed in Eq. (1) meets this requirement.

The proposed B-phase order parameter breaks the cubic symmetry more manifestly. Nevertheless, there is al-
most certainly a relationship between the A and B phase, particularly since the zero-field transition temperatures are so nearly equal. The simplest relationship consistent with the nodes at [001] and [001], despite requiring a hybrid representation, would suggest $|f| \sim 1 - \hat{k}_x^4$. This order parameter again would have a phase factor included in $f$ to ensure antisymmetry under interchange. These proposed order parameters are illustrated in Fig. 2 [17].

We note that while the B-phase is the prevalent phase in zero magnetic field, the A-phase exists at all temperatures below $T_c$ for fields between $H^*$ (the phase boundary) and $H_{c2}$.

Below is a comparison of the predicted B-phase DOS with scanning tunneling microscopy (STM) data taken by Suderow et al [18] at $T=0.19$ K. The predicted B-phase DOS differs somewhat from that presented in [7] due to the use of the angular-dependent quasiparticle density-of-states, as well as an accounting for the energy and directional resolution of the STM. Here we have assumed that the STM performed measurements along the nodal directions, where $\alpha$ is the size of the momentum cone within the STM’s spatial resolution. We note that the nodal structure can easily be masked by performing STM along a limited number of directions of single crystals. Here we have assumed $\Delta$ to take the B-phase weak-coupling value of 3.3 K. We observe fair agreement, with some differences apparent surrounding the quasiparticle peak at $E = \Delta$. In the following we analyze both phases over the entire temperature range from $T = 0$ to $T_c$.

2 Weak-coupling BCS Theory

We focus on the superconductivity in the A and B-phases of PrOs$_4$Sb$_{12}$, using the $\Delta(k)$ given by Eqs. 1 and 2 with $|d| = \Delta(T)$.
In the low-temperature regime $T / \Delta_0 < 4$ can be solved analytically. For $T < T_c$ where $N < 2^\gamma$ where $\gamma$ is the angular-dependent part of the order parameter and $N_0$ the normal state density of states at the Fermi level. For the A-phase, $< |f|^2 > = 3/7$, whereas for the B-phase, $< |f|^2 > = 32/45$. This yields two distinct condensation energies:

$$E_0^A = -1.17 N_0 (T_c^A)^2,$$

$$E_0^B = -1.32 N_0 (T_c^B)^2.$$
While there are a few reports of $H_c^2(T)$ for the A-phase and $H^*(T)$, the phase boundary between the A-phase and the B phase\cite{14,19,21,22,23}, no experimental data are available for $H_c(T)$. Finally the superfluid density is given by

$$\rho_{sA}(T) = 1 - \frac{\pi}{2} \left( \frac{T}{\Delta T} \right) + \ldots \quad (22)$$

$$\rho_{sBp}(T) = 1 - \frac{3\pi}{4} \left( \frac{T}{\Delta T} \right) + \ldots \quad (23)$$

$$\rho_{sBp}(T) = 1 - \frac{\pi^2}{16} \left( \frac{T}{\Delta T} \right)^2 + \ldots \quad (24)$$

Close to the transition temperature, we find

$$\rho_{sA}(T) \approx 6 < f^2 > \left( -\ln \frac{T}{T_c} \right) \quad (25)$$

$$= 1.393 \left( -\ln \frac{T}{T_c} \right) \quad (26)$$

$$\rho_{sBp}(T) \approx 17 \cdot 13 \left( -\ln \frac{T}{T_c} \right) \quad (27)$$

$$= 0.9567 \left( -\ln \frac{T}{T_c} \right) \quad (28)$$

where Re(...) refers to the real part, and the subscripts $\parallel$ and $\perp$ indicate parallel and perpendicular directions to the nodal points. The superfluid density, as expected, is isotropic for the cubic symmetry-retaining A-phase, but rather anisotropic for the B-phase. These superfluid densities are shown in Fig. 7. In the low-temperature regime ($T \ll \Delta$) both Eq. (20) and Eq. (21) can be expanded as
\[
\frac{\rho_{B\bot}(T)}{\rho_{s\bot}(0)} = \frac{31 \cdot 221}{45 \cdot T_c} (- \ln T/T_c) = 1.9772 (- \ln T/T_c)
\]

(29)

(30)

In the figure above we have compared \(\frac{\rho_{B\parallel}(T)}{\rho_{n\parallel}(0)}\) with the data taken from Chia et al., assuming that the nodal points in \(\Delta(k)\) are aligned parallel to \(\mathbf{H}\). Rather satisfactory agreement is observed for \(T < T_c/3\). But the theoretical \(\rho_{s\bot}(T)\) vanishes linearly with \(T_c - T\) in the vicinity of \(T = T_c\), whereas Chia et al. found a \(\rho_{s\bot}(T)\) which vanishes with essentially infinite slope at \(T_c\).

Recently Chia et al. also reported magnetic penetration depth measurements for a range of dopings \(x\) from 0.1 to 0.8 in the compound \(\text{Pr(Os}_4\text{Ru}_4\text{)}_4\text{Sb}_{12}\). Over the range from \(x = 0.4\) to \(x = 0.8\), exponential temperature dependence of the superfluid density was found, indicating an isotropic s-wave gap function in this regime. Of direct interest for this work, the superfluid density was found to go to zero linearly for all dopings, with no hint of the essentially infinite slope found in the pure case \((x=0)\). In addition, the slope of these linear curves at \(T_c\) does not increase dramatically from \(x=0.8\) to \(x=0.1\). Further experiments at doping ranges between \(x = 0\) and \(x = 0.1\) are highly desirable, to examine more closely the apparent transition from nodal to conventional superconductivity taking place in this system. It would also be of value to confirm the rather unusual “infinite-slope” behavior observed in the pure sample near \(T_c\).

3 Concluding Remarks

We have worked out the weak-coupling theory of the A and B phases of the heavy-fermion superconductor \(\text{PrOs}_4\text{Sb}_{12}\). A simple thermodynamic analysis offers an explanation for the appearance of the lower-symmetric B phase at lower temperatures. The present model leads to a fair description of STM data taken by Suderow et al. In addition, the present model for the B-phase describes the superfluid density determined by Chia et al. for the low-temperature regime, if we assume that the nodal points in the B-phase follow the magnetic field direction in the field cooled situation. Since the magnetic field is the only symmetry-breaking agent, this appears to be plausible. We will present the results of an analysis in the case of impurities shortly.

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