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Superconducting gap nodes in $PrOs_4Sb_{12}$

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Abstract

We examine the superconducting gap nodes in crystals with tetrahedral (T_h) symmetry. The $(0, 0, 1)$ phase of the three dimensional order parameter in the triplet channel has nodes in the [001] directions. Following a second order phase transition to the state $(0, i|\eta_2|, |\eta_1|)$, each node lifts away from the Fermi surface and splits into two deep dips. We discuss this scenario in the context of multiple superconducting phases in $PrOs_4Sb_{12}$.

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In the years since the discovery of multiple superconducting phases in $PrOs_4Sb_{12}$ experimental results concerning the symmetry of the superconducting states have proliferated, but so far no theoretical description is widely accepted. Our starting point is a strict analysis of symmetry and symmetry-breaking described by Landau theory [1,2]. This approach makes definite statements about the symmetry and gap nodes of possible superconducting states. In this proceedings, we extend this analysis to discuss the possible existence of deep dips in the gap function, and how they may be observed experimentally.

$PrOs_4Sb_{12}$ has two superconducting phases, as observed in thermal conductivity [3] and several other measurements [4–6], the 'A-phase', which borders the normal phase on the H-T phase diagram and the 'B-phase' which appears just below it. There are more experimental observations of the B-phase than the A-phase, in part because it occupies a much greater area of the phase diagram. Various measurements have determined that the B-phase has triplet pairing, breaks time-reversal symmetry [4] and has nodes or near-nodes in the [001] directions of the gap function [3,5]. Some experiments have interpreted the double transition in terms of multi-band superconductivity [7], such that the A-phase and B-phase possess the same symmetry. A third superconducting phase has been detected deep in the superconducting region of the H-T phase diagram, but its symmetry properties are presently unknown [8].

As the starting point of this discussion, we select from Table I of Ref. [2] the state which best matches the description of the B-phase. This table is a list of all possible superconducting states for crystals with tetrahedral symmetry with their corresponding gap nodes. Broken time-reversal symmetry is indicated by the absence of the element K in the symmetry groups. We also take into consideration the second order phase transition sequences, shown in Figs. 1 and 2 of Ref. [2]; the B-phase should be two steps away from the normal phase. The best choice for the B-phase is given by a three component order parameter, which transforms according to the 3D representation of the tetrahedral point group, with components $(0, i|\eta_2|, |\eta_1|)$, in the triplet channel. This phase breaks time reversal symmetry, and it is uniquely accessible both directly from the normal phase and from the phase $(0, 0, 1)$ by a second order phase transition. However, strictly speaking, this phase is nodeless. The A-phase is identified with the state $(0, 0, 1)$. The symmetry groups associated with $(0, 0, 1)$ and $(0, i|\eta_2|, |\eta_1|)$ are $D_2(C_2) \times K$ and $D_2(E)$ respectively [2]. Each of these includes non-trivial combinations of the D_2 point group operations, gauge elements and/or time reversal, and a group-subgroup relation exists between them.

Although a lowering of symmetry through the A-B transition is expected, the four-fold to two-fold symmetry lowering observed in a thermal conductivity experiment [3] is not described by this scenario. The probable existence of domains may account for the four-fold observation, espe-

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cially since in the tetrahedral point group there can be no four-fold symmetry, but then it is impossible to account for the two-fold observation. Clearly, confirmation of these results would be very useful.

The basis functions for the 3D representation in the triplet channel are

$$\{\mathbf{d}_1(\mathbf{k}), \mathbf{d}_2(\mathbf{k}), \mathbf{d}_3(\mathbf{k})\} =$$
$$\{a\hat{\mathbf{y}}k_z + b\hat{\mathbf{z}}k_y, a\hat{\mathbf{z}}k_x + b\hat{\mathbf{x}}k_z, a\hat{\mathbf{x}}k_y + b\hat{\mathbf{y}}k_x\},$$

where a and b are real numbers. Under octahedral symmetry, $|a| = |b|$. Since the Fermi surface is approximately octahedral [9], we will assume $|a| \approx |b|$. The gap functions are

$$\Delta_\pm(\mathbf{k}) = [|\mathbf{d}(\mathbf{k})|^2 \pm |\mathbf{d}(\mathbf{k}) \times \mathbf{d}^*(\mathbf{k})|]^{1/2},$$

where

$$\mathbf{d}(\mathbf{k}) = \sum_i \eta_i \mathbf{d}_i(\mathbf{k})$$

and η_i are the components of the order parameter. There are two different gap functions when $\mathbf{d}^*(\mathbf{k}) \neq \mathbf{d}(\mathbf{k})$, *i.e.* when time reversal symmetry is broken. In that case, usually only the '$-$' sign yields a gap function with nodes.

For the A-phase $(0,0,1)$, we have $\mathbf{d}(\mathbf{k}) = a\hat{\mathbf{x}}k_y + b\hat{\mathbf{y}}k_x$ with gap $[a^2k_y^2 + b^2k_x^2]^{1/2}$, which has two point nodes in the [001] directions, as shown in Fig. 1a). These nodes are a strict consequence of symmetry and are not an artifact of the choice of basis functions. The B-phase $(0, i|\eta_2|, |\eta_1|)$ emerges as a result of a second order phase transition, so $|\eta_2|$ is small close to the transition line. The gap function of the B-phase is

$$\Delta(\mathbf{k}) = [(|\eta_1|^2b^2 + |\eta_2|^a b^2)k_x^2 + |\eta_1|^2a^2k_y^2 + |\eta_2|^2b^2k_z^2$$
$$-2|\eta_1||\eta_2||k_x|\sqrt{a^2b^2k_x^2 + a^4k_y^2 + b^4k_z^2}]^{1/2}.$$

For small η_2, the nodes of the A-phase lift away from the Fermi surface, as expected, and split into two, as shown in Fig. 1b). Larger values of η_2 cause the dips to move around with respect to the Fermi surface, and the dips become less pronounced in general, as shown in Fig. 1c).

If the transition between the A-phase and the B-phase is second order then the gap minimum in the B-phase will be small in the vicinity of the phase boundary. Although in general, finite gaps will destroy power-law temperature dependencies in specific heat, *etc.*, at temperatures large compared to the gap minimum power laws may still be observe. [11]. As the temperature is lowered, two effects are at work, first, measurements become more sensitive to the finite energy gaps because of the reduced temperature and, second, the B-phase may evolve from a state with deep dips in the energy gap function and a small gap minimum toward a state in which the dips are less pronounced.

Experimentally, the situation is far from clear. Power law temperature dependencies are observed in the specific heat [14], thermal conductivity [3] and penetration depth [5]. On the other hand, nodelessness has been interpreted from nuclear quadrupole resonance [12], μSR [13] and tunneling spectroscopy [10]. Various temperature ranges were studied in each case. Each of these methods represents a different

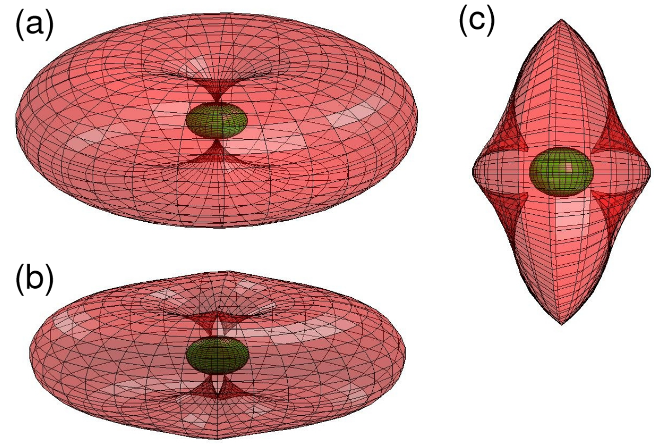

Fig. 1. Gap functions drawn over a spherical Fermi surface for $a = 1.2$ and $b = 1$. a) The A-phase, η_1 =1.1, $\eta_2 = 0$ with nodes in the [0, 0, 1] direction. b) The B-phase, $\eta_1 = 1$, $\eta_2 = 0.2$. c) The B-phase, $\eta_1 = 1$, $\eta_2 = 0.85$.

approach to the detection of quasiparticles in gap nodes. The cross-over between universal and non-universal scaling described in this proceedings would likely be observed differently in each experimental arrangement. To test the scenario put forward in this proceedings, evidence of a cross-over between universal and non-universal scaling behaviour should be sought within a single set-up. Of course, the ideal measurement would be a direct, directional-dependent detection of nodes or near nodes, especially of the splitting of nodes through the phase transition.

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