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Ultralow-temperature heat transport study of noncentrosymmetric superconductor CaPtAs

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The noncentrosymmetric superconductor CaPtAs with time-reversal symmetry breaking in its superconducting state was previously proposed to host nodal superconductivity. Here, by employing ultralow-temperature thermal conductivity measurement on CaPtAs single crystal, we study its superconducting gap structure. A negligible residual linear term of thermal conductivity (κ_0/T) in zero magnetic field and the field dependence of κ_0/T indicate that CaPtAs has multiple superconducting gaps with a dominant s-wave component. This is consistent with recent nuclear quadrupole resonance measurements on CaPtAs. Our work puts a strong constraint on the theories to describe the superconducting pairing symmetry of CaPtAs.

Keywords: noncentrosymmetric superconductor, thermal conductivity, superconducting gap structure

PACS: 74.25.fc, 74.25.Jb, 74.25.Op, 74.70.–b **DOI:** 10.1088/1674-1056/ad02e9

1. Introduction

Finding exotic superconductors and elucidating their superconducting pairing mechanism are important topics in condensed matter physics.[1] The noncentrosymmetric superconductors (NCSs) have attracted much attention since the discovery of unconventional superconductivity in $CePt_3Si$.[2,3] The existence of antisymmetric spin–orbit coupling (ASOC) leads to spin-split electron bands, which allows for the admixture of spin-singlet (s-wave) and spin-triplet (p-wave) pairing state.[4,5] Due to the strong electron correlation effect in this f-electron NCS, it is hard to study the role of ASOC in the superconducting state alone. Subsequently, many non-f-electron NCSs with weakly correlated electrons have been found, such as $Li_2(Pd_{1-x}Pt_x)_3B$,[4,5] $LaPt_3Si$ and $BaPt_3Si$.[6,7] Therefore, it is possible to disentangle ASOC from the correlation effects.[4,5,8] However, most weakly correlated NCSs exhibit the dominant s-wave superconducting state,[9–11] which raises the question of the exact role of ASOC in the superconducting pairing state.

Recently, a new NCS CaPtAs with weakly correlated effect has attracted considerable attention.[12] It has a transition temperature $T_c \approx 1.5$ K. Specific heat and muon-spin relaxation (μSR) measurements suggest nodes in the superconducting gap and broken time-reversal symmetry (TRS) in its superconducting state.[13] This has stimulated more theoretical works on CaPtAs, including spontaneous spin polarization, the origin of the gap nodes, and possible topological superconductivity.[14–16] However, more recent nuclear quadrupole resonance (NQR) measurements indicate that CaPtAs is a multigap superconductor with a large s-wave component.[17] In this context, more techniques are needed to clarify the superconducting state of CaPtAs.

Ultralow-temperature thermal conductivity is an established bulk technique to study the superconducting gap structure.[18] In this paper, we present ultralow-temperature thermal conductivity measurements on CaPtAs single crystal to investigate its superconducting gap structure. In zero magnetic field, a negligible residual linear term κ_0/T is observed, indicating a dominant s-wave pairing in its superconducting state. In magnetic fields, the field dependence of κ_0/T suggests CaPtAs has multiple superconducting gaps. These results are consistent with the NQR measurements in Ref. [17].

2. Materials and methods

CaPtAs single crystals were synthesized using a self-flux method.[12] The obtained single crystals have black

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metallic luster with mirror-like surfaces, as shown in the inset of Fig. 1(a). X-ray diffraction (XRD) measurement was performed with a D8 Advance x-ray diffractometer from Bruke. The sample for transport measurements was cut into a rectangular shape of 1.10×0.15 mm^2 with a thickness of 0.11 mm. Four silver leads were attached to the sample surface with silver paint, which were used for both resistivity and thermal conductivity measurements. The contact resistance is about 30 mΩ at 2 K. The in-plane resistivity was measured in a physical property measurement (PPMS, Quanutm Design) in a ^{3}He cryostat. The in-plane thermal conductivity was measured in a dilution refrigerator by using a standard four-wire steady-state method with two RuO_2 chip thermometers, calibrated *in situ* against a reference RuO_2 thermometer. Heat current was in the *ab* plane, and the magnetic field was applied along the *c* axis for all measurements. To ensure a homogeneous field distribution in the sample, all fields for resistivity and thermal conductivity measurements were applied above T_c.

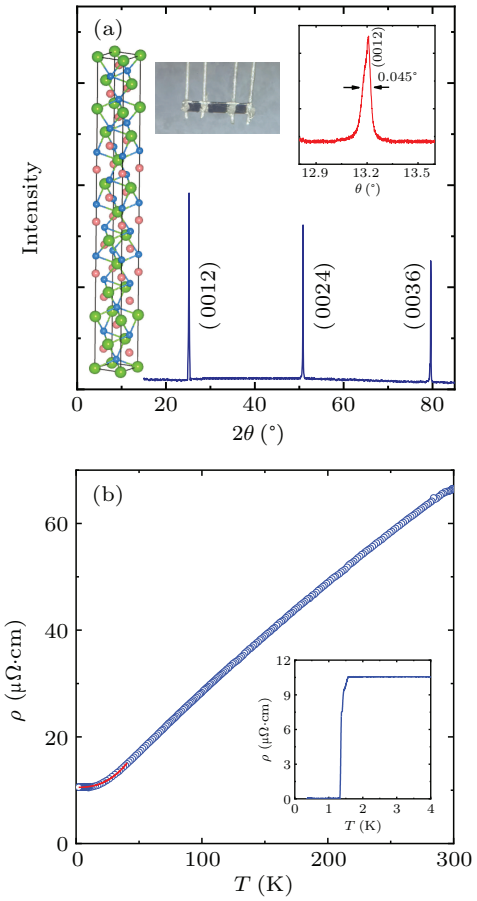


Fig. 1. (a) Room-temperature XRD pattern from the largest natural surface of CaPtAs single crystal. The left inset shows the chematic crystal structure for the orthorhombic GaPtAs (Ca: green; Pt: orange; As: blue) with space group $I4_1md$ (No. 109). The top inset is the optical image of CaPtAs single crystal with four electrodes and the rocking curve of the (0012) Bragg peak. (b) The temperature dependence of resistivity at zero magnetic field for CaPtAs single crystal, with current in (00*l*) plane. The red line is the fit of the normal-state resistivity to the Fermi-liquid behavior $\rho(T) = \rho_0 + AT^2$ from 1.5 K to 50 K. Inset: The resistive superconducting transition at low temperature.

3. Results and discussion

CaPtAs crystallizes in an orthorhombic structure with the space group $I4_1md$ (No. 109).[12,13] The large natural surface is identified to be the (00*l*) plane by XRD measurement, as illustrated in Fig. 1(a). The right inset of Fig. 1(a) shows the x-ray rocking curve of the (0012) Bragg peak. The full width at half-maximum (FWHM) is only about 0.045°, indicating the high quality of our CaPtAs single crystals. The in-plane resistivity of CaPtAs in zero field is plotted in Fig. 1(b). At low temperature, the width of the resistive superconducting transition (10%–90%) is 0.09 K, and the T_c is 1.36 K, defined at the 50% drop of the resistivity ($T_c^{50\%}$). The fit of the normal-state resistivity between 1.5 K and 50 K to Fermi-liquid behavior $\rho(T) = \rho_0 + AT^2$ yields $\rho_0 = 10.5$ μΩ·cm and $A = 2.6 \times 10^{-3}$ μΩ·cm·K^{-2}. The residual resistivity ratio $RRR = \rho(300\text{ K})/\rho_0$ is around 6.

Figure 2(a) shows the low-temperature resistivity of the CaPtAs single crystal in various magnetic fields up to 0.25 T. With increasing field, the superconducting transition is gradually suppressed to lower temperatures. To determine the upper critical field $\mu_0 H_{c2}(0)$, the T_cs at different fields are plotted in Fig. 2(b). An apparently linear temperature dependence of $\mu_0 H_{c2}$ can be seen. With a linear fit of the data, $\mu_0 H_{c2}^{10\%}(0) \approx 0.076$ T is roughly estimated, which is taken as the bulk upper critical field. Such a linear temperature dependence of H_{c2} has been previously observed in other superconductors, such as MgB_2,[19–21] UBe_{13},[22] YPtBi,[23] and pressurized Bi_2Se_3 and Cd_3As_2. For MgB_2, it may come from a two-band Fermi surface topology.[19–21] For heavy-fermion superconductor UBe_{13} and non-centrosymmetric superconductor YPtBi, it was considered as an indication of unconventional state.[22,23] While for pressurized topological insulator Bi_2Se_3 and Dirac semimetal Cd_3As_2, it probably relates to their topological bands.[24,25] Since density function theory calculations show that there are complex multiple electronic bands in CaPtAs[12] and CaPtAs is a non-centrosymmetric superconductor, the origin of its linear temperature dependence of $\mu_0 H_{c2}$ needs further investigation.

Figure 3 depicts the in-plane thermal conductivity of the CaPtAs single crystal in various magnetic fields. The measured thermal conductivity contains two contributions, $\kappa = \kappa_e + \kappa_p$, which comes from electrons and phonons, respectively. In order to separate the two contributions, all the curves below 0.5 K are fitted to $\kappa/T = a + bT^{\alpha-1}$.[26,27] aT and bT^α represent the contributions from electrons and phonons, respectively. The residual linear term $\kappa_0/T \equiv a$ is obtained by extrapolating κ/T to $T = 0$ K. Due to the specular reflections of phonons at the sample surface, the power α in the second term is typically between 2 and 3.[26,27] In zero field, the fitting gives $\kappa_0/T = 0.005 \pm 0.03$ mW·K^{-2}·cm^{-1}

and $\alpha = 2.85 \pm 0.09$. To show the data more clearly, κ/T vs. $T^{1.85}$ is plotted in Fig. 3(a). In consideration of our experimental error bar ± 5 μW·K^{-2}·cm^{-1}, the κ_0/T of CaPtAs in zero field is negligible. For s-wave nodeless superconductors, there are no fermionic quasiparticles to conduct heat as $T \to 0$, since all electrons participate in the formation of Cooper pairs.[18,26] Therefore, there is no residual linear term, as seen in V_3Si and $NbSe_2$.[26,28] However, for nodal superconductors, a substantial κ_0/T in zero field contributed by the nodal quasiparticles has been found.[18] For example, κ_0/T of the overdoped (T_c = 15 K) d-wave cuprate superconductor $Tl_2Ba_2CuO_{6+\delta}$ (Tl-2201) is 1.41 mW·K^{-2}·cm^{-1}.[29] Therefore, the negligible κ_0/T observed in CaPtAs indicates a dominant s-wave pairing in its superconducting state.

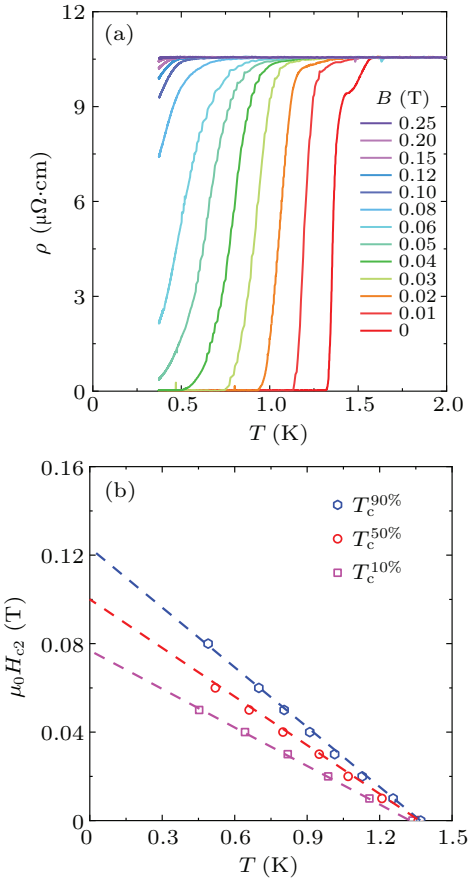


Fig. 2. (a) Low-temperature resistivity of CaPtAs single crystal in magnetic field up to 0.25 T. (b) Temperature dependence of the upper critical field $\mu_0 H_{c2}(T)$, the upper critical fields were defined by dropping to 90%, 50%, 10% normal-state resistivity, respectively. The magnetic fields were applied along the c axis. The dashed lines are the linear fit to the data, which point to $\mu_0 H_{c2}^{90\%}(0) = 0.124$ T, $\mu_0 H_{c2}^{50\%}(0) = 0.1$ T, and $\mu_0 H_{c2}^{10\%}(0) = 0.076$ T.

The field dependence of κ_0/T can provide further information on the superconducting gap structure.[18] The data in the magnetic fields $H = 0.01$ T, 0.02 T and 0.03 T are also fitted, as seen in Fig. 3(b). Above 0.03 T, the data become more and more noisy, which are not shown. The normalized $\kappa_0(H)/T$ as a function of H/H_{c2} ($\mu_0 H_{c2} = 0.076$ T) for CaPtAs is plotted in Fig. 4. For comparison, similar data of the clean s-wave superconductor Nb,[30] the dirty s-wave superconductor ally InBi,[31] the multiband s-wave superconductor $NbSe_2$,[28] and an overdoped d-wave cuprate superconductor Tl-2201[29] are also plotted. For single-band s-wave superconductor Nb, the $\kappa_0(H)/T$ changes not much even up to 40% H_{c2},[30] while for nodal superconductor Tl-2201, a small field can yield a quick growth in the quasiparticle density of state (DOS) due to the Volovik effect, and the low-field $\kappa_0(H)/T$ shows a roughly $\sqrt{H}$ dependence.[29] In the case of $NbSe_2$, the distinct $\kappa_0(H)/T$ behavior was well explained by multiple superconducting gaps with different magnitudes.[28]

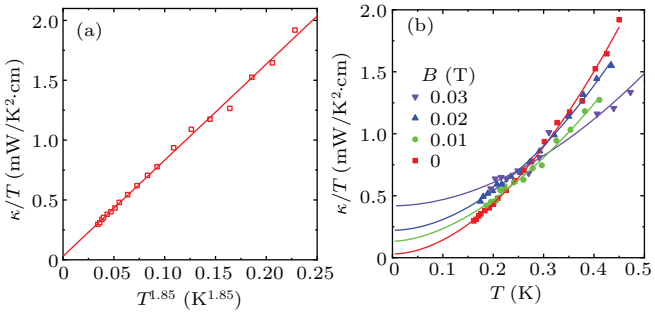


Fig. 3. The in-plane thermal conductivity of CaPtAs single crystal (a) in zero field, and (b) in magnetic field applied along the c axis. The solid lines represent the fits to $\kappa/T = a + bT^{\alpha-1}$ for the data in various magnetic fields.

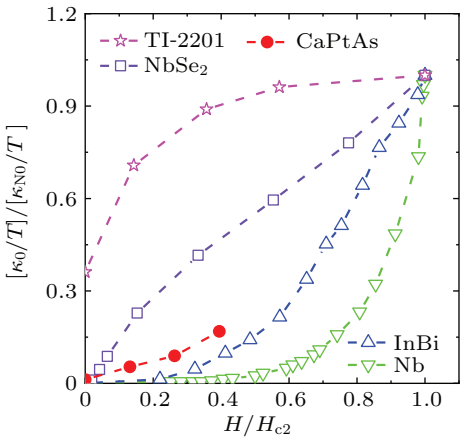


Fig. 4. Normalized residual linear term κ_0/T of CaPtAs as a function of H/H_{c2}, with bulk $\mu_0 H_{c2} = 0.076$ T. For comparison, similar data are shown for the clean s-wave superconductor Nb,[30] the dirty s-wave superconductor alloy InBi,[31] the multiband s-wave superconductor $NbSe_2$,[28] and an overdoped d-wave cuprate superconductor TI-2201.[29]

From Fig. 4, the field dependence of $\kappa_0(H)/T$ for CaPtAs grows slightly lower than that of the multiband s-wave superconductor $NbSe_2$ and faster than that of the dirty s-wave superconductor InBi. We check two possible scenarios for such a field dependence of $\kappa_0(H)/T$. One is that CaPtAs is an s-wave superconductor in the 'dirty' limit. To check whether CaPtAs is in the dirty limit, we estimate its superconducting coherence length ξ_0. From $\mu_0 H_{c2}(0) = 0.1$ T, we obtain $\xi_0 \approx$ 42 nm through the relation $H_{c2}(0) = \phi_0/(2\pi\xi_0^2)$. Recently,

magnetic penetration depth measurements found an electron mean free path $l \approx 1.5$ nm in CaPtAs.[13] $l \ll \xi_0$ indicates that CaPtAs is indeed in the 'dirty' limit. The other scenario is that CaPtAs is a multiband superconductor. Indeed, the electronic structure calculations of CaPtAs show multiple complex bands.[12] Therefore, the field dependence of $\kappa_0(H)/T$ in CaPtAs may result from both its dirtiness and multiple gaps.

For noncentrosymmetric superconductors, broken inversion symmetry and the accompanying antisymmetric spin-orbit coupling admix spin-singlet and spin-triplet pairing.[4] The typical examples are Li_2Pd_3B and Li_2Pt_3B.[4] The triplet contribution is weak in Li_2Pd_3B, leading to a wholly open but anisotropic gap.[4] However, the significantly larger spin–orbit coupling in Li_2Pt_3B allows the spin-triplet component to be larger in Li_2Pt_3B, producing line nodes in the energy gap.[4] Here for noncentrosymmetric superconductor CaPtAs, while the μSR measurements suggest nodes in the superconducting gap,[13] the latest NQR measurements[17] and our current ultralow-temperature thermal conductivity measurements indicate multiple superconducting gaps with a dominant s-wave component. In this sense, the spin-triplet component in CaPtAs may not be as large as that in Li_2Pt_3B.

4. Conclusion

In summary, we have measured the ultralow-temperature thermal conductivity of CaPtAs single crystal. The negligible residual linear term κ_0/T in zero field and the field dependence of κ_0/T suggest that CaPtAs has multiple superconducting gaps with a dominant s-wave component. These results are consistent with previous NQR measurements. More experimental and theoretical studies are desired to clarify the exact superconducting gap structure of this noncentrosymmetric superconductor.

Acknowledgements

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