Fermi surface and Berry phase in CaFeAsF, a variant of the 1111 parent compounds

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Introduction

Despite the fact that 1111-type iron arsenides hold the record transition temperature of iron-based superconductors, their electronic structures have not been studied much because of the lack of high-quality single crystals. Recently, Ma *et al*. have succeeded in growing large high-quality single crystals of CaFeAsF [1]. We have performed Shubnikov-de Haas (SdH) measurements on those crystals [2].

Experimental

We have performed standard four-contact resistivity measurements using a 20-T superconducting magnet at the NIMS and the 45-T Hybrid Magnet at the NHMFL.

Results and Discussion

Figure 1(a) shows the field derivative of magnetoresistivity for B // c (inset) and corresponding Fourier transform, where two frequencies α and β are resolved. Their field-angle dependences indicate that they are from two-dimensional cylinders. The carrier density is extremely small, $\sim 10^{-3}$ per Fe. The effective masses are estimated to be 0.383 and 0.92 m_e from the temperature dependences of the oscillations. We now determine the Berry phase. The SdH oscillation is given by $\Delta\rho = -C R_s \cos[2\pi(F/B - 1/2) + \varphi_D + \varphi_B]$, where C is a positive factor, $\varphi_D = 0$ (2D) or $+/-\pi/4$ (3D). When the double degeneracy of electronic bands due to spin degrees of freedom exits, which is the case for CaFeAsF, it is necessary to determine the sign of the spin reduction factor $R_s = \cos(\pi g \mu^*/2)$, where $\mu^* = m^*/m_e$, before the Berry phase φ_B (sign change in R_s is equivalent to a π phase shift). Figure 1(b) shows the analysis for the α oscillation. Plotted are the oscillatory part of resistivity after box-smoothing with a window size corresponding to one period of the β oscillation. The smoothing suppresses the β oscillation effectively, and the remaining oscillatory behavior is basically due to the α oscillation. Near $F_\alpha/B = 2$, a minimum is observed for $\theta \leq 48.3°$, while a maximum for $\theta \geq 57.4°$. Assuming $\mu^*(\theta) = \mu^*(0)/\cos\theta$, this observation indicates that $1.41 < g < 1.73$. For this range of g, $R_s > 0$ at $\theta = 0$. Since Δρ at $\theta = 0$ shows a minimum near $F_\alpha/B = 2$, the Berry phase is determined to be π (see the above formula), i.e., the α carriers are Dirac fermions. A similar analysis for the β oscillation indicates that the β carriers are normal fermions. Our band-structure calculation indicates that the Fermi surface consists of a pair of Dirac electron cylinders and a normal hole cylinder, corresponding nicely to the experimental α and β cylinders, respectively.

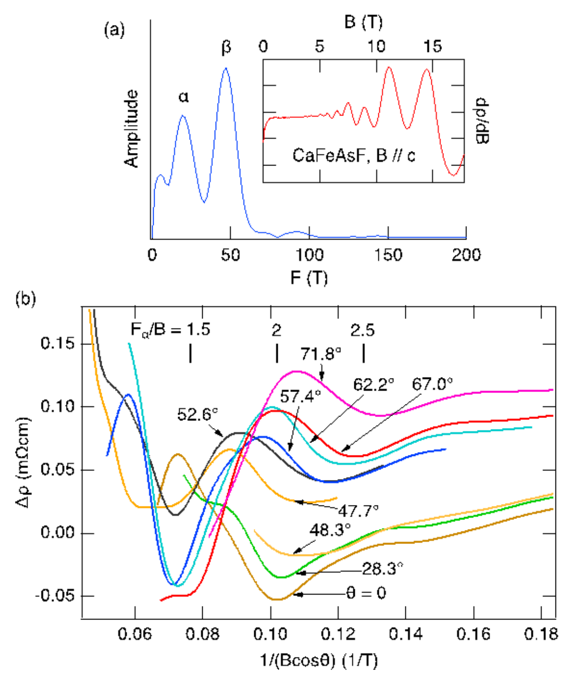

Fig.1 (a) Field-derivative of magnetoresistivity for B // c (inset) and corresponding Fourier transform. (b) Oscillatory part of resistivity after box-smoothing with a window size corresponding to one period of the β oscillation plotted against $1/B\cos\theta$. θ is the field angle measured from the c axis. Data for $\theta = 47.7°$ and $\theta \geq 52.6°$ were obtained with the Hybrid.

Conclusions

We have determined the Fermi surface in CaFeAsF completely and also demonstrated a nontrivial Berry phase associated with the α oscillation.

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References

[1] Ma, Y., *et al*., Supercond. Sci. Technol. **28**, 085008 (2015).

[2] Terashima, T., *et al*., arXiv:1710.03938.