Small and Nearly Isotropic Hole-Like Fermi Surfaces in LiFeAs Detected Through the de Haas–van Alphen Effect

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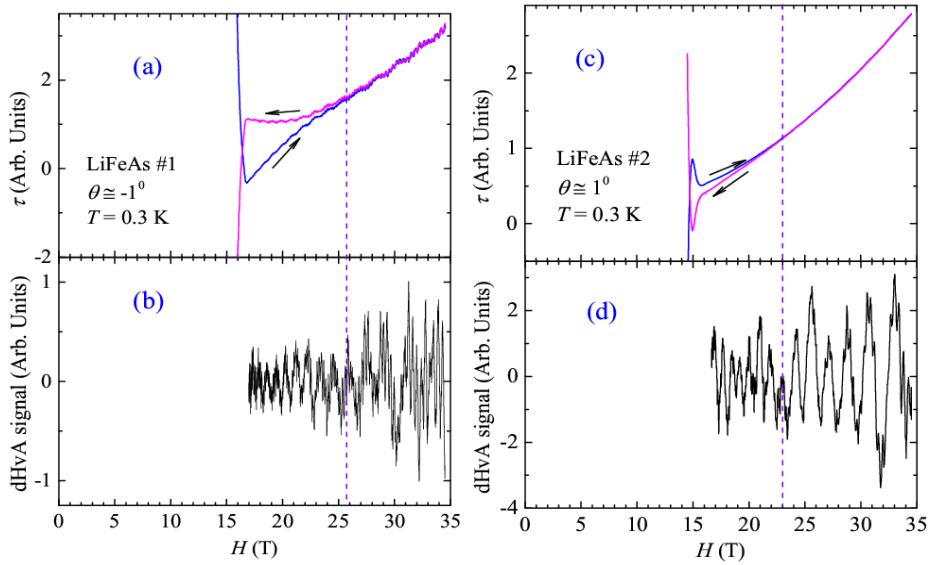
Introduction

LiFeAs is unique among the arsenic based Fe-pnictide superconductors because it is the only nearly stoichiometric compound which does *not* exhibit magnetic order. This is at odds with electronic structure calculations which find a very stable magnetic state and predict cylindrical hole- and electron-like Fermi surface sheets whose geometry suggests spin fluctuations and a possible instability toward long-range ordering at the nesting vector. In fact, a complex magnetic phase diagram is indeed observed in the isostructural NaFeAs compound. Previous angle-resolved photoemission (ARPES) experiments revealed the existence of both hole and electron-like surfaces, but with rather distinct cross-sectional areas and an absence of the nesting that is thought to underpin both magnetic order and superconductivity in the pnictide family of superconductors. These ARPES observations were challenged by subsequent de Haas–van Alphen (dHvA) measurements which detected a few, electron-like Fermi surface sheets in rough agreement with the original band calculations. Here, we show a detailed dHvA study unveiling additional, small and nearly isotropic Fermi surface sheets in LiFeAs single crystals, which ought to correspond to hole-like orbits, as previously observed by ARPES.

Experimental

We used cell 12 (35 T resistive magnet) in conjunction with a ^{3}He system to measure magnetic torque in LiFeAs single-crystals.



(a) Magnetic torque τ as a function of the magnetic field H for a LiFeAs single crystal (crystal 1) at a temperature T = 0.3 K and an angle $\theta \sim 1^\circ$ between H and the interplanar c axis. Blue and magenta lines indicate increasing and decreasing field sweeps. Notice how the large (and incomplete) hysteresis loop is followed at higher fields by a smaller one. (b) Same as in (a) but for a second LiFeAs single crystal (crystal 2). (c) The oscillatory component, or the de Haas–van Alphen effect, superimposed onto the τ (H) trace shown in (a) after the subtraction of a polynomial fit, and as a function of H. Vertical purple line indicates the irreversibility field. Hence, the quantum oscillatory phenomena is observed deep inside the irreversible superconducting region. (d) Same as in (c) but for the torque data in (b). Notice how the irreversibility field is higher for sample 1 when compared to 2, therefore indicating a higher sample quality.

Conclusions

Our detailed dHvA study unveiled additional, small and nearly isotropic Fermi surface sheets in LiFeAs single crystals, which ought to correspond to hole-like orbits, as previously observed by ARPES. Therefore, our results reconcile the apparent discrepancy between ARPES and the previous dHvA results.

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