Electronic and superconducting properties of Ce-based heavy-fermion compounds with quasi-two-dimensional Fermi surfaces

This research project appeared as a natural continuation of our long-standing collaboration with Prof. D. Aoki. Several new samples of heavy fermion compounds, such as Ce_2RhIn_8 and $CePt_2In_7$, were tested by quantum oscillation and thermodynamic measurements for future experiments in high magnetic fields. In addition, we have finalized the data analysis and discussed some of the previously obtained results. This gave rise, in particular, to a high-level publication related to a drastic change of the Fermi surface across the metamagnetic transition in $CeRh_2Si_2$ [1].

Quantum critical points (QCPs), i.e., continuous phase transitions at zero temperature, play a key role in the physics of heavy fermion (HF) compounds and other materials. Recent theoretical attempts to classify QCPs in HF systems rely on the knowledge of whether the *f* electrons are itinerant or localized on both sides of a QCP, i.e. whether or not they contribute to the Fermi surface (FS). This can be achieved by comparing experimentally established FS topology with the results of band structure calculations performed for both itinerant and localized f electrons. Magnetic quantum oscillations, such as the de Haas-van Alphen (dHvA) effect, are the most direct way to establish the FS topology of a metal.

We have tested and selected several new samples of Ce-based heavy fermion compounds for future high field dHvA measurements. In these materials, such as Ce_2RhIn_8 and $CePt_2In_8$, quantum critical points can be induced by either pressure or high magnetic field. Furthermore, we have finished the analysis and discussion of the results of our previous dHvA measurements in $CeRh_2Si_2$.

The tetragonal HF compound $CeRh_2Si_2$ with a moderate specific heat Sommerfeld coefficient γ = 22.8 mJ/K^2 mol orders antiferromagnetically at T_{N1} = 36 K. Its magnetic structure changes again at T_{N2} = 24 K. When the magnetic field is applied along the crystallographic *c* axis, a complex two-step first-order metamagnetic (MM) transition to a polarized paramagnetic state occurs at about 26 T at low temperatures. Previous low field dHvA measurements suggest that the *f* electrons are localized deep inside the antiferromagnetic phase.

We observed dHvA oscillations both below and above the metamagnetic transition, as shown in Fig. 1 for a magnetic field applied at 2° off the *c* axis. The fast Fourier transform (FFT) spectrum of the dHvA oscillations below the MM transition [Fig. 1 (b)] is dominated by a peak ν at 1.8 kT and its harmonics in good agreement with previous lower field results. We did not observe any dHvA frequencies above 6 kT in the AF state.

Above the MM transition, the amplitude of the dHvA oscillations is much smaller. Nonetheless, two high dHvA frequencies of 8.6 and 16.3 kT are clearly seen in the FFT spectrum [Fig. 1 (c)]. These frequencies are much higher than the frequencies observed below the transition both in our own and previously reported measurements for the same orientation of the magnetic field. This implies a drastic modification of the FS across the MM transition in $CeRh_2Si_2$.

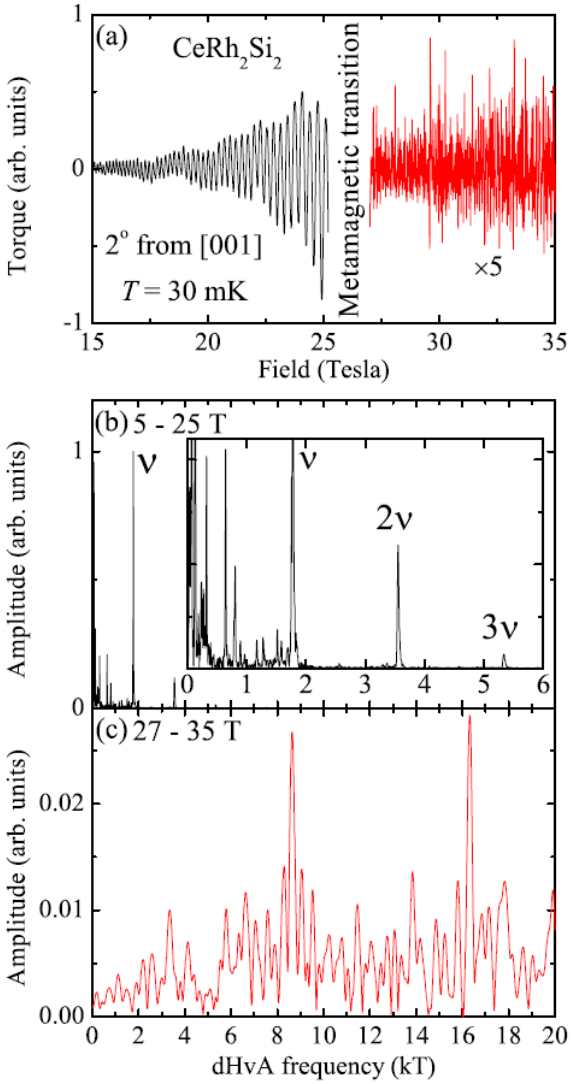

Fig. 1 (a) dHvA oscillations in $CeRh_2Si_2$ and the corresponding FFT spectra (b) below and (c) above the MM transition. The inset shows a zoom of the low frequency part of the FFT spectrum below the transition.

In order to figure out whether the f electrons are itinerant or localized above the MM transition, we compared the experimentally observed angular dependence of the dHvA frequencies with the results of band-structure calculations performed for both CeRh2Si2 (itinerant f electron model) and LaRh2Si2 (localized f electron model). In the latter case, the lattice parameters of CeRh2Si2 were used for the calculations. The calculated FSs are shown in Fig. 2. The comparison strongly suggests that the f electrons remain localized in the polarized paramagnetic state above the MM transition. Rather, a drastic change of the FS is caused by the modification of the Brillouin zone at the MM transition.

The FSs with localized and itinerant f electrons are commonly referred to as “small” and “large,” respectively, as in the latter case the *f* electrons effectively contribute to the FS. The example of the FS reconstruction in $CeRh_2Si_2$ from small to large without delocalization of the *f* electrons emphasizes the ambiguity of the commonly used simplistic conception of “small” and “large” FSs for localized and itinerant *f* electrons, respectively. The FS modification we observe here is different from that reported to occur at the pressure-induced QCP, where the *f* electrons do delocalize and become itinerant.

References

[1] K. Götze, D. Aoki, F. Lévy-Bertrand, H. Harima, and I. Sheikin, Phys. Rev. B **95**, 161107(R) (2017).

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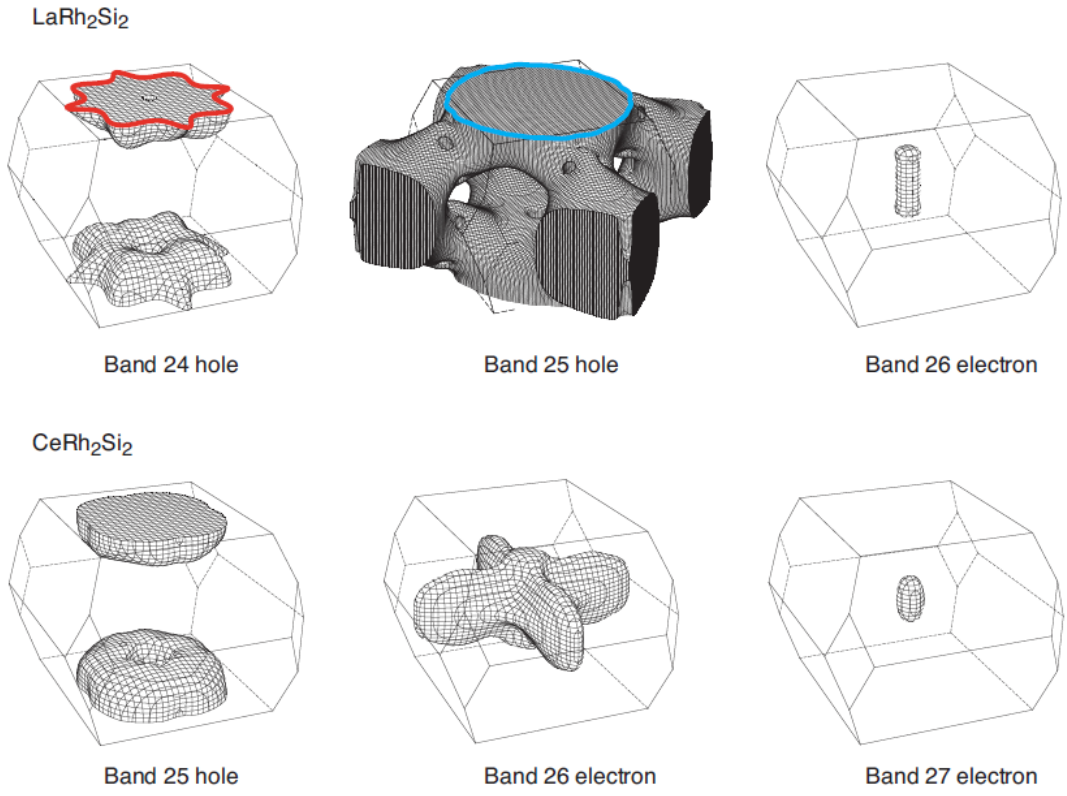

Fig. 2 Calculated Fermi surfaces of $LaRh_2Si_2$ and $CeRh_2Si_2$. For $LaRh_2Si_2$, the orbits giving rise to the experimentally observed high de Haas-van Alphen frequencies are shown.

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Dr. Ilya Sheikin (LNCMI-Grenoble, CNRS, Grenoble, France)
E-mail: ilya.sheikin@lncmi.cnrs.fr