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Electronic structure and de Haas-van Alphen quantities of $CeMIn_5$ (M = Co, Rh, and Ir) compounds

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Abstract

We report a critical analysis of the electronic structures and de Haas-van Alphen (dHvA) quantities of the heavy-fermion superconductors $CeCoIn_5$, $CeRhIn_5$, and $CeIrIn_5$. The ab initio calculated dHvA quantities are in good agreement with experimental data for $CeCoIn_5$ and $CeIrIn_5$, when we adopt the delocalized LSDA description for the Ce 4f states. For $CeRhIn_5$, however, a better agreement with experiment is obtained when the Ce 4f electron is treated as a localized core electron. The implications for an emerging picture of the localization behavior of the 4f electron in these materials are discussed.

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1. Introduction

A new group of fascinating heavy-fermion superconductors that crystallize in the $HoCoGa_5$ structure was discovered a few years ago [1]. $CeCoIn_5$ and $CeIrIn_5$ are superconductors at ambient pressure, with $T_c = 0.4$ and 2.3 K, respectively, whereas $CeRhIn_5$ becomes a superconductor (with $T_c = 2.1$ K) under pressure [2]. At ambient pressure $CeRhIn_5$ orders antiferromagnetically with an incommensurate spin spiral below the Néel temperature $T_N = 3.9$ K [3]. The entanglement of heavy-fermion behavior, antiferromagnetism, and superconductivity indicates an unconventional pairing mechanism, which was confirmed indeed [4]. An important issue which has become intensively debated is the role of the Ce 4f electrons and their degree of localization. De Haas-van Alphen (dHvA) measurements in connection with band-structure calculations are a very useful tool to analyze a multiband situation with a complicated Fermi surface [5].

2. Computational method

We use the full potential local orbital (FPLO) method in both the scalar-relativistic and the fully relativistic version [7–9], in combination with the local spin-density approximation [10]. In our calculations, the following basis sets were adopted for the valence states: the 4f; 5s5p5d; 6s6p states for Ce when the 4f are treated as

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valence states, while for Co, Rh, Ir and In we used 3s3p3d; 4s4p, 4s4p4d; 5s5p, 5s5p5d; 6s6p and 4d; 5s5p, respectively. The high lying 5s and 5p semicore states of Ce, which might hybridize with the 5d valence states, are thus included in the basis. The dHvA cyclotron frequency F, which is proportional to the Fermi surface cross section, and the cyclotron mass m of the extremal orbits are calculated numerically by discretizing the Fermi velocities on k-points along the orbit and by a subsequent Romberg integration [11]. For a detailed account of the computational method we refer to our previous work [12].

3. Band structure and extremal orbits

The compounds $CeMIn_5$ (M = Co, Rh, and Ir) crystallize in the tetragonal structure, space group P4/mmm (space group number 123) and are built of alternating stacks of $CeIn_3$ and MIn_2. We performed nonmagnetic band structure calculations for the experimental lattice parameters, which are (in atomic units): $a = 8.714a_0$ and $c = 14.264a_0$ ($CeCoIn_5$), $a = 8.791a_0$ and $c = 14.25a_0$ ($CeRhIn_5$), and $a = 8.818a_0$ and $c = 14.205a_0$ ($CeIrIn_5$). For the one special In-position we also adopted the experimental values.

The band structure of $CeCoIn_5$ computed with the fully relativistic scheme is presented in Fig. 1. We find for each of the Ce-115 systems using both FPLO codes three bands which cross the Fermi surface. These bands are denoted as Band 131, Band 133 and Band 135 (highlighted by the colors), according to their number in the valence band complex of the fully relativistic calculation counted from below.

Contrary to a recent study [6], we find only minor differences between the scalar and the fully relativistic calculations (Table 1). In Tables 2 and 3, we compare the calculated dHvA frequencies and effective masses with experimental values for the Ir- and Rh-compounds (for more details see Ref. [12]). Treating the 4f as valence states we find a good agreement for $CeCoIn_5$ and $CeIrIn_5$ but not for $CeRhIn_5$. In that case, the agreement can be improved by treating the Ce 4f electron as a core electron (4f-c, Fig. 2 and Table 3).

4. Discussion and conclusions

Our investigation of the electronic structures and dHvA quantum oscillations in the Ce-115 corroborate the following picture of these materials. In $CeCoIn_5$ and $CeIrIn_5$ the Ce 4f electrons appear to be rather delocalized. Therefore, treating the 4f electrons in these two compounds as itinerant states we do obtain a good description of the measured dHvA frequencies. However, the experimental effective masses of the extremal

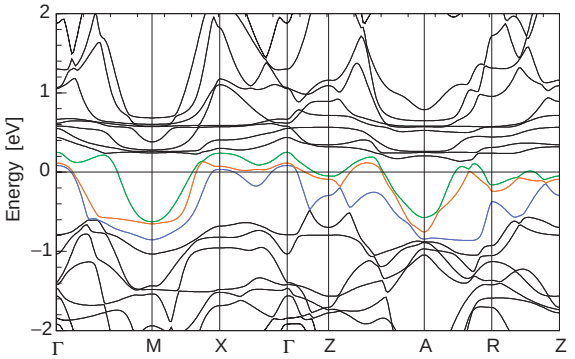

Fig. 1. The energy bands of nonmagnetic $CeCoIn_5$ calculated using the fully relativistic FPLO method.

Table 1
Calculated dHvA frequencies F (in kT) and effective masses m (in m_0) for $CeCoIn_5$ with $H \| c$

Symbol	Central point	Band no.	F (kT)		m (m_0)	
			sc-rel.	rel.	sc-rel.	rel.
g	Γ	131	0.809	0.761	−0.661	−0.814
h	X	131	0.460	0.438	−0.669	−0.974
β_1	M	133	12.910	12.680	2.279	2.314
β_2	A	133	6.312	6.295	1.232	1.474
c	A	133	13.496	13.113	−3.178	−3.645
α_1	$A'_{k_z=0.18}$	135	5.399	5.352	1.543	1.621
α_2	M	135	4.599	4.475	0.977	0.996
α_3	A	135	4.069	4.060	1.155	1.317
a_1	Z	135	1.280	1.264	1.445	1.536
a_2	R	135	1.186	1.136	0.909	0.946

The calculations were performed treating the Ce 4f electrons as delocalized and adopting either the scalar-relativistic or the fully relativistic approach.