Many-body effects in LuNi$_2$B$_2$C

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Abstract. We present de Haas–van Alphen measurements of the nonmagnetic borocarbide superconductor LuNi$_2$B$_2$C. The electronic band structure is extracted from the magnetic quantum oscillations in the normal state. In accordance with previous investigations we find a complex band structure with different open and closed Fermi-surface sheets. From the temperature dependence of the oscillations amplitude the effective mass of the single bands can be determined. Due to many-body interactions we observe enhancements of the effective masses compared to the results by full-potential-density-functional calculations. Therefore, we are able to determine the angular dependence of the interaction strength for the different bands separately.

1. Introduction

Even 50 years after Bardeen, Cooper, and Schrieffer formulated their pioneering theory of superconductivity, the BCS theory remains highly successful in describing many superconductors [1]. The theory covers most basic properties in assuming an isotropic phonon-mediated Cooper-pair coupling. However, for a deeper understanding of superconductivity a better knowledge of the band-resolved strength and anisotropy of the coupling is necessary. The determination of this important information for materials with involved band structures, such as LuNi$_2$B$_2$C, demands highly sophisticated efforts both from the experimental as well as from the theoretical side. The de Haas-van Alphen (dHvA) effect is an excellent tool to study these effects due to the possibility to examine the Fermi surface for all bands separately. From these field-dependent oscillations of the magnetization the Fermi-surface topology can be extracted and, furthermore, the effective band masses can be determined. In combination with full-potential local-orbital (FPLO) band-structure calculations which can model the ‘bare’ masses the mass enhancement due to the many-body effects can be obtained [2].

The quaternary borocarbides are a fascinating material class which allows to study the coexistence of superconductivity and magnetism [3]. The nonmagnetic superconductors
YNi$_2$B$_2$C and LuNi$_2$B$_2$C are of special interest due to their anisotropy of the superconducting gap function. Recent experiments point to several contrary coupling symmetries [4, 5, 6, 7]. Additionally, if the complicated band structure is taken into account [8, 9, 10, 11, 12], also multi-band superconductivity with different gaps belonging to different bands seems possible [13, 14, 15, 16, 17, 18].

2. Method
We present dHvA data on flux-grown single crystals of LuNi$_2$B$_2$C [19]. The measurements were carried out using a capacitance cantilever torquemeter on a rotatable set up in high magnetic fields up to 15 T in a superconducting magnet at the HLD Dresden, up to 32 T in the High Field Magnet Laboratory Nijmegen, and up to 28 T in the Grenoble High Magnetic Field Laboratory. Data were taken at low temperatures down to 20 mK in a dilution refrigerator and down to 0.4 K in a $^3$He cryostat. The effective masses of the Fermi sheets are obtained from the temperature dependence of the dHvA oscillation amplitude by use of the Lishitz-Kosevich formula [20]. The experimentally obtained effective masses, $m_{\text{exp}}$, are enhanced compared to the calculated ‘bare’ effective masses, $m_{\text{FPLO}}$. This enhancement $\lambda = m_{\text{exp}}/m_{\text{FPLO}} - 1$ is related to the many-body interaction of the electrons.

To calculate band structure, FS, and dHvA frequencies of LuNi$_2$B$_2$C, we applied the FPLO code (version 5.00-18) [2] in its scalar-relativistic version within the local-density approximation. We used the structural data of Ref. [21]. Further details of the calculations are provided in Ref. [8].

**Figure 1.** Fourier transform of the dHvA data. The inset shows dHvA data after background substraction obtained at 50 mK for the field aligned 3 deg with respect to [001] in the (100) plane.
3. Results

The band structure of LuNi$_2$B$_2$C consists of three closed (‘sphere’, ‘cube’, ‘cushion’) and one branched Fermi sheet [8]. Figure 1 shows typical dHvA data for LuNi$_2$B$_2$C for fields oriented 3 degrees with respect to the $c$-axis. For magnetic fields aligned close to the $c$-axis we find 13 different dHvA frequencies. By comparison with the band-structure calculations we are able to assign almost all observed dHvA frequencies to Fermi-surface branches. By that, we could identify the cubic and the cushion-like Fermi surface and even parts of the open (‘lemon’, ‘windmill’) Fermi sheets [8]. Until now, the peak at 7800 T could not be assigned to a certain part of the Fermi surface. The dHvA frequencies close to the ‘cushion’ frequency, might be due to corrugations of the Fermi sheets in this orientation. Their effective masses are similar to the effective mass extracted from the ‘main’ peak. For example, for the frequency at 5438 T which is assigned to the cushion sheet we find an effective mass of 4.25 $m_e$. The two nearby frequencies at 5170 and 5729 T reveal effective masses of 3.7 $m_e$ and 4.1 $m_e$, respectively (Fig. 2). Compared to the calculated FPLO ‘bare’ mass of 2 $m_e$ we find many-body interaction parameters of 0.85 and 1.05 instead of 1.1 for the main frequency. For orientations close to the $c$- and to the $a$-axis these effects appear to be especially pronounced.

The temperature dependence of the dHvA oscillation amplitudes for three selected dHvA frequencies is presented in Fig. 2. The data clearly follow the behavior predicted by the Lifshitz-Kosevich theory and, therefore, the effective masses can be obtained with high accuracy. The subsequent effective masses have been compared to the calculated ‘bare’ masses and from that
the many-body coupling interaction $\lambda$ has been determined. For LuNi$_2$B$_2$C the interaction is mainly electron-phonon like. Therefore, the mass enhancement, or coupling strength, is most probably directly related to the Cooper-pair coupling parameter [22]. This kind of analysis has been performed for all observed frequencies and for several orientations of the sample [8]. The resulting angular dependence of $\lambda$ shown in the inset of Fig. 2. We find different coupling anisotropies and different absolute values for the observed Fermi sheets resulting in different contributions of the bands to the superconductivity and supports a multiband scenario for the superconductivity in LuNi$_2$B$_2$C. The weakest coupling is found for the spherical Fermi surface. This band has the lowest contribution to the total density of states (DOS) and, therefore, it is of minor relevance for the superconductivity. The cube Fermi surface is most strongly coupled along the $c$-axis. This sheet contributes only by 10 percent to the DOS and, in addition, due to interband scattering it is supposed to be connected with the other Fermi surfaces. Consequently, although the coupling is strong in one direction, it does not yield higher transition temperatures. Other experimental methods provide averaged coupling strength parameters between 0.5 and 1.2 [5, 17, 23]. If we average our data over all bands and orientations our mean coupling-strength is consistent with these numbers.

In conclusion, we investigated the many-body coupling interactions for all the bands separately and for different orientations. We find distinct coupling strengths and anisotropies for different bands which strongly points to a multi-band character of the superconductivity.

Acknowledgments

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