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Fermi surfaces of PrOs$_4$Sb$_{12}$ based on the LDA+$U$ method

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Abstract

Fermi surfaces of PrOs$_4$Sb$_{12}$ are investigated based on the LDA+$U$ method with many $U$ values. The 4$f^2$ electrons in PrOs$_4$Sb$_{12}$ are experimentally suggested to be localized, in contrast with other heavy fermion superconductors. This study has revealed that the 4$f^2$ electrons remain localized with small $U = 0.4\text{Ry}$, then become itinerant with $U = 0.05\text{Ry}$, where the topology of the Fermi surfaces are changed and no longer explains the dHvA measurement.

Key words: PrOs$_4$Sb$_{12}$, LDA+$U$ method, Fermi surface

The filled skutterudite compounds with a general formula $RT_4X_{12}$ ($R$= Rare earth, Th and U; $T$= Fe, Ru and Os; $X$= P, As and Sb) have recently attracted much attention for the variety of the electrical and magnetic properties. Among them, PrOs$_4$Sb$_{12}$ has been reported to undergo superconductivity at $T_c = 1.85\text{K}$ with the large electronic specific heat coefficient $\gamma = 350 - 700\text{mJ/mol K}^2$.[1,2]. Unconventional superconducting properties have been reported from the thermal conductivity,[3], the NMR measurement[4] and the $\mu$SR measurement[5]. In applied magnetic fields, another ordered phase appears above the upper critical field [6]. The neutron measurement has suggested that quadrupole interactions should play a crucial role in the field induced ordered phase[7].

The measurements of the de Haas-van Alphen (dHvA) effects have revealed that the topology of Fermi surface (FS) of PrOs$_4$Sb$_{12}$ is very similar to that of the reference compound LaOs$_4$Sb$_{12}$.[8] It indicates that the 4$f^2$ electrons in PrOs$_4$Sb$_{12}$ are well localized, in contrast with other heavy fermion superconductors. The LDA+$U$ method can treat such localized electrons in a unfilled shell within a band picture. The ground state of 4$f^2$ in PrOs$_4$Sb$_{12}$ suggested to be a singlet and such the localized singlet ground state can be obtained without any symmetry breaking. In fact, the FSs obtained by the LDA+$U$ method with a parameter $U = 0.4\text{Ry}$, have explained well the angular dependence of the dHvA experiments.[8] In the bandstructure, 4$f^2$ electrons are located below the Fermi level and well localized. Therefore, the density of states at the Fermi level contains only a small amount of $f$ component (a few %), though the measured cyclotron masses are largely enhanced in PrOs$_4$Sb$_{12}$. Then the question arises how the $U$ value affects the topology of the FSs and the mass enhancement. In this study, the $U$ dependence of the electronic bandstructures have been investigated. Calculations with $U = 0.4\text{Ry}, 0.3\text{Ry}, 0.2\text{Ry}, 0.1\text{Ry}, 0.05\text{Ry}$ and $0\text{Ry}$ (LDA) have been performed self-consistently.

Figure 1 (a) shows the bandstructure in the vicinity of the Fermi level with $U = 0.4\text{Ry}$, which is very similar to the case of non $f$ reference LaOs$_4$Sb$_{12}$.[9] The hole FSs around the N points is observed as the $\gamma$ branch, and the cyclotron masses are the most largely enhanced.[8] As shown in Fig. 1 (b), the bandstructure near the Fermi level remains unchanged with down to $U = 0.10\text{Ry}$. The electronic specific heat coefficient (the density of states at the Fermi level) $\gamma$ is 43.3 mJ/mol-K$^2$ and the $f$-component is still less than 10%. As shown in Fig. 2 (a), the main part of the $f$-
components are located well below and above the Fermi level, so the f-electrons are regarded as still localized.

When $U$ is set as $0.05\text{Ry}$, the FSs are topologically changed, i.e. the hole FSs around the $N$ points disappear. The $f$-components are situated on the Fermi level, then affect the FSs (see Fig. 1(c) and Fig. 2(b)). This corresponds the $f$-itinerant picture. The $\gamma$ value becomes large as $81.5\text{ mJ/mol-K}^2$ in which the $f$-component is about 50%. However, the FSs containing such large $f$-component could not explain the angular dependence of the dHvA measurements.

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Fig. 1. The LDA+$U$ bandstructures for PrOs$_4$Sb$_{12}$ with $U = 0.40\text{Ry}$ (a), $U = 0.10\text{Ry}$ (b) and $U = 0.05\text{Ry}$ (c). Note that the topology of FSs are changed between (b) and (c).

Fig. 2. The LDA+$U$ density of states for PrOs$_4$Sb$_{12}$ with $U = 0.10\text{Ry}$ (a) and $U = 0.05\text{Ry}$ (b). $f$-components are indicated by grey parts.

References