Research Article

Giant Sommerfeld coefficient in the heavy-fermion YbBiPt

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It has been derived that the Sommerfeld coefficient γ as large as 25 J/K^{2}mol can be theoretically accounted for provided the charge f-electron fluctuations are substantially suppressed. This result enables the understanding of the heavy-fermion YbBiPt (γ =8 J/K^{2}mol) as the spin fluctuator and should stimulate the experimental specific-heat research at low temperatures.

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In 1991 Fisk *et al.* [1] discovered that YbBiPt has the linear-temperature specific-heat coefficient (Sommerfeld coefficient) γ of 8 J/K^{2}mol. It is the largest value measured up to now - in the highest heavy-fermion systems a value up to 1.6 J/K^{2}mol has been found ($CeAl_3$). The origin of such the giant value is still the subject of extensive theoretical studies and long-lasting discussions [1–5]. In fact, this discussion concentrates on the role played by $4f$ electrons and the way how to treat them. One school considers the f electrons as the part of the core whereas the second one treats them as itinerant band–like electrons.

The aim of this Letter is to show that a giant value of 25 J/K^{2}mol for the Sommerfeld coefficient can be derived using the method described in Ref. [2] provided the charge f-electron fluctuations are strongly suppressed.

In the theoretical paper of Ref. [2] it has been concluded that the band-structure LSDA+U calculations provide the single-particle density of states that i) is peak-like at the Fermi level E_F and ii) its value

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of about 200 states per eV yields the Sommerfeld coefficient γ of 0.25 J/K^2mol. Moreover, in order to make this value closer to the experimental one of 8 J/K^2mol in Ref. [2] iii) an enhancement by the factor $(1\text{-}n_f)^{-1}$ has been invoked. This factor has been introduced to the charge-fluctuation model for heavy-fermion phenomena in Ref. [4] and is due to the suppression of the f occupation fluctuations. In Ref. [2] the n_f has been assumed as 0.9. It increases the bare LSDA+U Sommerfeld-coefficient value by factor of 10 to γ of 2.5 J/K^2mol. The large density of states at E_F in the heavy-fermion system YbBiPt found in Ref. [1] has been recently confirmed by the ab initio self-interaction correction to the local-spin density approximation (SIC-LSDA) calculations of Temmerman *et al.* [7], though in this approximation the f electrons are not part of the core.

According to me in the approach described in Ref. [2] there is no justification for the assumed value of 0.9 for n_f. In fact, basing on the original approach to YbBiPt [1] the value of n_f of 0.99 seems to be much more realistic. It is also in agreement with the suppresion of the charge fluctuations already in temperatures above 10 K where the full trivalent ytterbium moment is seen in the susceptibility *vs* temperature plot [1, 3]. Such the value for n_f yields so giant Sommerfeld coefficient as 25 J/K^2mol. I predict that such the large Sommerfeld-coefficient value will be experimentally detected for ytterbium/cerium/samarium systems with the characteristic temperatures below 0.1 K. (In YbBiPt the Sommerfeld coefficient of 8 J/K^2mol occurs below 0.4 K). Values of such order has been found already for ^{3}He below 0.2 K [8, 9].

In conclusion, I have derived that the Sommerfeld coefficient as large as 25 J/K^2mol can be theoretically accounted for provided the charge f-electron fluctuations are substantially suppressed. This result enables the understanding of the heavy-fermion YbBiPt (γ =8 J/K^2mol) as almost spin-fluctuating system (the f electrons are part of the core) and should stimulate the experimental specific-heat research at low temperatures. According to Refs [5] and [6] these spin fluctuations are related with the atomic scale Kramers doublet ground state of the trivalent ytterbium ions.

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