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Journal

Physica B: Physics of Condensed Matter, 199-200(C)

ISSN

0921-4526

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Publication Date

1994-04-02

DOI

10.1016/0921-4526(94)91879-1

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Peer reviewed

Charge dynamics in the Kondo insulator $\text{Ce}_3\text{Bi}_4\text{Pt}_3$

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Abstract

We report the reflectivity and optical conductivity of the Kondo insulator $\text{Ce}_3\text{Bi}_4\text{Pt}_3$. For temperatures less than 100 K, depletion of the conductivity below about 300 cm^{-1} signifies the development of a charge gap. The temperature dependence of the disappearance of the spectral weight scales with the quenching of the Ce 4f moments.

Some mixed valent compounds show a semiconducting behavior at low temperatures. Recently, renewed interest has been focused on the nature of the small gap responsible for the insulating ground state [1]. Since the periodic Kondo Hamiltonian has been used to describe the mixed valent compounds, the notion Kondo insulator has been coined.

We address the crucial issue about the nature of the Kondo insulator gap. With no electron–electron correlation ($U = 0$), a small gap is expected due to the coherent hybridization between d and f bands [2]. Essentially, this gap is not different from bonding–antibonding gaps of conventional band structure calculations. When the correlation is switched on ($U_{\text{ff}} \neq 0$), the Kondo coupling J disturbs the conduction electrons and strongly effects the gap value. In that case the temperature dependence of the magnetic interaction may correlate with the temperature dependence of the gap. By far infrared measurements [3], we probe the temperature-dependent evolution of the charge response ($\sigma_1(\omega)$) and the gap formation for the Kondo insulator $\text{Ce}_3\text{Bi}_4\text{Pt}_3$.

In Fig. 1(a) the infrared reflectivity is shown for selected temperatures. In the high-temperature region

(100–300 K) the reflectivity does not show much temperature dependence. Below 100 K the reflectivity begins to show strong temperature dependence, and exhibits characteristics of gap development at low frequency. In Fig. 1(b) the real part of the optical conductivity, $\sigma_1(\omega)$, is shown as a function of frequency. Between about 100 and 300 K the conductivity is nearly constant as a function of frequency in the far infrared. Changes of the conductivity are modest above 100 K; however, below this temperature spectral weight begins to disappear from the low-frequency region signifying the development of a charge gap or pseudogap.

The conductivity is strongly depleted up to a characteristic frequency of about 300 cm^{-1} at low temperature, which corresponds to roughly 400 K. The data show, however, that the development of the gap primarily occurs only below the much lower temperature of 100 K indicating a severe departure from a picture of gap disappearance based on rigid bands and simple thermal activation of carriers.

$\text{Ce}_3\text{Bi}_4\text{Pt}_3$ exhibits the gradually magnetic – nonmagnetic transition of mixed valent, dense Kondo systems [4]. In addition, inelastic neutron scattering measurements [5] have detected a spin gap at an energy of $\Delta_s = 160\text{ cm}^{-1}$ opening at temperatures below 100 K. The simultaneous formation of spin and charge gap

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Fig. 1(a). Far infrared reflectivity of $\text{Ce}_3\text{Bi}_4\text{Pt}_3$ at selected temperatures (from bottom to top: 25, 50, 75, 100 and 300 K). (b) Real part of the optical conductivity $\sigma_1(\omega)$ for different temperatures (from below: 25, 50, 75, 100 and 300 K). A gap is opening below 100 K; the prominent feature Δ_C seems to be independent of temperature.

below 100 K provokes the proposition that the charge gap is triggered by the magnetic–nonmagnetic transition. On assuming the Curie law with a temperature-dependent magnetic moment $\mu_{\text{eff}}(T)$,

$$\chi = \frac{\mu_{\text{eff}}^2(T)}{3k_B T}, \quad (1)$$

we can calculate the effective magnetic moment $\mu_{\text{eff}}(T)$ of the localized, magnetic 4f states exploiting the experimental [4] magnetic susceptibility χ (see Fig. 2). The optical sum rule provides a formula to calculate the number of localizing charge carriers upon the gap (singlet) formation:

$$\frac{\Delta n(T)}{m^*} \propto \int_0^{\Delta_C} \sigma_1(\omega, T) d\omega - \int_0^{\Delta_C} \sigma_1(\omega, 300 \text{ K}) d\omega. \quad (2)$$

Proposing that the opening of the charge gap, i.e., the localization of charge carrier is due to the involvement of the d-electrons into the singlet formation, the number of disappearing charge carriers should scale with the amount of the quenched magnetic moment μ_{eff} . Indeed

Fig. 2. Left axis: Effective magnetic moment μ_{eff} on the Ce ions of $\text{Ce}_3\text{Bi}_4\text{Pt}_3$ in units of the Bohr magneton μ_B . The dashed line gives the magnetic susceptibility data from Ref. [4]; the round points are from the neutron data of Ref. [5]. Right axis: The diamond-shaped points represent the localized charge carrier as a function of temperature as calculated by the optical sum rule (Eq. (2)). The thin line indicates the linear temperature dependence below T^* .

a convincing agreement has emerged as depicted in Fig. 2.

In contrast to ordinary heavy fermions where the local 4f states delocalize below the coherence temperature T^* , the Kondo insulators show a localization of the charge carrier to the local moments.

We now address the physical nature of Δ_C . Theoretical estimations of hybridization gaps give a direct gap Δ^{direct} of the order of tenths of eV and an indirect gap $\Delta^{\text{indirect}} \sim 1/2 (\Delta^{\text{direct}})^2/D \sim T_K$, with D the width of the conduction band [6]. With $T_K = 320 \text{ K}$ for $\text{Ce}_3\text{Bi}_4\text{Pt}_3$ [4] and the gap temperature $\Delta_C/k_B = 450 \text{ K}$, the arguing of the optical gap coinciding with the transport gap seems reasonable. On the other hand, the linear extrapolation of the steep part of $\sigma_1(\omega)$ to zero gives a value of the order of 100 K. Similar temperatures of the transport gap have been predicted on suggesting an opening transport gap [7]. Another possibility is to interpret Δ_C as the energy needed to excite a bound charge out from a local Kondo singlet ($\Delta_C \sim k_B T_K$). The temperature independence of Δ_C is explained by the fixed Kondo energy T_K .

In conclusion, we have presented explicitly the formation of a charge gap for the mixed valent Kondo insulator $\text{Ce}_3\text{Bi}_4\text{Pt}_3$ at low temperature. The gap formation is characterized by (i) a temperature-independent gap with a energy Δ_C similar to the single ion Kondo energy $k_B T_K$ and (ii) a loss of spectral weight scaling with the quenching of the local 4f moments.

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- [7] M. Hundley, *Physica B 199&200 (1994) 443*. From the Arrhenius plot of the resistivity the gap value cannot be extracted straightforward if the gap is changing with temperature. Indeed, the resistivity data of $\text{Ce}_3\text{Bi}_4\text{Pt}_3$ might be interpreted by an opening of the transport gap below 100 K although extrinsic effects become dominant below 50 K.