Two-channel conduction in YbPtBi

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We investigated transport, magnetotransport, and broadband optical properties of the half-Heusler compound YbPtBi. Hall measurements evidence two types of charge carriers: highly mobile electrons with a temperature-dependent concentration and low-mobile holes; their concentration stays almost constant within the investigated temperature range from 2.5 to 300 K. The optical spectra (10 meV – 2.7 eV) can be naturally decomposed into contributions from intra- and interband absorption processes, the former manifesting themselves as two Drude bands with very different scattering rates, corresponding to the charges with different mobilities. These results of the optical measurements allow us to separate the contributions from electrons and holes to the total conductivity and to implement a two-channel-conduction model for description of the magnetotransport data. In this approach, the electron and hole mobilities are found to be around 50000 and 10 cm²/Vs at the lowest temperatures (2.5 K), respectively.

Introduction. For 25 years YbPtBi was renowned as a heavy-fermion compound that exhibits one of the highest effective electron masses among the strongly correlated electron systems [1,2]. Its Kondo temperature is around 1 K; in addition an antiferromagnetic transition is observed at 0.4 K. So far, most of the experimental studies on YbPtBi explore its heavy-fermion state and a possible quantum critical point; hence they focus on temperatures below 2 K [1,4].

More recently, however, it has been emphasized that YbPtBi belongs to the large family of intermetallic ternary, so-called half-Heusler, compounds, which demonstrate a variety of rather interesting electronic properties. Several half-Heuslers are predicted to exhibit band inversion at the Γ point, leading to topologically non-trivial states [8–11]. Due to the combination of diverse electronic properties and non-trivial band topology, half-Heuslers are currently recognized as extremely promising objects in the research towards functioning materials. This calls for a more comprehensive look on the electronic properties of YbPtBi, beyond the heavy-fermion state.

In our present study, we concentrate on the temperature range well above the Kondo temperature, i.e. 2.5 to 300 K, where from our magnetotransport and optical measurements we can draw conclusions on the carrier dynamics. We present evidence that two types of charge carriers coexist in this compound: highly mobile electrons with a temperature-dependent carrier concentration of the order of 10¹⁸ cm⁻³ and holes with a rather high and basically temperature-independent concentration of 10²⁰ cm⁻³ that possess a very low mobility. We find the values of electron mobility in YbPtBi to be record high for half-Heuslers. The presence of the highly mobile carriers is typical for materials with linear bands [12,13]. Possible presence of such bands in YbPtBi has been noticed e.g. in Ref. [8], but still remains an open issue. The found very high mobility in YbPtBi indicates that Dirac physics might indeed be relevant for this compound, however more studies in this regard are certainly necessary.

Experiment. YbPtBi single crystals were grown by the solution growth method, where Bi acts as a flux. Stoichiometric quantities of freshly polished pieces of elements Yb, Pt, and Bi of purity > 99.99% in the atomic ratio of 0.7:0.7:10 were put in a tantalum crucible and then sealed in a dry quartz ampoule under 3–5 mbar argon pressure. The filled ampoules were heated at a rate of 100 K/h up to 1473 K, followed by 12 hours of soaking; after that the furnace temperature was decreased to 1373 K. For crystal growth, the temperature was slowly reduced from 1373 K to 873 K by 2 K/h and the surplus of Bi flux was removed by decanting the ampoule at 873 K. Using this method, we obtained 3–5 mm regular triangular shaped crystals, with a preferred growth in the (111)-direction. The general crystal growth procedure was followed from literature [14]. The space group and lattice parameters are found to be Fmmm (cubic face-centered) and 6.591 Å, respectively, consistent with previous reports [15,17].

Specimens of appropriate shapes were cut from a single crystal, e.g. Hall bars for (magneto)transport experiments and a large-surface sample for optical reflectivity. Direct-current resistivity measurements were performed in a custom-made setup by cooling from room temperature down to 2.5 K. Transversal magnetoresistance (MR) and Hall resistivity measurements were conducted at the same temperatures in magnetic fields B of up to 6.5 T. The voltages/currents were measured/applied within the (111) plane and magnetic field was along the [111] axis.

The optical reflectivity R(ν) was measured from the (111) plane in the temperature range between T = 12 and 300 K using two Fourier-transform infrared spectrometers, a Bruker IFS 113v and a Bruker Vertex 80v equipped with an infrared microscope. This way we co-
showed the frequency range from $\nu = \omega/(2\pi) = 100$ to 22\,000 cm$^{-1}$ ($h\nu = 12 - 2700$ meV). The sample for the optical experiments had lateral dimensions of roughly 2 by 2 mm and a typical thickness of 0.5 mm; all optical experiments were performed on freshly cleaved (111) surfaces. For low frequencies (50 - 1000 cm$^{-1}$), an in-situ gold evaporation technique \cite{18} was utilized for reference measurements. Freshly evaporated gold and protected-silver mirrors served as references at higher frequencies. In accord with the cubic face-centered crystal structure, measurements with linearly polarized light revealed isotropic optical properties.

From the measured reflectivity $R(\nu)$, the optical conductivity, $\sigma(\nu) = \sigma_1(\nu) + i\sigma_2(\nu)$, and dielectric function, $\varepsilon(\nu) = 1 - 2\sigma(\nu)/\nu = \varepsilon_1(\nu) + i\varepsilon_2(\nu)$, were extracted via the Kramers-Kronig relations \cite{19}. In the course of the paper, we express our optical results in terms of $\sigma_1(\nu)$ and $\varepsilon_2(\nu)$. For a Kramers-Kronig analysis, the measured data have to be extrapolated to zero and high frequencies. It turns out that in the case of our measurements the commonly applied Hagen-Rubens extrapolation to zero frequency is not adequate because a very narrow Drude component is present in the spectra with a scattering rate comparable to our lowest measurement frequency, $\nu_{\text{min}} \approx 100$ cm$^{-1}$. Thus, we used a set of Lorentzians instead – some at a finite, some at zero frequency – to fit the measured reflectivity. Between $\nu = 0$ and $\nu_{\text{min}}$ these Drude-Lorentz fits were utilized as zero-frequency extrapolations. On the high-frequency side ($\nu \to \infty$), the x-ray atomic scattering functions were employed according to Tanner \cite{20}.

**Magnetotransport.** The dc resistivity $\rho_{\text{dc}}$ and conductivity, $\sigma_{\text{dc}} = 1/\rho_{\text{dc}}$, are displayed in Fig. 1 versus temperature. Upon cooling, $\rho_{\text{dc}}(T)$ continuously decreases; the residual resistivity ratio is 8, comparable to the values reported earlier \cite{1, 3}. In $\rho_{\text{dc}}(T)$, a point of inflection, tentatively attributed to the influence of crystalline-electric-field effects \cite{2}, is observed around $T = (90 \pm 5)$ K.

Fig. 2 shows the results of our magnetotransport experiments by plotting the field-dependent resistivity taken at different temperatures. The MR curves are supplemented by data of Mun et al. \cite{3} taken at $T = 1$ K. At all temperatures the magnetoresistance sharply increases with $B$ in the range of low magnetic fields. It then flattens out for elevated temperatures, eventually reaching almost 60% as $B \to 6.5$ T. Such sharp increase in MR at low fields and its high-field saturation can be interpreted as localization of carriers with low scattering rate (i.e. with high mobility) in the fields of $\sim 0.5$ T, while other type of carriers, with high scattering rates and low mobility, still provides the dc transport. For $T < 20$ K the magnetoresistance is not monotonic anymore: a pronounced maximum is observed that shifts to lower fields as temperature decreases. At very low temperatures, $T \leq 2.5$ K, MR changes sign: at $B = 3.5$ T for $T = 2.5$ K and around 0.5 T for the 1 K data of Mun et al. \cite{3}. The position of the maximum in the MR-versus-$B$ curves follows a power-law temperature dependence, $T^n$, with $n = 1.2 \pm 0.1$. Negative MR in YbPtBi is usually discussed in terms related to Kondo physics \cite{1, 3}, though no in-depth discussion is available so far. It is worth to note here, that similar, but somewhat different, results on transversal MR are reported recently for related compounds, ScPtBi \cite{20} and HoPdBi \cite{21}. In ScPtBi, no negative MR is observed in the whole range of measured fields (0 – 10 T) and temperatures (2 – 300 K), but the shape of the MR-versus-$B$ curves is very similar to our high-temperature results. In HoPdBi, the negative MR

![FIG. 1: Temperature-dependent four-point resistivity $\rho_{\text{dc}}$ (black line, left scale) and dc conductivity, $\sigma_{\text{dc}} = 1/\rho_{\text{dc}}$, (red line, right axis) of YbPtBi. In addition, the bold dots correspond to the values obtained as $\nu \to 0$ extrapolations of the two Drude contributions, broad and narrow, to the optical conductivity, and to the sum of the two, see text. The inset shows $d\rho_{\text{dc}}/dT$.](image1)

![FIG. 2: Magnetoresistance of YbPtBi as measured between 2.5 and 300 K. The 1 K data are extracted from Ref. \cite{3}.](image2)
sets in already at 50 K in 7 T and the overall shape of the lower temperature MR curves are similar to our results for $T < 20$ K, but the temperature dependencies of the MR maximum is different.

The results of the Hall measurements on YbPtBi, i.e. the Hall resistance, $R_{xy}(B,T)$, and the Hall coefficient, $R_H(B,T) = \rho_{xy}/B$, are plotted in Fig. 3 as the functions of applied magnetic field for various temperatures as indicated. The low-field behavior is magnified in the inset in order to demonstrate that $R_H$ is always negative in low fields. As the field increases, the Hall coefficient eventually changes sign: electrons get localized and the Hall response becomes dominated by holes (accordingly, the MR saturates, as discussed). Within our range ($B < 6.5$ T), $R_H$ turns positive for all temperatures below 260 K and saturates at 0.015 cm$^2$/C$^{-1}$. Obviously, this very value would be reached at all temperatures up to 300 K, if we could go to higher magnetic fields, as demonstrated in the inset of the bottom panel. Thus, we conclude that the hole concentration $n_h$ is temperature independent and equal to $(5.2 \pm 0.6) \times 10^{20}$ cm$^{-3}$.

Oppositely, the electron concentration $n_e$ demonstrates a strong temperature dependence. We calculate $n_e(T)$ from $R_H = 1/(n_e \cdot e)$, taking into account only the initial slop in $\rho_{xy}(B)$ at low fields, and plot the results in Fig. 3(a).

The two-carrier-type scenario for YbPtBi does not allow us to calculate the carrier mobility in a straightforward fashion because at this stage we cannot separate the contributions of each carrier type to the total conductivity $\sigma_{dc}$. In the so-called one-carrier-type (OCT) approach (i.e. if we use the total measured $\sigma_{dc}$ to compute both, electron and hole, mobilities from the corresponding Hall coefficients), one can though estimate roughly the mobilities: $\mu_e^{\text{OCT}} = R_H^{\text{OCT}} \cdot \sigma_{dc} \approx 53,000$ cm$^2$/Vs and $\mu_h^{\text{OCT}} = R_H^{\text{OCT}} \cdot \sigma_{dc} \approx 200$ cm$^2$/Vs at $T = 10$ K. This estimate not only provides the upper limits for the mobilities, but also shows that the mobilities of electrons and holes in YbPtBi differ from each other by orders of magnitude. Below we will describe, how our optical measurements provide additional information in order to separate the electron and hole contributions to the conductivity and thus to get more accurate values of the carrier mobilities.

**Optics.** Fig. 5 displays the results of our optical investigations. The measured reflectivity spectra $R(\nu)$ are plotted in panel (a) for various temperatures. The
Drude-like interband contributions below 2000 cm$^{-1}$ are separated from the interband transitions at higher frequencies. The characteristic downturn in $R(\nu)$ near the plasma edge ($\sim$ 1000 cm$^{-1}$), however, reaches only 0.45, indicating some overlap of the intra- and interband contributions in the mid-infrared region.

Panel (c) of Fig. 5 shows the optical conductivity as derived from the Kramers-Kronig analysis of the reflectivity data. Here not only the absorption bands due to the intra- and interband transitions can be separated; it also becomes apparent that the low-frequency response consists of two Drude-like terms.

The dielectric constant $\varepsilon_1(\nu)$ is presented in Fig. 5(b). It is negative below approximately 1000 cm$^{-1}$ due to the free-carrier (Drude) contributions and reveals a broad maximum at around 3500 cm$^{-1}$ signaling an interband absorption edge at somewhat lower frequencies.

FIG. 5: Frequency-dependent reflectivity (a), dielectric constant (b), and optical conductivity (c) of YbPtBi for selected temperatures between 12 and 300 K. The inset in panel (b) zooms in $\varepsilon_1(\nu)$ near the zero crossing. Panel (d): fit of the optical conductivity at 300 K using a Drude-Lorentz model. The intraband conductivity can be represented with two Drude components. The reflectivity and dielectric constant are fitted using the same Drude-Lorentz model (fits are not shown).

and confirming the assignment of the optical-conductivity modes above 2000 cm$^{-1}$ to interband transitions. At $T < 100$ K, i.e. in the same temperature range, where $\rho_{dc}(T)$ demonstrates the inflection point, a shoulder in $\varepsilon_1(\nu)$ appears at approximately 1600 cm$^{-1}$. The shoulder becomes more pronounced as the temperature decreases. It likely corresponds to an additional interband transition and hence indicates a possible band-structure modification at around $T \approx 90$ K.

Zero-line crossings of the $\varepsilon_1(\nu)$ curves (the inset of Fig. 5(b)) shift towards higher frequencies as $T$ increases. This reflects the increased carrier concentration at higher temperatures: the zero-line crossings of $\varepsilon_1(\nu)$ can be taken as a measure of the screened plasma frequency, $\omega_{pl}^{scr}/2\pi$, which in turn is proportional to the carrier concentration.

In order to get more insight into the charge carrier dynamics, we simultaneously fit the experimental spectra of $\sigma_1(\nu)$, $\varepsilon_1(\nu)$, and $R(\nu)$ for each temperature by the Lorentz-Drude model. Results of these fits are exemplified in the panel (d) for $\sigma_1$ at $T = 300$ K. For the entire temperature range of our measurements, we were not able to describe the observed conductivity with a single Drude term, but obtained a satisfactory description only for two such contributions. These Drude terms have very different (by more than an order of magnitude) scattering rates, $1/\tau$.

Analysis of Shubnikov–de Haas oscillations in YbPtBi yields the effective carrier masses $m^*$ close to the free-electron mass $m_e$ for any band, ranging from $\sim$ 0.5 to 1.5$m_e$. Thus, the large difference between the electron and hole mobilities in YbPtBi should be mostly related to the difference in the scattering rates ($\mu = e\tau/m^*$) and one can ascribe the Drude term with the smaller scattering rate (the narrow Drude) to the highly mobile electrons and the term with larger scattering rate (the broad Drude) to the holes with low mobility.

The optical fits with the two Drude terms allow us to separate the contributions from the electrons and holes into the total conductivity. The bold dots in Fig. 5(d) correspond to the values obtained as $\nu \rightarrow 0$ extrapolations of the two Drude contributions. As one can see from the Figure, their sum nicely follows the dc-conductivity curve. It is also apparent that at low temperatures electrons dominate the conductivity, while as $T \rightarrow 300$ K, the contributions of electrons and holes to $\sigma_{dc}$ become comparable, the electrons still providing a larger contribution.

Using the interpolations between the points, obtained from the optical-data fits, and the carrier concentrations, obtained from the Hall measurements, we calculate the carrier mobilities of electrons, $\mu_e$, and holes, $\mu_h$. The electron mobility is plotted in Fig. 5(b). As the hole contribution to the dc conductivity is (much) lower than the electron contribution (Fig. 5(b)), the values for electron motility do not differ much from the values, obtained using the one-carrier-type approximation. However, the
hole mobility, calculated with the use of the optical fits, is much lower than the one obtained in the one-carrier-type approach. We find $\mu_h = (10 \pm 5) \text{ cm}^2/\text{Vs}$, being basically temperature independent. However, we cannot exclude a weak temperature dependence of $\mu_h$ within the given error bar: the hole scattering rate changes somewhat as a function of $T$.

As one can see from Fig. 4b, the electron mobility shoots up exponentially as $T$ decreases [28]. We could fit $\mu_e$ with $\mu_e(T) = \mu_e(0) \exp(-T/T_0)$ in the entire temperature range. We have found $\mu_e(0) = 50\,000 \text{ cm}^2/\text{Vs}$ and $T_0 = 70 \text{ K}$. The exponential behavior of $\mu_e$ is quite remarkable: usually, even in the materials with the highest reported mobilities, such as e.g. the Weyl semimetal NbP, $\mu(T)$ saturates at temperatures below some $20-30 \text{ K}$ [12]. The exponential behavior of $\mu_e(T)$ in YbPtBi persists down to our lowest temperature (2.5 K) despite leveling off the electron concentration at $T < 100 \text{ K}$, Fig. 1a. This signals collapsing of the electron scattering in YbPtBi at low temperatures. The electron concentration as a function of temperature does not show a sign of Arrhenius behavior at any $T$, the flat behavior at low temperatures being followed by a power law, $\mu_e \propto T^2$, at $T > 100 \text{ K}$.

**Conclusions.** From our transport, magnetotransport, and optical investigations of the half-Heusler compound YbPtBi at $T \geq 2.5 \text{ K}$ (i.e. not in the heavy-fermion state), we can separate two conduction channels caused by electrons and holes. Electrons posses a temperature-dependent concentration, high mobility, and low scattering rates. Holes form the second channel with the concentration and mobility that are basically temperature independent. While at high temperatures, i.e. 200 – 300 K, both channels provide comparable contributions to the dc transport, at low temperatures the electron channel dominates overwhelmingly. This is due to very high mobility, $\mu_e(T = 2.5 \text{ K}) = 50\,000 \text{ cm}^2/\text{Vs}$, and low scattering of the electrons at $T < 100 \text{ K}$. To the best of our knowledge, the values of electron mobility in YbPtBi, are record high for half-Heusler compounds.

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