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On the temperature dependence of the Hall constant in some heavy-fermion compounds: a qualitative theory

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Abstract. The non-linear temperature dependence of the Hall constant in heavy-fermion compounds is explained on the basis of the self-consistent temperature shift of the chemical potential within the two-band hybridization model without explicit reference to any magnetic (Kondo) interaction.

1. Introduction

The objective of this work is a qualitative explanation of the anomalous temperature dependence of the Hall constant $R_H(T)$ in some heavy-fermion compounds (HFCs) [1, 2] (figure 1). The consistent theory must explain such experimental facts as

- (i) the mainly positive sign of $R_H(T)$ in the whole temperature range,
- (ii) the maximum at a temperature $T \approx 10-100$ K,
- (iii) the rapid decrease in $R_H(T)$ at higher temperatures and
- (iv) a possible sign change at the ascending (as in UAl_2) or descending (as in $Ce_xLa_{1-x}Cu_6$) branch of the $R_H(T)$ curve and, in the latter case, the dependence of transition temperature T_{tr} , on the concentration of the f element (table 1).

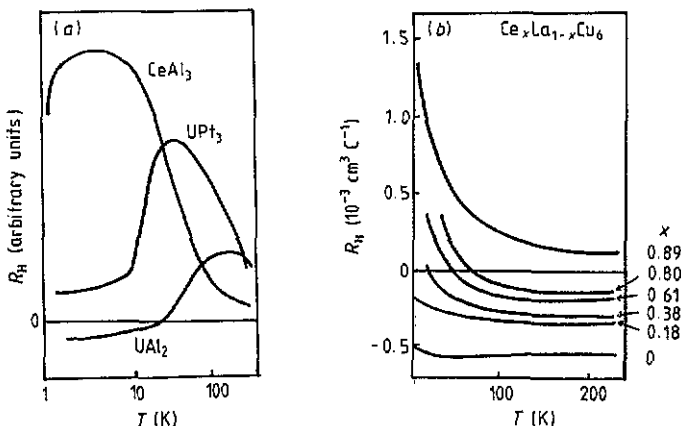


Figure 1. Temperature dependences of the Hall constant R_H in HFCs: (a) $CeAl_3$, UPt_3 and UAl_2 [2]; (b) $Ce_xLa_{1-x}Cu_6$ [1].

Table 1. The concentration dependence of the Hall constant transition temperature in $\text{Ce}_x\text{La}_{1-x}\text{Cu}_6$ (after [1]).

x	T_{tr} (K)	$\delta x/x_0$	$\delta T/T_0$	$C \equiv (\delta T/T_0)/(\delta x/x_0)$
$0.80 \equiv x_0$	$\approx 65 \equiv T_0$	—	—	—
0.61	≈ 40	-0.24	-0.38	1.58
0.38	≈ 15	-0.53	-0.77	1.45

In the present work we show that these demands are met by the two-band hybridization model of HFCs and that this model can be used to explain the anomalous temperature dependences of the thermodynamic and kinetic coefficients in these systems [3-5].

2. Formulation of model: validity of band description of HFCs

The above-mentioned model considers two bare electron bands (s and f electrons) hybridized to form two new bands (lower and upper bands in figure 2(a)). The model Hamiltonian is

$$H = \sum_{k,\sigma} \left[\epsilon_s(k) a_{k,\sigma}^{(s)+} a_{k,\sigma}^{(s)} + \epsilon_f(k) a_{k,\sigma}^{(f)+} a_{k,\sigma}^{(f)} \right] + V \sum_{k,\sigma} \left(a_{k,\sigma}^{(s)+} a_{k,\sigma}^{(f)} + a_{k,\sigma}^{(f)+} a_{k,\sigma}^{(s)} \right). \quad (1)$$

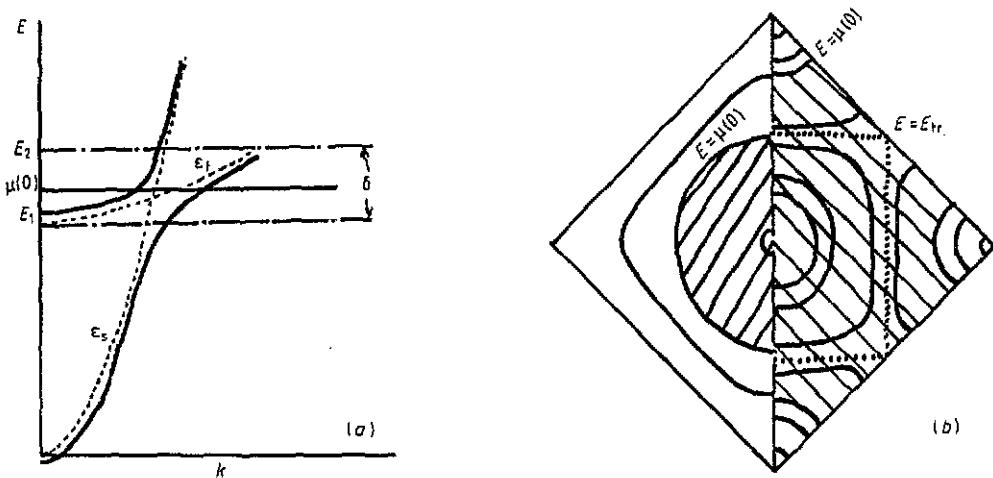


Figure 2. (a) The two-band hybridization model of HFC electronic structure: ϵ_s and ϵ_f , dispersion laws in the bare bands; δ , width of the bare narrow (f) band; E_1 , the bottom of the upper hybridized band; E_2 , the top of the lower hybridized band; $\mu(0)$, the position of the chemical potential at zero temperature. (b) The Brillouin zone filling at zero temperature: E_{tr} , the energy of the critical orbit dividing the electron-like states and the hole-like states in the lower band.

Here ϵ_s and ϵ_f denote the dispersion law curves in the s and f bands, respectively, $a_{k,\sigma}^{(s)+}$ and $a_{k,\sigma}^{(f)+}$ are the electron creation operators in the s or f bands, respectively, and V is the interband hybridization potential.

The typical bare width δ of the f band is estimated to be of the order of 10–100 K (see, e.g., the review in [6]). We stress that an effective f band is considered, its origin being left beyond the scope of our paper. The hybridization potential V is asserted to be of the order of 0.1 eV [7].

According to [3], all the anomalous temperature dependences of HFCs are attributed to the density of states (DOS), the carrier group velocity and inverse mass tensor being the sharp functions of energy on the scale of δ (see figure 2(a)). This statement needs an additional comment. Indeed, at first sight it seems almost evident that the only energy scale in theory is $V \simeq 10^3$ K, and the narrow region of width about δ is simply absorbed by it, but this is not the general situation. Let us analyse the hybridized dispersion law $E(k)$ (two possible solutions correspond to upper and lower hybridized bands):

$$E(k) = \epsilon_s(k) + V^2/[E(k) - \epsilon_f(k)] \tag{2}$$

and the ensuing DOS function

$$N(E) = (1/\pi^2 \hbar^3) k^2(E) dk/dE \\ = N_{s0}(E)[1 + V^2/(E - \epsilon_f)^2]/\{1 + [u_f(E)/u_s(E)]V^2/(E - \epsilon_f)^2\}. \tag{3}$$

Here u_s and u_f denote the group velocities in the bare s and f bands, respectively, and $N_{s0}(E)$ is the DOS in the bare s band. One can easily see that, when the inequality

$$(u_f/u_s)(V^2/\delta^2) \ll 1 \tag{4}$$

holds, the density of states is peaked within the energy interval of the order of δ , and not V !

The band theory of HFCs claims that at zero the chemical potential $\mu(0)$ of HFCs lies within the bare f band. Then $\mu(T)$ acquires a significant temperature shift, mainly an almost linear fall with the tangent dependent on its initial value $\mu(0)$ [3–5]. This shift provides the valuable variation in the charge-carrier parameters in the effective energy layer, $k_B T$, and proves to be the main reason for the anomalous temperature dependences of various HFC characteristics. The possible dehybridization mechanism in the two-band model [8] would manifest itself at higher temperatures $T \sim V$.

Since pioneer theoretical papers on the HFCs it has been commonly accepted that we treat f electrons as being strongly Coulomb correlated. The corresponding Hamiltonian contains a Hubbard term with the repulsion constant $u_Q \sim e^2/a \gg \delta$ (a is the interatomic distance). As a result, f electrons turned out to be strongly localized; they could be regarded as the local magnetic moments giving rise to the well known Kondo effect.

Our model (1), on the contrary, considers f electrons as free particles, thus neglecting Coulomb splitting of the band states. Such a description is justified by a correct treatment of Debye screening in a system with a gigantic DOS.

The trivial calculation in the free-gas approximation yields

$$r_D^{-1} = \max \left\{ (2e/\pi \hbar) k_F^{(\pm)} [N^{(\pm)}(\mu)]^{1/2} \right\} \simeq (r_D^{(0)})^{-1} [u_s(\mu)/u_f(\mu)]^{1/2} \gg (r_D^{(0)})^{-1}. \tag{5}$$

Here r_D is the Debye radius, $r_D^{(0)}$ is one for bare s electrons, and $k_F^{(\pm)}$ and $N^{(\pm)}(\mu)$ are the Fermi momenta and DOS for the upper and lower hybridized bands correspondingly. Because $r_D^{(0)} \sim a$, the true estimate of the Coulomb potential is

$$u_Q \simeq (e^2/a) \exp \left[-\lambda \sqrt{u_s(\mu)/u_t(\mu)} \right] \quad (6)$$

where $\lambda = a/r_D^{(0)} \simeq 1$. The quantity (6) can be easily made much less than δ by a proper choice of bare band parameters. (The question of why the model parameters have particular numerical values is outside our phenomenological considerations.) Finally, the condition $\delta \gg u_Q$ is natural for a typical HFC having $u_s/u_t \gtrsim 10^2$.

3. Calculation of the Hall resistance

The galvanomagnetic parameter $\gamma = |e|H\tau/m^*c$, where τ is the collision time and m^* is the cyclotron mass, is small in the experiments considered. Indeed, γ can be rewritten as the ratio $\gamma \simeq (H/n|e|c)/\rho < 10^{-4}H$ (kOe), for the HFC resistivity $\rho \simeq 10^{-4} \Omega \text{ cm}$ and carrier density $n > 10^{22} \text{ cm}^{-3}$ [1, 2]. At the magnetic fields actually applied in experiments, $\gamma \ll 1$, and in the τ -approximation the solution to the kinetic equation is given by the Jones-Zener series over γ [9] as follows:

$$f(\mathbf{k}) = f_0(\epsilon_{\mathbf{k}} - \mu) + (1 - \hat{\Omega} + \hat{\Omega}^2 - \dots)(-\tau e \mathbf{E} \cdot \mathbf{v} \partial f_0 / \partial \epsilon_{\mathbf{k}}). \quad (7)$$

Here $f_0(\epsilon - \mu)$ is the Fermi distribution function, and $\hat{\Omega}$ stands for the operator ($\hbar = 1$)

$$\hat{\Omega} = (e\tau/c)[\mathbf{v} \times \mathbf{H}] \cdot \partial / \partial \mathbf{k}.$$

In the linear approximation over H , the Hall constant (in geometry $j \parallel O x, \mathbf{H} \parallel O z$) is given by the expression [9]

$$R_H = \frac{e^3 \tau^2}{c} \rho_0^2 \int d\mathbf{k} \left(-\frac{\partial f_0}{\partial \epsilon_{\mathbf{k}}} \right) (v_x^2 M_{yy}^{-1} - v_x v_y M_{yx}^{-1}) \quad (8)$$

where $v_\alpha = (\partial \epsilon_{\mathbf{k}} / \partial k_\alpha)$ is the carrier group velocity, $M_{\alpha\beta}^{-1} = (\partial v_\alpha / \partial k_\beta)$ is the inverse effective mass tensor and $\rho_0(T)$ is the zero-field resistivity. The integral is taken over all the bands.

Consider the charge carriers in the model sketched in figure 2. At zero temperature the Fermi level lies inside the bare narrow band. Then the lower hybridized band is almost filled and its conductivity is due to hole states in the corners of the Brillouin zone. The upper hybridized band conducts owing to the electron states. To estimate $R_H(T)$ we regard the inverse mass tensor as the isotropic tensor

$$M_{\alpha\beta,\pm}^{-1} \simeq \delta_{\alpha\beta} [1/m_\pm^*(\epsilon)]. \quad (9)$$

Here $m_\pm^*(\epsilon)$ is the energy-dependent effective mass in the lower (-) or upper (+) band; $-1/m_-^*(E_1) \simeq 1/m_+^*(E_2) \simeq 1/M$, and $-1/m_-^*(E_1 - \delta) \simeq 1/m_+^*(E_2 + \delta) \simeq$

$1/m$, where m and $M \gg m$ are the 'light' and 'heavy' effective masses of carriers. Utilizing (9) in equation (8), we get eventually

$$R_H(T) \simeq \frac{e^3 \tau^2(T)}{3c} \rho_0^2(T) \sum_s A_s(\mu(T)) \frac{v_s(\mu(T))}{m_s^*(\mu(T))}. \quad (10)$$

(Here $A_s(\epsilon)$ is the area of the surface $E(k) = \epsilon$ in the s th band.)

The main temperature dependence comes from the interplay between the electron-phonon collision time $\tau(T)$, which decreases rapidly with increasing temperature (e.g. $\tau(T) \sim (\omega_0/2T)/\sinh^2(\omega_0/2T)$ in the Einstein model of phonons with frequency ω_0), and of the zero-field HFC resistivity $\rho_0(T)$, which increases at low T ($< T_{\max} \simeq \delta$) and then saturates or decreases [2].

At low temperatures the Hall constant would be small, since all the terms in (4) are small. Its sign is defined by $\mu(0)$; if $\mu(0)$ lies in the region where $m_+^* < |m_-^*|$, the electron state contribution to (10) dominates. This is the case for UAl_2 (figure 1(a)). At higher temperatures the hole contribution dominates in any case. The position of the $R_H(T)$ maximum is defined by the concurrence between the increasing scattering rate and the carrier group velocity.

The maximum temperature is estimated to be

$$T_{\max} \simeq \delta/|d\mu/dT|. \quad (11)$$

At $T > T_{\max}$, $R_H(T)$ decreases mainly owing to the scattering, and its sign can alter again because of the transition from the hole states to the electronic states occurring in the lower band at sufficiently low $\mu(T)$ -value, say $\mu \leq E_{tr}$ (see figure 2(b)). At these energies the effective mass alters its sign: $1/m_-^*(\epsilon) \propto E_{tr} - \epsilon$, and so the Hall constant does too. The crossover is possible at some reasonable temperature T_{tr} if initially the chemical potential does not lie too high. That is, $\mu(0)$ is near the very bottom of the lower band, and the influence of the upper band can be neglected. The ascending branch of the $R_H(T)$ curve can be totally absent if $\mu(0)$ is in the region where the $v_+ (\mu(T))/|m_+^* (\mu(T))|$ -dependence is not yet too sharp to beat the rapid fall in the $\tau^2(T)$ -factor. This is the way that $Ce_xLa_{1-x}Cu_6$ compounds behave.

The estimate for the transition temperature is

$$T_{tr} \sim [\mu(0) - E_{tr}]/|d\mu/dT|. \quad (12)$$

It can be easily seen that, for a given concentration x of the f element, the R_H -sign transition temperature $T_{tr}(x)$ obeys the rule

$$[T_{tr}(x) - T_0]/T_0 \sim C(x - x_0)/x_0, \quad C \sim 1 \quad (13)$$

where x_0 is the f element concentration for which the sign alteration occurs at T_0 . This rule seems to agree with the experimental data on $Ce_xLa_{1-x}Cu_6$ [1] (see figure 1 and table 1). For $x = 1$ or 0.89, the chemical potential at zero temperature lies too high to reach the transition point while, for $x = 0.18$, the f band does not reveal itself.

Our model predicts the approximately universal connection of the relative shift of the peculiarity temperature for different HFC characteristics with the variation in $\mu(0)$ [5]:

$$\delta T/T \simeq \alpha(\delta\mu)/\delta \quad (14)$$

where $\alpha \simeq 1$ depends on the material and the parameter measured. Then under a pressure P , both the characteristic temperatures T_{\max} and T_{tr} for R_{H} (if the transition occurs) will change approximately as

$$\delta T/T \simeq \frac{2}{3}[\mu(0)/\delta]\kappa P \quad (15)$$

where $\kappa \equiv -(1/V)(\partial V/\partial P) \simeq 10^{-3} \text{ kbar}^{-1}$ is the compressibility. For $\mu/\delta \simeq 10^2$ the estimated shift would be $\delta T/T \simeq 0.1 P$ (kbar). Similar pressure dependences of the $\rho_0(T)$ maximum temperature were reported for CeCu_6 [10, 11] and UBe_{13} [12]†.

More exact predictions allowing quantitative comparison with the experimental data need full-scale numerical calculations for a given HFC and will be published elsewhere.

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† Recently such a change in the temperature dependence of a Hall constant under pressure was actually observed in an HFC, CeRu_2Si_2 [13]. The shift $\delta T_{\max}/T_{\max}$ of the maximum temperature is about 1.1 under a pressure of 19 kbar, while our estimate in the text gives $\delta T_{\max}/T_{\max} \simeq 0.9$, in good accordance with reality. The estimates based on skew scattering theory [14] give a shift at least twice that observed.