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Philips Research Laboratories, N. V. Philips' Gloeilampenfabrieken, Eindhoven

Study of the Temperature Dependence of the Resistivity in the Kondo Side-Band Model

By

F. E. Maranzana and P. Bianchessi

The influence of the crystal field on the Kondo effect in a magnetically non-dilute intermetallic compound is analysed. An expression for the resistivity versus temperature is obtained. Some resistivity versus temperature curves are reported and discussed.

L'influence du champ cristallin sur l'effet Kondo est analysée dans un composé intermétallique magnétiquement non dilué. Une expression est obtenue pour la résistivité en fonction de la température. Quelques courbes de résistivité en fonction de la température sont calculées numériquement et discutées.

1. Introduction

The present article contains a detailed analysis of the temperature dependence of the resistivity within the Kondo side-band model [1]. A second order perturbational calculation has been carried out in order to establish the effect on the resistivity of the scattering of the conduction electrons by magnetic ions subject to a crystal field. This calculation has been completed by a numerical study that has supplied a set of resistivity versus temperature curves. The numerical calculation has been performed assuming that the magnetic ion has a total angular momentum equal to 5/2 and it is under the influence of a hexagonal crystal field. The curves obtained show as a function of temperature either one or two maxima whose positions and widths vary as a function of the crystal field parameters and of the exchange constant proper to the curve under consideration. These maxima are in general the consequence of the existence of Kondo side-bands in the expression of the relaxation time of the conduction electrons as a function of energy. Kondo side-bands are obtained when the perturbation expansion is carried up to second order. A set of crystal field parameters can be chosen, however, in a rather narrow range such that a maximum followed by a minimum can be obtained already as a consequence of first-order contributions. This first order effect adds up constructively in this range to Kondo side-band effects, and it will be discussed in some detail in the following sections.

The results presented here can be applied in our opinion to magnetically non-dilute compounds. A question that arises of course is how does the correlation between the motion of different localized angular momenta influence the Kondo effect. In agreement with the traditional molecular field theory we think we can neglect correlations when a material is paramagnetic. There may be valid reasons to do this. In the first place the present theory is meant to be applied to rare-earth intermetallic compounds. The limited spatial extension of the 4f electrons, as compared to the d electrons of the transition-metal ions, appreciably reduces the possibility of the existence of correlations in the rare-earth compounds. Furthermore in a compound the magnetic moments are separated from each other by the non-magnetic anion, and thus random internal magnetic fields seem negligible. The present point of view is not in agreement with the opinions stated by other authors [2]. We expect the magnetic transition temperature in our systems to be smaller than the Kondo temperature, while the opposite is true for the alloys considered by the authors just cited.

Besides this introduction, this article contains two other sections. Section 2 contains the calculation of the resistivity as a function of temperature for the Kondo side-band model. It is an adaptation to our model of Kondo's original calculation [3]. Section 3 of this paper contains a discussion of the numerical results.

2. Description of the Model and Calculation

The model to be considered consists of a gas of charge carriers and of a periodic array of spins. We shall indicate in this context with the word "spin" a total angular momentum. Indeed in the case of intermetallic compounds of the rare-earths the "spins" are total angular momenta that result from the L–S coupling in the presence of the spin–orbit interaction. The spin–orbit interaction is much larger than the interactions acting on the spins, so that the length of the spins can be considered a good quantum number. In particular we are thinking for example of the cerium ion, which has a "spin" $S = 5/2$, and thus possesses six degenerate levels, which are labelled by the six values of the z-component S_z of the spin. The degeneracy is partially raised by the presence of the crystal field interaction:

$$H_{\mathrm{mag}} = N\, H_{\mathrm{cf}}\,. \tag{1}$$

N is the number of spins present in the crystal. H_{cf} is the crystal field Hamiltonian proper to the symmetry of the site of a spin. We shall take the z-axis appearing in H_{cf} as the axis of quantization for the spins S. H_{mag} is the unperturbed Hamiltonian of the array of spins. It can be diagonalized and one obtains the energy levels E_m ($m = 1, 2, \ldots, 6$ for the cerium ion). We assume that no interaction is present between the spins, so that in particular no spontaneous magnetization is expected. Our results should be applied only in the paramagnetic region.

We shall now turn our attention to the charge carrier system. The charge carriers are described by creation and annihilation operators $a^+_{k\uparrow}\, a_{k\uparrow}$, $a^+_{k\downarrow}$, $a_{k\downarrow}$. $\boldsymbol{k}$ is the wave vector, and the arrow indicates the direction of the spin with respect to the z-axis. As the magnetic system is paramagnetic the charge carriers of opposite spin reside in the same band. This band extends from $-E_1$ to E_1, where we have chosen $E_{\mathrm{F}} = 0$ as the zero of the energies. We shall also assume that the density-of-states function of the band is equal to a constant $n(E_{\mathrm{F}})$.

The eigenfunctions of the Hamiltonians now described are the product of a Slater determinant of kets $|\boldsymbol{k}, \uparrow\rangle$, $|\boldsymbol{k}, \downarrow\rangle$ times a product of eigenfunctions $|E^r_m\rangle$ relative to the mth energy level of the rth ion. We shall take these eigenfunctions as the unperturbed eigenfunctions of the model under consideration. The perturbation Hamiltonian is the s–d Hamiltonian [4]:

$$H' = -\left(\frac{J}{N}\right) \sum_{\boldsymbol{k}\boldsymbol{k}'r} \exp\left[i\,(\boldsymbol{k} - \boldsymbol{k}') \cdot \boldsymbol{R}_r\right] \times$$
$$\times \ \{S^r_z\,(a^+_{\boldsymbol{k}'\uparrow}\,a_{\boldsymbol{k}\uparrow} - a^+_{\boldsymbol{k}'\downarrow}\,a_{\boldsymbol{k}\downarrow}) + S^r_+\,a^+_{\boldsymbol{k}'\downarrow}\,a_{\boldsymbol{k}\uparrow} + S^r_-\,a^+_{\boldsymbol{k}'\uparrow}\,a_{\boldsymbol{k}\downarrow}\}\ . \tag{2}$$

The matrix elements of the perturbation H' between the above-defined unperturbed states are

$$\langle \boldsymbol{k}', \uparrow\downarrow\,;\, E^1_{m_1}, \ldots, E^r_{m'_r}, \ldots, E^N_{m_N}|\ H'\ |\boldsymbol{k}, \uparrow\downarrow; E^1_{m_1}, \ldots, E^r_{m_r}, \ldots E^N_{m_N}\rangle =$$
$$= -\left(\frac{J}{N}\right)(\pm 1)\exp\left[i\,(\boldsymbol{k} - \boldsymbol{k}') \cdot \boldsymbol{R}_r\right]\langle E^r_{m'_r}|\,S^r_z\,|E^r_{m_r}\rangle, \tag{3a}$$

$$\langle \boldsymbol{k}', \uparrow; E^1_{m_1}, \ldots, E^r_{m'_r}, \ldots, E^N_{m_N}|\ H'|\boldsymbol{k}, \downarrow\,;\, E^1_{m_1}, \ldots, E^r_{m_r}, \ldots, E^N_{m_N}\rangle =$$
$$= -\left(\frac{J}{N}\right)\exp\left[i\,(\boldsymbol{k} - \boldsymbol{k}') \cdot \boldsymbol{R}_r\right]\langle E^r_{m'_r}|\ S^r_-\,|E^r_{m_r}\rangle, \tag{3b}$$

$$\langle \boldsymbol{k}', \downarrow; E^1_{m_1}, \ldots, E^r_{m'_r}, \ldots, E^N_{m_N}|\ H'\ |\boldsymbol{k}, \uparrow; E^1_{m_1}, \ldots, E^r_{m_r}, \ldots, E^N_{m_N}\rangle =$$
$$= -\left(\frac{J}{N}\right)\exp\left[i\,(\boldsymbol{k} - \boldsymbol{k}') \cdot \boldsymbol{R}_r\right]\langle E^r_{m'_r}|\,S^r_+\,|E^r_{m_r}\rangle. \tag{3c}$$

These matrix elements are introduced in the following formula that gives the transition probability up to terms cubic in H':

$$W\,(a \to b) = W^{(1)}\,(a \to b) + W^{(2)}\,(a \to b)\ ,$$
$$W^{(1)}(a \to b) = \left(\frac{2\,\pi}{\hbar}\right)\delta\,(E_a - E_b)\,H'_{ab}\,H'_{ba}\ ,$$
$$W^{(2)}\,(a \to b) = \left(\frac{2\,\pi}{\hbar}\right)\delta\,(E_a - E_b)\sum_{c \neq a}\{[H'_{ac}\,H'_{cb}\,H'_{ba}\,(E_a - E_c)^{-1}] + \text{c.c.}\}\ . \tag{4}$$

We shall concern ourselves with the first terms in W, which are quadratic in H'. The $W^{(1)}$'s are

$$W^{(1)}\,(\boldsymbol{k}\uparrow\downarrow, m \to \boldsymbol{k}'\uparrow\downarrow, m') = \left(\frac{2\,\pi}{\hbar}\right)\left(\frac{J}{N}\right)^2\sum_r \delta\,(E_{\boldsymbol{k}} - E_{\boldsymbol{k}'} + E^r_{m_r} - E^r_{m'_r}) \times$$
$$\times\ \langle E^r_{m'_r}|\ S^r_z\ |E^r_{m_r}\rangle\langle E^r_{m_r}|\ S^r_z\ |E^r_{m'_r}\rangle, \tag{5a}$$

$$W^{(1)}\,(\boldsymbol{k}\uparrow, m \to \boldsymbol{k}'\downarrow, m') = \left(\frac{2\,\pi}{\hbar}\right)\left(\frac{J}{N}\right)^2\sum_r \delta\,(E_{\boldsymbol{k}} - E_{\boldsymbol{k}'} + E^r_{m_r} - E^r_{m'_r}) \times$$
$$\times\ \langle E^r_{m'_r}|\ S^r_+\ |E^r_{m_r}\rangle\langle E^r_{m_r}|\ S^r_-\ |E^r_{m'_r}\rangle, \tag{5b}$$

$$W^{(1)}\,(\boldsymbol{k}\downarrow, m \to \boldsymbol{k}'\uparrow, m') = \left(\frac{2\,\pi}{\hbar}\right)\left(\frac{J}{N}\right)^2\sum_r \delta\,(E_{\boldsymbol{k}} - E_{\boldsymbol{k}'} + E^r_{m_r} - E^r_{m'_r}) \times$$
$$\times\ \langle E^r_{m'_r}|\ S^r_-\ |E^r_{m_r}\rangle\langle E^r_{m_r}|\ S^r_+\ |\ E^r_{m'_r}\rangle. \tag{5c}$$

In the equations just written the summation over r is easily performed in view of the fact that the states $|E^r_m\rangle$ are the same for every r. One can then omit the index r and one obtains

$$W^{(1)}(\boldsymbol{k}\uparrow\downarrow, m \to \boldsymbol{k}'\uparrow\downarrow, m') = \left(\frac{2\pi}{\hbar}\right)\left(\frac{J}{N}\right)^2 N\,\delta(E_k - E_{k'} + E_m - E_{m'})\,|\langle E_{m'}|\,S_z\,|E_m\rangle|^2, \quad (6\text{a})$$

$$W^{(1)}(\boldsymbol{k}\uparrow, m \to \boldsymbol{k}'\downarrow, m') = \left(\frac{2\pi}{\hbar}\right)\left(\frac{J}{N}\right)^2 N\,\delta(E_k - E_{k'} + E_m - E_{m'})\,|\langle E_{m'}|\,S_+\,|E_m\rangle|^2, \quad (6\text{b})$$

$$W^{(1)}(\boldsymbol{k}\downarrow, m \to \boldsymbol{k}'\uparrow, m') = \left(\frac{2\pi}{\hbar}\right)\left(\frac{J}{N}\right)^2 N\,\delta(E_k - E_{k'} + E_m - E_{m'})\,|\langle E_{m'}|\,S_-\,|E_m\rangle|^2. \quad (6\text{c})$$

These transition probabilities should finally be averaged over the occupation of the initial state E_m and summed over the final states $E_{m'}$:

$$W^{(1)}(\boldsymbol{k}\uparrow\downarrow \to \boldsymbol{k}'\uparrow\downarrow) = \left(\frac{2\pi}{\hbar}\right)\left(\frac{J}{N}\right)^2 N \left[\sum_m \exp\left(-\frac{E_m}{k_{\mathrm{B}}T}\right)\right]^{-1} \times$$
$$\times \left[\sum_{m m'} \exp\left(-\frac{E_m}{k_{\mathrm{B}}T}\right)\delta(E_k - E_{k'} + E_m - E_{m'})\,|\langle E_{m'}|\,S_z\,|E_m\rangle|^2\right], \quad (7\text{a})$$

$$W^{(1)}(\boldsymbol{k}\uparrow \to \boldsymbol{k}'\downarrow) = \left(\frac{2\pi}{\hbar}\right)\left(\frac{J}{N}\right)^2 N \left[\sum_m \exp\left(-\frac{E_m}{k_{\mathrm{B}}T}\right)\right]^{-1} \times$$
$$\times \left[\sum_{m m'} \exp\left(-\frac{E_m}{k_{\mathrm{B}}T}\right)\delta(E_k - E_{k'} + E_m - E_{m'})\,|\langle E_{m'}|\,S_+\,|E_m\rangle|^2\right], \quad (7\text{b})$$

$$W^{(1)}(\boldsymbol{k}\downarrow \to \boldsymbol{k}'\uparrow) = \left(\frac{2\pi}{\hbar}\right)\left(\frac{J}{N}\right)^2 N \left[\sum_m \exp\left(-\frac{E_m}{k_{\mathrm{B}}T}\right)\right]^{-1} \times$$
$$\times \left[\sum_{m m'} \exp\left(-\frac{E_m}{k_{\mathrm{B}}T}\right)\delta(E_k - E_{k'} + E_m - E_{m'})\,|\langle E_{m'}|\,S_-\,|E_m\rangle|^2\right]. \quad (7\text{c})$$

We shall now consider the contribution to the transition probability (4) from terms cubic in H'. The transition probability that an electron of wave vector $\boldsymbol{k}$ and spin up is scattered to a state of wavevector $\boldsymbol{k}'$ and spin up, is a sum of four terms, resulting from four different processes. This transition probability is

$$W^{(2)}(\boldsymbol{k}\uparrow, m \to \boldsymbol{k}'\uparrow, m') = \left(\frac{2\pi}{\hbar}\right)\delta(E_k - E_{k'})\left(-\frac{J}{N}\right)^3 N \times$$
$$\times \Big\{\sum_{k'' m''} [(1 - f_{k''})(E_k - E_{k''} + E_m - E_{m''} + i\,\eta)^{-1} + \text{c.c.}] \times$$
$$\times [\langle E_{m''}|\,S_z\,|E_m\rangle\langle E_{m'}|\,S_z\,|E_{m''}\rangle\langle E_m|\,S_z\,|E_{m'}\rangle +$$
$$+ \langle E_{m''}|\,S_+\,|E_m\rangle\langle E_{m'}\,|S_-|\,E_{m''}\rangle\langle E_m\,|S_z\,|E_{m'}\rangle] -$$
$$- \sum_{k'' m''} [f_{k''}(E_{k''} - E_{k'} + E_m - E_{m''} + i\,\eta)^{-1} + \text{c.c.}] \times$$
$$\times [\langle E_{m''}|\,S_z\,|E_m\rangle\langle E_{m'}|\,S_z\,|E_{m''}\rangle\langle E_m|\,S_z\,|E_{m'}\rangle +$$
$$+ \langle E_{m''}|\,S_-\,|E_m\rangle\langle E_{m'}|\,S_+\,|E_{m''}\rangle\langle E_m|\,S_z\,|E_{m'}\rangle]\Big\}. \quad (8)$$

For $T \to 0$ the summation over k'' can be carried out in (8). Terms $E_k + E_m - E_{m''}$ are neglected with respect to E_1. One sums further over m' and averages over the states E_m. The following result is obtained:

$$W^{(2)}\,(\boldsymbol{k}\uparrow \to \boldsymbol{k}'\uparrow) = \left(\frac{2\,\pi}{\hbar}\right)\left(-\frac{J}{N}\right)^3 N\, n(E_\mathrm{F}) \left[\sum_m \exp\left(-\frac{E_m}{k_\mathrm{B}T}\right)\right]^{-1} \times$$
$$\times \left[\sum_{mm'm''} \exp\left(-\frac{E_m}{k_\mathrm{B}T}\right) \delta\,(E_k - E_{k'} + E_m - E_{m'}) \times\right.$$
$$\times \{\ln |(E_k + E_m - E_{m''})\, E_1^{-1}|\, \langle E_m|\, S_z\, |E_{m'}\rangle\, (\langle E_{m''}|\, S_z\, |E_m\rangle\, \langle E_{m'}|\, S_z\, |E_{m''}\rangle +$$
$$+ \langle E_{m''}|\, S_+\, |E_m\rangle\, \langle E_{m'}|\, S_-\, |E_{m''}\rangle) - \ln |(E_k + E_{m''} - E_{m'})\, E_1^{-1}| \times$$
$$\times \langle E_m\, |S_z|\, E_{m'}\rangle\, (\langle E_{m''}\, |S_z|\, E_m\rangle\, \langle E_{m'}\, |S_z|\, E_{m''}\rangle +$$
$$\left. + \langle E_{m''}|\, S_-\, |E_m\rangle\, \langle E_{m'}|\, S_+\, |E_{m''}\rangle)\}\right]. \tag{9}$$

We shall now consider the transition probability that an electron of wave-vector $\boldsymbol{k}$ and spin up is scattered to a state of wave vector $\boldsymbol{k}'$ and spin down. This transition probability equals

$$W^{(2)}\,(\boldsymbol{k}\uparrow, m \to \boldsymbol{k}'\downarrow, m') = \left(\frac{2\,\pi}{\hbar}\right) \delta\,(E_k - E_{k'} + E_m - E_{m'}) \left(-\frac{J}{N}\right)^3 N \times$$
$$\times \left\{ \sum_{k''m''} [(1 - f_{k''})\,(E_k - E_{k''} + E_m - E_{m''} + i\,\eta)^{-1} + \text{c.c.}] \times\right.$$
$$\times [\langle E_{m''}\, |S_z\, |E_m\rangle\, \langle E_{m'}\, |S_+\, |E_{m''}\rangle\, \langle E_m\, |S_-|\, E_{m'}\rangle - \langle E_{m''}\, |S_+\, |E_m\rangle\, \langle E_{m'}\, |S_z\, |E_{m''}\rangle \times$$
$$\times \langle E_m|\, S_-\, |E_{m'}\rangle] - \sum_{k''m''} [f_{k''}\,(E_{k''} - E_{k'} + E_m - E_{m''} + i\,\eta)^{-1} + \text{c.c.}\,] \times$$
$$\times [\langle E_{m''}\, |S_+\, |E_m\rangle\, \langle E_{m'}|\, S_z\, |E_{m''}\rangle\, \langle E_m|\, S_-\, |E_{m'}\rangle -$$
$$\left. - \langle E_{m''}|\, S_z\, |E_m\rangle\, \langle E_{m'}|\, S_+\, |E_{m''}\rangle\, \langle E_m|\, S_-\, |E_{m'}\rangle] \right\}. \tag{10}$$

By performing the summation over k'' at $T \to 0$ and by neglecting the energy differences between different levels as done above, and by finally averaging, one obtains

$$W^{(2)}\,(\boldsymbol{k}\uparrow \to \boldsymbol{k}'\downarrow) = \left(\frac{2\,\pi}{\hbar}\right)\left(-\frac{J}{N}\right)^3 N\, n(E_\mathrm{F}) \left[\sum_m \exp\left(-\frac{E_m}{k_\mathrm{B}T}\right)\right]^{-1} \times$$
$$\times \left[\sum_{m\,m'\,m''} \exp\left(-\frac{E_m}{k_\mathrm{B}T}\right) \delta\,(E_k - E_{k'} + E_m - E_{m'}) \times\right.$$
$$\times [\ln |(E_k + E_m - E_{m''})\, E_1^{-1}| + \ln |(E_k + E_{m''} - E_{m'})\, E_1^{-1}|]\, \langle E_m|\, S_-\, |E_{m'}\rangle \times$$
$$\left. \times (\langle E_{m''}|\, S_z\, |E_m\rangle\, \langle E_{m'}|\, S_+\, |E_{m''}\rangle - \langle E_{m''}|\, S_+\, |E_m\rangle\, \langle E_m\, |\, S_z\, |E_{m''}\rangle) \right]. \tag{11}$$

Consider equations (9) and (11), valid as $T \to 0$. The interesting feature of these equations is the presence of logarithmic terms that diverge when the energy of the scattered charge carriers equals one of the energy differences between the energy levels of the scattering spins. These logarithmic terms converge to the usual ln E term when the crystal field Hamiltonian (1) tends to zero. When, however, the crystal field Hamiltonian is not zero, the logarithmic terms make the transition probability diverge at finite charge carrier energies. These divergencies we call Kondo side-bands. When $T \neq 0$, the summation over k'' cannot be performed in closed form. As implied above, when $T \to 0$ the Fermi-Dirac distribution function in (8) and (10) is a stepfunction and the sum over k'' gives the logarithms of (9) and (11). Otherwise, at finite T, the summation over k'' gives numerically a sort of smoothed-out logarithm, the smoothing taking place in an interval of length $2\,T$ around the value of the energy for which the argument of the logarithm is zero. Equation (8) and (10) are sufficient to compute the resistivity of a paramagnet.

In the absence of spontaneous magnetization, as remarked above, the distribution function f_k of charge carriers with spin up is equal to the distribution of charge carriers with spin down. The relaxation times for the two types of electrons are equal. The calculation of the resistivity can be copied from van Peski-Tinbergen and Dekker [4]. The change in the distribution function as a consequence of collisions is [4]:

$$\left.\frac{\partial f_k}{\partial t}\right]_{\text{coll}} = \sum_{k'} \{- W(\boldsymbol{k}\uparrow \to \boldsymbol{k}'\uparrow)\, f_k (1 - f_{k'}) + W(\boldsymbol{k}'\uparrow \to \boldsymbol{k}\uparrow)\, f_{k'} (1 - f_k) - {}$$
$$- W(\boldsymbol{k}\uparrow \to \boldsymbol{k}'\downarrow)\, f_k (1 - f_{k'}) + W(\boldsymbol{k}'\uparrow \to \boldsymbol{k}\downarrow)\, f_{k'} (1 - f_k)\} \,. \tag{12}$$

By considering the principle of detailed balance in the absence of electric fields, and by introducing the deviation g_k from the equilibrium distribution function f_k^0 caused by the electric field F_x one obtains the following:

$$\left.\frac{\partial f_k}{\partial t}\right]_{\text{coll}} = -\frac{g_k}{\tau_k} = -g_k \sum_{k'} \left[1 - f_k^0 \left(1 - \exp\left[\frac{E_k - E_{k'}}{k_B T}\right]\right)\right]^{-1} \times$$
$$\times \left(1 - \frac{k'_x}{k_x}\right) [W(\boldsymbol{k}\uparrow \to \boldsymbol{k}'\uparrow) + W(\boldsymbol{k}\uparrow \to \boldsymbol{k}'\downarrow)] \,. \tag{13}$$

The deduction of (13) from (12) can be followed in detail in the reference cited above. When one substitutes the transition probabilities obtained above in (13) the desired expression for the relaxation time in the case of isotropic scattering is:

$$\frac{1}{\tau_k} = \frac{1}{\tau_k^{(1)}} + \frac{1}{\tau_k^{(2)}},$$

$$\frac{1}{\tau_k^{(1)}} = \left(\frac{2\pi}{\hbar}\right)\left(\frac{J}{N}\right)^2 N\, n(E_F) \left[\sum_m \exp\left(-\frac{E_m}{k_B T}\right)\right]^{-1} \times$$
$$\times \left\{\sum_{m\,m'} \left[(1 - f_k^0) \exp\left(\frac{E_m}{k_B T}\right) + f_k^0 \exp\left(\frac{E_{m'}}{k_B T}\right)\right]^{-1} \times\right.$$
$$\left.\times \left[|\langle E_{m'}|\, S_z\, |E_m\rangle|^2 + |\langle E_{m'}|\, S_+\, |E_m\rangle|^2\right]\right\},$$

$$\frac{1}{\tau_k^{(2)}} = \left(\frac{2\pi}{\hbar}\right)\left(-\frac{J}{N}\right)^3 N\, n^2(E_F) \left[\sum_m \exp\left(-\frac{E_m}{k_B T}\right)\right]^{-1} \times$$
$$\times \left\{\sum_{m\,m'\,m''} \left[(1 - f_k^0) \exp\left(\frac{E_m}{k_B T}\right) + f_k^0 \exp\left(\frac{E_{m'}}{k_B T}\right)\right]^{-1} \times\right.$$
$$\times \left[\left(\int_{-E_1}^{E_1} \mathrm{d}E_{k''}\, (1 - f_{k''})\, (E_k - E_{k''} + E_m - E_{m''})^{-1}\right) \langle E_m|\, S_z\, |E_{m'}\rangle \times\right.$$
$$\times (\langle E_{m''}|\, S_z\, |E_m\rangle \langle E_{m'}|\, S_z\, |E_{m''}\rangle + \langle E_{m''}|\, S_+\, |E_m\rangle \langle E_{m'}|\, S_-\, |E_{m''}\rangle) -$$
$$- \left(\int_{-E_1}^{E_1} \mathrm{d}E_{k''}\, f_{k''}\, (E_{k''} - E_k + E_{m'} - E_{m''})^{-1}\right) \langle E_m|\, S_z\, |E_{m'}\rangle \times$$

$$\times (\langle E_{m''}|\, S_z\, |E_m\rangle \langle E_{m'}|\, S_z\, |E_{m''}\rangle + \langle E_{m''}|\, S_-\, |E_m\rangle \langle E_{m'}|\, S_+\, |E_{m''}\rangle) +$$

$$+ \left(\int_{-E_1}^{E_1} \mathrm{d}E_{k''}\, (1 - f_{k''})\, (E_k - E_{k''} + E_m - E_{m''})^{-1} + \right.$$

$$\left. + \int_{-E_1}^{E_1} \mathrm{d}E_{k''}\, f_{k''}\, (E_{k''} - E_k + E_{m'} - E_{m''})^{-1} \right) \langle E_m|\, S_-\, |E_{m'}\rangle \times$$

$$\times (\langle E_{m''}|\, S_z\, |E_m\rangle \langle E_{m'}|\, S_+\, |E_{m''}\rangle - \langle E_{m''}|\, S_+\, |E_m\rangle \langle E_{m'}|\, S_z\, |E_{m''}\rangle) \Big]\Big\}. \quad (14)$$

When an expression for the relaxation time is available, the conductivity is obtained by applying

$$\sigma \sim \int \mathrm{d}E_k \tau_k \frac{\partial f_k}{\partial E_k}. \quad (15)$$

The whole calculation presented here is of course non-sensical, like all perturbation calculations, when $1/\tau_k^{(2)} \gg 1/\tau_k^{(1)}$. This is epitomized, as usual, by the fact that, for instance, $1/\tau_k$ can become negative if $J > 0$.

3. Numerical Calculation and Discussion of the Results

In order to obtain numerically the temperature dependence of the resistivity from equation (15), we have to specify in greater detail the properties of the scattering system. We have therefore to refer to a particular intermetallic compound. We have chosen a hexagonal material containing Ce ions as trivalent ions. It is well known that a hexagonal crystal field splits the six degenerate levels of the Ce ion spin into three doublets that are eigenstates of S_z: $|\pm 1/2\rangle$, $|\pm 3/2\rangle$, $|\pm 5/2\rangle$. We have performed the calculation of equation (15) considering the three doublets' energies as parameters. We shall report the results obtained for a few particular choices of these parameters.

The numerical calculations were performed on the Philips Electrologica X8 computer of our laboratory. The computation of equation (15) at finite temperatures requires a double integration, one over E_k appearing explicitly in (15) and one on the energy $E_{k''}$ of the intermediate state. In order to maintain our computing times within reasonable limits, we approximated the integrals on $E_{k''}$ in the following way:

$$\int_{-E_1}^{E_1} \mathrm{d}E_{k''}\, f_{k''}\, (E_{k''} - E_{k'} + E_{m'} - E_{m''})^{-1} = \begin{cases} \ln\left(\dfrac{T}{E_1}\right) & \text{if } |E_{k'} + E_{m'} - E_{m''}| < T, \\ \ln[|(E_{k'} + E_{m'} - E_{m''})\, E_1^{-1}|] & \text{otherwise,} \end{cases} \quad (16)$$

that is, a "chopped" logarithmic function. We have computed the integral (15) exactly and checked that the approximation (16) is justified.

The parameter $(-J/N)\, n(E_F)$ has been given a maximum value of 0.1, which is a limit for the present perturbation theory because the terms $1/\tau_k^{(1)}$ and $1/\tau_k^{(2)}$ are of the same order of magnitude when $(-J/N)\, n(E_F)$ is 0.1. The limits of the band, E_1 and $-E_1$, have been given the absolute value of 10000 °K.

Fig. 1 shows a set of resistivity versus temperature curves. These curves refer to a situation in which the $\pm 5/2$ doublet lies lowest and the $\pm 1/2$ doublet

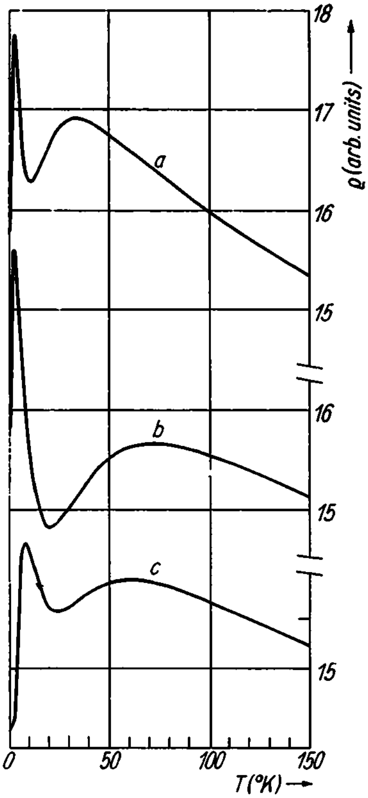

Fig. 1. Resistivity vs. temperature curves computed with the following choice of energy levels: curve a: (0, 5, 50); curve b: (0, 5, 100); curve c: (0, 15, 100). The numbers in brackets express, in degrees Kelvin, the energy of the levels ±5/2, ±3/2, ±1/2, respectively

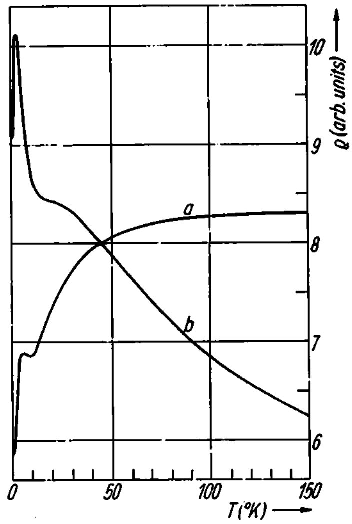

Fig. 2. ϱ vs. T curves obtained by setting, in formula (14), $1/\tau_k = 1/\tau_k^{(1)}$ (curve a) and setting $1/\tau_k = 0.1 \times 1/\tau_k^{(2)}$ (curve b). The choice of energy levels is the same as in curve a of Fig. 1

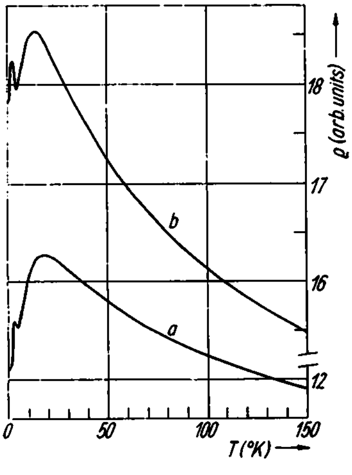

Fig. 3. ϱ vs. T curves computed with the following choice of energy levels (see caption to Fig. 1): (0, 3, 20). The parameter $(-J/N)\, n(E_F)$ has been set equal to 0.05 for curve a and equal to 0.1 for curve b

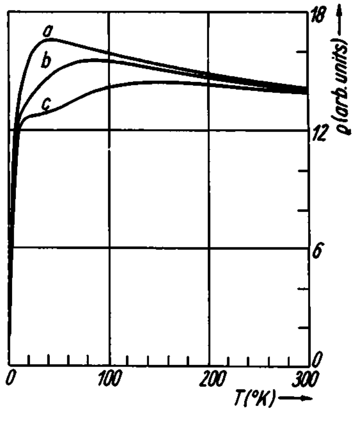

Fig. 4. ϱ vs. T curves computed with the following choice of energy levels (see caption to Fig. 1): curve a: (5, 0, 50); curve b: (5, 0, 100); curve c: (5, 0, 200)

lies highest. The energies of these doublets chosen for the different curves are given in the caption of Fig. 1. In each curve we see two maxima, whose position changes when the value of the doublets' energy levels is changed. We have plotted in Fig. 2 the resistivity versus temperature curves that are obtained from first order processes only (setting $1/\tau_k^{(2)} = 0$) and from second order processes only (setting $1/\tau_k^{(1)} = 0$). From Fig. 2b we observe that the maxima in Fig. 1 are a consequence of the existence of Kondo side-bands in the energy dependence of the relaxation time. Moreover the Kondo side-band effects are amplified by a first order effect which is visible in Fig. 2a in the form of a maximum at the place of the first Kondo side-band. This first-order effect is peculiar to the situation in which the $\pm 5/2$ doublet is lowest and it appears only for certain choices of the doublets energy levels. It follows probably from a competing effect of elastic and inelastic first order processes.

Fig. 3 gives an idea of the change of the resistivity behaviour as a function of temperature when the parameter $(-J/N)\,n(E_F)$ is changed. We observe that by proper adjustment of this parameter the relative height of the two resistivity maxima can be modified within a certain range of values. It has to be noted that in this figure our arbitrary units scale of the ϱ-axis is not the same one for case a) and case b). This follows obviously from the fact that the normalization factor $(J^2/N)\,n(E_F)$ has been varied in the two curves.

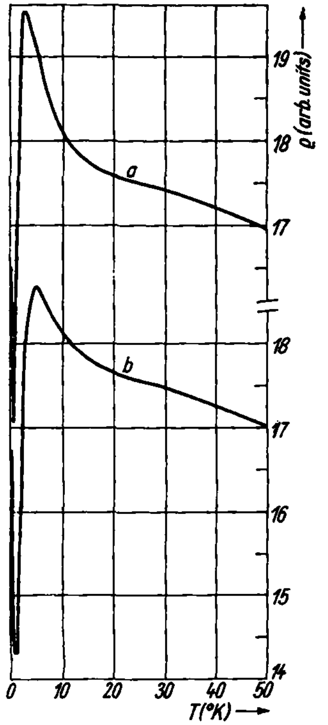

Fig. 5. ϱ vs. T curves computed with the following choice of energy levels (see caption to Fig. 1): curve a: (50, 3, 0); curve b: (50, 5, 0)

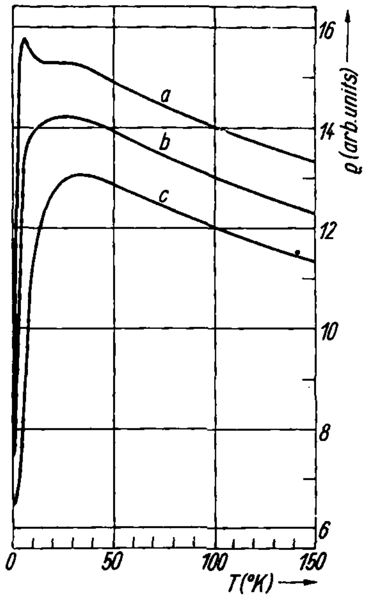

Fig. 6. ϱ vs. T curves computed with the following choice of energy levels (see caption to Fig. 1): curve a: (50, 0, 3); curve b: (50, 0, 5); curve c: (50, 0, 10)

Fig. 4, 5, and 6 give resistivity versus temperature curves relative to other choices of the order in which the doublets appear on the energy scale. We see here again that the position of the resistivity maxima is correlated to the position of the Kondo side-bands. In certain cases, (see for instance Fig. 6) we observe that the maxima overlap each other to form one broad maximum. This process takes place when the relative position of the doublets on the energy scale is varied continuously.

In Fig. 5 we notice that the well-known Kondo divergence at $T = 0$ reappears when the $\pm 1/2$ doublet lies lowest. This is quite obvious: spin-flip scattering can take place within the doublet, i.e. without energy expenditure, so that the typical Kondo central band is present at $E = 0$.

In conclusion it appears that the Kondo side-band model allows sufficient freedom to obtain quite different types of resistivity versus temperature behaviour. Experimental results of resistivity measurements on intermetallic compounds containing cerium are available, and a comparison between this theory and the existing evidence will be made in the near future.

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