# Kondo effect in dilute Y-Ce alloys[*]

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The influence of the hexagonal crystal field on the magnetic susceptibility and electrical resistivity of the Kondo system Y-Ce is studied in the framework of the $s$-$f$ exchange model. The second-order-perturbation-theory magnetic susceptibility is computed exactly in the whole range of temperatures and the results of the calculation are compared with the available experimental data. From the theoretical behavior of the magnetic susceptibility the general conclusion that no "Kondo sidebands" are present in the susceptibility-vs-$T$ curve is inferred. The third-order-perturbation-theory resistivity is computed exactly within the "usual" $f_k = 1/2$ approximation and a Kondo temperature of 1.4 K is estimated.

## I. INTRODUCTION

It is now well established that dilute Y-Ce alloys exhibit anomalous low-temperature properties[1-3] analogous to the Kondo effect of dilute alloys of noble metals with transition-metal impurities. Recently, Sugawara and Yoshida[3] carried out a detailed experimental study of the magnetic susceptibility and electrical resistivity of dilute Y-Ce alloys using single crystals. These results were interpreted in terms of the crystal-field splitting of the $^2F_{5/2}$ state of the cerium ion and the Kondo effect. However, owing to the lack of an adequate theory for the crystal-field effects in dilute Kondo systems, their phenomenological treatment was necessarily insufficient to give a reliable account for the whole matter. On the other hand, a considerable amount of theoretical work has been recently accomplished by several authors[4-9] in order to elucidate the role of the crystal field in explaining some properties of alloys and compounds with cerium impurities. This subject was first discussed by Maranzana[4] and by Maranzana and Bianchessi,[5] who, taking crystal-field splitting into account, showed the presence of sidebands in the resistivity versus temperature curve of a Kondo system.

More recently, a complete analysis of the crystal-field effects on the resistivity of cerium alloys and compounds has been made by Cornut and Coqblin,[6] using the Schrieffer-Wolff transformation in the framework of the Anderson model, and by the present authors using the usual $s$-$f$-exchange Hamiltonian.[7,8]

As far as the crystal-field effects on the magnetic susceptibility of a Kondo system are concerned, a theoretical treatment was given in a recent paper by the present authors.[9] The case of a cerium ion in a cubic crystal field was examined and the theoretical results were compared with the experimental data on the La-Ce system. Owing to the difficulty of the algebraic calculation, only diver-

gent $\ln(k_B T)$ terms were taken into account and the other terms were neglected under the assumption that they are of some relevance only at relatively high temperatures, where the entire (second-order) exchange contribution was reasonably estimated to be negligible with respect to the zero-order one.

However, in this way, the possible existence of anomalous features, e.g., Kondo sidebands, in the magnetic susceptibility curve was completely ignored. This being the present state of the matter, an exact calculation of the crystal-field effects on the magnetic susceptibility of the Y-Ce dilute alloy would account for the experimental data[3] and, at the same time, provide useful information on the general theoretical behavior of the magnetic susceptibility in rare-earth Kondo systems.

In the Y-Ce alloy, the hexagonal crystal field splits the $^2F_{5/2}$ ground state of the cerium ion into three doublets which are eigenstates of $J_z$ (the component of the angular momentum parallel to the $c$ axis of the crystal). Due to this favorable feature, the algebraic calculation of the magnetic susceptibility in the direction parallel to the $c$ axis is more tractable than the calculation for a cubic crystal field. Here we present the theoretical calculation of the magnetic susceptibility (in the $z$ direction) for the Y-Ce system.

The crystal-field effects are taken into account with no approximation in the whole range of temperatures. Moreover, we evaluate the exchange resistivity for the Y-Ce dilute alloy; for simplicity the usual $f_k = \frac{1}{2}$ approximation will be used. The exchange resistivity evaluated in this manner is accurate in the whole range of temperatures except for $T$ close to the values of the crystal-field splitting.[6]

The theoretical results on the magnetic susceptibility are then compared with the available experimental data,[3] and the exchange-resistivity expression is used to estimate the Kondo temperature $T_K$. Finally we wish to point out that, even if this

work is mainly devoted to the Y-Ce system, the theoretical results we obtain are clearly suitable to the general case of a cerium impurity in an hexagonal crystal field.

The calculation of the magnetic susceptibility is carried out in Sec. II. Section III reports on the results for the exchange resistivity. Section IV is devoted to a comparison with experiments and concluding remarks.

## II. CALCULATION OF THE MAGNETIC SUSCEPTIBILITY

As reported in Ref. 9, the magnetic susceptibility (in the $z$ direction), assuming the $g$ value of the conduction electrons is zero, is calculated with the formula[10]

$$\chi_{\parallel} = (g\mu_B)^2 \int_0^\beta d\lambda \langle e^{\lambda H} J_z e^{-\lambda H} J_z \rangle . \quad (2.1)$$

Here the Hamiltonian $H$ is given by

$$H = H_{fe} + H_{cf} + H_{sf} ,$$

where $H_{fe}$ is the free-electron Hamiltonian, $H_{sf}$ is the exchange interaction, which is conventionally written as $H_{sf} = -\Gamma \vec{J} \cdot \vec{S}$, and $H_{cf}$ is the hexagonal-crystal-field Hamiltonian which is diagonal with respect to the eigenstates of $J_z$ (see Ref. 3 for further details).

In Eq. (2.1), $\beta = 1/k_B T$ and

$$\langle O \rangle \equiv \mathrm{Tr}(Oe^{-\beta H})/\mathrm{Tr}(e^{-\beta H}) . \quad (2.2)$$

By expanding the ordered exponentials in Eq. (2.1) up to second order in $\Gamma$ and by rearranging various terms, the lowest-order term which we obtain is

$$\chi^{(0)} = (g\mu_B)^2 \int_0^\beta d\lambda \langle J_z J_z \rangle_0 , \quad (2.3)$$

where $\langle \rangle_0$ denotes a thermal average in absence of the $s$-$f$ interaction.

The next nonvanishing terms which are second order in $\Gamma$ are

$$\chi_A^{(2)} = (g\mu_B)^2 \int_0^\beta d\lambda \int_0^\lambda du_1 \int_\lambda^\beta du_2$$
$$\times \langle H_{sf}(u_2)[J_z, H_{sf}(u_1)] J_z \rangle_0 , \quad (2.4)$$

$$\chi_C^{(2)} = (g\mu_B)^2 \int_0^\beta d\lambda \int_0^\beta du_1 \int_0^{u_1} du_2$$
$$\times \langle H_{sf}(u_1) H_{sf}(u_2) J_z J_z \rangle_0 , \quad (2.5)$$

$$\chi_D^{(2)} = -(g\mu_B)^2 \int_0^\beta d\lambda \langle J_z J_z \rangle_0 \int_0^\beta du_1 \int_0^{u_1} du_2$$
$$\times \langle H_{sf}(u_1) H_{sf}(u_2) \rangle_0 , \quad (2.6)$$

where $H_{sf}(u) = e^{uH_0} H_{sf} e^{-uH_0}$ and $H_0 = H_{fe} + H_{cf}$. Owing to the commutativity between $H_{cf}$ and $J_z$ the term $\chi_B^{(2)}$ of Ref. 9 does not contribute to $\chi^{(2)}$.

We would note that the calculation of $\chi_\perp$ (the magnetic susceptibility perpendicular to the $c$ axis of the crystal) should require the substitution of $J_z$ by
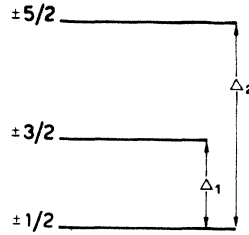
$J_x$ ($J_y$) in Eq. (2.1). Even if, in this case, an exact calculation could be still possible in principle, a much larger amount of algebraical work would be required owing to the noncommutativity between $H_{cf}$ and $J_x$ ($J_y$). Now we want to evaluate these various contributions for the Y-Ce system.

Since the spin-orbit coupling is strong in cerium, the ground state $^2F_{5/2}$ and the next excited state $^2F_{7/2}$ are very distant in energy (about 2200 cm$^{-1}$). For this reason one can assume $J^2 = $ const. at ordinary temperature, and limit oneself to the subspace with $J = \frac{5}{2}$.

In an hexagonal crystal field the six degenerate states of cerium are split into three doublets with $J_z = \pm \frac{1}{2}; \pm \frac{3}{2}; \pm \frac{5}{2}$. A point-charge calculation gives for the energy-level diagram the result reported on Fig. 1 where, following the theoretical treatment by Kasuya,[11] $\Delta_1$ and $\Delta_2$ are easily evaluated in terms of the effective charge number $Z'$ of the Y ions as[3] (in degrees Kelvin)

$$\Delta_1 = 106(\tfrac{1}{3}Z') \text{ and } \Delta_2 = 247(\tfrac{1}{3}Z') .$$

However, these values are not completely reliable since they are based upon a point-charge calculation. An exact calculation should also take covalency effects into account and, consequently, could alter this level scheme in a substantial way. For this reason, in the following we shall take $\Delta_1$ and $\Delta_2$ as disposable parameters. On the other hand, we assume the $J_z = \pm \frac{1}{2}$ doublet to be the ground state, as this is confirmed by the experimental results.[3]

The zero-order term $\chi^{(0)}$ simply gives the crystal-field contribution as obtained by Sugawara and Yoshida[3]:

$$\chi^{(0)} = \frac{C}{T} \frac{3}{35} \frac{1 + 9e^{-\beta\Delta_1} + 25e^{-\beta\Delta_2}}{1 + e^{-\beta\Delta_1} + e^{-\beta\Delta_2}} , \quad (2.7)$$

where $C = (g\mu_B)^2 J(J+1)/3k_B$ is the Curie constant for one cerium ion per volume unit, $g = \frac{6}{7}$, and $J = \frac{5}{2}$. Now we introduce $e^{\beta\epsilon_k} = (1 - f_k)/f_k$, where $f_k$ is the Fermi function. From Eq. (2.4) we obtain after some algebraic calculations in which the position of the dummy variables have been rearranged:

$$\chi_A^{(2)} = (g\mu_B)^2 \Gamma^2 (1 + e^{-\beta\Delta_1} + e^{-\beta\Delta_2})^{-1} \sum_{k,k'} f_k (1 - f_{k'}) \left[ -9 \left( \frac{\beta}{(\epsilon_k - \epsilon_{k'})^2} + \frac{2}{(\epsilon_k - \epsilon_{k'})^3} \right) - 8 \left( \frac{\beta}{(\epsilon_k - \epsilon_{k'} - \Delta_1)^2} \right. \right.$$

$$+ \frac{2}{(\epsilon_k - \epsilon_{k'} - \Delta_1)^3}\Big) - 8e^{-\beta\Delta_1}\Big(\frac{\beta}{(\epsilon_k - \epsilon_{k'} + \Delta_1)^2} + \frac{2}{(\epsilon_k - \epsilon_{k'} + \Delta_1)^3}\Big) - 5e^{-\beta\Delta_1}\Big(\frac{\beta}{(\epsilon_k - \epsilon_{k'} + \Delta_1 - \Delta_2)^2}$$

$$+ \frac{2}{(\epsilon_k - \epsilon_{k'} + \Delta_1 - \Delta_2)^3}\Big) - 5e^{-\beta\Delta_2}\Big(\frac{\beta}{(\epsilon_k - \epsilon_{k'} + \Delta_2 - \Delta_1)^2} + \frac{2}{(\epsilon_k - \epsilon_{k'} + \Delta_2 - \Delta_1)^3}\Big)\Big] . \tag{2.8}$$

In a similar way we obtain from Eqs. (2.5) and (2.6),

$$\chi_C^{(2)} + \chi_D^{(2)} = (g\mu_B)^2 \Gamma^2 (1 + e^{-\beta\Delta_1} + e^{-\beta\Delta_2})^{-2}\beta \sum_{k,k'} f_k(1 - f_{k'})\Big((10e^{-\beta\Delta_1} - 18e^{-\beta\Delta_2} - 32e^{-\beta(\Delta_1+\Delta_2)})\frac{\beta}{\epsilon_k - \epsilon_{k'}}$$

$$+ 16(e^{-\beta\Delta_1} + 3e^{-\beta\Delta_2})\frac{\beta}{\epsilon_k - \epsilon_{k'} - \Delta_1} + 16(2e^{-\beta(\Delta_1+\Delta_2)} - e^{-\beta\Delta_1})\frac{\beta}{(\epsilon_k - \epsilon_{k'} + \Delta_1)} + 16(1 + e^{-\beta\Delta_1} + e^{-\beta\Delta_2})$$

$$\times\frac{1}{(\epsilon_k - \epsilon_{k'} - \Delta_1)^2} - 16(1 + e^{-\beta\Delta_1} + e^{-\beta\Delta_2})\frac{e^{-\beta\Delta_1}}{(\epsilon_k - \epsilon_{k'} + \Delta_1)^2} + 10(2e^{-\beta(\Delta_1+\Delta_2)} - e^{-\beta\Delta_1})\frac{\beta}{\epsilon_k - \epsilon_{k'} + \Delta_1 - \Delta_2}$$

$$- 10(3e^{-\beta\Delta_2} + 2e^{-\beta(\Delta_1+\Delta_2)})\frac{\beta}{\epsilon_k - \epsilon_{k'} + \Delta_2 - \Delta_1} + 20e^{-\beta\Delta_1}(1 + e^{-\beta\Delta_1} + e^{-\beta\Delta_2})\frac{1}{(\epsilon_k - \epsilon_{k'} + \Delta_1 - \Delta_2)^2}$$

$$- 20e^{-\beta\Delta_2}(1 + e^{-\beta\Delta_1} + e^{-\beta\Delta_2})\frac{1}{(\epsilon_k - \epsilon_{k'} + \Delta_2 - \Delta_1)^2}\Big) . \tag{2.9}$$

The evaluation of $\chi^{(2)}$ depends on the three functions

$$S_1(\Delta) = \sum_{k,k'} \frac{f_k(1 - f_{k'})}{(\epsilon_k - \epsilon_{k'} + \Delta)^2} , \tag{2.10}$$

$$S_2(\Delta) = \sum_{k,k'} \frac{f_k(1 - f_{k'})}{\epsilon_k - \epsilon_{k'} + \Delta}$$

$$\equiv S_2(0) - \int_0^\Delta d\Delta' S_1(\Delta') , \tag{2.11}$$

$$S_3(\Delta) = \sum_{k,k'} \frac{f_k(1 - f_{k'})}{(\epsilon_k - \epsilon_{k'} + \Delta)^3}$$

$$\equiv -\frac{1}{2}\frac{\partial S_1(\Delta')}{\partial(\Delta')}\Big|_{\Delta'=\Delta} . \tag{2.12}$$

By assuming the charge carriers to reside in a band extending from $-D$ to $D$ with a constant density of states $n(E_F)$, where the Fermi level $E_F$ has been chosen as the zero of energy, we obtain

$$S_1(\Delta) \equiv -n^2(E_F)J_1(\Delta)$$

$$= -n^2(E_F)\Big[I_1\Big(\frac{\Delta}{k_BT}\Big) + \ln\Big|\frac{2k_BT(2D - \Delta)}{(D - \Delta)^2}\Big|\Big] , \tag{2.13}$$

where

$$I_1\Big(\frac{\Delta}{k_BT}\Big) = \int\int \frac{\partial f_k}{\partial\epsilon_k}\frac{\partial f_{k'}}{\partial\epsilon_{k'}}\ln\Big|\frac{\epsilon_k - \epsilon_{k'} + \Delta}{2k_BT}\Big| d\epsilon_k d\epsilon_{k'}$$

has been previously computed. [12] The functions $S_2(\Delta)$ and $S_3(\Delta)$ are then easily evaluated as

$$S_2(\Delta) - S_2(0) \equiv \frac{n^2(E_F)}{\beta} J_2(\Delta)$$

$$= \frac{n^2(E_F)}{\beta}\Big[I_2\Big(\frac{\Delta}{k_BT}\Big)$$

$$+ \frac{\Delta}{k_BT}\Big(1 + \ln\Big|\frac{2k_BT(2D - \Delta)}{(D - \Delta)^2}\Big|\Big)$$

$$- \frac{2D}{k_BT}\ln\Big|\frac{2D - \Delta}{2(D - \Delta)}\Big|\Big] , \tag{2.14}$$

$$S_3(\Delta) \equiv \frac{1}{2}n^2(E_F)\beta J_3(\Delta) = \frac{n^2(E_F)}{2}\beta\Big[I_3\Big(\frac{\Delta}{k_BT}\Big)$$

$$+ k_BT\frac{3D - \Delta}{(2D - \Delta)(D - \Delta)}\Big] , \tag{2.15}$$

where

$$I_2(\alpha) = \int_0^\alpha d\alpha' I_1(\alpha') , \quad I_3(\alpha) = \frac{\partial I_1(\alpha')}{\partial\alpha'}\Big|_{\alpha'=\alpha} ,$$

and $\alpha = \Delta/k_BT$.

As far as the term $S_2(0)$ is concerned, a simple calculation gives $S_2(0) = -n^2(E_F)D\ln4$. However, as is easily seen from Eq. (2.9), this constant term does not give any contribution to $\chi^{(2)}$, therefore it will be ignored in the following.

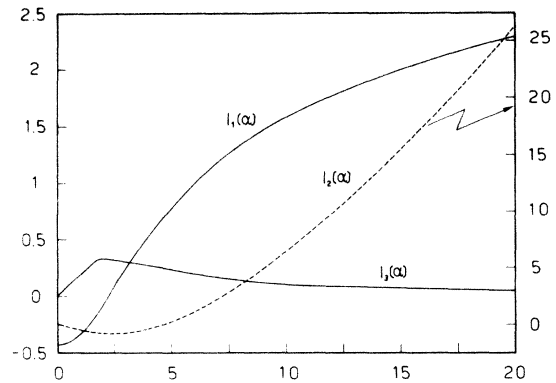The functions $I_1$, $I_2$, $I_3$ are plotted in Fig. 2 for positive values of the argument $\alpha$. For negative

FIG. 2. Functions $I_1(\alpha)$, $I_2(\alpha)$, and $I_3(\alpha)$, where $\alpha = \Delta/k_BT$.

values of the argument, it is easily seen that
$I_1(-\alpha) = I_1(\alpha)$, $I_2(-\alpha) = -I_2(\alpha)$, $I_3(-\alpha) = -I_3(\alpha)$. For completeness here we report the values of the functions $J_1$, $J_2$, $J_3$ for the zero value of the argument. We have

$$J_1(0) = -0.432 + \ln|4k_BT/D| = \ln|2.62 k_BT/D| \ ,$$

$$J_2(0) = 0 \ ,$$

$$J_3(0) = 3k_BT/2D \ .$$

$J_3(0)$ is usually negligible since $k_BT \ll D$ at ordinary temperature. In terms of the $J_1$, $J_2$, $J_3$ functions we obtain after some straightforward calculations

$$\chi_A^{(2)} = \frac{C}{T}[2n(E_F)\Gamma]^2 \varphi_1(T) \ , \tag{2.16}$$

where

$$\varphi_1(T) = \tfrac{3}{35}(1 + e^{-\beta\Delta_1} + e^{-\beta\Delta_2})^{-1}\{9[J_1(0) - J_3(0)] + 8[J_1(-\Delta_1) - J_3(-\Delta_1)] + 8e^{-\beta\Delta_1}[J_1(\Delta_1) - J_3(\Delta_1)] + 5e^{-\beta\Delta_1}[J_1(\Delta_1 - \Delta_2)$$
$$- J_3(\Delta_1 - \Delta_2)] + 5e^{-\beta\Delta_2}[J_1(\Delta_2 - \Delta_1) - J_3(\Delta_2 - \Delta_1)]\} \tag{2.17}$$

and

$$\chi_C^{(2)} + \chi_D^{(2)} = \frac{C}{T}[2n(E_F)\Gamma]^2 \varphi_2(T) \ , \tag{2.18}$$

where

$$\varphi_2(T) = \tfrac{6}{35}(1 + e^{-\beta\Delta_1} + e^{-\beta\Delta_2})^{-2}\{(e^{-\beta\Delta_1} + 3e^{-\beta\Delta_2})[8J_2(-\Delta_1) - 5J_2(\Delta_2 - \Delta_1)] + e^{-\beta\Delta_1}(2e^{-\beta\Delta_2} - 1)[8J_2(\Delta_1) + 5J_2(\Delta_1 - \Delta_2)$$
$$- 5J_2(\Delta_2 - \Delta_1)] + 2(1 + e^{-\beta\Delta_1} + e^{-\beta\Delta_2})[-4J_1(-\Delta_1) + 4e^{-\beta\Delta_1}J_1(\Delta_1) - 5e^{-\beta\Delta_1}J_1(\Delta_1 - \Delta_2) + 5e^{-\beta\Delta_2}J_1(\Delta_2 - \Delta_1)]\} \ . \tag{2.19}$$

It is easily seen from Eqs. (2.16)–(2.19) that the correct limit is obtained in the absence of the crystal field as $\varphi_1(T)$ goes to $\ln(2.62\,k_BT/D)$ (apart from a term of order $k_BT/D$ which is usually neglected), and $\varphi_2(T)$ goes to zero.

In the opposite limit at low temperatures ($\beta\Delta_1$, $\beta\Delta_2 \to \infty$), we obtain

$$\varphi_1(T) + \varphi_2(T)$$

$$\approx \tfrac{3}{35}[9\ln(2.62\,k_BT/D) - 8\ln(2\Delta_1/D)] \ , \quad T \to 0 \ ;$$

so that the logarithmic divergent term is clearly predominant in the low-temperature region.

### III. CALCULATION OF THE RESISTIVITY

Now we present the calculation of the resistivity for a cerium ion in an hexagonal crystal field inside the third-order approximation. Numerical calculations on this subject have been already carried out by Maranzana and Bianchessi[5] and by van Daal et al.[13] in the framework of the s-f exchange coupling and by Cornut and Coqblin[6] in the framework of the Anderson model. Since in the present paper we are mainly interested in obtaining an analytical expression for the Kondo temperature $T_K$, we will evaluate the exchange resistivity using the usual $f_k = \tfrac{1}{2}$ approximation. We do this since this restriction does not alter in a substantial way the conclusions of the work and, at the same time, allows for a great simplification of the calculations.

The results, which we will obtain, can be considered as reliable in the whole range of temperatures except for $T$ close to the values of the crystal-field splitting.[6] The relaxation time $\tau_k$ is given up to third order in $\Gamma$ by

$$1/\tau_k = 1/\tau_k^{(1)} + 1/\tau_k^{(2)} \ , \tag{3.1}$$

where $1/\tau_k^{(1)}$ and $1/\tau_k^{(2)}$ are the reciprocal relaxation times proportional to $\Gamma^2$ and $\Gamma^3$, respectively. Expressions of $1/\tau_k^{(1)}$ and $1/\tau_k^{(2)}$ have been reported by several authors.[5–8] Inside the $f_k = \tfrac{1}{2}$ approximation the term $1/\tau_k^{(1)}$ is independent of the electron wave vector $k$, so that the correct expression of the magnetic resistivity is given by

$$\rho = \rho_0 \left[1 + \tau^{(1)}\int_{-D}^{D}\left(-\frac{\partial f_k}{\partial\epsilon_k}\right)\frac{1}{\tau_k^{(2)}}\,d\epsilon_k\right] \ , \tag{3.2}$$

where $\rho_0 = (m/ne^2)(1/\tau^{(1)})$ is the spin-disorder resistivity. The evaluation of the resistivity $\rho$ depends on the calculation of the typical integral

$$F(\Delta) = \int_{-D}^{D}\left(-\frac{\partial f_k}{\partial\epsilon_k}\right)d\epsilon_k$$
$$\times \int_{-D}^{D}f_{k'}\frac{1}{\epsilon_{k'} - \epsilon_k + \Delta}\,d\epsilon_{k'} \ . \tag{3.3}$$

When $D$ is sufficiently large compared to $\Delta$ and $k_BT$, as it is in the present case, the integral can be easily evaluated as

$$F(\Delta) = F(-\Delta) = \ln(2\,k_BT/D) + I_1(\Delta/k_BT) \ , \tag{3.4}$$

where the $I_1(\Delta/k_BT)$ function has been previously reported. Then, after some algebraical calculations, we obtain

$$\rho = \rho_0(T)[1 + 4n(E_F)\Gamma\,\Psi(T)] \ , \tag{3.5}$$

where the spin-disordered resistivity is given by

$$\rho_0(T) = \frac{2\pi}{\hbar}\frac{m}{ne^2}n(E_F)\Gamma^2 J(J+1)$$
$$\times(1 + e^{-\beta\Delta_1} + e^{-\beta\Delta_2})^{-1}\frac{R(T)}{35} \ , \tag{3.6}$$

where
$$R(T) = 19 + 9e^{-\beta\Delta_1} + 25e^{-\beta\Delta_2} + 64(1 + e^{\beta\Delta_1})^{-1}$$
$$+ 40(e^{\beta\Delta_1} + e^{\beta\Delta_2})^{-1} \quad . \quad (3.7)$$

In presence of the crystal-field splitting $\Psi(T)$ replaces the Kondo divergent term $\ln k_B T/D$. We obtain

$$\Psi(T) = [R(T)]^{-1}\{[27 + 32(1 + e^{\beta\Delta_1})^{-1} + 20(e^{\beta\Delta_1} + e^{\beta\Delta_2})^{-1}]F(0) + [24e^{-\beta\Delta_1} + 32(1 + e^{\beta\Delta_1})^{-1} - 8]F(\Delta_1)$$

$$+ [25e^{-\beta\Delta_2} + 20(e^{\beta\Delta_1} + e^{\beta\Delta_2})^{-1} - 15e^{-\beta\Delta_1}]F(\Delta_2 - \Delta_1)\} \quad . \quad\quad (3.8)$$

It is easily seen that the correct limits are obtained for $\Delta_1, \Delta_2 \to 0$. The Kondo temperature $T_K$ is obtained, as usual, by writing that the third-order term of $\rho$ is two times the second-order term $\rho_0$. So $T_K$ is given by the equation

$$2n(E_F)\Gamma\Psi(T_K) = 1 \quad . \quad\quad (3.9)$$

## IV. COMPARISON WITH EXPERIMENTS AND CONCLUDING REMARKS

The observed solute susceptibility per g of alloy per at.% Ce has been reported by Sugawara and Yoshida.[3] Here we try to compare these experimental data with the theoretical evaluated susceptibility which is given by the Eqs. (2.7), (2.16), and (2.18). Of the four disposable parameters $\Delta_1, \Delta_2, D, |n(E_F)\Gamma|$, which appear in the expression of the magnetic susceptibility, the half-bandwidth $D$ does not greatly affect the physical results. We assume $D$ to be in a range typical of the rare-earth alloys[6-8]: $D = 600$–$1000$ K. As far as the other parameters are concerned we note that, as a general trend, the value of $|n(E_F)\Gamma|$ influences the magnitude of the susceptibility mainly in the low-temperature region ($T \lesssim 20$ K). On the other hand, the influence of the crystal-field splittings $\Delta_1$ and $\Delta_2$ is appreciable at relatively higher temperatures.

Allowing for a variation of $\Delta_1$ and $\Delta_2$ in a broad range of temperatures (from 30 to 300 K) and assuming $|n(E_F)\Gamma|$ in the region of typical values (from 0.05 to 0.10), we first obtain a rough fit to the experimental high-temperature values ($T > 50$ K) for $\Delta_1 = 80$–$90$ K and $\Delta_2 = 230$–$250$ K. The best fit to the experimental data, in the whole temperature range, is then obtained for the following values of the parameters: $D = 800$ K, $\Delta_1 = 87$ K, $\Delta_2 = 240$ K, $|n(E_F)\Gamma| = 0.065$. We note that the level sequence which we obtain agrees with the point-charge calculation. Also we obtain for the $\Delta_2/\Delta_1$ ratio a value 2.76 which is in a reasonable agreement with the point-charge value 2.33, even if slightly larger. The other hypothetical level diagram, with $\Delta_1 > \Delta_2$, never allows for a good fit to the experimental data. The experimental points and theoretical curve for the reciprocal magnetic susceptibility (in the direction parallel to the $c$ axis of the crystal) are given in Fig. 3.

In order to provide useful information on the general theoretical behavior of the magnetic sus-

ceptibility, Fig. 4 reports on the various terms contributing to the susceptibility.

The zero-order contribution $\chi^{(0)}$ appears to be largely dominant everywhere but in the very-low-temperature range. The second-order contributions $\chi_A^{(2)}$ and $\chi_{C+D}^{(2)}$ are opposite in sign among them and go rapidly to zero as soon as a temperature of few degrees Kelvin is reached.

Even if these features are probably strongly dependent on the magnitude of the $n(E_F)\Gamma$ parameter, it is likely to be generally true that no "Kondo side-bands" are present in the magnetic-susceptibility-vs-$T$ curve.

As far as the exchange resistivity is concerned, we see from Eq. (3.5) it to be isotropic in the whole range of temperatures. This result agrees with the experimental behavior since the observed high-temperature anisotropy of the total Y-Ce resistivity can be attributed to the anisotropy of the phonon resistivity.[3]

Owing to the approximation used in the resistivity calculation, we do not try a comparison with the available experimental data. On the other hand to make a comparison with experiments one must be able to extract the "experimental" magnetic contribution from the total-resistivity data. Even if, as in the case of Y-Ce alloys, the phonon contribution by the host is known, it must be noted that deviations from Matthiessen's rule can make this a difficult task.[14,15] For these reasons we limit our-
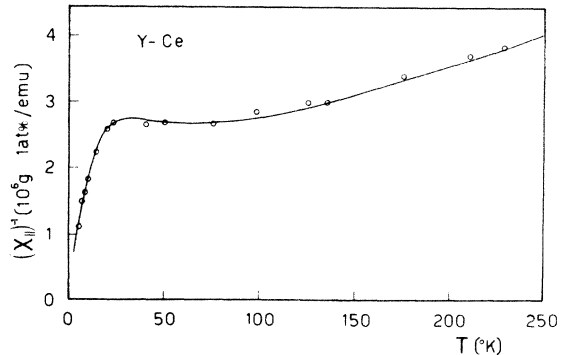


FIG. 3. Temperature variation of the reciprocal solute susceptibility for the direction parallel (H∥c) to the $c$ axis of the crystal. The experimental points are taken from Ref. 3. The continuous curve gives the predictions of the theory.
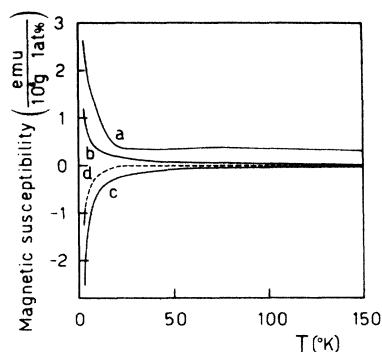
FIG. 4. Contributions to the magnetic susceptibility vs $T$ for the following choice of the parameters: $\Delta_1$ = 87 K, $\Delta_2 = 240$ K, $n(E_F)\Gamma = 0.065$, and $D = 800$ K. (a) Zero-order contribution $\chi^{(0)}$, (b) second-order contribution $\chi_C^{(2)} + \chi_D^{(2)}$, (c) second-order contribution $\chi_A^{(2)}$, and (d) total second-order contribution.

selves to simply give an estimate of the Kondo temperature $T_K$, or the temperature where perturbation theory breaks down.

Inserting the previously determined values of the parameters $\Delta_1$, $\Delta_2$, $n(E_F)\Gamma$, $D$ in Eq. (3.9) we obtain $T_K = 1.4$ K. This value of $T_K$ appears to be somewhat smaller than previously reported values, which were found in the range 4–40 K.[3] However, previous values cannot be considered as completely reliable since they were obtained on a phenomenological basis. As previously noted,[6] the introduction of the crystal-field splitting considerably increases the range of validity of the perturbative approach.

In conclusion, our calculation examines the role played by the crystal field both for resistivity and susceptibility of Y-Ce alloys, explains susceptibility measurements on Y-Ce alloys, and provides useful information on the general theoretical behavior of the magnetic susceptibility in rare-earth Kondo systems. Further theoretical work is required in order to examine the influence of the crystal field on other properties of the Kondo systems.

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