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Anisotropy of the resistivity and susceptibility of Kondo systems

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Previous models for the anisotropy of the resistivity and susceptibility of Kondo systems are based on the Anderson model, which includes a crystal-field term and isotropic mixing. We determine the effects of anisotropic hybridization on the resistivity and susceptibility of Kondo systems and find that there are significant differences between the results of the two models.

I. INTRODUCTION

The primary focus of the theoretical studies of Kondo-type systems has been to understand the crossover from weak to strong coupling. This has largely been achieved on the single-impurity problem and is still an active area of investigations for the lattice problem. Another characteristic of these systems, in particular the cerium Kondo-type compounds, has been their magnetic anisotropy as displayed by interalia, the resistivity and susceptibility, e.g., for $CeAl_3$, $CeCu_6$, and $CeCu_2Si_2$.[1-4] The explanation for the anisotropy of the resistivity is usually based on a combination of a crystalline electric field and the resonant Kondo scattering as first given by Cornut and Coqblin[5] for high temperature, as compared to the Kondo temperature T_K, and more recently further developed by Hanzawa *et al.*[6] for $T \ll T_K$. The ingredient that is missing in previous treatments of the anisotropy of Kondo-type systems is the anisotropy of the conduction-local state mixing interaction. Takahashi and Kasuya proposed anisotropic *p*-*f* mixing to explain the anomalous magnetic properties of the cerium monopnictides;[7] recently we showed that quite aside from the crystalline electric field, the anisotropy of the mixing interaction alone is able to account for the splitting of the *f* levels in cerium Kondo compounds.[8] Also, Schmidt, Ulrich, and Müller-Hartmann have just considered the orbital anisotropy of Kondo ions.[9]

Here we will derive the anisotropic resistivity and susceptibility of Kondo compounds containing cerium that come solely from the mixing interaction. It is natural to anticipate that the resistivity will be anisotropic if the mixing interaction is, because this mixing is the source of scattering, and thereby resistivity, in the Anderson model of Kondo systems. The other major source of anisotropy is the crystalline electric field. As we are unable to reliably estimate this in metallic systems, we will not include it; rather we focus on the anisotropy of the mixing interaction. In the following section we derive the density of states for the local $4f$ electron that is needed to calculate the resistivity and susceptibility. In Sec. III we calculate the resistivity parallel and perpendicular to the principal symmetry axis of a single crystal with tetragonal or hexagonal symmetry, and consider in particular cerium in $LaAl_3$, and in Sec. IV we do the same for the susceptibility. In the concluding section we discuss our results, and compare them with previous theoretical results. We find that the contributions of anisotropic hybridization are significant.

II. MODEL HAMILTONIAN

To describe cerium Kondo systems we use the Anderson model with infinite U (intra-atomic Coulomb energy) and anisotropic mixing,[8]

$$H=\sum_{\mathbf{k}\sigma}\varepsilon_k C^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}+\sum_{i,m}\varepsilon_{fm}f^{i+}_{m}f^{i}_{m}+\frac{1}{\sqrt{N_s}}\sum_{\mathbf{k}im}V_m e^{i\mathbf{k}\cdot\mathbf{R}_i}c^{\dagger}_{\mathbf{k}m}b^{i+}f^{i}_{m}+\text{H.c.}\ , \tag{2.1}$$

where m represents a linear combination of cerium $4f^1|j=\frac{5}{2},m_j\rangle$ states which transform according to the irreducible representations of the point-group symmetry at the sites of the local states. The anisotropy of the mixing parameters V_m is given by its dependence on the index m. This was recently calculated for $CeAl_2$ and $CeAl_3$.[8] The relation between $c^{\dagger}_{\mathbf{k}\sigma}$ and $c^{\dagger}_{\mathbf{k}m}$ is

$$c^{\dagger}_{\mathbf{k}\sigma}=\sqrt{4\pi}\sum_{m,m_j}\langle\sigma|m_j\rangle\langle m_j|m\rangle Y_3^{m_j-\sigma}(\hat{\mathbf{k}})c^{\dagger}_{\mathbf{k}m}\ , \tag{2.2a}$$

where

$$\langle\sigma|m_j\rangle\equiv\langle l=3,s=\tfrac{1}{2},m_l=m_j-\sigma,m_s=\sigma|j=\tfrac{5}{2},m_j\rangle$$

is a Clebsch-Gordan coefficient, and $\langle m_j|m\rangle$ represents the linear combination of $|m_j\rangle$ states in $|m\rangle$. We can also relate $c^{\dagger}_{\mathbf{k}m}$ to $c^{i\dagger}_{km}$ by

$$c^{i\dagger}_{km}=\int d\,\Omega_k e^{i\mathbf{k}\cdot\mathbf{R}_i}c^{\dagger}_{\mathbf{k}m}\ . \tag{2.2b}$$

In our treatment we will neglect the correlation between local states as well as the interference terms coming from scatterings at different sites. Furthermore, we set $\varepsilon_{fm}=\varepsilon_f$ and focus on the splitting coming from the anisotropy of the mixing interaction. From our previous studies,[8] we find this is reasonable as the anisotropy from the mixing interaction is able to account for the $4f$-level splittings observed in Kondo-type systems.

For the Hamiltonian, Eq. (2.1), the fully dressed conduction-electron propagator is

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$$G_{\mathbf{k}\sigma}^{-1}(\varepsilon)=G_{\mathbf{k}\sigma}^{0-1}(\varepsilon)-4\pi c_i \sum_{m_j m'_j m} \langle\sigma|m_j\rangle\langle m_j|m\rangle\langle\sigma|m'_j\rangle\langle m'_j|m\rangle Y_3^{m_j-\sigma *}(\hat{\mathbf{k}})Y_3^{m'_j-\sigma}(\hat{\mathbf{k}})V_m^2 G_{fm}(\varepsilon)\ , \tag{2.3}$$

where $G_{fm}(\varepsilon)$ is the local $4f$ propagator for the state $|m\rangle$, and $c_i=N_i/N_s$ is the concentration of the Kondo ions. The spectral function $\rho_{fm}(\varepsilon)$ is approximately calculated by $1/N$ expansion methods.[10] To order $1/N$, we can write it as a sum of spin (Kondo) and charge resonances

$$\begin{aligned}\rho_{fm}(\varepsilon)&=-\frac{1}{\pi}\mathrm{Im}G_{fm}(\varepsilon)\\ &\approx A_m^s\frac{\Gamma_m^*}{(\varepsilon-\varepsilon_m^*)^2+\Gamma_m^{*2}}+A_m^c\frac{N\Gamma}{(\varepsilon-\tilde{\varepsilon}_f)^2+(N\Gamma)^2}\ ,\end{aligned} \tag{2.4}$$

where $\tilde{\varepsilon}_f\approx\varepsilon_f$, $\varepsilon_m^*\equiv\varepsilon_m-E_0$, and A_m^s, A_m^c are the weights of the spin and charge resonances. Here E_0 is the ground-state energy of the model Hamiltonian, Eq. (2.1),[8]

$$\begin{aligned}E_0&=\varepsilon_f+\min[\Sigma_m(\varepsilon_f)-T_m]\\ &\equiv\varepsilon_f+\Sigma_0(\varepsilon_f)-T_0\ ,\end{aligned} \tag{2.5a}$$

where

$$T_m\approx\frac{De^{-\pi|\varepsilon_m|/N_m\Gamma_m}}{\prod\limits_{m'\neq m}\left|\dfrac{\Sigma_m(\varepsilon_f)-\Sigma_{m'}(\varepsilon_f)-T_m}{D}\right|^{N_{m'}\Gamma_{m'}/N_m\Gamma_m}}\ ,$$

$$\varepsilon_m\equiv\varepsilon_f+\Sigma_m(\varepsilon_f)\ ,$$

$$\Gamma_m\equiv\pi N(0)|V_m|^2\ ,$$

$$\sum_m N_m\Gamma_m\equiv N\Gamma\ ,$$

where $N(0)$ is the single-particle density of states, N_m the degeneracy of the mth level, D the half-width of the conduction band that is taken to be flat, and T_0 the low-temperature Kondo energy scale. It is found by evaluating Eq. (2.5b) for the ground state designated by "0", i.e., $T_0=T_{m=0}$. It is *different* from the $T_0\approx De^{-\pi|\varepsilon_f|/N\Gamma}$ used in Ref. 8, where it represents the Kondo energy scale for an *isotropic* (unsplit) system.

If the $4f$-level splittings are much larger than the Kondo energy scale, i.e., if $\Delta_{m0}\equiv\Sigma_m-\Sigma_0\gg T_0$, $-\varepsilon_f\gg\varepsilon_m^*$, and if the widths Γ_m^* are $O(1/N)$ of ε_m^*, then the *individual* spectral densities ρ_{fm} satisfy the sum rules at $T=0$ K:[10]

$$\int_{-\infty}^{0}d\varepsilon\,\rho_{fm}(\varepsilon)=\pi A_m^c=n_f(0)/N$$

and

$$\int_0^{\infty}d\varepsilon\,\rho_{fm}(\varepsilon)=\pi A_m^s=1-n_f(0)\ . \tag{2.6}$$

By placing these weights in Eq. (2.4) and summing over f levels we find the total spectral density of f states is

$$\begin{aligned}\rho_f=\Sigma_m\rho_{fm}&\approx\frac{1-n_f(0)}{\pi}\sum_m\frac{N_m\Gamma_m^*}{(\varepsilon-\varepsilon_m^*)^2+\Gamma_m^{*2}}\\ &\quad+\frac{n_f(0)}{\pi}\frac{N\Gamma}{(\varepsilon-\varepsilon_f)^2+(N\Gamma)^2}\ ,\end{aligned} \tag{2.7}$$

The valence of the f electron n_f can be calculated from $n_f=-\partial E_0/\partial\varepsilon_f$.[10] For $\varepsilon_{m\neq 0}^*\gg\varepsilon_0^*\equiv T_0$ we find to $O(1)$

$$n_f(0)=\frac{N_0\Gamma_0/\pi T_0}{(1+N_0\Gamma_0/\pi T_0)}\ . \tag{2.8}$$

III. RESISTIVITY

To demonstrate that the anisotropy of the mixing interaction produces anisotropy of the resistivity for Kondo-type compounds we neglect the interaction between Kondo ions and assume the scattering from different sites are *uncorrelated*. Thus our results are only valid for *dilute* systems. In the linear response regime the conductivity is given by the standard formula[12]

$$\sigma_{\mu\nu}=\left[\frac{e\hbar}{m}\right]^2\frac{1}{V}\sum_\sigma\int k_\mu k_\nu\left[-\frac{\partial f(\varepsilon_k)}{\partial\varepsilon_k}\right]\tau_{k\sigma}(\varepsilon_k)d^3k\ , \tag{3.1}$$

where $\tau_{k\sigma}(\varepsilon_k)$ is the relaxation time of conduction electrons,

$$\tau_{k\sigma}^{-1}(\varepsilon_k)=-\frac{2}{\hbar}\mathrm{Im}G_{k\sigma}^{-1}(\varepsilon_k)\ . \tag{3.2}$$

It is important to stress that this is the correct formula for the conductivity of Kondo systems, even in the presence of *inelastic* scattering due to crystal-field splittings.[12] By using Eq. (2.3) we find

$$\begin{aligned}\tau_{k\varepsilon}^{-1}(\varepsilon_k)=\frac{8\pi^2}{\hbar}c_i\sum_{m_j m'_k m}&\langle\sigma|m_j\rangle\langle m_j|m\rangle\langle\sigma|m'_j\rangle\langle m'_j|m\rangle\\ &\times Y_3^{m_j-\sigma *}(\hat{k})\\ &\times Y_3^{m'_j-\sigma}(\hat{k})V_m^2\rho_{fm}(\varepsilon_k)\end{aligned} \tag{3.3}$$

where $\rho_{fm}(\varepsilon)$ is given by Eq. (2.4). In general the integral over energy in Eq. (3.1) is difficult. To facilitate our calculation we limit ourselves to $T=0$ K, where
K, where

$$-\frac{\partial f(\varepsilon_k)}{\partial\varepsilon_k}\bigg|_{T=0\mathrm{K}}=\delta(\varepsilon_k)\ ,$$

and we find

$$\sigma_{\mu\nu}(T=0)=\left[\frac{e\hbar}{m}\right]^2\frac{\hbar N(0)k_f^2}{4\pi V}\sum_\sigma\int\hat{k}_\mu^2 d\Omega_k\left[8\pi^2 c_i\sum_{m_j m}\langle\sigma|m_j\rangle^2\langle m_j|m\rangle^2|Y_l^{m_j-\sigma}(\hat{k})|^2V_m^2\rho_{fm}(0)\right]^{-1}\delta_{\mu\nu}\ . \tag{3.4}$$

The condition $\delta_{\mu\nu}$ is found when integrating over the angle ϕ_k. We find for $\mu \neq \nu$ and $m_j' \neq m_j$ in Eq. (3.3) that $\sigma_{\mu\nu}=0$.

As an example of the effects of anisotropic mixing on the resistivity we consider systems having either tetragonal ($CeCu_2Si_2$) or hexagonal ($CeAl_3$) site symmetry. As our formula for the conductivity is valid only for dilute systems we are thinking about, e.g., cerium in $LaAl_3$. In these systems the ground state of the $4f^1$ electron may be a state that is nearly pure $|\pm m_j\rangle$, where $m_j = \frac{1}{2}, +\frac{3}{2}$, or $\frac{5}{2}$. The conductivities parallel and perpendicular to the symmetry axis of the crystal are

$$\frac{\sigma_{zz}}{\sigma_0} = \lambda_f \int_0^{\pi/2} \frac{24\cos^2\theta \sin\theta \, d\theta}{2\lambda_{1/2}(\sin^4\theta + 4\cos^4\theta) + \lambda_{3/2}\sin^2\theta(1+15\cos^2\theta) + 5\lambda_{5/2}\sin^4\theta}$$

and (3.5)

$$\frac{\sigma_{xx}}{\sigma_0} = \lambda_f \int_0^{\pi/2} \frac{12\sin^3\theta \, d\theta}{2\lambda_{1/2}(\sin^4\theta + 4\cos^4\theta) + \lambda_{3/2}\sin^2\theta(1+15\cos^2\theta) + 5\lambda_{5/2}\sin^4\theta} \, .$$

The isotropic conductivity σ_0 is

$$\sigma_0 = \frac{2\pi N(0) n e^2 \hbar}{m c_i N_f \sin^2\eta_3} \, , \tag{3.6}$$

where η_3 is the phase shift in the $j=\frac{5}{2}$ channel, $\eta_3 = \pi n_f / N_f$,

$$\lambda_{m_j} = N_{m_j} V_{m_j}^2 \rho_{f m_j}(0) \, ,$$

and

$$\lambda_f = N_f V^2 \rho_f(0) \, , \tag{3.7a}$$

where V^2 and $\rho_f(0)$ are the isotropic mixing parameter and $4f$ density of states *per channel,* i.e.,

$$N_f V^2 = \sum_m N_m |V_m|^2 \, . \tag{3.7b}$$

We can parametrize these conductivities as

$$\frac{\sigma_{\mu\mu}}{\sigma_0} = \frac{N_f}{N_g} \frac{\sin^2(\pi n_f / N_f)}{\sin^2(\pi n_f / N_g)} I_\mu \, , \tag{3.8}$$

where

$$I_\mu \equiv \int_0^{\pi/2} \frac{12(\sin^2\theta \delta_{\mu x} + 2\cos^2\theta \delta_{\mu z})\sin\theta \, d\theta}{2\Lambda_{1/2}(\sin^4\theta + 4\cos^4\theta) + \Lambda_{3/2}\sin^2\theta(1+15\cos^2\theta) + 5\Lambda_{5/2}\sin^4\theta} \, ,$$

$$\Lambda_{m_f} \equiv \lambda_{m_j} / \lambda_g \, , \tag{3.9}$$

λ_g is the ground doublet λ, $N_g = 2$ for a doublet, and we used for the $4f$ spectral density at the Fermi surface

$$\rho_{f m_j}(0) = \frac{1}{\pi \Gamma_{m_j}} \sin^2 \left[\frac{\pi n_f}{N_{m_j}} \right] \, . \tag{3.10}$$

From Eq. (3.8) we see that the conductivity depends on three factors: the degeneracy of the ground-state N_g, the phase shift at the Fermi level $\eta_3(0) = \pi n_f / N_g$, and the angular integral I_μ.

When all the levels are degenerate $N_g = N_f$, the λ_{m_j}'s are all equal, and $\Lambda_{m_j} = 1$. Then the angular integral $I_\mu = 1$ and we find $\sigma_{\mu\mu} = \sigma_0$. The opposite extreme is when one of the doublets $|\pm m_j\rangle$ is lowest and the others are much higher in energy, i.e., $\Lambda_{m_j} \approx \delta_{m_j g}$. In this limit

$$\frac{\sigma_{\mu\mu}^{(m_j)}}{\sigma_0} = \frac{2j+1}{2} \frac{\sin^2[\pi n_f / (2j+1)]}{\sin^2(\pi n_f / 2)} I_\mu^{(m_j)} \, . \tag{3.11}$$

Whereas the first two factors do not depend on the nature of the ground doublet, the angular integral varies dramatically with m_j.[6] We find

$$I_x^{(1/2)} = 4.3 \, ,$$

$$I_z^{(1/2)} = 2.8 \, ,$$

$$I_x^{(3/2)} = 4.1 \, ,$$

$I_z^{(3/2)}$ diverges as $\log x$,

$I_x^{(5/2)}$ diverges as $\log x$,

and

$I_z^{(5/2)}$ diverges as x^{-2} . (3.12)

Therefore in addition to making the conductivities anisotropic, anisotropic mixing alters their *magnitudes* dramatically. In particular when the ground state is nominally $|\pm\frac{5}{2}\rangle$ or $|\pm\frac{3}{2}\rangle$ it is important to consider all

Λ_{m_j} and not to approximate them as above i.e., $\Lambda_{m_j} \approx \delta_{m_j g}$.

To illustrate the above we consider cerium in $LaAl_3$. In this system the ground state of the $4f^1$ electron is *nearly* $|\pm\frac{3}{2}\rangle$, the first excited state $|\pm\frac{1}{2}\rangle$ is at $\Delta_{10}=60$ K, and the uppermost $|\pm\frac{5}{2}\rangle$ state is at $\Delta_{20}=88$ K.[13] From our previous work on the anisotropy of the mixing, we determined for $CeAl_3$ that[14]

$$\begin{aligned} &V_1^2/V_0^2=1.35 \ , \\ &V_2^2/V_0^2=1.49 \ , \\ &T_0=3.14 \text{ K} \ , \\ &\Gamma_0^* \approx 5 \text{ K} \ , \\ &\Gamma_1^* \approx \Gamma_2^* \approx 25 \text{ K} \ . \end{aligned} \tag{3.13}$$

where 0, 1, and 2 are the ground and two excited states. By placing these values in Eqs. (3.7a) and (3.9) we find for Ce in $LaAl_3$

$$\begin{aligned} &\Lambda_0=1 \ , \\ &\Lambda_1=\frac{V_1^2}{V_0^2}\frac{\rho_{f_1}(0)}{\rho_{f_0}(0)}=\frac{V_1^2}{V_0^2}\frac{\Gamma_1^*/(\Delta_{10}^2+\Gamma_1^{*2})}{\Gamma_0^*/(T_0^2+\Gamma_0^{*2})}=0.056 \ , \end{aligned} \tag{3.14}$$

and similarly

$$\Lambda_2=\frac{V_2^2}{V_0^2}\frac{\rho_{f_2}(0)}{\rho_{f_0}(0)}=0.031 \ .$$

Although Λ_1 and Λ_2 are small they should not be set to zero as the ground state is nominally $|\pm\frac{3}{2}\rangle$; therefore the angular integral I_μ is sensitive to nonzero values of Λ_1 and Λ_2. For the above values of Λ_m we find

$$I_z=3.8 \tag{3.15}$$

and

$$I_x=3.2 \ .$$

On comparing with Eqs. (3.12) for $m_j=\frac{3}{2}$ we note these values lie between the two extremes of isotropy $I_\mu=1$ and an isolated $|\pm\frac{3}{2}\rangle$ ground state. By placing these values for I_μ in Eq. (3.11), we find the conductivities parallel and perpendicular to the c axis of the crystal are

$$\begin{aligned} &\sigma_{zz}=2.85\sigma_0 \ , \\ &\sigma_{xx}=2.4\sigma_0 \ , \end{aligned} \tag{3.16}$$

and

$$\sigma_{zz}/\sigma_{xx}=1.19 \ .$$

For cerium in $LaAl_3$ we find the resistivity or conductivity is not that anisotropic. On the contrary, the main effect of the anisotropy of the mixing interaction in this system is to change the *magnitude* of the resistivity by about a factor of 3. As we will discuss in the concluding section the major role of anisotropic mixing is to alter the parameters Λ_{m_j}, Eqs. (3.14), entering the angular integrals I_μ, so that they are radically different from those one would find from a model which had crystalline field splittings but *isotropic* mixing parameters.

At the present time it is not possible to compare our results for the conductivities, Eqs. (3.16), with experimental data, because data do not exist for temperatures small compared to $T_0=3.14$ K. The extant data[1] is for $T \geq 10$ K, where $T > T_0$. Therefore the effects to the Kondo scattering are minimal, and our theory does not readily distinguish itself from others which have isotropic mixing with crystal-field-split levels.

We have not evaluated the conductivity, Eq. (3.8), for $CeCu_2Si_2$ because the mixing parameters V_m have not been determined. For this structure there are too many independent variables to reliably determine the V_m's. Once they are available we can readily calculate the anisotropy of the resistivity by using the formulas in this section.

IV. SUSCEPTIBILITY

To obtain the magnetic susceptibility we take two derivatives of the ground-state energy of the Hamiltonian for our systems, Eq. (2.1), with respect to the field. We previously found this energy E_0 in the absence of a field.[8] When we focus on the susceptibility coming from the local f electrons,[10,11] the ground-state energy in the presence of a field for the Hamiltonian Eq. (2.1) is

$$E_0 \approx \sum_m \frac{\Gamma_m}{\pi}\int_{-D}^{D}\frac{f(\varepsilon_k-\boldsymbol{\alpha}_m\cdot\mathbf{H}-\mathbf{H}\cdot\overleftrightarrow{\beta}_m\cdot\mathbf{H})d\varepsilon_k}{E_0-\epsilon_f+\epsilon_k-\Sigma_m(\varepsilon_f)} \ , \tag{4.1}$$

where

$$\begin{aligned} &\boldsymbol{\alpha}_m=g\mu_B\langle m|\mathbf{J}|m\rangle \\ &\overleftrightarrow{\beta}_m=(g\mu_B)^2\sum_{m'\neq m}\langle m|\mathbf{J}|m'\rangle\langle m'|\mathbf{J}|m\rangle/(E_m-E_{m'}) \ , \end{aligned} \tag{4.2}$$

and we have neglected the term of $O(H^3)$.

As it is defined E_0 is an intrinsic function of the field H. By taking two derivatives with respect to the field and using Eq. (2.5), we find the zero-field susceptibility at $T=0$ K is given as

$$\begin{aligned} \chi_{\mu\mu}(T=0) &= -\frac{\partial^2 E_0}{\partial H_\mu^2}\Big|_{H=0} \\ &= \left[1+\frac{\pi T_0}{N_0\Gamma_0}+\sum_{m\neq 0}\frac{N_m}{N_0}\frac{T_0}{\Delta_{m0}}\frac{\Gamma_m}{\Gamma_0}\right]^{-1}\left[\left[\frac{(\alpha_0^\mu)^2}{T_0}-2\beta_0^{\mu\mu}\right]+\sum_{m\neq 0}\frac{N_m}{N_0}\frac{T_0}{\Delta_{m0}}\frac{\Gamma_m}{\Gamma_0}\left[\frac{(\alpha_m^\mu)^2}{\Delta_{m0}}-2\beta_m^{\mu\mu}\right]\right] \ , \end{aligned} \tag{4.3}$$

where $\Delta_{m0} \equiv \Sigma_m - \Sigma_0$ are the $4f$-level splittings, and $\alpha_m^{\mu}, \beta_m^{\mu\mu}$ are components of $\boldsymbol{\alpha}_m$ and $\overleftrightarrow{\beta}_m$, see Eq. (4.2). When $\Delta_{m0} \gg T_0$ we can identify the term proportional to $(\alpha_0^{\mu})^2/T_0$ as the Kondo-type susceptibility, while the remaining terms are Van Vleck–type corrections due to the upper f levels removed from the ground state in our model by the anisotropy of the mixing interaction.[8] When there is no splitting of the $4f$ level, the above formula reduces to the isotropic susceptibility at $T=0$ K

$$\chi_0(T=0) = \tfrac{1}{3} j(j+1)(g\mu_B)^2/T_0 \ . \qquad (4.3a)$$

Our result, Eq. (4.3), is in overall agreement with the susceptibility derived by Hanzawa *et al.*[15] Differences appear because our treatment of the Kondo effect is different from theirs.

By using Eq. (4.3) we have calculated the susceptibility of CeAl$_3$ at $T=0$ K for the magnetic field parallel and perpendicular to the c axis of this compound. As the susceptibility is more sensitive to the precise composition of the states than the resistivity we use the following states for the ground, first, and second excited states of CeAl$_3$ (Ref. 13)

$$\begin{aligned} |0\rangle &= a|\pm\tfrac{5}{2}\rangle + b|\mp\tfrac{3}{2}\rangle \ , \\ |1\rangle &= |\pm\tfrac{1}{2}\rangle \ , \\ |2\rangle &= a|\pm\tfrac{3}{2}\rangle - b|\mp\tfrac{5}{2}\rangle \ , \end{aligned} \qquad (4.4)$$

where $a=0.97$ and $b=0.24$. These states are spatially quantized along the c axis of the crystal; therefore, we must be careful when the field is perpendicular to the c axis to use the proper linear combinations of these states, so that the perturbation, i.e., $g\mu_B H J_x$, does not connect degenerate states. This is readily done for the previous states by taking the symmetric and antisymmetric combinations (properly normalized by $1/\sqrt{2}$) of the states $|\pm m_j\rangle$ in Eqs. (4.4). For the field parallel to the c axis we find

$$\begin{aligned} \alpha_0^{\parallel} &= \pm(\tfrac{5}{2}a^2 - \tfrac{3}{2}b^2) g\mu_B \ , \\ \alpha_1^{\parallel} &= \pm\tfrac{1}{2} g\mu_B \ , \\ \alpha_2^{\parallel} &= \pm(\tfrac{3}{2}a^2 - \tfrac{5}{2}b^2) g\mu_B \ , \\ \beta_0^{\parallel} &= -\beta_2^{\parallel} = -\frac{(4ab)^2}{\Delta_{20}}(g\mu_B)^2 \ , \end{aligned} \qquad (4.5)$$

and

$$\beta_1^{\parallel} = 0 \ ,$$

while for the field perpendicular to the c axis we find

$$\begin{aligned} \alpha_0^{\perp} &= \alpha_2^{\perp} = \sqrt{5}\, ab g\mu_B \ , \\ \alpha_1^{\perp} &= \tfrac{3}{2} g\mu_B \ , \\ \beta_0^{\perp} &= -\left[\frac{2b^2}{\Delta_{10}} + \frac{5}{4}\frac{(a^2-b^2)^2}{\Delta_{20}}\right](g\mu_B)^2 \ , \\ \beta_1^{\perp} &= \left[\frac{2b^2}{\Delta_{10}} - \frac{2a^2}{\Delta_{21}}\right](g\mu_B)^2 \ , \end{aligned} \qquad (4.6)$$

and

$$\beta_2^{\perp} = \left[\frac{2a^2}{\Delta_{21}} + \frac{5}{4}\frac{(a^2-b^2)^2}{\Delta_{20}}\right](g\mu_B)^2 \ .$$

By using the T_0 and Γ_m we previously found for CeAl$_3$,[8] see Eq. (3.13), and the *actual* splittings $\Delta_{10}=60$ K and $\Delta_{20}=88$ K,[13] we find

$$\chi_{\parallel} = 0.53(g\mu_B)^2/K \ ,$$

and (4.7)

$$\chi_{\perp} = 0.15(g\mu_B)^2/K \ .$$

The ratio of the susceptibilities,

$$\frac{\chi_{\parallel}}{\chi_{\perp}} = 3.5 \ , \qquad (4.8)$$

is in excellent agreement with the experimental value extrapolated to zero temperature of (3.6), but the absolute values are about twice as large as the experimental ones.[1]

We have repeated this calculation for CeCu$_2$Si$_2$. For this compound with tetragonal symmetry there are three doublet as for CeAl$_3$ with $a=0.83$ and $b=0.56$, see Eqs. (4.4), $\Delta_{10}=140$ K, $\Delta_{20}=364$ K, and $T_0=10$ K.[16] As $\Delta_{10}, \Delta_{20} \gg T_0$ we can neglect the contributions to the susceptibility from the excited states, i.e., the $\sum_{m\neq 0}$ in Eq. (4.3), and we find

$$\chi_{\mu\mu}(T=0) \approx \frac{(\alpha_0^{\mu})^2}{T_0} - 2\beta_0^{\mu\mu} \ . \qquad (4.9)$$

By using this abridged formula we find

$$\begin{aligned} \chi_{\parallel} &= 0.16(g,u_B)^2/K \ , \\ \chi_{\perp} &= 0.11(g\mu_B)^2/K \ , \\ \frac{\chi_{\parallel}}{\chi_{\perp}} &= 1.45 \ . \end{aligned} \qquad (4.10)$$

The experimental data of the susceptibility for CeCu$_2$Si$_2$ are[17]

$$\begin{aligned} \chi_{\parallel} &= 0.062(g\mu_B)^2/K \ , \\ \chi_{\perp} &= 0.048(g\mu_B)^2/K \ , \\ \frac{\chi_{\parallel}}{\chi_{\perp}} &\approx 1.2 \ . \end{aligned} \qquad (4.11)$$

Our calculated ratio of the susceptbilities parallel and perpendicular to the principal axis is in good agreement with the observed ratio. However, the absolute values of the susceptibilities are about twice as large as those measured.

We note that our calculated values for the susceptibilities of *both* CeAl$_3$ and CeCu$_2$Si$_2$ are about twice as large as those observed. We do not have an explanation for this.

V. DISCUSSION OF RESULTS

We have determined the effects of anisotropic hybridization on the resistivity and susceptibility of Kondo systems. As the conduction electrons are scattered by the mixing interaction in the Anderson model, it is natural to expect that the resistivity would be anisotropic. In addition, we previously found that anisotropic mixing was a major source of the $4f$-level splittings observed in cerium Kondo systems. Systems with crystal-field-split magnetic ions are known to yield anisotropic resistivities and susceptibilities. Therefore the question arises whether one could explain these properties for Kondo systems on the basis of *crystal-field*-split levels (of arbitrary origin) with an *isotropic* mixing interaction. Indeed this is the model used up until now to explain the anisotropy of the resistivity, e.g., see Refs. 5 and 6, and the susceptibility Ref. 15. In such a model all the mixing parameters V_m are the same so that the parameters $\Gamma_m = \pi N(0)|V_m|^2$ are identical. When the degeneracies of all the split levels are the same, as they are for the cases we are considering (they are all doublets), the parameters Λ_{m_f}, Eq. (3.14), are given by

$$(\Lambda_{m_j})_{\rm iso} = \frac{(\Gamma^*_{m_j})_{\rm iso}}{(\Gamma^*_0)_{\rm iso}} \frac{T_0^2+(\Gamma^*_0)^2_{\rm iso}}{\Delta^2_{m_j0}} \tag{5.1}$$

for $\Delta^2_{m_j0} \gg (\Gamma^*_{m_j})^2_{\rm iso}$. The $(\Gamma^*_{m_j})_{\rm iso}$ are determined from Eq. (12) of Ref. 8 with the *same Kondo temperature* T_0 *and crystal-field-splittings* Δ_{m_j0} that we used in the calculation with anisotropic mixing, and we find

$$\begin{aligned}(\Gamma^*_0)_{\rm iso} &= 4.5\ \text{K} , \\ (\Gamma^*_1)_{\rm iso} &\approx (\Gamma^*_2)_{\rm iso} \approx 14\ \text{K} , \\ (\Gamma^*_{1,2})_{\rm iso}/(\Gamma^*_0)_{\rm iso} &\approx 3 .\end{aligned} \tag{5.2}$$

The equivalent expression when anisotropic mixing is present, see Eqs. (3.14), can be written as

$$\Lambda_{m_j} = \left[\frac{V_{m_j}}{V_0}\right]^2 \frac{\Gamma^*_{m_j}}{\Gamma^*_0} \frac{T_0^2+\Gamma_0^{*2}}{\Delta^2_{m_j0}} , \tag{5.3}$$

where we took $\Delta^2_{m_j0} \gg \Gamma^2_{m_j}$, and from Eq. (3.13) we have

$$\left[\frac{V_{1,2}}{V_0}\right]^2 \approx 1.5 , \tag{5.4}$$

and

$$\frac{\Gamma^*_{1,2}}{\Gamma^*_0} \approx 5 .$$

By inserting the same Kondo temperature and crystal-field splittings in the two expressions, Eqs. (5.1) and (5.3), we find the Λ_{m_j}'s for the isotropic mixing are $2\frac{1}{2}$ times *smaller* than for those with anisotropic mixing.

With the model used in Ref. 6, we find

$$\Lambda_{m_j} = \left[\frac{T_0}{2\Delta_{m_j0}}\right]^2 , \tag{5.5}$$

and we find this is about 60 times *smaller* than the correct parameters, Eqs. (3.14). As the angular integral I_z diverges for the ground state of cerium in LaAl_3 when $\Lambda_1=\Lambda_2=0$, a finite conductivity along the z axis depends critically on the small but finite values of these Λ's. Even though the Λ_{m_j}'s are small for the model with anisotropic mixing, $\Lambda_1=0.056$ and $\Lambda_2=0.031$, the models with isotropic mixing have even *smaller* parameters. Therefore the conductivity σ_{zz} will be considerably larger in these models. The integral I_x converges even for a pure $|\pm\frac{3}{2}\rangle$ ground state, $I_x^{(3.2)}=4.1$ [see Eq. (3.12)], and for cerium in LaAl_3 we find $I_x=3.2$. Therefore the smaller parameters Λ_{m_j} in the models with isotropic mixing change I_x by at most from 3.2 to 4.1.

We conclude that by fixing the Kondo temperature and crystal-field splittings, the models with isotropic mixing have much larger conductivities than the model with anisotropic mixing, particularly along the c direction (z axis), thereby increasing the anisotropy of the conductivity. On the other hand the susceptibility, see Eq. (4.3), is relatively unaffected by the anisotropy of the mixing interaction provided one accounts for the crystal-field splittings. If one reverses this procedure, i.e., uses known data to fix the model parameters Λ_{m_j}, we would find that the ratios $(T_0/\Delta_{m_j0})^2$ found by using isotropic mixing, see Eqs. (5.1) and (5.5), are 2.5–60 times *larger* than for the model with anisotropic mixing, Eq. (5.3).

To summarize, the Anderson model of Kondo systems with anisotropic mixing produces an anisotropy of the resistivity, which is quite different from the model in which one splits the $4f$ level, and uses an isotropic mixing interaction. As data on the conductivities are unavailable, we are unable to decide which model is better. A more realistic calculation in which we relax our assumption $\varepsilon_{fm}=\varepsilon_f$ will no doubt yield better results; after all, one has additional parameters to play with. The one thing that is clear at this time is that the isotropic mixing interaction yields linewidths Γ^*_m, Eq. (5.2), which are too small. Anisotropic mixing is an effect that should be considered in any crystal-electric-field-type calculation of heavy fermions.

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