

el and with an isotropic exchange interaction. The contribution to the anisotropy per ion of Ru^{3+} in YIG is very large, about 2 to 3 times larger than that of Co^{2+} . The value of v/ξ is negative in agreement with ESR measurements on YGaG and amounts to -1 . The exchange interaction between Ru^{3+} and Fe^{3+} is found to be substantially larger than that between the iron ions. It should be noted that the error due to the relatively large uncertainty in the concentration of Ru^{3+} ions does not affect the obtained values of v/ξ and gH_e because they are deduced from the ratio $\Delta K_2/\Delta K_1$. It may be mentioned that these results do not only apply for the ruthenium-doped YIG, but in the main also for ruthenium-doped lithium ferrite.²¹ Here, ΔK_1 also is positive and ΔK_2 negative, and thus the value of

v/ξ is negative.

Above room temperature, the agreement of theory and experiment is not as good, but in this range it is no longer justified to neglect the temperature dependence of the exchange field.

By additionally incorporating Ca, Mg,¹⁷ or Zn,²⁰ it could be found that the concentration of Ru^{4+} ions is negligible and, therefore, Fe^{4+} ions are probably present.^{22,23}

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Influence of Spin-Orbit Scattering on the s - d Exchange Model

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Starting with an Anderson Hamiltonian for a metallic system with impurities, adding to it a spin-orbit scattering term for the conduction electrons, and performing a Schrieffer-Wolff canonical transformation, one induces an s - d model which takes into account spin-orbit scattering in a consistent fashion. The Hamiltonian derived in this way is used to discuss the alteration of the Kondo effect to lowest order in perturbation theory (for $T \gg T_K$) and the EPR residual linewidth.

I. INTRODUCTION

Since Kondo's¹ discovery of a logarithmic divergence in perturbation theory for the scattering of

conduction electrons from magnetic impurities in metals, a large amount of experimental and theoretical work has been devoted to this problem.² Recently, Heeger² suggested that the Kondo effect

can be interpreted as arising from an indirect electron-interaction via the magnetic impurity. From this point of view, he speculated that spin-lattice relaxation of this localized spin should destroy this effective interaction, and therefore the Kondo effect.

As demonstrated by McElroy and Heeger,³ one can induce a spin-lattice relaxation of a localized spin by introducing impurities in the lattice. This arises from the admixture of conduction electrons wave function, as will be demonstrated from a more general point of view in this paper.

To test these ideas further, Gainon and Heeger⁴ doped a $CuMn$ alloy (a Kondo system with $T_k = e^{-1/N(0)|J|} \sim 0.05^\circ K$) with Pt impurities and showed experimentally that the anomalous term in the resistivity fitted a

$$\rho(T) \sim \ln(T^2 + \theta^2) \quad (1)$$

law. Surprisingly, θ is not a linear function of the concentration of the heavy impurities used to induce spin-orbit scattering, but a more complicated function. The purpose of this paper is to discuss a possible explanation for this behavior.

In Sec. II, the effect of impurities on the localized wave function is discussed, and an effective Hamiltonian is derived which describes the relaxation of the localized spins. In Sec. III, this Hamiltonian is used to calculate the self-energy of the localized level. In Sec. IV, it is demonstrated that this self-energy is essentially equal to the θ measured by Gainon and Heeger. These results are discussed in Sec. V; in particular it is demonstrated that only part of this θ can be seen in an EPR experiment.

II. DERIVATION OF THE EFFECTIVE HAMILTONIAN

We want to discuss the effect of heavy impurities on the magnetic-moment problem, for example the effect of Pt impurities on the $CuMn$ system. We start from a slightly modified Anderson Hamiltonian

$$\mathcal{H} = \mathcal{H}_A + \mathcal{H}_{so}, \quad \mathcal{H}_A = \mathcal{H}_0 + \mathcal{H}_v, \quad (2)$$

$$\mathcal{H}_0 = \sum_{\vec{k}, \sigma} \epsilon_{\vec{k}} n_{\vec{k}\sigma} + U n_d n_{d'} + E \sum_{\sigma} n_{d\sigma}, \quad (3)$$

$$\mathcal{H}_v = \sum_{\vec{k}, \sigma} V_{\vec{k}d} c_{\vec{k}\sigma}^\dagger d_{\sigma} + c. c., \quad (4)$$

$$\mathcal{H}_{so} = \sum_{i, \vec{k}, \vec{k}'} W_{\vec{k}\vec{k}', \sigma\sigma'}(\vec{R}_i) c_{\vec{k}\sigma}^\dagger c_{\vec{k}'\sigma'}, \quad (5)$$

$$W_{\vec{k}\vec{k}', \sigma\sigma'}(\vec{R}_i) = i(\vec{k} \times \vec{k}') \cdot \vec{\sigma}_{\sigma\sigma'} b(|\vec{k} - \vec{k}'|) e^{+i(\vec{k} - \vec{k}') \cdot \vec{R}_i}. \quad (6)$$

\mathcal{H}_A is the Anderson Hamiltonian, and all quantities are as defined in his paper.⁵ \mathcal{H}_{so} is the spin-orbit interaction of the conduction electrons, \vec{R}_i denotes the sites of the heavy impurities, and $b(|\vec{k}|)$ is the spin-orbit potential. As demonstrated by Schrieffer

and Wolff,⁶ the Hamiltonian \mathcal{H}_A is not written in the best possible variables, at least from the historical point of view, when one discusses the extreme magnetic limit $U \gg \pi N(0)|V|^2$ [where $N(0)$ is the density of states at the Fermi surface and V is an average matrix element $\langle V_{\vec{k}d} \rangle_{av}$].

Going to the new basis functions,

$$\bar{d}_{\sigma} = e^{-S} d_{\sigma} e^S, \quad \bar{c}_{\vec{k}\sigma} = e^{-S} c_{\vec{k}\sigma} e^S, \quad (7)$$

chosen so as to eliminate \mathcal{H}_v to the first order from \mathcal{H}_A , one gets the result that \mathcal{H}_A is equivalent to an exchange-type Hamiltonian (with a negative exchange constant) written in the new variables $\bar{d}_{\sigma}, \bar{c}_{\vec{k}\sigma}$,

$$\mathcal{H}_A(c_{\vec{k}\sigma}, d_{\sigma}) \rightarrow \mathcal{H}_0(\bar{c}_{\vec{k}\sigma}, d_{\sigma}) + \mathcal{H}_{ex}(\bar{c}_{\vec{k}\sigma}, d_{\sigma}) + \text{higher-order terms}, \quad (8)$$

where \mathcal{H}_0 is defined by (3) and

$$\mathcal{H}_{ex} = -\frac{1}{4} \sum_{\vec{k}, \vec{k}', \sigma, \sigma'; s, s'} J_{\vec{k}\vec{k}'} (d_{\sigma}^\dagger \bar{\sigma}_{\sigma\sigma'} d_{\sigma'}) (c_{\vec{k}s}^\dagger \bar{\sigma}_{ss'} c_{\vec{k}'s'}). \quad (9)$$

If one assumes, as is generally accepted, that the Anderson Hamiltonian describes the fundamental physics of the problem, and if one wishes to discuss the Kondo effect or EPR measurements in terms of an exchange-type Hamiltonian when spin-orbit scattering is present in the system, one has therefore to consistently start with the Hamiltonian (2) and then transform it in terms of the variables (7). To do this we simply calculate, in analogy with Ref. 6,

$$\bar{\mathcal{H}} = e^S \mathcal{H} e^{-S},$$

taking

$$S = \sum_{\vec{k}\sigma\alpha} \frac{V_{\vec{k}d}}{\epsilon_{\vec{k}} - \epsilon_{\alpha}} n_{d-\sigma}^\dagger c_{\vec{k}\sigma}^\dagger d_{\sigma} - c. c.,$$

where the quantities are as defined in Appendix A. Keeping only the dominant terms, one gets⁷ (see Appendix A)

$$\bar{\mathcal{H}} = \mathcal{H}_0 + \mathcal{H}_{ex} + \mathcal{H}_{so} + \mathcal{H}'_{so} + \mathcal{H}''_{so}, \quad (10)$$

where \mathcal{H}_{ex} is the usual exchange-type Hamiltonian [Eq. (9)] and⁸

$$\mathcal{H}'_{so} = \sum_{\alpha\alpha'\sigma\sigma'} W'_{\vec{k}\alpha\sigma\sigma'}(\vec{R}_i) c_{\vec{k}\sigma}^\dagger d_{\sigma'} n_{d-\sigma'}^\alpha + c. c., \quad (11)$$

$$\mathcal{H}''_{so} = \sum_{\alpha\alpha'\sigma\sigma'} W''_{\alpha\alpha'\sigma\sigma'}(\vec{R}_i) n_{d-\sigma}^\alpha d_{\sigma'}^\dagger n_{d-\sigma'}^{\alpha'} d_{\sigma'} + c. c., \quad (12)$$

where W' and W'' are given by

$$W'_{\vec{k}\alpha\sigma\sigma'}(\vec{R}_i) = - \sum_{\vec{k}'} W_{\vec{k}\vec{k}', \sigma\sigma'}(\vec{R}_i) V_{\vec{k}'d} (\epsilon_{\vec{k}'} - \epsilon_{\alpha})^{-1}, \quad (13)$$

$$W''_{\alpha\alpha'\sigma\sigma'}(\vec{R}_i) = \frac{1}{2} \sum_{\vec{k}, \vec{k}'} W_{\vec{k}\vec{k}', \sigma\sigma'}^*(\vec{R}_i) \frac{V_{\vec{k}d} V_{\vec{k}'d}^*}{(\epsilon_{\vec{k}} - \epsilon_{\alpha})(\epsilon_{\vec{k}'} - \epsilon_{\alpha'})} \quad (14)$$

One might be tempted at this point to perform a

second canonical transformation \vec{S} to eliminate \mathcal{H}'_{s_0} which indeed looks very much like \mathcal{H}_0 . One of the particular properties, however, that gives the Schrieffer-Wolff transformation a good physical sense is that the total magnetization operator \vec{M} commutes with S (when the conduction electron and the localized electron have the same g value),

$$[\vec{M}, S] = 0.$$

This ensures that the magnetization described by $\mathcal{H}_0(\vec{c}_k, \vec{d})$ still obeys a Curie law plus a Pauli susceptibility.

In contrast, \vec{S} does not commute with \vec{M} (as can be seen by explicit calculation) and therefore the Kubo formula for the susceptibility of the conduction electron, for instance, written in the basis functions $\vec{c}_k = e^{-\vec{S}} \vec{c}_k e^{\vec{S}}$, has a very complicated form.

III. CALCULATION OF THE SELF-ENERGY OF THE LOCALIZED LEVEL

As we shall see in Sec. IV, the function θ measured by Gainon and Heeger [Eq. (1)] is given by the self-energy of the localized level for $U=0$. More precisely, if one defines

$$\mathcal{G}_{d\sigma}(\omega) = -i \int dt e^{i\omega t} \langle\langle [d_\sigma(t), d_\sigma^\dagger(0)] \rangle\rangle \theta(r) \\ = [\omega - E - \Sigma_d(\omega)]^{-1}, \quad (15)$$

$$\theta \simeq 2 \text{Im} \Sigma_d(E) \Big|_{U=0}. \quad (16)$$

The self-energy Σ_d has three sources, \mathcal{H}_{ex} , \mathcal{H}'_{s_0} , and \mathcal{H}_{s_0} .

Let us first look at \mathcal{H}'_{s_0} . Taking into account the definition of $n_{d\sigma}^\alpha$ [see Eq. (A4)], one finds

$$\mathcal{H}'_{s_0} = \sum_i W''_{-\sigma\sigma}(\vec{R}_i) d_{i\sigma}^\dagger d_{-\sigma} + c. c. \\ + \sum_{\alpha, i} W''_{\alpha\alpha\sigma\sigma}(\vec{R}_i) n_{d-\sigma}^\alpha n_{d\sigma} + c. c. \quad (17)$$

Since $\langle n_{d-\sigma} n_{d\sigma} \rangle \simeq 0$ in a magnetic state, we can write the second part of Eq. (17) as

$$\sim \sum W''_{-\sigma\sigma}(\vec{R}_i) n_{d\sigma} + c. c.,$$

which is just a renormalization of E . We therefore write

$$\mathcal{H}'_{s_0} \sim \sum W''_{\sigma\sigma}(\vec{R}_i) d_{i\sigma}^\dagger d_{-\sigma} + c. c. \quad (18)$$

with

$$W''_{\sigma\sigma}(\vec{R}_i) = W''_{-\sigma\sigma}(\vec{R}_i). \quad (19)$$

As for \mathcal{H}'_{s_0} , in order to simplify the problem, we shall treat it in the Hartree-Fock approximation, and write

$$\mathcal{H}'_{s_0} \simeq \sum_{\vec{k}\alpha\sigma\sigma' i} W'_{\vec{k}\alpha\sigma\sigma'}(\vec{R}_i) c_{\vec{k}\sigma}^\dagger d_{\sigma'} \langle n_{d-\sigma'}^\alpha \rangle + c. c. \\ \simeq \frac{1}{2} \sum_{\vec{k}\alpha\sigma\sigma' i} W'_{\vec{k}\alpha\sigma\sigma'}(\vec{R}_i) c_{\vec{k}\sigma}^\dagger d_{\sigma'} + c. c. \quad (20)$$

These approximations are justified because we

only want to investigate orders of magnitude and temperature and concentration dependence.

We turn now to the evaluation of $\Sigma_d(\omega)$, using \mathcal{H}_{ex} , \mathcal{H}'_{s_0} [Eq. (18)], and \mathcal{H}_{s_0} [Eq. (20)]. An important point here is that the simple average over the heavy impurities of the matrix elements $W'_{\vec{k}\alpha\sigma\sigma'}$ and $W''_{\sigma\sigma'}$ vanishes because of the form (6). We have, therefore, to coherently average over pairs of impurities, as in the resistivity problem.⁹

We now write the self-energy as a sum of three terms¹⁰

$$\Sigma_d = \Sigma'_d + \Sigma''_d + \Sigma_d^{\text{ex}} \quad (21)$$

due, respectively, to the interactions \mathcal{H}'_{s_0} , \mathcal{H}_{s_0} , and \mathcal{H}_{ex} . These three terms are shown pictorially in Figs. 1–4. Their calculation is straightforward, using standard perturbation theoretic methods.⁹

The results are

$$\Sigma'_d = ivc, \quad (22)$$

where c is the concentration of heavy impurities and

$$v = \frac{1}{4} \pi N(0) N \sum_{\sigma'} \int d^3r W'_{\vec{k}\sigma\sigma\sigma'}(\vec{r}) W'^*_{\vec{k}\sigma\sigma\sigma'}(\vec{r}), \quad (23)$$

$$\Sigma''_d = cw/(\omega - E - \Sigma_d), \quad (24)$$

where

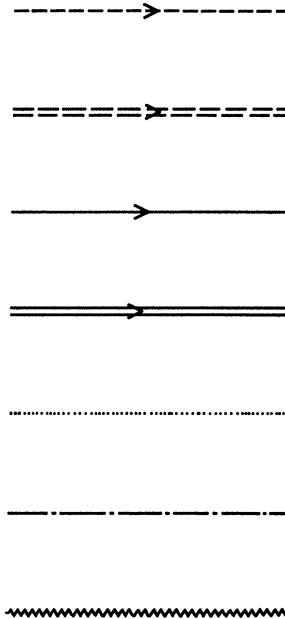


FIG. 1. Perturbation theoretic symbols: (a) bare d -electron propagator; (b) renormalized d -electron propagator; (c) bare conduction-electron propagator; (d) renormalized conduction-electron propagator; (e) interaction line corresponding to \mathcal{H}'_{s_0} ; (f) interaction line corresponding to \mathcal{H}_{s_0} ; (g) interaction line corresponding to \mathcal{H}_{ex} .

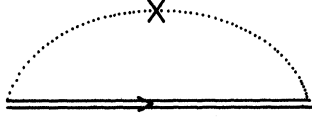


FIG. 2. Self-energy Σ_d' of the localized electron. The cross in the interaction line means coherent averaging over two impurities.

$$w = N \int d^3r W_{\sigma}''(\vec{r}) W_{\sigma}''^*(\vec{r}). \quad (25)$$

Finally, (we put the Boltzman constant equal to unity)

$$\Sigma_d^{\text{ex}} = izT \quad (26)$$

is one-fourth of the Korringa relaxation, where

$$z = \frac{1}{4}\pi [N(0)J]^2.$$

Putting together Eq. (22), (24), and (26), we get the self-consistent equations (on the energy shell)

$$\Sigma_d(\omega = E) = cw / [-\Sigma_d(\omega - E)] + ivc + izT, \quad (27)$$

which gives

$$\text{Re}\Sigma_d(\omega = E) = 0, \quad (28)$$

$$\text{Im}\Sigma_d(\omega = E) = \frac{1}{2}(zT + vc) + \frac{1}{2}[(zT + vc)^2 + 4cw]^{1/2}.$$

This is the main result of this paper. Before discussing it, we must first show that $\text{Im}\Sigma_d = \theta$.

IV. RELATION BETWEEN THE SELF-ENERGY AND θ

In order to discuss the Kondo effect by perturbation theory, Brenig and Götze introduced an elegant representation¹¹ which envisions the magnetic impurities as a dilute gas of (in the limit) infinitely heavy particles. In absence of spin-orbit scattering, the transformed Anderson Hamiltonian (8) does not contain any transfer (or mixing terms) to order V^3 . If one neglects these higher-order terms, the localized and itinerant electrons form two distinct systems; one can then think of the localized electron as a different kind of particle, with its own chemical potential. The extreme dilution limit is then equivalent to the magnetic limit, the pseudoparticles being kept apart by the dilution rather than by a potential U .

The self-energy of these pseudoparticles is then clearly to be identified with the one-particle self-energy of the d electron. Since the terms propor-

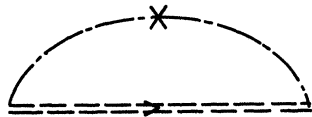


FIG. 3. Self-energy Σ_d' of the localized electron.

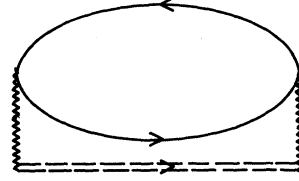


FIG. 4. Self-energy Σ_d^{ex} of the localized electron.

tional to U in this self-energy are proportional to c_i^2 (c_i is the concentration of d electrons), one can put $U=0$ in this calculation.

In our case, this procedure would be rigorously correct if $\mathcal{H}'_{\text{so}} + \mathcal{H}''_{\text{so}}$ did not contain any transfer terms. Since \mathcal{H}'_{so} does contain such terms, however, this procedure is only approximately correct, but it seems clear from a physical point of view that it is a good approximation. It corresponds to taking into account only the most important correlations induced by U , namely, those contained implicitly in \mathcal{H}_{ex} .

In the Brenig-Götze representation, the exchange Hamiltonian (8) is written

$$\mathcal{H} = \mathcal{H}_e + \mathcal{H}_i + \mathcal{H}_{e_i}, \quad (29)$$

$$\mathcal{H}_e = \sum_{\vec{k}, \sigma} \epsilon_{\vec{k}\sigma} n_{\vec{k}\sigma}, \quad (30)$$

$$\mathcal{H}_i = \sum_{\vec{p}, \kappa} \omega_{\vec{p}} b_{\vec{p}\kappa}^{\dagger} b_{\vec{p}\kappa} \quad (31)$$

$$\mathcal{H}_{e_i} = \sum_{\substack{\vec{k}, \vec{k}', \sigma, \sigma' \\ \vec{p}, \vec{p}', \kappa, \kappa'}}} \langle \vec{k}\sigma, \vec{p}\kappa | V_J | \vec{k}'\sigma', \vec{p}'\kappa' \rangle b_{\vec{p}\kappa}^{\dagger} b_{\vec{p}'\kappa'} c_{\vec{k}\sigma}^{\dagger} c_{\vec{k}'\sigma'}, \quad (32)$$

$$\langle \vec{k}\sigma, \vec{p}\kappa | V_J | \vec{k}'\sigma', \vec{p}'\kappa' \rangle = J \delta_{\vec{k}+\vec{p}, \vec{k}'+\vec{p}'} \delta_{\sigma\sigma'} \delta_{\kappa\kappa'} \vec{S}_{\vec{k}\kappa}. \quad (33)$$

Perturbation theory for the conduction-electron self-energy $\Sigma(\vec{k}, z)$ is straightforward, and leads, for the lowest-order divergent contribution, to the Feynman diagrams shown in Fig. 5. To each of these Feynman diagrams corresponds six Goldstone (time-ordered) graphs. As shown by Brenig and Götze¹² only part of these graphs contribute to

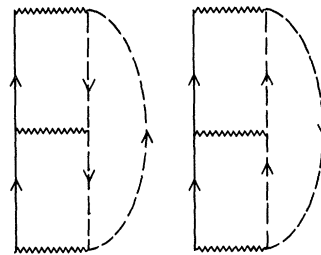


FIG. 5. Lowest divergent diagrams. In these diagrams $---$ represents a heavy particle in the Brenig-Götze picture.

the self-energy in lowest order of the magnetic impurity concentration c_i . These (time-ordered) graphs are shown in Fig. 6. Calculating these graphs with the usual rules, one gets the $\ln T$ law for the imaginary part of the self-energy $\Sigma(\vec{k}, T)$ when $T \gg z$.

As we have seen in Sec. III, \mathcal{K}'_{so} and \mathcal{K}''_{so} induce an effective "two-body interaction" due to the coherent averaging over impurities. In addition to self-energy corrections, we should therefore consider vertex corrections. We will assume, however, that these will essentially renormalize J , and therefore alter the Kondo temperature. This was not observed in experiment, and we will therefore not consider these terms in the present work.

We now slightly generalize Brenig and Götze calculations to allow for spin-flip scattering. Specifically, we write Lorentzian one-particle density of states for both the conduction electron and the heavy particles,

$$A_e(\vec{k}, \omega) = \frac{\text{Im}\Sigma_e/\pi}{(\omega - \epsilon_k - \text{Re}\Sigma_e)^2 + (\text{Im}\Sigma_e)^2}, \quad (34)$$

$$A_i(\vec{p}, \omega) = \frac{\text{Im}\Sigma_d/\pi}{(\omega - \omega_p)^2 + (\text{Im}\Sigma_d)^2}, \quad (35)$$

and calculate the first divergent terms in the conduction-electron self-energy. One finds (see Appendix B) for the anomalous term in the resistivity

$$\rho(T) \sim \ln[T^2 + 4(\text{Im}\Sigma_d)^2], \quad (36)$$

while Σ_e drops out of the result.

V. DISCUSSION

The coefficients v and w are difficult to calculate from first principles with meaningful accuracy, and we will therefore consider them as parameters to be determined experimentally.

It is easy to see that a form like the one given in Eq. (28) fits roughly the experimental curve of Gainon and Heeger. But a detailed comparison is not possible at this point, for the following reasons: Our calculation predicts that θ should be both concentration *and* temperature dependent, whereas Gainon and Heeger give θ as a function of the concentration only. Note that at zero concentration

$$\ln(T^2 + z^2 T^2)^{1/2} = \ln T + \frac{1}{2} \ln(1 + z^2),$$

and the Korringa term does not contribute to the temperature-dependent part of the resistivity. At finite concentration this argument does not work, however, and since $z \sim 0.2$ in CuMn , one expects this term to have some influence on the experimental results. One seems, therefore, to be in need of a more detailed experimental analysis of $\theta(c, T)$.

It is interesting to note that $\theta(c, T)$ is very dif-

ferent from the linewidth one would measure in a resonance experiment. First $4zT$ is *unbottlenecked* and therefore usually larger than the resonance Korringa linewidth. Second, \mathcal{K}''_{so} alone has no influence on the EPR resonance, because

$$[\vec{M}, \mathcal{K}''_{so}] = 0. \quad (37)$$

Only when another relaxation mechanism is at work can this "bottleneck" be broken, but then the term $(wc)^{1/2}$ is probably small anyway.

A comparison of our results with the calculation of McElroy and Heeger³ is in order. Their expression corresponds to

$$\text{Im}\Sigma_d'' = \text{Im} \frac{cw}{(\omega - E) - i\Delta_A}, \quad (38)$$

where

$$\Delta_A = \pi N(0) |V|^2 \quad (39)$$

is the width of the d state for the Anderson Hamiltonian. One can see, however, by the more detailed analysis given above that it is the width of the transformed states

$$\vec{d} = e^{-S} d e^S$$

that should enter Eq. (38), and this leads to the self-consistent Eq. (24).

In conclusion, the main contribution of this paper is to show that spin-orbit scattering induces a spin-flip relaxation rate on the localized d level, and that this rate alters the Kondo anomalous term in the resistivity. The alteration of the Kondo term is given by Eqs. (28) and (36). The quantity z appearing in Eq. (27) is given by $z = \frac{1}{4}\pi[N(0)J]^2$, whereas the quantities v and w are to be determined experimentally. Since, however, v is also related to the

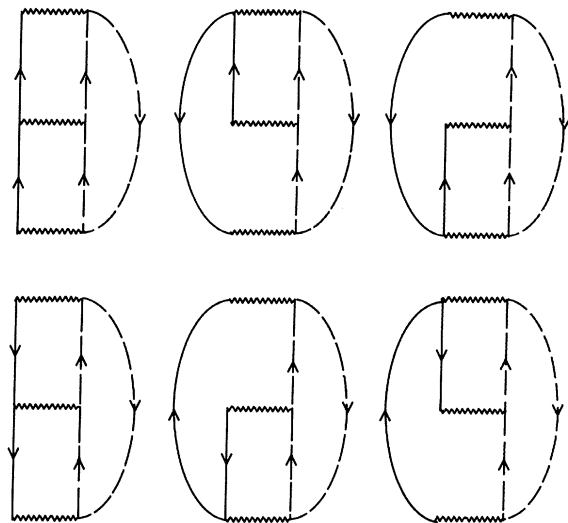


FIG. 6. Time-ordered graphs corresponding to the Feynman graphs shown in Fig. 5.

residual linewidth in an EPR experiment,

$$(1/T_2)_{\text{res}} = 2\nu c ,$$

there is only one free parameter w , and the theory can be meaningfully tested.

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APPENDIX A

We perform a Schrieffer-Wolff canonical transformation on \mathcal{H}

$$\bar{\mathcal{H}} = e^S \mathcal{H} e^{-S} \quad (\text{A1})$$

with the condition

$$[\mathcal{H}_0, S] = \mathcal{H}_v , \quad (\text{A2})$$

where \mathcal{H}_0 and \mathcal{H}_v are defined in Eqs. (3) and (4). This leads to⁶

$$S = \sum_{\mathbf{k}\sigma\alpha} \frac{V_{\mathbf{k}d}}{\epsilon_{\mathbf{k}} - \epsilon_{\alpha}} n_{d-\sigma}^{\alpha} c_{\mathbf{k}\sigma}^{\dagger} d_{\sigma} - \text{c. c.} , \quad (\text{A3})$$

where

$$\epsilon_{\alpha} = \begin{cases} E + V, & \alpha = + \\ E, & \alpha = - \end{cases} \quad n_{d\sigma}^{\alpha} = \begin{cases} n_{d\sigma}, & \alpha = + \\ 1 - n_{d\sigma}, & \alpha = - \end{cases} \quad (\text{A4})$$

are as defined in Ref. 6.

With condition (A2), Eq. (A1) has the following expansion:

$$\bar{\mathcal{H}} = \mathcal{H}_0 + \mathcal{H}_{\text{so}} + \frac{1}{2}[S, \mathcal{H}_v] + [S, \mathcal{H}_{\text{so}}] + \frac{1}{2}[S, \mathcal{H}_{\text{so}}] + \dots \quad (\text{A5})$$

The third term on the right-hand side gives the usual exchange Hamiltonian. It might seem inconsistent to neglect the term $\frac{1}{2}[S, [S, \mathcal{H}_v]]$ and retain the term $\frac{1}{2}[S, [S, \mathcal{H}_{\text{so}}]]$. These two terms correspond to two completely different physical effects. The former, if taken into account, would describe spin-fluctuation effects and its importance depends on the ratio $V^2 N(0)/U$, whereas the latter, depending on the ratio $[VN(0)]^2 w/U$, is important because of the peculiar dependence on $c^{1/2}$ which it produces in the self-energy [Eq. (28)]. Both terms are potentially important, but we are, in this paper interested only on the effect of the heavy impurities on the Kondo effect, not the effect of the spin fluctuations, which is a separate and difficult problem.¹³

The calculation of the fourth term is straightforward and gives

$$[S, \mathcal{H}_{\text{so}}] = \mathcal{H}'_{\text{so}} ,$$

$$\mathcal{H}'_{\text{so}} = \sum_{\mathbf{k}\alpha\sigma\sigma'} W'_{\mathbf{k}\alpha\sigma\sigma'}(\vec{\mathbf{R}}_i) c_{\mathbf{k}\sigma}^{\dagger} d_{\sigma} n_{d-\sigma'}^{\alpha} + \text{c. c.} , \quad (\text{A6})$$

where

$$W'_{\mathbf{k}\alpha\sigma\sigma'}(\vec{\mathbf{R}}_i) = - \sum_{\mathbf{k}'} W_{\mathbf{k}\mathbf{k}'\sigma\sigma'}(\vec{\mathbf{R}}_i) V_{\mathbf{k}'d} (\epsilon_{\mathbf{k}'} - \epsilon_{\alpha})^{-1} , \quad (\text{A7})$$

$$\frac{1}{2}[S, [S, \mathcal{H}_{\text{so}}]] = \mathcal{H}''_{\text{so}} + \mathcal{H}'''_{\text{so}} , \quad (\text{A8})$$

$$\mathcal{H}''_{\text{so}} = \sum_{\alpha\alpha'\sigma\sigma'} W''_{\alpha\alpha'\sigma\sigma'}(\vec{\mathbf{R}}_i) n_{d-\sigma}^{\alpha} d_{\sigma}^{\dagger} n_{d-\sigma'}^{\alpha'} d_{\sigma'} + \text{c. c.} , \quad (\text{A9})$$

where

$$W''_{\alpha\alpha'\sigma\sigma'}(\vec{\mathbf{R}}_i) = \frac{1}{2} \sum_{\mathbf{k}\mathbf{k}'} \frac{V_{\mathbf{k}d} V_{\mathbf{k}'d}}{(\epsilon_{\mathbf{k}} - \epsilon_{\alpha})(\epsilon_{\mathbf{k}'} - \epsilon_{\alpha'})} \times W_{\mathbf{k}\mathbf{k}'\sigma\sigma'}^*(\vec{\mathbf{R}}_i) , \quad (\text{A10})$$

$$\begin{aligned} \mathcal{H}'''_{\text{so}} = & \sum_{\mathbf{k}\mathbf{k}'\sigma\sigma', i} W_{\mathbf{k}\mathbf{k}'\sigma\sigma', i}'''(1)(\vec{\mathbf{R}}_i) c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}'\sigma'}^{\dagger} d_{-\sigma} d_{\sigma} + \text{c. c.} \\ & + \sum_{\alpha\mathbf{k}\mathbf{k}'\sigma\sigma', i} W_{\alpha\mathbf{k}\mathbf{k}'\sigma\sigma', i}'''(2)(\vec{\mathbf{R}}_i) n_{d-\sigma}^{\alpha} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}'\sigma'}^{\dagger} + \text{c. c.} \\ & + \sum_{\mathbf{k}\mathbf{k}'\sigma\sigma', i} W_{\mathbf{k}\mathbf{k}'\sigma\sigma', i}'''(3)(\vec{\mathbf{R}}_i) d_{-\sigma}^{\dagger} d_{\sigma} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}'\sigma'} + \text{c. c.} , \end{aligned} \quad (\text{A11})$$

where

$$W_{\mathbf{k}\mathbf{k}'\sigma\sigma', i}'''(1)(\vec{\mathbf{R}}_i) = - \frac{1}{2} \sum_{\alpha\alpha'} \frac{V_{\mathbf{k}d} V_{\mathbf{k}'d}}{(\epsilon_{\mathbf{k}} - \epsilon_{\alpha})(\epsilon_{\mathbf{k}'} - \epsilon_{\alpha'})} \times W_{\mathbf{k}\mathbf{k}'\sigma\sigma', i}(\vec{\mathbf{R}}_i) \{ \alpha' \delta_{\alpha, -} - \alpha \delta_{\alpha', -} \} , \quad (\text{A12})$$

$$W_{\alpha\mathbf{k}\mathbf{k}'\sigma\sigma', i}'''(2)(\vec{\mathbf{R}}_i) = - \frac{1}{2} \sum_{\mathbf{k}'} \frac{V_{\mathbf{k}d} V_{\mathbf{k}'d}}{(\epsilon_{\mathbf{k}} - \epsilon_{\alpha})(\epsilon_{\mathbf{k}'} - \epsilon_{\alpha'})} \times W_{\mathbf{k}\mathbf{k}'\sigma\sigma', i}(\vec{\mathbf{R}}_i) , \quad (\text{A13})$$

$$W_{\mathbf{k}\mathbf{k}'\sigma\sigma', i}'''(3)(\vec{\mathbf{R}}_i) = \frac{1}{2} \sum_{\mathbf{k}'', \alpha, \alpha'} \frac{V_{\mathbf{k}d} V_{\mathbf{k}''d}}{(\epsilon_{\mathbf{k}} - \epsilon_{\alpha})(\epsilon_{\mathbf{k}''} - \epsilon_{\alpha'})} \times W_{\mathbf{k}\mathbf{k}''\sigma\sigma', i}(\vec{\mathbf{R}}_i) (\alpha \delta_{\alpha', -} + \alpha' \delta_{\alpha, +}) . \quad (\text{A14})$$

We will neglect $\mathcal{H}'''_{\text{so}}$ altogether for the following reasons: the first term, because it involves two electron transfers and occurs only in higher-order diagrams, the second and the third because they are essentially of the same type as \mathcal{H}_{so} and \mathcal{H}_{ex} , respectively, but smaller by a factor of the order V^2/E_f^2 and W/E_f , respectively. We keep, however, the term (A9) because it is of a qualitatively different type than \mathcal{H}_{so} , \mathcal{H}'_{so} , or \mathcal{H}_{ex} .

APPENDIX B

The rules for calculating a time-ordered diagram contributing to $\Sigma(\vec{\mathbf{k}}, z)$ and containing dressed lines are the following.

(i) To each propagator line, associate a wave vector, a spin direction, and a frequency. Wave vectors and spin are conserved at each vertex.

(ii) To each upward (downward) running internal electron propagators carrying frequency ω and wave vectors \vec{k} , associate a factor

$$[1 - f_e(\omega)] A_e(\vec{k}, \omega) [-f_e(\omega) A_e(\vec{k}, \omega)].$$

Correspondingly to each upward (downward) running internal heavy-particle propagator carrying frequency ω and wave vector \vec{p} , associate a factor

$$[1 - f_i(\omega)] A_i(\vec{p}, \omega) [-f_i(\omega) A_i(\vec{p}, \omega)].$$

In this, A_e and A_i are the corresponding single-particle density-of-states function

$$f_e(\omega) = [1 + e^{\beta(\omega - \mu_e)}]^{-1}, \quad f_i(\omega) = [1 + e^{\beta(\omega - \mu_i)}]^{-1}.$$

(iii) Associate with each cut an energy factor N , where N^{-1} is the sum of the frequencies of the downward running propagators minus the sum of the frequencies of the upward running propagators. The external line must be considered as closed and carrying frequency z .

(iv) Include the vertices.

(v) Sum over the internal variables, and multiply the graph by $(-1)^L$, where L is the number of fermion loops.

Applying these rules to Fig. 2(a) gives

$$\Sigma^{2a} = -J^3 S(S+1) \int d\omega_1 d\omega_2 d\omega_3 d\omega_4 d\omega_5 [1 - f_e(\omega_1)] [1 - f_e(\omega_2)] f_i(\omega_3) [1 - f_i(\omega_4)] [1 - f_i(\omega_5)] A_e(\vec{k}_1, \omega_1) A_e(\vec{k}_2, \omega_2) \\ \times A_i(\vec{p}_1, \omega_3) A_i(\vec{p}_1 + \vec{k} - \vec{k}_1, \omega_4) A_i(\vec{k} + \vec{p}_1 - \vec{k}_2, \omega_5) \{z - \omega_1 + \omega_3 - \omega_4\}^{-1} \{z - \omega_2 - \omega_5 + \omega_3\}^{-1} (d^3 k_1 d^3 k_2 d^3 p_1) / (2\pi)^9,$$

where

$$A_e(\vec{k}, \omega) = \frac{\text{Im}\Sigma_e/\pi}{(\omega - \epsilon_{\vec{k}} - \text{Re}\Sigma_e)^2 + (\text{Im}\Sigma_e)^2}, \quad (\text{B1})$$

$$A_i(\vec{p}, \omega) = \frac{\text{Im}\Sigma_d/\pi}{(\omega - \omega_{\vec{p}}}^2 + (\text{Im}\Sigma_d)^2}, \quad (\text{B2})$$

and Σ_e and Σ_d are the self-energies of the conduction electrons and of the heavy particles, respectively.

If one restricts the integration for the conduction electron to one band, it is clear that in the limit $m \rightarrow \infty$, the variables \vec{k}_1 and \vec{k}_2 can be neglected in A_i . Furthermore, for $m \rightarrow \infty$, and for $\Sigma_d < T$,

$$f_i(\omega_3) \sim f_i(\omega_{\vec{p}_1}), \quad f_i(\omega_4) \sim f_i(\omega_{\vec{k} + \vec{p}_1 - \vec{k}_1}),$$

$$f_i(\omega_5) \sim f_i(\omega_{\vec{p}_1 + \vec{k}_1 - \vec{k}_2})$$

to a good approximation. All the remaining integrals are then trivial, and one gets, for $\omega \ll T$ and in lowest order of c_i the magnetic impurity concentration,

$$\text{Im}\Sigma^{2a}(T) \sim \ln(T^2 + 4\text{Im}\Sigma_d^2), \quad (\text{B3})$$

while Σ_e drops out of the result. The other diagrams give similar results.

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⁷Similar results have been derived independently by H. Spencer (private communication).

⁸ $\bar{c}_{\vec{k}\sigma}$ and \bar{d}_σ are now replaced by $c_{\vec{k}\sigma}$ and d_σ for convenience.

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¹⁰There are of course self-energy terms which involve several pieces of the interaction Hamiltonian in a more-complicated way, and cannot therefore be written in a form like Eq. (21), but these come in higher order in the interaction, and we will therefore neglect them.

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