Contributions from two-particle scattering to the extraordinary Hall effect in Kondo systems

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The contributions of skew scattering to the extraordinary Hall effect (EHE) in Kondo-type systems have been evaluated by using current-current correlation functions. By using this formalism we take account of two-electron scattering processes that are neglected in the conventional one-electron scattering theory of the EHE. We evaluate the correlation functions for dilute Kondo systems by considering only independent single-site scattering. We find there are two types of contributions to the EHE. Type-I terms come from diagrams in which the energies of the propagators are held fixed. We find that these type-I contributions reproduce the EHE found by the one-electron formalism, i.e., the elastic impurity- or potential-scattering contribution; in addition, there is a spin-scattering contribution which was not previously incorporated in the one-electron scattering formalism. The type-II contributions come from diagrams in which energy is *exchanged* between resonant and nonresonant scattering channels. These contributions to the EHE are new, i.e., they require two-electron scattering processes, and therefore perforce cannot be accounted for in a one-electron formalism. We find the type-II contributions to the EHE are as large as those of type I at low temperatures $T < T_0$, where T_0 is the characteristic energy scale of the single-ion Kondo problem; at high temperatures $T \gg T_0$, they are negligible compared with type-I contributions. To obtain the Hall effect we must have scattering in two partial-wave channels whose orbital angular momenta differ by $1\hbar$. To account for the dominant resonant Kondo scattering, we use the Anderson mixing interaction and consider the local electron is in a spin-orbit-coupled j state. In the nonresonant channel we consider two-electron charge- and spin-scattering terms whose origins could be, *interalia*, the direct and exchange parts of the Coulomb interaction between local and conduction electrons.

I. INTRODUCTION

The Hall effect is a particularly effective probe of conduction-electron scattering in Kondo-type compounds. In particular, the extraordinary Hall effect (EHE) probes the scattering of conduction electrons by the orbital angular momentum of localized electrons. The contributions of skew scattering to the Hall effect have been considered within a one-electron scatter formalism.[1] While this approach produces the correct variation of the Hall constant at high temperatures, it is inadequate at low temperatures, i.e., for $T < T_0$, where T_0 is the temperature characteristic of the Kondo scale of energies. There are at least two ingredients that have been left out in our model calculations. First, there are contributions from anomalous velocity to the Hall constant; this is also known as the side-jump contribution. We have evaluated these terms and find they are quite large in concentrated Kondo-type compounds at low temperatures.[2] The second feature left out of previous calculations is the two-electron scattering processes, i.e., we were limited to impurity scattering, because the formalism we used is applicable only to one-electron scattering processes.

Here we consider the spin-flip and two electron-charge-scattering processes neglected in previous approaches. To incorporate these two-electron scattering processes we use the Kubo formalism which gives the conductivity in terms of current-current correlation functions.[3] This formalism has been previously used to calculate the resistivity of Kondo systems.[4] A special feature of Kondo scattering is the resonant nature of the scattering for one partial-wave channel of the conduction electrons, e.g., for Kondo systems with rare-earth ions, the $l = 3$ partial wave of conduction electrons is resonantly scattered by the $4f$ electrons. This selectivity is readily explained by the Anderson mixing interaction. In the approximation of considering only *spherical* mixing, the local $4f$ state mixes or hybridizes only with the partial-wave component of the conduction electrons that has the same $l = 3$ symmetry. When scattering is confined to one angular-momentum channel there are no vertex corrections, i.e., there are no correlations between the electron-hole pair excitations of the Fermi sea that produce the resistivity. Therefore, the resistivity calculated by the Kubo formalism reproduces that which one finds using the Boltzmann transport equation with one-electron impurity scattering. The additional two-electron scattering processes present in a complete quantum-transport theory do not lead to additional contributions to the resistivity.

On the contrary, we find that two-electron scattering processes yield important contributions to the Hall effect in Kondo systems. In particular, the inelastic vertex corrections which enter the *Hall* resistivity (conductivity) make large contributions at low temperatures $T < T_0$. The reason vertex corrections enter the Hall conductivity is that *a priori* one must have scattering in channels with

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opposite parity in order to obtain the transverse drift which gives rise to a Hall voltage.[1] By using the Kubo formalism we find that in addition to the contribution from one-electron impurity scattering there are elastic contributions to the EHE from spin-dependent scattering, and inelastic vertex corrections coming from two-electron-charge and spin-scattering processes. The contributions from two-electron-charge scattering are by far the largest contribution, and at low temperatures they are as large as the EHE due to impurity scattering.

In the next section we derive the Hall conductivity due to skew scattering by using the Kubo formalism. We evaluate the different contributions to the EHE in Secs. III and IV. To obtain the variation of the Hall constant with temperature requires a self-consistent procedure, e.g., the self-consistent large-N expansion [or noncrossing approximation (NCA)].[5] In Sec. V we present analytic results for the EHE in the limits of weak coupling $T \gg T_0$ and strong coupling at $T=0$ K. In the last section we summarize and discuss our results. We stress that our results are derived on the basis of the single-ion Anderson model, and the impurity-averaging procedure we use is applicable to the dilute limit, i.e., we do not consider interference between scattering at different sites. Therefore our results can at best be compared to the EHE in Kondo systems in which the scattering is *incoherent.*

II. DERIVATION OF HALL CONSTANT

The linear Hall constant is defined as

$$R_H \equiv \frac{\rho_H}{H} \approx \frac{1}{H}\frac{\sigma_H}{\sigma_N^2} , \tag{2.1}$$

where ρ_H is the Hall resistivity, σ_H is the Hall conductivity, σ_N is the normal resistivity, and H is the magnetic field. We define the off-diagonal Hall conductivity as

$$\mathbf{J}_{\text{Hall}} \equiv \sigma_H \mathbf{E}\times\hat{\mathbf{h}} , \tag{2.2}$$

and the normal conductivity as

$$\mathbf{J}_N \equiv \sigma_N \mathbf{E} , \tag{2.3}$$

and we find the Hall resistivity by inverting the conductivity tensor

$$\rho_H = \frac{\sigma_H}{\sigma_N^2+\sigma_H^2} . \tag{2.4}$$

To leading order in the magnetic field we can neglect the Hall conductivity in the denominator; then we find the linear Hall constant given by Eq. (2.1).

In the linear-response regime, transport properties can be expressed in terms of current-current or two-particle correlation functions by using the Kubo formalism.[3] The dc conductivity tensor can be written as

$$\sigma_{\alpha\beta} = -\lim_{\omega\to 0}\left[\frac{1}{\omega}\text{Im}\Pi_{\alpha\beta}(\omega)\right] , \tag{2.5}$$

where $\Pi_{\alpha\beta}(\omega)$ is the Fourier transform of the current-current correlation function

$$\Pi_{\alpha\beta}(\tau) = -\langle \mathcal{T}_\tau[J_\alpha^\dagger(\tau)J_\beta]\rangle \tag{2.6}$$

and the current operator is

$$\mathbf{J}_\alpha = -\frac{e}{m}\sum_{(\mathbf{k},\sigma)}\mathbf{k}_\alpha c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} . \tag{2.7}$$

We take the sign convention $e>0$, and consider the system to have unit volume. Also, we set $\hbar=1$ throughout the calculation, and insert it only in our final results. By placing the current operator in the correlation function and taking the Fourier transform, we find

$$\Pi_{\alpha\beta}(\omega) = -\frac{e^2}{m^2}\sum_{(\mathbf{k},\sigma),(\mathbf{k}',\sigma')} k_\alpha k'_\beta C(i\nu_m)|_{i\nu_m=\omega+i0^+} , \tag{2.8}$$

where

$$C(i\nu_m) = \int_0^\beta d\tau\, e^{i\nu_m\tau}\langle \mathcal{T}_\tau[c_{\mathbf{k}\sigma}^\dagger(\tau)c_{\mathbf{k}\sigma}(\tau) \times c_{\mathbf{k}'\sigma'}^\dagger(0)c_{\mathbf{k}'\sigma'}(0)]\rangle$$

and β is inverse of the temperature.

In zero magnetic field, the conductivity tensor for a system of random impurities is diagonal and $k_\alpha k'_\beta$ is replaced by $\frac{1}{3}\mathbf{k}\cdot\mathbf{k}'$. For impurity or single-ion Kondo systems there is a resonant scattering of conduction electrons by the local electrons in one partial-wave channel. For this case the vertex corrections which couple the currents $\mathbf{J}_\alpha(\tau)$ and $\mathbf{J}_\beta$ vanish, because they are proportional to $\mathbf{k}\cdot\mathbf{k}'$ and odd rank harmonics $\hat{\mathbf{k}} \sim Y_1(\hat{\mathbf{k}})$ have no matrix elements in a manifold of definite angular momentum. Therefore, for Kondo systems, the transport relaxation time reduces to the lifetime of the conduction electrons. The correlation function reduces to[5]

$$\Pi_{\alpha\beta}(i\nu_m) = \frac{2e^2}{3m^2}\delta_{\alpha\beta}\sum_{\mathbf{k}}\mathbf{k}^2\frac{1}{\beta}\sum_n G_k(i\omega_n+i\nu_m)G_k(i\omega_n) , \tag{2.9}$$

where G_k is the fully dressed conduction-electron band propagator and $i\omega_n$, $i\nu_m$ are Matsubara frequencies. By analytically continuing this expression to the real axis one finds that the isotropic conductivity in zero field [see Eqs. (2.3) and (2.5)] is

$$\sigma_N = \frac{2e^2}{3m^2}\int d\varepsilon_k n(\varepsilon_k)\left[-\frac{\partial f(\varepsilon_k)}{\partial\varepsilon_k}\right]\mathbf{k}^2\tau_0(\varepsilon_k,\sigma) , \tag{2.10}$$

where τ_0 is the isotropic relaxation time, $n(\varepsilon_k)$ is the density of states for conduction electrons, and f is the Fermi function. When we model the resonant scattering in Kondo systems, e.g., for a rare-earth system with local $4f$ electrons, by using the single-ion Anderson model,[5] the isotropic relaxation rate is given as

$$\tau_0^{-1}(\varepsilon_k,\sigma) = -c|V_k|^2\,\text{Im}G_0(\varepsilon_k)$$
$$= \frac{cN_f\Gamma}{\pi N(0)}\rho_f(\varepsilon_k)+O(H^2) , \tag{2.11}$$

where

$$G_0 \equiv \sum_m G_m^{4f} = N_f G^{4f} + O(H^2) \ ,$$

$$\Gamma = \pi N(0) |V_k|^2 \ ,$$

and c is the concentration of Kondo ions, V_k is the Anderson mixing parameter, G^{4f} is the local $4f$ propagator in zero field, ρ_f is its spectral function, N_f is the degeneracy of the local state, and finally $N(0)$ is the single-particle density of states for conduction electrons at the Fermi surface,

$$N(\varepsilon) = \frac{n(\varepsilon)}{N_s} \ , \tag{2.12}$$

where N_s is the number of sites in the lattice. By placing Eq. (2.11) in (2.10), and evaluating the integral,[6] we find

$$\sigma_N = \frac{2}{N_f \Gamma} \frac{\pi N(0) n e^2}{mc} \rho_f^{-1}(0) \equiv \frac{n e^2 \tau}{m} \ , \tag{2.13}$$

where we have defined the *mean* relaxation time τ as

$$\tau = \frac{2\pi N(0)}{c N_f \Gamma} \rho_f^{-1}(0) \ . \tag{2.14}$$

At low temperatures $T \ll T_0$ the $4f$ spectral density at the Fermi surface is dominated by the Abrikosov-Suhl-Kondo peak, so that for $T = 0$ K (Ref. 5)

$$\rho_f(0) = \frac{1}{\Gamma} \sin^2 \left[\frac{\pi n_f(0)}{N_f} \right] \ , \tag{2.15a}$$

where $n_f(0)$ is the occupancy of the local f state at $T = 0$ K. At temperatures high compared to T_0, it is only the tail of the Friedel-Anderson charge peak that exists at the Fermi surface and we have

$$\rho_f(0) = \frac{\Gamma}{|\varepsilon_f|^2} \ , \tag{2.15b}$$

where ε_f is the position of the f level relative to the Fermi surface.

The Hall conductivity, Eq. (2.2), can be written in terms of the components of the conductivity tensor [see Eqs. (2.5) and (2.8)] as

$$\sigma_H = \tfrac{1}{2}(\sigma_{xy} - \sigma_{yx}) = \frac{e^2}{m^2} \sum_{(\mathbf{k},\sigma),(\mathbf{k}',\sigma')} \tfrac{1}{2}(k_x k_y' - k_y k_x') \times \lim_{\omega \to 0} \left[\frac{1}{\omega} \mathrm{Im} C(\omega + i0^+) \right] . \tag{2.16}$$

We rewrite the Cartesian components of the wave vectors $\mathbf{k}, \mathbf{k}'$ in terms of spherical harmonics as

$$\tfrac{1}{2}(k_x k_y' - k_y k_x') = -\frac{4\pi i}{\sqrt{6}} k k' \sum_m \begin{bmatrix} 1 & 1 & 1 \\ m & -m & 0 \end{bmatrix} \times Y_1^m(\hat{\mathbf{k}}) Y_1^{-m}(\hat{\mathbf{k}}') , \tag{2.17}$$

where the expression in large parentheses is a 3-j symbol. We can now see that the Hall effect exists only when the expectation values of $\langle Y^1(\hat{\mathbf{k}}) \rangle$ and $\langle Y^1(\hat{\mathbf{k}}') \rangle$ are nonzero. This assumes we have made a random-phase approximation in averaging $C(\omega)$ over the positions of the Kondo ions; see the discussion below. As these are proportional to integrals over three spherical harmonics, this occurs only if we consider that scattering occurs in two channels of *opposite* parity and differing by one. Therefore, if the resonant scattering of conduction electrons occurs in the $l = 3$ channel, e.g., for rare-earth Kondo systems, then we must consider either the $l = 2$ or $l = 4$ channel to obtain a Hall effect. We limit our attention to the nonresonant $l = 2$ channel, as most of the rare-earth Kondo compounds have conduction bands with far larger $l = 2$ partial-wave character than $l = 4$. As the expectation value $\langle k_\alpha k_\beta' \rangle$ exists for $k \neq k'$ in order to obtain a Hall effect, we immediately note that there are *vertex corrections* to the Hall conductivity for Kondo systems even though there were none for the normal conductivity.

To evaluate the correlation function Eq. (2.8) we must sum over the scattering sites as they enter in the Heisenberg representation of the conduction-electron operators $c_{\mathbf{k}}^\dagger(\tau)$ and $c_{\mathbf{k}}(\tau)$. We will consider that the Kondo ions are randomly distributed on a regular lattice and we neglect (1) interactions between Kondo ions, and (2) the interference terms coming from scatterings at different sites. Therefore, we make the random-phase approximation in evaluating the correlation function $C(\omega)$, and we can write

$$C(\omega) \equiv N_i C_i(\omega) \tag{2.18}$$

where N_i is the number of Kondo ions ("impurities") on the lattice and $C_i(\omega)$ is the correlation function for *one site*. This approximation becomes exact when $N_i \ll N_s$, i.e., in the dilute limit. We continue to use it for moderately dense Kondo systems as long as the scattering is *incoherent*, i.e., uncorrelated from one site to another.

The one-site correlation function can be written as[3]

$$C_i(i\nu_m) = \frac{1}{\beta^2} \sum_{i\omega_1, i\omega_2} G_{\mathbf{k}\sigma}(i\omega_1) G_{\mathbf{k}\sigma}(i\nu_m + i\omega_1) \times G_{\mathbf{k}',\sigma'}(i\omega_2) G_{\mathbf{k}'\sigma'}(i\nu_m + i\omega_2) \times \Gamma(i\nu_m, i\omega_1, i\omega_2) \ , \tag{2.19}$$

where $1/\beta$ is the temperature and Γ is s four-point vertex function. There are two types of contributions to the Hall effect which we will refer to as types I and II.

Type-I contributions are those for which there is no transfer of energy between the electron and hole propagators. For these we write the correlation function (a two-particle propagator) as a product of two single-particle propagators (see Fig. 1). In this case the vertex function Γ reduces to the product of two T matrices. To obtain a Hall effect we must consider that the two single-particle propagators correspond to conduction electrons in partial-wave channels of opposite parity, e.g., $l = 2$ and 3. Therefore we can write the vertex function for type-I contributions as

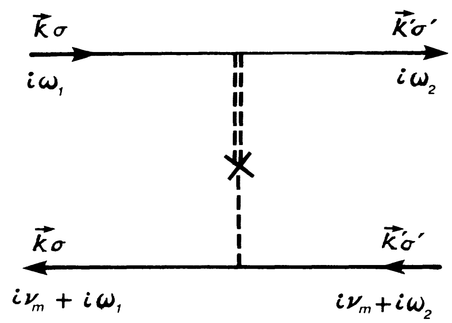

FIG. 1. The vertex function for type-I contributions. In this diagram the upper propagator is for the $l=3$ channel and the scattering due to the Anderson mixing interaction is described by the T matrix $T^{(3)}_{k'\sigma',\mathbf{k}\sigma}(i\omega_1)$. The lower propagator is for the nonresonant $l=2$ channel; the scattering comes from the two-electron interaction H_2 [see Eq. (3.4)] when it is reduced to a one-electron scattering potential and is described by $T^{(2)}_{\mathbf{k}\sigma,\mathbf{k}'\sigma'}(i\nu_m+i\omega_2)$. The cross signifies both scatterings occur at the *same* site. Note there are no energy transfers for type-I processes, thus the scatterings are *elastic* $\omega_1=\omega_2$. A second diagram with $l=2$ on top and $l=3$ on bottom also contributes to the Hall constant.

$$\Gamma_{\mathrm{I}}(i\nu_m,i\omega_1,i\omega_2)=\beta T^{(3)}_{\mathbf{k}'\sigma',\mathbf{k}\sigma}(i\omega_1)\times T^{(2)}_{\mathbf{k}\sigma,\mathbf{k}'\sigma'}(i\nu_m+i\omega_2)\delta_{\omega_1,\omega_2}\ , \quad (2.20)$$

where the $T^{(l)}$ are the on-shell (*elastic* scattering) T matrices for the conduction-electron partial-wave channels $l=2$ and 3. We use the convention

$$T_{k',k}\equiv\langle k'|T|k\rangle=T_{k\to k'}\ . \quad (2.20a)$$

As we show in the next section, this contribution to the Hall effect reproduces the skew-scattering contributions found by using the Boltzmann transport equation.[1] Also, it picks up a spin-dependent contribution when we consider spin scattering in the nonresonant $l=2$ channel.

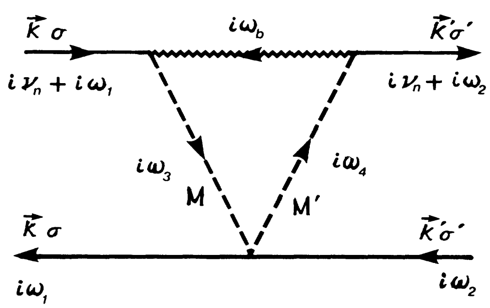

FIG. 2. The vertex function for type-II contributions. The boson frequency is given as $i\omega_b=i\omega_3-i\omega_1-i\nu_n$, and $i\omega_4=i\omega_3+i\omega_2-i\omega_1$. Here, there are energy transfers between the resonant $l=3$ (the top propagator) and the nonresonant $l=2$ channel. The solid lines are conduction-electron propagators $G_{\mathbf{k}\sigma}$, the dashed lines are pseudo-f propagators G_m, and the wiggly line is a boson propagator D. The scattering into and out of the resonant channel comes from the Anderson mixing interaction [Eq. (3.3)] and the two-electron scattering in the $l=2$ channel is described by Eq. (3.4). A second diagram with $l=2$ on top and $l=3$ on bottom also contributes to the Hall constant.

The type-II contributions come from vertex corrections with energy exchange between the electron-hole propagators (see Fig. 2). As we show in Sec. IV these terms lead to entirely new contributions to the EHE which are totally unaccounted for in the semiclassical approach which uses the conventional Boltzmann transport equation.

III. EVALUATION OF TYPE-I CONTRIBUTIONS

To calculate the correlation functions [Eq. (2.8) or (2.19)] needed for the Hall effect we use the Anderson mixing interaction to produce resonant scattering in one channel. We will consider local f states, therefore it is the $l=3$ partial-wave channel of the conduction electrons which are resonantly scattered by the mixing interaction. For the scattering in the nonresonant $l=2$ channel we use a two-electron scattering term. This term could come from the direct and exchange Coulomb interaction between local and conduction electrons; however, this detail is not needed, and we merely introduce an unknown parameter to represent the scattering in the nonresonant channel. This parameter is determined by fitting to the data on the Hall constant.[1]

The single-ion Anderson Hamiltonian for a local f orbital in a spin-orbit-coupled j state in the limit of infinite U (intra-atomic Coulomb energy),[7] together with an additional scattering term in the nonresonant channels is given as

$$H=H_0+H_{\mathrm{mix}}+H_2\ , \quad (3.1)$$

where

$$H_0=\sum_{(\mathbf{k},\sigma)}\varepsilon_{\mathbf{k}}c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}+\varepsilon_f\sum_m f^{\dagger}_m f_m\ , \quad (3.2)$$

$$H_{\mathrm{mix}}=\frac{1}{(N_s)^{1/2}}\sum_{(\mathbf{k},\sigma),m}V_{\mathbf{k}\sigma,m}c^{\dagger}_{\mathbf{k}\sigma}b^{\dagger}f_m+\mathrm{H.c.}\ , \quad (3.3)$$

and

$$H_2=\frac{1}{N_s}\sum_{(\mathbf{k},\sigma)m;(\mathbf{k}',\sigma'),m'}J(k)Y_2(\hat{\mathbf{k}})\cdot Y_2(\hat{\mathbf{k}}')\times\langle\sigma'm'|a+b\mathbf{s}\cdot\mathbf{J}|\sigma m\rangle\times c^{\dagger}_{\mathbf{k}'\sigma'}c_{\mathbf{k}\sigma}f^{\dagger}_{m'}f_m\ . \quad (3.4)$$

In this limit of infinite U an auxiliary or slave boson has been introduced in the mixing term to keep track of the occupancy of the f level.[8] We note no bosons enter the two-particle interaction H_2 because it does not change the number of f electrons. To obtain a contribution to the EHE we must explicitly consider the dependence of the mixing interaction $V_{\mathbf{k}\sigma,m}$ on $\hat{\mathbf{k}}$ and m when the local f orbital is in a spin-orbit-coupled j state.[7] When we make the approximation of *spherical* symmetry for the mixing interaction, we scatter that part of a plane wave which has the same symmetry as the local state it is mixing with, i.e.,

$$\langle kjm|\mathbf{k}\sigma\rangle=(-1)^{l-1/2+m}\sqrt{4\pi(2j+1)}i^{l}\times\sum_{m'}Y_l^{m'}(\hat{\mathbf{k}})\begin{bmatrix} l & \frac{1}{2} & j \\ m' & \sigma & -m\end{bmatrix} . \tag{3.5}$$

For cerium $l=3$ and $j=\frac{5}{2}$, we find

$$V_{\mathbf{k}\sigma,m}=(-1)^{7/2+m}\sqrt{24\pi}iV_k\times\sum_{m_1}\begin{bmatrix} 3 & \frac{1}{2} & \frac{5}{2} \\ m_1 & \sigma & -m\end{bmatrix}Y_3^{m_1}(\hat{\mathbf{k}}) . \tag{3.3'}$$

Also, the Hall effect occurs in the presence of a magnetic field. The dominant effect of the field will be on the local f state, and we include this in the local f propagator $G^{4f}_{mm'}(i\omega_1)$. It is this field that makes $G^{4f}_{mm'}$ dependent on the orbital indices m and m'. When we choose the direction of the magnetic field as the axis of spatial quantization for our states, the propagator is diagonal in m, and the T matrix describing the scattering of conduction electrons in the resonant channel due to the mixing interaction [Eq. (3.3)] is given as

$$T^{(3)}_{\mathbf{k}'\sigma',\mathbf{k}\sigma}(i\omega_1)=\sum_m V^*_{\mathbf{k}\sigma,m}V_{\mathbf{k}'\sigma',m}G^{4f}_m(i\omega_1)$$
$$=\frac{24\pi|V_k|^2}{N_s}\sum_m G^{4f}_m(i\omega_1)\sum_{m_1,m_2}\begin{bmatrix} 3 & \frac{1}{2} & \frac{5}{2} \\ m_1 & \sigma & -m\end{bmatrix}\begin{bmatrix} 3 & \frac{1}{2} & \frac{5}{2} \\ m_2 & \sigma' & -m\end{bmatrix}[Y_3^{m_1}(\hat{\mathbf{k}})]^*Y_3^{m_2}(\hat{\mathbf{k}}') . \tag{3.6}$$

To obtain the T matrix in the nonresonant channel we take the expectation values of the f-electron operators in the two-particle scattering interaction [Eq. (3.4)]:

$$\langle f^\dagger_{m'}f_m\rangle=n_{fm}\delta_{mm'} . \tag{3.7}$$

To first order in the coupling constant $J(k)$, the scattering matrix is

$$t^{(2)}_{\mathbf{k}\sigma,\mathbf{k}'\sigma'}=\frac{J(k)}{N_s}Y_2(\hat{\mathbf{k}})\cdot Y_2(\hat{\mathbf{k}}')\sum_m(a+b\sigma m)n_{fm}\delta_{\sigma\sigma'}$$
$$=\frac{J(k)}{N_s}Y_2(\hat{\mathbf{k}})\cdot Y_2(\hat{\mathbf{k}}')(an_f+b\sigma\overline{m})\delta_{\sigma\sigma'} , \tag{3.8}$$

where

$$n_f\equiv\sum_m n_{fm}$$

and

$$\overline{m}\equiv\sum_m mn_{fm}=-\frac{M}{g\mu_B} .$$

Here n_f is the number of electrons in the f level, and $\overline{m}$ is, to within $g\mu_B$ ($\mu_B>0$), the magnetization. As we show later on when we obtain the full T matrix to all orders in the charge scattering, the exchange constant is *complex*; therefore we represent it in general as $\tilde{J}(\varepsilon)$. From Eq. (3.8) we note that while these are spin-dependent terms they are *not* spin-flip terms $\sigma'\neq\sigma$.

When we place these T matrices in the correlation function [see Eqs. (2.19) and (2.20)] and if we consider *isotropic* band propagators, i.e., $G_{\mathbf{k}\sigma}(\varepsilon)=G_{k\sigma}(\varepsilon)$, we find the contribution to the Hall conductivity [Eq. (2.16)] from this diagram (see Fig. 1) is given as

$$\sigma_H(1)=\frac{e^2}{m^2}\mathrm{Im}\Bigg[-\frac{4\pi i}{\sqrt{6}}\frac{24\pi}{N_s^2}N_i\sum_\sigma(an_f+b\sigma\overline{m})\sum_{m_1,m_2,m_3}\begin{bmatrix} 3 & \frac{1}{2} & \frac{5}{2} \\ m_1 & \sigma & -m_3\end{bmatrix}\begin{bmatrix} 3 & \frac{1}{2} & \frac{5}{2} \\ m_2 & \sigma & -m_3\end{bmatrix}\sum_{m',m_4}\begin{bmatrix} 1 & 1 & 1 \\ m' & -m' & 0\end{bmatrix}$$
$$\times\int\frac{d\Omega_k}{4\pi}[Y_3^{m_1}(\hat{\mathbf{k}})]^*Y_2^{m_4}(\hat{\mathbf{k}})Y_1^{m'}(\hat{\mathbf{k}})\int\frac{d\Omega_{k'}}{4\pi}Y_3^{m_2}(\hat{\mathbf{k}}')[Y_2^{m_4}(\hat{\mathbf{k}}')]^*Y_1^{-m'}(\hat{\mathbf{k}}')\sum_{k,k'}|V_k|^2kk'$$
$$\times\lim_{\omega\to0}\frac{1}{\omega}\left\{\frac{1}{\beta}\sum_{i\omega_1}G_{k\sigma}(i\omega_1)G_{k\sigma}(i\nu_m+i\omega_1)G_{k'\sigma}(i\omega_1)G_{k'\sigma}(i\nu_m+i\omega_1)G^{4f}_{m_3}(i\omega_1)\tilde{J}(i\nu_m+i\omega_1)|_{i\nu_m=\omega+i0^+}\right\}\Bigg] . \tag{3.9}$$

We have replaced the sum over $\mathbf{k}$ as an angular integration and a sum over the magnitude k. By evaluating the integrals over the spherical harmonics and by recoupling the 3-j symbols,[9] we find

$$6\sum_{m_3}G^{4f}_{m_3}\sum_{m_1,m_2,\sigma}\begin{bmatrix} 3 & \frac{1}{2} & \frac{5}{2} \\ m_1 & \sigma & -m_3\end{bmatrix}\begin{bmatrix} 3 & \frac{1}{2} & \frac{5}{2} \\ m_2 & \sigma & -m_3\end{bmatrix}\sum_m(a+b\sigma m)n_{fm}$$
$$\times\sum_{m',m_4}\begin{bmatrix} 1 & 1 & 1 \\ m' & -m' & 0\end{bmatrix}\int d\Omega_k[Y_3^{m_1}(\hat{\mathbf{k}})]^*Y_2^{m_4}(\hat{\mathbf{k}})Y_1^{m'}(\hat{\mathbf{k}})\int d\Omega_{k'}Y_3^{m_2}(\hat{\mathbf{k}}')[Y_2^{m_4}(\hat{\mathbf{k}}')]^*Y_1^{-m'}(\hat{\mathbf{k}}')$$
$$=\frac{\sqrt{6}}{49\pi}(an_fG_1-\tfrac{7}{12}b\overline{m}G_0-\tfrac{1}{24}b\overline{m}G_2)$$
$$\equiv-\frac{\sqrt{6}}{49\pi}\tilde{G} , \tag{3.10}$$

where

$$G_r \equiv \sum_m O_0^r(m) G_m \ , \tag{3.11}$$

and $O_0^r(m)$ are rth-rank polynomials whose traces, except for $r=0$, are zero; e.g., for $j=\frac{5}{2}$, $O_0^0=1$, $O_0^1=m$, and $O_0^2=3m^2-\frac{35}{4}$. By placing this in Eq. (3.9) we find

$$\sigma_H(1)=\frac{c}{49\pi}\frac{e^2}{m^2N_s}\sum_{k,k'}|V_k|^2 kk' \mathrm{Im} \lim_{\omega\to 0}\left[\frac{1}{\omega}\left[\frac{i}{\beta}\sum_{i\omega_1} G_{k\sigma}(i\omega_1)G_{k\sigma}(i\nu_m+i\omega_1)G_{k',\sigma}(i\omega_1)G_{k'\sigma}(i\nu_m+i\omega_1) \times \tilde{G}(i\omega_1)\tilde{J}(i\nu_m+i\omega_1)|_{i\nu_m=\omega+i0^+}\right]\right] , \tag{3.12}$$

where we have defined the concentration $c\equiv N_i/N_s$. The sum over the Matsubara frequencies has been evaluated in a manner analogous to that given in Ref. 3. When we consider the type-I diagram with the $l=2$ and $l=3$ reversed we obtain a second contribution which is identical to the first. Thus the total contribution from type-I diagrams to the Hall conductivity is

$$\sigma_H(\mathrm{I})=\frac{4c}{49\pi}\frac{e^2}{m^2N_s}\sum_{k,k'}|V_k|^2 kk'\int\frac{d\varepsilon}{2\pi}\left[-\frac{\partial f(\varepsilon)}{\partial\varepsilon}\right]\mathrm{Im}[G^R_{\mathbf{k}\sigma}(\varepsilon)G^R_{k'\sigma}(\varepsilon)i\tilde{G}(\varepsilon)]\mathrm{Im}[G^R_{\mathbf{k}\sigma}(\varepsilon)G^R_{k'\sigma}(\varepsilon)\tilde{J}(\varepsilon)] , \tag{3.13}$$

where $G^R(\varepsilon)$ is the retarded propagator.

In the case of single-ion Kondo scattering, i.e., in the dilute limit, the spectral functions for the conduction electrons are δ functions:

$$\mathrm{Im}G^R_{k\sigma}(\varepsilon)=-\pi\delta(\varepsilon-\varepsilon_{k\sigma}) . \tag{3.14}$$

We evaluate Eq. (3.13) in the dilute limit as shown in Ref. 3, and find

$$\sigma_H(\mathrm{I})=\frac{8\pi c}{49}\frac{e^2}{m^2N_s}\sum_{k,k'}|V_k|^2 kk'\int\frac{d\varepsilon}{2\pi}\left[-\frac{\partial f(\varepsilon)}{\partial\varepsilon}\right]\tau_0(\varepsilon_k)\tau_0(\varepsilon_{k'})\delta(\varepsilon-\varepsilon_k)\delta(\varepsilon-\varepsilon_{k'})\mathrm{Im}[\tilde{G}(\varepsilon)\tilde{J}(\varepsilon)] , \tag{3.15}$$

where the relaxation time is given by Eq. (2.11). We replace the sums over k and k' by integrals and take the temperature low compared to the Fermi energy so that we can *approximately* replace the derivative of the Fermi function by a δ function at the Fermi surface $\delta(\varepsilon)$. This approximation is valid for $T>T_0$ and for $T=0$ K; however, it should not be used for $0<T<T_0$. By evaluating the integral in Eq. (3.15) we find that the contribution to the Hall conductivity from type-I diagrams in the dilute limit is

$$\sigma_H(\mathrm{I})=\frac{c}{49}\frac{n^2(0)e^2\tau^2}{m^2N_s}|V_{k_F}|^2 k_F^2\mathrm{Im}[\tilde{G}(0)\tilde{J}(0)] . \tag{3.16}$$

For a band of free electrons we use $n(0)=3n/2E_F$, where n is the number of conduction electrons per unit volume *and* spin direction, $k_F^2=2mE_F$, $n(0)=N(0)N_s$ [Eq. (2.12)], and $\pi N(0)|V_{k_F}|^2=\Gamma$. Finally, we find

$$\sigma_H(\mathrm{I})=\frac{3c}{49\pi}\frac{ne^2\tau^2}{m}\Gamma\,\mathrm{Im}[\tilde{G}(0)\tilde{J}(0)] . \tag{3.17}$$

By using Eqs. (2.1) and (2.13), we find the Hall constant from type-I contributions in the dilute limit is

$$R_H(\mathrm{I})=\frac{3}{49\pi}\frac{mc}{ne^2\hbar}\frac{\Gamma}{H}\mathrm{Im}[\tilde{G}(0)\tilde{J}(0)] . \tag{3.18}$$

Note we have inserted $\hbar$ to obtain the proper units for the Hall constant.

To first order in the two-particle scattering, $\tilde{J}(0)\equiv J$ is real, and the contribution to the Hall constant is

$$R_H(\mathrm{I})=-\frac{3}{49}\frac{mc}{\pi ne^2\hbar}\Gamma J\left[an_f(\rho_1/H)+\frac{b}{12}(\chi/g\mu_B)(7\rho_0+\tfrac{1}{2}\rho_2)\right] , \tag{3.19}$$

where $\rho_r=-\mathrm{Im}G_r(0)$ are the spectral densities of the functions Eq. (3.11) and χ is the magnetic susceptibility. The charge- (impurity-) scattering contribution which is proportional to a is identical to that previously found by using the Boltzmann equation if we set $n_f=1$.[1] The spin (exchange) contribution is new. By using Eq. (2.13) it can be written as

$$R_H^{\mathrm{spin}}(\mathrm{I})=-\frac{J_{\mathrm{ex}}N(0)}{14}\left[1+\frac{1}{14}\frac{\rho_2}{\rho_0}\right]\frac{\chi}{g\mu_B}\rho_{\mathrm{iso}} , \tag{3.20}$$

where we used $bJ\equiv J_{\mathrm{ex}}$, $\rho_0=N_f\rho_f$, and $\rho_{\mathrm{iso}}=\sigma_N^{-1}$ [see Eq. (2.13)]. For the linear Hall constant we can neglect ρ_2 as it is proportional to H^2. Then we find the temperature dependence of the spin contribution from type-I diagrams to the linear Hall constant is *completely* given by the susceptibility and normal resistivity.

The on-shell (elastic scattering) T matrix for the nonresonant channel to all orders in the *charge* scattering and first order in the spin scattering is[10]

$$T^{(2)}_{\mathbf{k}\sigma,\mathbf{k}'\sigma'}=-\frac{4}{n(\varepsilon_k)}e^{-i\eta_2(\varepsilon_k)}\sin[\eta_2(\varepsilon_k)]\times\left[1-\frac{J_{\rm ex}}{\Delta_2}\bar{m}\sigma e^{-i\eta_2(\varepsilon_k)}\sin[\eta_2(\varepsilon_k)]\right]\times Y_2(\hat{\mathbf{k}})\cdot Y_2(\hat{\mathbf{k}}')\delta_{\sigma\sigma'}\ , \quad (3.21)$$

where $J_{\rm ex}=bJ$, η_2 is the phase shift in the nonresonant channel, and Δ_2 is the half-width of the virtual bound state formed by the charge scattering.[10] When we use this T matrix instead of Eq. (3.8) we make the following replacements:

$$\tilde{J}(k)\rightarrow-\frac{4}{N(\varepsilon_k)}e^{-i\eta_2(k)}\sin[\eta_2(k)]\ ,$$

$$an_f\rightarrow 1\ , \quad (3.22)$$

and

$$b\rightarrow-\frac{J_{\rm ex}}{\Delta_2}e^{-i\eta_2(k)}\sin[\eta_2(k)]\ .$$

By placing these in Eq. (3.18) we find that the charge scattering gives a type-I contribution to the Hall constant of

$$R_H^{\rm charge}({\rm I})=\frac{12}{49}\frac{mc}{\pi N(0)ne^2\hbar}\frac{\Gamma}{H}\times\sin\eta_2(\rho_1\cos\eta_2+R_1\sin\eta_2)\ , \quad (3.23)$$

where $R_r\equiv{\rm Re}G_r(0)$. This expression is *identical* to that previously found.[1] The spin-or exchange-scattering contribution to the linear Hall constant is given as

$$R_H^{\rm spin}({\rm I})=-\frac{1}{7}\frac{J_{\rm ex}}{\Delta_2}\frac{mc\Gamma}{\pi N(0)ne^2\hbar}\frac{\chi}{g\mu_B}\times\sin^2\eta_2(\rho_0\cos2\eta_2+R_0\sin2\eta_2)\ . \quad (3.24)$$

When we write the normal resistivity [see Eq. (2.13)] as

$$\rho_{\rm iso}=\frac{\rho_0}{2}\frac{mc\Gamma}{\pi N(0)ne^2\hbar} \quad (3.25)$$

and define $R_{\rm iso}$ in a similar way with R_0 instead of ρ_0, we find

$$R_H^{\rm spin}({\rm I})=-\frac{2}{7}\frac{J_{\rm ex}}{\Delta_2}\frac{\chi}{g\mu_B}\sin^2\eta_2(\rho_{\rm iso}\cos2\eta_2+R_{\rm iso}\sin2\eta_2)\ . \quad (3.26)$$

We note from Eq. (3.20) that the major modification of the spin contribution to the Hall constant when we include the effects of charge scattering is to reduce it by

$$\frac{1}{\Delta_2 N(0)}\sin^2\eta_2\ .$$

For small phase shifts $\eta_2\sim\Delta_2/O(E_F)$ and as $N(0)\sim1/E_F$, we find the reduction is $\sim O(\Delta_2/E_F)$.

IV. TYPE-II CONTRIBUTIONS

The vertex function for type-II diagrams is found from Fig. 2 to be

$$\Gamma_2(i\nu_n,i\omega_1,i\omega_2)=\frac{1}{\beta}\sum_{i\omega_3}D(i\omega_3-i\omega_1-i\nu_n)\sum_{m,m'}G_m(i\omega_3)G_{m'}(i\omega_3+i\omega_2-i\omega_1)V^*_{\mathbf{k}\sigma,m}V_{\mathbf{k}'\sigma',m'}\langle\sigma m'|H_2|\sigma'm\rangle\ , \quad (4.1)$$

where the $V_{\mathbf{k}\sigma,m}$ and H_2 are defined by Eqs. (3.3') and (3.4), the $D(i\omega_n)$ is a renormalized f^0 or slave boson propagator, and $G_m(i\omega_n)$ is a pseudo-f-electron propagator.[11] By placing this vertex function in Eq. (2.19) we find that the one-site correlation function *without* the coupling constants V_k and J is

$$C^{(2)}_{mm'}(\omega)=\left[\frac{1}{\beta}\right]^3\sum_{i\omega_1,i\omega_2,i\omega_3}G_{\mathbf{k}\sigma}(i\omega_1)G_{\mathbf{k}\sigma}(i\nu_n+i\omega_1)G_{\mathbf{k}'\sigma'}(i\omega_2)G_{\mathbf{k}'\sigma'}(i\nu_n+i\omega_2)\times D(i\omega_3-i\omega_1-i\nu_n)G_m(i\omega_3)G_{m'}(i\omega_3+i\omega_2-i\omega_1)|_{i\nu_n=\omega+i0^+}\ . \quad (4.2)$$

In Appendix A we have evaluated the sums over the Matsubara frequencies. The ensuing general expressions are unwieldy and we have immediately considered the case of single-ion Kondo scattering, i.e., the dilute limit, where Eq. (3.14) applies. We can already see from Eq. (3.9) that the only complex number entering σ_H besides $C^{(2)}_{mm'}(\omega)$ is the imaginary term entering from Eq. (2.17). Therefore we find

$$\lim_{\omega\rightarrow0}\left[{\rm Im}\frac{iC^{(2)}_{mm'}(\omega)}{\omega}\right]=-\int\frac{d\varepsilon}{2\pi}\left[-\frac{\partial f(\varepsilon)}{\partial\varepsilon}\right]\int\frac{d\varepsilon'}{\pi}f(\varepsilon')(1-e^{\beta(\varepsilon'-\varepsilon)})\times\int\frac{d\varepsilon''}{\pi}\frac{e^{-\beta\varepsilon''}}{Z_{4f}}\bar{G}_{k\sigma}(\varepsilon)\bar{G}_{k'\sigma'}(\varepsilon')B(\varepsilon''-\varepsilon')A_{m'}(\varepsilon'')A_m(\varepsilon''-\varepsilon'+\varepsilon)\ , \quad (4.3)$$

where

$$\bar{G}_{k\sigma}(\varepsilon)\equiv G^R_{k\sigma}(\varepsilon)G^A_{k\sigma}(\varepsilon)\ , \quad (4.4a)$$

that is, a product of a retarded and advanced propagator for the conduction electron, Z_{4f} is the $4f$ partition function, and $A_m(\varepsilon)$ and $B(\varepsilon)$ are spectral functions of the pseudo-f-electron and boson propagators.[11] In the dilute limit (see Appendix A) the function $\bar{G}_{k\sigma}$ reduces to

$$\bar{G}_{k\sigma}(\varepsilon)=2\pi\tau_0(\varepsilon)\delta(\varepsilon-\varepsilon_{k\sigma}) . \tag{4.4b}$$

We place the result [Eq. (4.3)] together with the coupling constants $V_{k\sigma,m}$ and J in the expression for the Hall conductivity [Eqs. (2.16) and (2.17)], and multiply our result by 2 to take account of a similar type-II contribution where the role of the $l=2$ and 3 channels is interchanged. Then we find that the contribution to the Hall conductivity from these two type-II diagrams is

$$\begin{aligned}\sigma_H(\mathrm{II})=&\frac{e^2}{m^2}\frac{8\pi}{\sqrt{6}}\frac{24\pi|V_k|^2N_i}{N_s^2}\sum_{m,m',\sigma,\sigma'}(-1)^{m'-m}\langle\sigma m'|a+b\mathbf{s}\cdot\mathbf{J}|\sigma' m\rangle\\ &\times\sum_{m_1,m_2,m_3}\begin{bmatrix}3 & \frac{1}{2} & \frac{5}{2}\\ m_1 & \sigma & -m\end{bmatrix}\begin{bmatrix}3 & \frac{1}{2} & \frac{5}{2}\\ m_2 & \sigma' & -m'\end{bmatrix}\begin{bmatrix}1 & 1 & 1\\ m_3 & -m_3 & 0\end{bmatrix}\sum_{m_4}\int\frac{d\Omega_k}{4\pi}[Y_3^{m_1}(\hat{\mathbf{k}})]^*Y_2^{m_4}(\hat{\mathbf{k}})Y_1^{m_3}(\hat{\mathbf{k}})\\ &\times\int\frac{d\Omega_{k'}}{4\pi}Y_3^{m_2}(\hat{\mathbf{k}}')[Y_2^{m_4}(\hat{\mathbf{k}}')]^*Y_1^{-m_3}(\hat{\mathbf{k}}')\int d\varepsilon_k\,n(\varepsilon_k)kJ(k)\int d\varepsilon_{k'}\,n(\varepsilon_{k'})k'\\ &\times\int\frac{d\varepsilon}{2\pi}\left[-\frac{\partial f(\varepsilon)}{\partial\varepsilon}\right]\int\frac{d\varepsilon'}{\pi}f(\varepsilon')(1-e^{\beta(\varepsilon'-\varepsilon)})\int\frac{d\varepsilon''}{\pi}\frac{e^{-\beta\varepsilon''}}{Z_{4f}}\bar{G}_{k\sigma}(\varepsilon)\bar{G}_{k'\sigma'}(\varepsilon')B(\varepsilon''-\varepsilon')A_{m'}(\varepsilon'')A_m(\varepsilon''-\varepsilon'+\varepsilon) .\end{aligned} \tag{4.5}$$

By evaluating the integrals over the spherical harmonics and recoupling the 3-j symbols we find[9]

$$\begin{aligned}\sum_{m_3,m_4}\begin{bmatrix}1 & 1 & 1\\ m_3 & -m_3 & 0\end{bmatrix}&\int d\Omega_k[Y_3^{m_1}(\hat{\mathbf{k}})]^*Y_2^{m_4}(\hat{\mathbf{k}})Y_1^{m_3}(\hat{\mathbf{k}})\int d\Omega_{k'}Y_3^{m_2}(\hat{\mathbf{k}}')[Y_2^{m_4}(\hat{\mathbf{k}}')]^*Y_1^{-m_3}(\hat{\mathbf{k}}')\\ &=-\frac{3}{4\pi}\sqrt{2/7}(-1)^{m_1}\begin{bmatrix}3 & 3 & 1\\ -m_1 & m_2 & 0\end{bmatrix} .\end{aligned} \tag{4.6}$$

The matrix elements for the potential- or charge-scattering term are

$$\langle\sigma m'|a|\sigma' m\rangle=a\delta_{\sigma\sigma'}\delta_{mm'} . \tag{4.7}$$

By recoupling the 3-j symbols in Eqs. (4.5) and (4.6) with the above condition we find

$$\begin{aligned}\sum_{m_1,m_2}(-1)^{m_1}&\begin{bmatrix}3 & \frac{1}{2} & \frac{5}{2}\\ m_1 & \sigma & -m\end{bmatrix}\begin{bmatrix}3 & \frac{1}{2} & \frac{5}{2}\\ m_2 & \sigma & -m\end{bmatrix}\begin{bmatrix}3 & 3 & 1\\ -m_1 & m_2 & 0\end{bmatrix}\\ &=(-1)^{1+m-\sigma}\sum_{s,j}(2s+1)(2j+1)\begin{Bmatrix}1 & s & j\\ 3 & \frac{1}{2} & \frac{5}{2}\\ 3 & \frac{1}{2} & \frac{5}{2}\end{Bmatrix}\begin{bmatrix}1 & s & j\\ 0 & 0 & 0\end{bmatrix}\begin{bmatrix}\frac{5}{2} & \frac{5}{2} & j\\ -m & m & 0\end{bmatrix}\begin{bmatrix}\frac{1}{2} & \frac{1}{2} & s\\ \sigma & -\sigma & 0\end{bmatrix} ,\end{aligned} \tag{4.8}$$

where the expression in curly brackets is a 9-j symbol.[9] By using Eq. (4.8) we sum over m and σ in Eq. (4.5) and find that the type-II charge-scattering contribution to the Hall conductivity is

$$\begin{aligned}\sigma_H^{\mathrm{charge}}(\mathrm{II})=&-\frac{c}{49\pi}\frac{e^2}{m^2}\frac{a|V_k|^2}{N_s}\int d\varepsilon_k\,kJ(k)n(\varepsilon_k)\int d\varepsilon_{k'}\,k'n(\varepsilon_{k'})\int\frac{d\varepsilon}{2\pi}\left[-\frac{\partial f(\varepsilon)}{\partial\varepsilon}\right]\\ &\times\int\frac{d\varepsilon'}{\pi}f(\varepsilon')(1-e^{\beta(\varepsilon'-\varepsilon)})\int\frac{d\varepsilon''}{\pi}\frac{e^{-\beta\varepsilon''}}{Z_{4f}}B(\varepsilon''-\varepsilon')\left[\sum_\sigma\bar{G}_{k\sigma}(\varepsilon)\bar{G}_{k'\sigma}(\varepsilon')\sum_m m\,A_m(\varepsilon'')A_m(\varepsilon''-\varepsilon'+\varepsilon)\right.\\ &\left.-\tfrac{7}{3}\sum_\sigma\sigma\bar{G}_{k\sigma}(\varepsilon)\bar{G}_{k'\sigma}(\varepsilon')\left[\sum_m A_m(\varepsilon'')A_m(\varepsilon''-\varepsilon'+\varepsilon)+\tfrac{1}{14}\sum_m O_0^2(m)A_m(\varepsilon'')A_m(\varepsilon''-\varepsilon'+\varepsilon)\right]\right] .\end{aligned} \tag{4.9}$$

To obtain the linear Hall constant we keep only the leading-order terms in the magnetic field. The field enters the pseudo-$4f$ spectral functions and energies of the conduction electrons [see Eq. (4.4b)]. To leading order in the field we find

$$\sum_\sigma\bar{G}_{k\sigma}(\varepsilon)\bar{G}_{k'\sigma}(\varepsilon')=\tfrac{1}{2}\bar{G}_k^0(\varepsilon)\bar{G}_{k'}^0(\varepsilon')+O(H^2) , \tag{4.10a}$$

$$\sum_m m A_m(\varepsilon'')A_m(\varepsilon''-\varepsilon'+\varepsilon)=\frac{1}{N_f}[A^1(\varepsilon'')A^0(\varepsilon''-\varepsilon'+\varepsilon)+A^0(\varepsilon'')A^1(\varepsilon''-\varepsilon'+\varepsilon)]+O(H^3)\ , \tag{4.10b}$$

$$\sum_\sigma \sigma\overline{G}_{k\sigma}(\varepsilon)\overline{G}_{k'\sigma}(\varepsilon')=\tfrac{1}{2}[\overline{G}\,^1_k(\varepsilon)\overline{G}\,^0_{k'}(\varepsilon')+\overline{G}\,^0_k(\varepsilon)\overline{G}\,^1_{k'}(\varepsilon')]+O(H^3)\ , \tag{4.10c}$$

$$\sum_m A_m(\varepsilon'')A_m(\varepsilon''-\varepsilon'+\varepsilon)=\frac{1}{N_f}A^0(\varepsilon'')A^0(\varepsilon''-\varepsilon'+\varepsilon)+O(H^2)\ , \tag{4.10d}$$

and

$$\sum_m O_0^2(m)A_m(\varepsilon'')A_m(\varepsilon''-\varepsilon'+\varepsilon)=O(H^2)\ , \tag{4.10e}$$

where

$$A^r\equiv\sum_m O_0^r(m)A_m$$
$$\overline{G}\,^r_k\equiv\sum_\sigma \sigma^r\overline{G}_{k\sigma}(\varepsilon),\quad r=0,1 \tag{4.11}$$

and the $O_0^r(m)$ are defined in Eq. (3.11). These quantities have the property that $A^r\sim H^r$ and $\overline{G}\,^r\sim H^r$; therefore to obtain the linear Hall constant we must have either A^1 or $\overline{G}\,^1$ appear *once*, while all other quantities are either A^0 or $\overline{G}\,^0$. Finally we use Eq. (4.4b) to write

$$\sum_\sigma \overline{G}_{k\sigma}(\varepsilon)\overline{G}_{k'\sigma}(\varepsilon')=8\pi^2\tau_0(\varepsilon)\tau_0(\varepsilon')\delta(\varepsilon-\varepsilon_k)\delta(\varepsilon'-\varepsilon_{k'})\ , \tag{4.12}$$

where we drop the spin index on the energy as these functions are in zero field. We will neglect the terms coming from Eq. (4.10c) as they depend on the polarization of the conduction band which is the order of $g\mu_B H/E_F$. This is considerably smaller than the other part coming from the polarization of the local state which is the order of $g\mu_B H/k_B T_0$, where $k_B T_0$ is the characteristic low-temperature energy scale for the Kondo problem. With these simplifications we find that the type-II contribution from charge scattering to the *linear* Hall conductivity is

$$\sigma_H^{\text{charge}}(\text{II})=-\tfrac{24}{49}c\frac{ne^2}{m}\frac{aJ(0)\Gamma}{N_f}\int\frac{d\varepsilon}{2\pi}\left[-\frac{\partial f(\varepsilon)}{\partial\varepsilon}\right]\tau_0(\varepsilon)\int\frac{d\varepsilon'}{\pi}f(\varepsilon')(1-e^{\beta(\varepsilon'-\varepsilon)})\tau_0(\varepsilon')$$
$$\times\int\frac{d\varepsilon''}{\pi}\frac{e^{-\beta\varepsilon''}}{Z_{4f}}B(\varepsilon''-\varepsilon')[A^0(\varepsilon'')A^1(\varepsilon''-\varepsilon'+\varepsilon)+A^1(\varepsilon'')A^0(\varepsilon''-\varepsilon'+\varepsilon)]+O(H^3)\ , \tag{4.13}$$

where we set the conduction electron's density of states $n(\varepsilon)$ and the nonresonant coupling parameter $J(k)$ equal to their value at the Fermi surface; these quantities vary slowly over the range of integration. To arrive at the prefactor we used the same free-electron model as for Eq. (3.16), i.e., $n(0)=3n/2E_F$, $k_F^2/m=2E_F$, as well as Eq. (2.12), $n(0)=N(0)N_s$, and $\pi N(0)|V_k|^2=\Gamma$.

Now, the matrix element for the exchange or spin scattering in terms of 3-j symbols is[9]

$$\langle\sigma m'|b\mathbf{s}\cdot\mathbf{J}|\sigma' m\rangle=(-1)^{1-\sigma-m'}\tfrac{3}{2}\sqrt{5\times7}\,b\sum_{m_3}(-1)^{m_3}\begin{bmatrix}\frac12 & 1 & \frac12\\ -\sigma & m_3 & \sigma'\end{bmatrix}\begin{bmatrix}\frac52 & 1 & \frac52\\ -m' & -m_3 & m\end{bmatrix}. \tag{4.14}$$

By placing this and Eq. (4.6) in the expression for the type-II Hall conductivity [Eq. (4.5)] we find

$$\sigma_H^{\text{spin}}(\text{II})=\frac{9\sqrt{15}}{2\pi}\frac{e^2}{m^2}\frac{c|V_k|^2b}{N_s}\int d\varepsilon_k\,kJ(k)n(\varepsilon_k)$$
$$\times\int d\varepsilon_{k'}\,k'n(\varepsilon_{k'})\int\frac{d\varepsilon}{2\pi}\left[-\frac{\partial f(\varepsilon)}{\partial\varepsilon}\right]\int\frac{d\varepsilon'}{\pi}f(\varepsilon')(1-e^{\beta(\varepsilon'-\varepsilon)})\int\frac{d\varepsilon''}{\pi}\frac{e^{-\beta\varepsilon''}}{Z_{4f}}B(\varepsilon''-\varepsilon')$$
$$\times\sum_{\sigma,\sigma'}\overline{G}_{k\sigma}(\varepsilon)\overline{G}_{k'\sigma'}(\varepsilon')\sum_{m,m'}A_{m'}(\varepsilon'')A_m(\varepsilon''-\varepsilon'+\varepsilon)$$
$$\times\sum_{m_1,m_2m_3}(-1)^{m_1+m_3-m-\sigma}\begin{bmatrix}3 & \frac12 & \frac52\\ m_1 & \sigma & -m\end{bmatrix}\begin{bmatrix}3 & \frac12 & \frac52\\ m_2 & \sigma' & -m'\end{bmatrix}\begin{bmatrix}3 & 3 & 1\\ -m_1 & m_2 & 0\end{bmatrix}\begin{bmatrix}\frac52 & 1 & \frac52\\ -m' & -m_3 & m\end{bmatrix}\begin{bmatrix}\frac12 & 1 & \frac12\\ -\sigma & m_3 & \sigma'\end{bmatrix}. \tag{4.15}$$

In Appendix B we recouple the 3-j symbols so that the sums over the propagators and spectral functions which depend on the orbital and spin indices m and σ can be written in their *irreducible* forms G^r and A^r [see Eqs. (3.11) and (4.11)]. Whereas the highest-rank polynomial to enter the charge contribution was $r=2$ [see Eq. (4.9)], spectral functions A^r up to $r=5$ enter the spin contribution to the Hall conductivity. However, to lowest order in the magnetic field we want $r=1$ to appear only *once*, and all other ranks are $r=0$. Then the *integrand* in the expression for the spin contribution [Eq. (4.15)] that is *linear* in the field is

$$\sigma_H^{\rm spin}({\rm II})\sim\frac{1}{2^3\times3^3\times7^2}\sqrt{5/3}\{\bar G_k^0(\varepsilon)\bar G_{k'}^0(\varepsilon')[A^0(\varepsilon'')A^1(\varepsilon''-\varepsilon'+\varepsilon)+A^1(\varepsilon'')A^0(\varepsilon''-\varepsilon'+\varepsilon)]$$
$$-\tfrac{7}{3}[\bar G_k^0(\varepsilon)\bar G_{k'}^1(\varepsilon')+\bar G_k^1(\varepsilon)\bar G_{k'}^0(\varepsilon')]A^0(\varepsilon'')A^0(\varepsilon''-\varepsilon'+\varepsilon)\}\ . \tag{4.16}$$

By using Eq. (4.4b) for the functions $\bar G_{k'}^r$ [see Eq. (4.11)] we find

$$\bar G_k^0(\varepsilon)\bar G_{k'}^0(\varepsilon')=16\pi^2\tau_0(\varepsilon)\tau_0(\varepsilon')\delta(\varepsilon-\varepsilon_k)\delta(\varepsilon'-\varepsilon_{k'})\ . \tag{4.17}$$

With the same simplifications we made in Eq. (4.9) to arrive at Eq. (4.13) for the charge contribution, we find that the spin contribution from type-II diagrams to the linear Hall conductivity is

$$\sigma_H^{\rm spin}({\rm II})=\tfrac{5}{49}c\frac{ne^2}{m}bJ(0)\Gamma\int\frac{d\varepsilon}{2\pi}\left[-\frac{\partial f(\varepsilon)}{\partial\varepsilon}\right]\tau_0(\varepsilon)\int\frac{d\varepsilon'}{\pi}f(\varepsilon')(1-e^{\beta(\varepsilon'-\varepsilon)})\tau_0(\varepsilon')$$
$$\times\int\frac{d\varepsilon''}{\pi}\frac{e^{-\beta\varepsilon''}}{Z_{4f}}B(\varepsilon''-\varepsilon')[A^0(\varepsilon'')A^1(\varepsilon''-\varepsilon'+\varepsilon)+A^1(\varepsilon'')A^0(\varepsilon''-\varepsilon'+\varepsilon)]+O(H^3)\ . \tag{4.18}$$

By combining this with the charge contribution and dividing by the normal conductivity squared, we find that the total of the type-II contributions to the linear Hall constant [see Eqs. (2.1) and (2.13)] is

$$R_H({\rm II})=-\frac{1}{49}\frac{mc}{ne^2\hbar}\frac{\Gamma J(0)}{H}\left[\frac{6a}{N_f}-\tfrac{5}{4}b\right]\rho_f^2(0)\int\frac{d\varepsilon}{2\pi}\left[-\frac{\partial f(\varepsilon)}{\partial\varepsilon}\right]\rho_f^{-1}(\varepsilon)\int\frac{d\varepsilon'}{\pi}f(\varepsilon')(1-e^{\beta(\varepsilon'-\varepsilon)})\rho_f^{-1}(\varepsilon')$$
$$\times\int\frac{d\varepsilon''}{\pi}\frac{e^{-\beta\varepsilon''}}{Z_{4f}}B(\varepsilon''-\varepsilon)[A^0(\varepsilon'')A^1(\varepsilon''-\varepsilon'+\varepsilon)+A^1(\varepsilon'')A^0(\varepsilon''-\varepsilon'+\varepsilon)]+O(H^3)\ , \tag{4.19}$$

where we used the relation

$$\frac{\tau_0(\varepsilon)}{\tau}=\frac{\rho_f(0)}{2\rho_f(\varepsilon)} \tag{4.20}$$

which is found by comparing Eqs. (2.11) and (2.14).

To first order in the field,

$$A_0(\varepsilon'')A^1(\varepsilon''-\varepsilon'+\varepsilon)=\sum_{m,m'}m'A_m(\varepsilon'',H)A_{m'}(\varepsilon''-\varepsilon'+\varepsilon,H)$$
$$=g\mu_BHN_fR_0\left.\left[A_m(\varepsilon'',H)\frac{\partial}{\partial\varepsilon_m}[A_m(\varepsilon''-\varepsilon'+\varepsilon,H)]\right]\right|_{H=0} \tag{4.21}$$

and

$$A^1(\varepsilon'')A^0(\varepsilon''-\varepsilon'+\varepsilon)=g\mu_BHN_fR_0\left.\left[\frac{\partial}{\partial\varepsilon_m}[A_m(\varepsilon'',H)]A_m(\varepsilon''-\varepsilon'+\varepsilon,H)\right]\right|_{H=0}\ ,$$

where $R_0\equiv\sum_m m^2$ and $\varepsilon_m\equiv g\mu_BHm$. The combination of these entering Eq. (4.19) can be rewritten as

$$A^0(\varepsilon'')A^1(\varepsilon''-\varepsilon'+\varepsilon)+A^1(\varepsilon'')A^0(\varepsilon''-\varepsilon'+\varepsilon)=g\mu_BHN_fR_0\frac{\partial}{\partial\varepsilon_m}\{A_m(\varepsilon'',H)A_m(\varepsilon''-\varepsilon'+\varepsilon,H)\}\Big|_{H=0} \tag{4.22}$$

so we can rewrite the expression for the Hall constant as

$$R_H({\rm II})=-\frac{1}{49}\frac{mc}{ne^2\hbar}g\mu_BR_0\Gamma J(0)(6a-\tfrac{5}{4}N_fb)I\ , \tag{4.23}$$

where

$$I \equiv \rho_f^2(0) \int \frac{d\varepsilon}{2\pi} \left[-\frac{\partial f(\varepsilon)}{\partial \varepsilon} \right] \rho_f^{-1}(\varepsilon)$$
$$\times \int \frac{d\varepsilon'}{\pi} f(\varepsilon')(1-e^{\beta(\varepsilon'-\varepsilon)})\rho_f^{-1}(\varepsilon') \int \frac{d\varepsilon''}{\pi} \frac{e^{-\beta\varepsilon''}}{Z_{4f}} B(\varepsilon''-\varepsilon') \frac{\partial}{\partial \varepsilon_m} [A_m(\varepsilon'',H) A_m(\varepsilon''-\varepsilon'+\varepsilon,H)] \Big|_{H=0} . \tag{4.24}$$

There are no analytical solutions for the spectral densities that are valid for all temperatures, therefore it is not possible to write down expressions for the Hall constant of Kondo systems that are valid for all temperatures. In the next section we evaluate the expressions we derived for $R_H(\mathrm{I})$ and $R_H(\mathrm{II})$ in the limits of weak coupling $T \gg T_0$, and strong coupling at $T=0$ K.

V. RESULTS

In Appendixes C and D we have evaluated the integral I [Eq. (4.24)] in the limits of weak and strong coupling. By placing the solution [Eq. (C13)] in Eq. (4.23) we find that the contribution to the Hall constant from type-II diagrams at high temperatures is

$$R_H^{\mathrm{II}}(T \gg T_0) \approx \frac{1}{49\pi^2} \frac{39}{40} \frac{mc}{ne^2\hbar} \left[\frac{\Gamma}{E_f} \right]^2 \left[\frac{T_0}{T} \right]^2 \times \frac{g\mu_B}{k_B T} R_0 (J_{\mathrm{ch}} - \tfrac{5}{24} N_f J_{\mathrm{ex}}) , \tag{5.1}$$

where $J_{\mathrm{ch}} = aJ(0)$ and $J_{\mathrm{ex}} = bJ(0)$.

We immediately note that this contribution is smaller than that from type I at high temperatures[1] by $(T_0/T)^2$; therefore for $T \gg T_0$, type-II contributions are negligible compared to type I. Also, while the temperature dependence is correct, the precise constant depends on our approximating the Lorentzians in Eq. (C3) by rectangular functions [Eq. (C4)], thus this should not be taken too seriously.

To write the Hall constant as a dimensionless ratio we use[6,12]

$$f \equiv g\mu_B \frac{R_H}{\rho_{\mathrm{iso}} \chi} \tag{5.2}$$

where χ is the magnetic susceptibility and ρ_{iso} is given by Eq. (3.25). In weak coupling the susceptibility is given as[12]

$$\chi = \frac{(g\mu_B)^2}{k_B T} \frac{R_0}{N_f} \tag{5.3}$$

and the resistivity [Eq. (3.25)] with $\rho_0 = N_f \Gamma / \varepsilon_f^2$ is

$$\rho_{\mathrm{iso}} = \frac{N_f}{2} \frac{mc}{\pi N(0) ne^2\hbar} \left[\frac{\Gamma}{\varepsilon_f} \right]^2 . \tag{5.4}$$

The dimensionless ratio for type-II contributions in weak coupling is

$$f_{\mathrm{II}} \equiv \frac{1}{49\pi} \frac{39}{20} \left[\frac{T_0}{T} \right]^2 N(0)(J_{\mathrm{ch}} - \tfrac{5}{24} N_f J_{\mathrm{ex}}) , \tag{5.5}$$

while that for type-I contributions [see Eq. (3.19)] is

$$f_{\mathrm{I}} \equiv \tfrac{3}{49} N(0)(n_f J_{\mathrm{ch}} - \tfrac{7}{6} J_{\mathrm{ex}}) , \tag{5.6}$$

where we used

$$\frac{\rho_1}{H} = -\frac{1}{2} \frac{\chi}{g\mu_B} \frac{N_f \Gamma}{|\varepsilon_f|^2}$$

and

$$\rho_0 = \frac{N_f \Gamma}{|\varepsilon_f|^2} .$$

The salient difference between the type-I and -II contributions in weak coupling is the factor $(T_0/T)^2$ which is small for $T_0 \ll T$.

By placing the result, Eq. (D17), in Eq. (4.23) we find the contribution of type-II diagrams to the Hall constant at $T=0$ K is

$$R_H^{\mathrm{II}}(0) = \frac{3}{2 \times 49\pi^2} \frac{mc}{ne^2\hbar} \frac{g\mu_B}{\Gamma^*} R_0 \sin^4[\eta_3(0)] \times \left[A + \frac{p_1 N_f}{\pi} \sin[2\eta_3(0)] \right] \times (J_{\mathrm{ch}} - \tfrac{5}{24} N_f J_{\mathrm{ex}}) , \tag{5.7}$$

where A and p_1 are numbers of order 1 (see Appendix D). The phase shift at the Fermi surface at $T=0$ K is given by the Friedel-Langreth sum rule:[5,11]

$$\eta_3(0) = \frac{\pi n_f(0)}{N_f} . \tag{5.8}$$

The magnetic susceptibility at $T=0$ K is[5,11,12]

$$\chi = \frac{(g\mu_B)^2 \sin^2[\eta_3(0)]}{\pi \Gamma^*} R_0 , \tag{5.9}$$

while the resistivity [see Eq. (3.25)] is

$$\rho_{\mathrm{iso}} = \frac{N_f}{2} \frac{mc}{\pi N(0) ne^2\hbar} \sin^2[\eta_3(0)] , \tag{5.10}$$

where we used, for $T=0$ K,

$$\rho_0 = \frac{N_f}{\Gamma} \sin^2[\eta_3(0)] .$$

The dimensionless ratio [Eq. (5.2)] for type-II contributions in strong coupling at $T=0$ K is

$$f_{\mathrm{II}}(0) = \frac{3}{49} \frac{N(0)}{N_f} \left[A + \frac{p_1 N_f}{\pi} \sin[2\eta_3(0)] \right] \times (J_{\mathrm{ch}} - \tfrac{5}{24} N_f J_{\mathrm{ex}}) , \tag{5.11}$$

while that for type-I contributions [see Eq. (3.19)] is

$$f_{\rm I}(0)=\frac{6}{49}\frac{N(0)}{N_f}\left[\pi\frac{\sin[2\eta_3(0)]}{\sin^2[\eta_3(0)]}n_f J_{\rm ch}-\tfrac{7}{12}N_f J_{\rm ex}\right] , \tag{5.12}$$

where we used

$$\frac{\rho_1}{H}=-\frac{1}{\Gamma}\frac{g\mu_B}{\Gamma^*}R_0\sin[2\eta_3(0)]\sin^2[\eta_3(0)] , \tag{5.13}$$

and neglected the nonlinear contribution from ρ_2.

VI. DISCUSSION OF RESULTS AND CONCLUSIONS

We have extended Luttinger's one-electron theory of the Hall effect in metallic alloys to take account of two-electron scattering processes for Kondo-type compounds. In addition to reiterating the one-electron results we have found new contributions that are important in the strong-coupling limit at low temperatures $T<T_0$. The Kubo formalism which gives the Hall current that is linear in the *electric* field has been used to write the conductivity in terms of current-current correlation functions. These functions were evaluated in the dilute limit where the number of Kondo ions is small compared to the available lattice sites. To apply this formalism to more concentrated (dense) Kondo systems, it will be necessary to take into account (1) interference terms between scattering at different sites, (2) the interactions between Kondo ions at different sites, and (3) the renormalization of the conduction electrons due to the Kondo scattering.

In the present treatment we considered both two-particle charge and spin scattering in the nonresonant channel. As charge scattering is much stronger than the spin, we evaluated the type-I contributions to the extraordinary Hall effect to all orders in this scattering [see Eqs. (3.23), (3.24), and (3.26)]. For the type-II contributions we limited ourselves to vertex corrections that are first order in the *nonresonant* two-particle charge and spin scatterings. In a future development it would be useful to extend this to all orders in the charge scattering by using a ladder approximation for the four-point electron-hole vertex function entering the type-II contributions (see Fig. 2). Finally, we limited our investigation to the contributions from skew scattering; we are presently using the Kubo formalism to evaluate the anomalous velocity or side-jump contributions to the EHE. These terms have been evaluated by using Luttinger's one-electron theory, and have been found to give important contributions to the EHE at low temperatures.[2,6] As we have found that two-electron scattering processes lead to new and important contributions due to skew scattering, we anticipate that the anomalous velocity mechanism will also contribute new and equally important contributions.[13]

By comparing the new contributions we found by using the Kubo formalism to those previously found,[1,12] we conclude that type-II contributions arising from energy transfers between the resonant $l=3$ and nonresonant $l=2$ channels [see Eq. (5.11)] are as large as type-I contributions at low temperatures $T<T_0$ [Eq. (5.12)]. However, at high temperatures $T\gg T_0$, type-II contributions to the EHE [Eq. (5.5)] are smaller than the *elastic* scattering type-I terms [Eq. (5.6)] by a factor $(T_0/T)^2$. By considering two-electron scattering processes we have also found spin- or exchange-scattering contributions that were not previously accounted for. The type-I contribution to the EHE due to spin scattering is directly proportional to the product of the magnetic susceptibility and resistivity, i.e., $f_{\rm I}^{\rm spin}(T)=$const. However, as the spin scattering is an order of magnitude smaller than charge scattering, this proportionality will be masked by the temperature-dependent ratios $f_{\rm I,II}^{\rm charge}(T)$ coming from charge scattering. Indeed, the experimental data on the EHE in Kondo-type compounds can be parametrized in terms of *two* different parameters $f_1(T>T_0)$ and $f_2(T_{\rm coh}<T<T_0)$, over limited ranges of temperatures.[1]

We reiterate that in their present form our expressions for the EHE are applicable only to *dilute* Kondo systems. We are presently evaluating the role of two-electron scattering processes in the anomalous velocity contribution to the Hall effect.[13] Once this is completed we will be able to compare the results of the two contributions (skew scattering and anomalous velocity), which are based on our impurity-scattering model, to experimental data on *dilute* or impurity Kondo systems. In the future we plan to extend our results to dense Kondo systems by incorporating some features mentioned earlier that have been neglected in the present treatment. Then we will be able to compare our results to concentrated Kondo-type compounds.

APPENDIX A: TWO-PARTICLE CORRELATION FUNCTION

The two-particle correlation function for type-II diagrams [Eqs. (2.19) and (4.2)] can be written as

$$C^{(2)}_{mm'}(i\nu_n)=\left[\frac{1}{\beta}\right]^2\sum_{i\omega_1,i\omega_2}G_{\mathbf{k}\sigma}(i\omega_1)G_{\mathbf{k}\sigma}(i\omega_1+i\nu_n)G_{\mathbf{k}'\sigma'}(i\omega_2)G_{\mathbf{k}'\sigma'}(i\omega_2+i\nu_n)\Gamma^{(2)}_{mm'}(i\nu_n,i\omega_1,i\omega_2) \tag{A1}$$

where the vertex function $\Gamma^{(2)}_{mm'}(i\nu_n,i\omega_1,i\omega_2)$ is defined as

$$\Gamma^{(2)}_{mm'}(i\nu_n,i\omega_1,i\omega_2)=\frac{1}{\beta}\sum_{i\omega_3}D(i\omega_3-i\omega_1-i\nu_n)G_{m'}(i\omega_3+i\omega_2-i\omega_1)G_m(i\omega_3) . \tag{A2}$$

The sum over complex frequencies can be expressed in terms of a contour integral as follows:[14]

$$\Gamma^{(2)}_{mm'}(i\nu_n,i\omega_1,i\omega_2,)=-\frac{1}{Z_{4f}}\int_\Gamma \frac{dz}{2\pi i}e^{-\beta z}D(z-i\omega_1-i\nu_n)G_{m'}(z+i\omega_2-i\omega_1)G_m(z)$$
$$=\frac{1}{Z_{4f}}\int\frac{d\varepsilon}{\pi}e^{-\beta\varepsilon}[D(\varepsilon-i\omega_1-i\nu_n)G_{m'}(\varepsilon+i\omega_2-i\omega_1)A_m(\varepsilon)+D(\varepsilon-i\omega_2-i\nu_n)G_m(\varepsilon-i\omega_1-i\omega_2)A_{m'}(\varepsilon)-G_{m'}(\varepsilon+i\omega_2+i\nu_n)G_m(\varepsilon+i\omega_1+i\nu_n)B(\varepsilon)]\ . \tag{A3}$$

We define

$$\gamma_1(i\omega_1,i\omega_1+i\nu_n)=\frac{1}{\beta}\sum_{i\omega_2}G_{\mathbf{k}'\sigma'}(i\omega_2)G_{\mathbf{k}'\sigma'}(i\omega_2+i\nu_n)\Gamma^{(2)}_{mm'}(i\nu_n,i\omega_1,i\omega_2)$$
$$\equiv\frac{1}{\beta}\sum_{i\omega_2}P_1(i\omega_1,i\omega_1+i\nu_n,i\omega_2,i\omega_2+i\nu_n)\ . \tag{A4}$$

By using the contour-integral representation, the γ function is

$$\gamma_1(i\omega_1,i\omega_1+i\nu_n)=-\int\frac{d\varepsilon'}{2\pi i}f(\varepsilon')[P_1(i\omega_1,i\omega_1+i\nu_n,\varepsilon'+i\delta,\varepsilon'+i\nu_n)-P_1(i\omega_1,i\omega_1+i\nu_n,\varepsilon'-i\delta,\varepsilon'+i\nu_n)+P_1(i\omega_1,i\omega_1+i\nu_n,\varepsilon'-i\nu_n,\varepsilon'+i\delta)-P_1(i\omega_1,i\omega_1+i\nu_n,\varepsilon'-i\nu_n,\varepsilon'-i\delta)]\ . \tag{A5}$$

The two-particle correlation function $C^{(2)}_{mm'}$ can be expressed in terms of γ_1 [see Eqs. (A1) and (A4)] as follows:

$$C^{(2)}_{mm'}(i\nu_n)=\frac{1}{\beta}\sum_{i\omega_1}G_{\mathbf{k}\sigma}(i\omega_1)G_{\mathbf{k}\sigma}(i\omega_1+i\nu_n)\gamma_1(i\omega_1,i\omega_1+i\nu_n)$$
$$=\frac{i}{\beta}\sum_{i\omega_1}P_2(i\omega_1,i\omega_1+i\nu_n)$$
$$=-\int\frac{d\varepsilon}{2\pi i}f(\varepsilon)[P_2(\varepsilon+i\delta,\varepsilon+i\nu_n)-P_2(\varepsilon-i\delta,\varepsilon+i\nu_n)+P_2(\varepsilon-i\nu_n,\varepsilon+i\delta)-P_2(\varepsilon-i\nu_n,\varepsilon-i\delta)]. \tag{A6}$$

When we analytically continue $i\nu_n$ to the real axis, we take $i\nu_n\to\omega+i\delta$, and find

$$C^{(2)}_{mm'}(\omega)=-\int\frac{d\varepsilon}{2\pi}f(\varepsilon)[P_2(\varepsilon+i\delta,\varepsilon+\omega+i\delta)-P_2(\varepsilon-i\delta,\varepsilon+\omega+i\delta)+P_2(\varepsilon-\omega-i\delta,\varepsilon+i\delta)-P_2(\varepsilon-\omega-i\delta,\varepsilon-i\delta)]\ ,$$

where

$$P_2(\varepsilon+i\delta,\varepsilon+\omega+i\delta)=G^R_{\mathbf{k}\sigma}(\varepsilon)G^R_{\mathbf{k}\sigma}(\varepsilon+\omega)\gamma_1(\varepsilon+i\delta,\varepsilon+\omega+i\delta)\ ,$$
$$P_2(\varepsilon-\omega-i\delta,\varepsilon-i\delta)=G^A_{\mathbf{k}\sigma}(\varepsilon-\omega)G^A_{\mathbf{k}\sigma}(\varepsilon)\gamma_1(\varepsilon-\omega-i\delta,\varepsilon-i\delta)\ ,$$
$$P_2(\varepsilon-i\delta,\varepsilon+\omega+i\delta)=G^A_{\mathbf{k}\sigma}(\varepsilon)G^R_{\mathbf{k}\sigma}(\varepsilon+\omega)\gamma_1(\varepsilon-i\delta,\varepsilon+\omega+i\delta)\ ,$$

and (A7)

$$P_2(\varepsilon-\omega-i\delta,\varepsilon+i\delta)=G^A_{\mathbf{k}\sigma}(\varepsilon-\omega)G^R_{\mathbf{k}\sigma}(\varepsilon)\gamma_1(\varepsilon-\omega-i\delta,\varepsilon+i\delta)\ .$$

If one uses this result for $C^{(2)}_{mm'}$ to calculate the conductivity, one finds an unwieldy expression. To make it manageable, we consider the expression in the dilute limit.

In the dilute limit, terms like $G^R_{\mathbf{k}\sigma}(\varepsilon)G^R_{\mathbf{k}\sigma}(\varepsilon+\omega)$ and $G^A_{\mathbf{k}\sigma}(\varepsilon)G^A_{\mathbf{k}\sigma}(\varepsilon+\omega)$ go to zero, therefore in Eqs. (A7) only $\gamma_1(\varepsilon-i\delta,\varepsilon+\omega+i\delta)$ and $\gamma_1(\varepsilon-\omega-i\delta,\varepsilon+i\delta)$ need to be calculated. The γ function [Eq. (A5)] can be analytically continued to the real axis, i.e., set $i\nu_n\to\omega+i\delta$, and for ω approaching zero $\gamma_1(\varepsilon-i\delta,\ \varepsilon+\omega+i\delta)$ is (see Ref. 14)

$$\gamma_1(\varepsilon-i\delta,\varepsilon+\omega+i\delta)|_{\omega=0}=\frac{1}{Z_{4f}}\int\frac{d\varepsilon''}{\pi}e^{-\beta\varepsilon''}\int\frac{d\varepsilon'}{\pi}G^A_{\mathbf{k}'\sigma'}(\varepsilon')G^R_{\mathbf{k}'\sigma'}(\varepsilon')\times\frac{1-e^{-\beta(\varepsilon'-\varepsilon)}}{1+e^{\beta\varepsilon'}}A_{m'}(\varepsilon'')D^A(\varepsilon''-\varepsilon')A_m(\varepsilon''-\varepsilon'+\varepsilon) \tag{A8}$$

and

$$\gamma_1(\varepsilon-\omega-i\delta,\varepsilon+i\delta)|_{\omega=0}=\gamma_1(\varepsilon-i\delta,\varepsilon+\omega+i\delta)|_{\omega=0}\ . \tag{A9}$$

When we place these expressions for the dilute limit, and for $\omega\approx0$ in Eq. (A7), we find

$$\lim_{\omega\to 0}\left[\mathrm{Im}\frac{iC^{(2)}_{mm'}(\omega)}{\omega}\right]=\lim_{\omega\to 0}\left[-\int\frac{d\varepsilon}{2\pi}\left[\frac{f(\varepsilon)-f(\varepsilon+\omega)}{\omega}\right]G^R_{\mathbf{k}\sigma}(\varepsilon)G^A_{\mathbf{k}\sigma}(\varepsilon)\mathrm{Im}\gamma_1(\varepsilon-i\delta,\varepsilon+i\delta)\right]$$

$$=-\int\frac{d\varepsilon}{2\pi}\left[-\frac{\partial f(\varepsilon)}{\partial\varepsilon}\right]\int\frac{d\varepsilon'}{\pi}\int\frac{d\varepsilon''}{\pi}\frac{e^{-\beta\varepsilon''}}{Z_{4f}}G^R_{\mathbf{k}\sigma}(\varepsilon)G^A_{\mathbf{k}\sigma}(\varepsilon)G^R_{\mathbf{k}'\sigma'}(\varepsilon')G^A_{\mathbf{k}'\sigma'}(\varepsilon')$$

$$\times\frac{1-e^{\beta(\varepsilon'-\varepsilon)}}{1+e^{\beta\varepsilon'}}A_{m'}(\varepsilon'')B(\varepsilon''-\varepsilon')A_m(\varepsilon''-\varepsilon'+\varepsilon)\ . \qquad (A10)$$

This is just the result quoted in Eq. (4.3) when we use the equations defined in Eq. (4.4a).

APPENDIX B: SPIN OR EXCHANGE CONTRIBUTION

In evaluating the spin or exchange contribution from type-II diagrams to the Hall conductivity in Sec. IV, we find the sum over five 3-j symbols [see Eq. (4.15)]:

$$J_{m\sigma,m'\sigma'}\equiv\sum_{m_1,m_2,m_3}(-1)^{m_1+m_3-m-\sigma}\begin{pmatrix}3&\frac{1}{2}&\frac{5}{2}\\ m_1&\sigma&-m\end{pmatrix}\begin{pmatrix}3&\frac{1}{2}&\frac{5}{2}\\ m_2&\sigma'&-m'\end{pmatrix}$$

$$\times\begin{pmatrix}3&3&1\\ -m_1&m_2&0\end{pmatrix}\begin{pmatrix}\frac{5}{2}&1&\frac{5}{2}\\ -m'&-m_3&m\end{pmatrix}\begin{pmatrix}\frac{1}{2}&1&\frac{1}{2}\\ -\sigma&m_3&\sigma'\end{pmatrix}\ . \qquad (B1)$$

Here we show how these symbols are recoupled so that we isolate the dependence of J on each index.

We start by recoupling[9]

$$\sum_{m_1,m_2}(-1)^{m_1-m-\sigma}\begin{pmatrix}1&3&3\\ 0&-m_1&m_2\end{pmatrix}\begin{pmatrix}3&\frac{1}{2}&\frac{5}{2}\\ -m_1&-\sigma&m\end{pmatrix}\begin{pmatrix}3&\frac{1}{2}&\frac{5}{2}\\ m_2&\sigma'&-m'\end{pmatrix}$$

$$=-\sum_{b,c,\beta,\gamma}[b][c]\begin{pmatrix}1&b&c\\ 0&\beta&\gamma\end{pmatrix}\begin{pmatrix}b&\frac{1}{2}&\frac{1}{2}\\ \beta&-\sigma&\sigma'\end{pmatrix}\begin{pmatrix}c&\frac{5}{2}&\frac{5}{2}\\ \gamma&m&-m'\end{pmatrix}\begin{Bmatrix}1&b&c\\ 3&\frac{1}{2}&\frac{5}{2}\\ 3&\frac{1}{2}&\frac{5}{2}\end{Bmatrix}\ , \qquad (B2)$$

where $[b]\equiv 2b+1$. As two rows of the 9-j symbol are identical, the sum of the elements must be even,[9] therefore $b+c$ must be *odd*. As $b=0,1$, it follows that we have the following possibilities:

$$b=0,\quad c=1$$

and (B3)

$$b=1,\quad c=0,2\ .$$

Next we recouple the spin indices as follows:

$$\begin{pmatrix}b&\frac{1}{2}&\frac{1}{2}\\ \beta&-\sigma&\sigma'\end{pmatrix}\begin{pmatrix}1&\frac{1}{2}&\frac{1}{2}\\ -m_3&\sigma&-\sigma'\end{pmatrix}=\sum_{a',b',c',\alpha',\beta',\gamma}[a'][b'][c']\begin{Bmatrix}a'&b'&c'\\ b&\frac{1}{2}&\frac{1}{2}\\ 1&\frac{1}{2}&\frac{1}{2}\end{Bmatrix}$$

$$\times\begin{pmatrix}a'&b'&c'\\ \alpha'&\beta'&\gamma'\end{pmatrix}\begin{pmatrix}a'&b&1\\ \alpha'&\beta&-m_3\end{pmatrix}\begin{pmatrix}b'&\frac{1}{2}&\frac{1}{2}\\ \beta'&-\sigma&\sigma\end{pmatrix}\begin{pmatrix}c'&\frac{1}{2}&\frac{1}{2}\\ \gamma'&\sigma'&-\sigma'\end{pmatrix}\ , \qquad (B4)$$

and the orbital indices in an analogous fashion:

$$\begin{pmatrix}c&\frac{5}{2}&\frac{5}{2}\\ \gamma&m&-m'\end{pmatrix}\begin{pmatrix}1&\frac{5}{2}&\frac{5}{2}\\ m_3&-m&m'\end{pmatrix}=\sum_{a'',b'',c'',\alpha'',\beta'',\gamma''}[a''][b''][c'']\begin{Bmatrix}a''&b''&c''\\ c&\frac{5}{2}&\frac{5}{2}\\ 1&\frac{5}{2}&\frac{5}{2}\end{Bmatrix}$$

$$\times\begin{pmatrix}a''&b''&c''\\ \alpha''&\beta''&\gamma''\end{pmatrix}\begin{pmatrix}a''&c&1\\ \alpha''&\gamma&m_3\end{pmatrix}$$

$$\times\begin{pmatrix}b''&\frac{5}{2}&\frac{5}{2}\\ \beta''&m&-m\end{pmatrix}\begin{pmatrix}c''&\frac{5}{2}&\frac{5}{2}\\ \gamma''&-m'&m'\end{pmatrix}\ . \qquad (B5)$$

Finally, we sum over the indices m_3, β, and γ, and find

$$\sum_{m_3,\beta,\gamma}(-1)^{m_3}\begin{pmatrix}1 & b & c\\ 0 & \beta & \gamma\end{pmatrix}\begin{pmatrix}a' & b & 1\\ \alpha' & \beta & -m_3\end{pmatrix}\begin{pmatrix}1 & a'' & c\\ m_3 & \alpha'' & \gamma\end{pmatrix}=(-1)^{a'+b+1}\begin{pmatrix}a'' & a' & 1\\ \alpha'' & \alpha' & 0\end{pmatrix}\begin{Bmatrix}a'' & a' & 1\\ b & c & 1\end{Bmatrix}, \quad \text{(B6)}$$

where the term in curly brackets is a 6-j symbol. From the 3-j symbols in Eqs. (B4)–(B6) we find

$$\beta'=\gamma'=\beta''=\gamma''=0 , \quad \text{(B7)}$$

and it follows that

$$\alpha'=\alpha''=0 .$$

By substituting Eqs. (B2)–(B7) into Eq. (B1) we find

$$J_{m\sigma,m'\sigma'}=\sum_{b,c;a',b',c';a'',b''c''}[b][c][a'][b'][c'][a''][b''][c'']$$
$$\times\begin{Bmatrix}1 & b & c\\ 3 & \frac{1}{2} & \frac{5}{2}\\ 3 & \frac{1}{2} & \frac{5}{2}\end{Bmatrix}\begin{Bmatrix}a' & b' & c'\\ b & \frac{1}{2} & \frac{1}{2}\\ 1 & \frac{1}{2} & \frac{1}{2}\end{Bmatrix}\begin{Bmatrix}a'' & b'' & c''\\ c & \frac{5}{2} & \frac{5}{2}\\ 1 & \frac{5}{2} & \frac{5}{2}\end{Bmatrix}(-1)^{a'+b}\begin{Bmatrix}a'' & a' & 1\\ b & c & 1\end{Bmatrix}\begin{pmatrix}a' & a'' & 1\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}a' & b' & c'\\ 0 & 0 & 0\end{pmatrix}$$
$$\times\begin{pmatrix}a'' & b'' & c''\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}\frac{5}{2} & \frac{5}{2} & b''\\ m & -m & 0\end{pmatrix}\begin{pmatrix}\frac{5}{2} & \frac{5}{2} & c''\\ -m' & m' & 0\end{pmatrix}\begin{pmatrix}\frac{1}{2} & \frac{1}{2} & b'\\ -\sigma & \sigma & 0\end{pmatrix}\begin{pmatrix}\frac{1}{2} & \frac{1}{2} & c'\\ \sigma' & -\sigma' & 0\end{pmatrix}. \quad \text{(B8)}$$

The quantity entering the exchange or spin contribution [see Eq. (4.15)] is

$$\sum_{m,m',\sigma,\sigma'}J_{m\sigma,m'\sigma'}A_m(\varepsilon''-\varepsilon'+\varepsilon)A_{m'}(\varepsilon'')\bar{G}_{k\sigma}(\varepsilon)\bar{G}_{k'\sigma'}(\varepsilon')$$
$$\equiv\sum_{b',c',b'',c''}\Gamma_{b''c'',b'c'}\tilde{A}^{(b'')}(\varepsilon''-\varepsilon'+\varepsilon)\tilde{A}^{(c'')}(\varepsilon'')\tilde{G}_k^{(b')}(\varepsilon)\tilde{G}_{k'}^{(c')}(\varepsilon') , \quad \text{(B9)}$$

where

$$\Gamma_{b''c'',b'c'}=\sum_{b,c;a',a''}(-1)^{b+b'+b''}[b][c][a'][b'][c'][a''][b''][c'']$$
$$\times\begin{Bmatrix}1 & b & c\\ 3 & \frac{1}{2} & \frac{5}{2}\\ 3 & \frac{1}{2} & \frac{5}{2}\end{Bmatrix}\begin{Bmatrix}a' & b' & c'\\ b & \frac{1}{2} & \frac{1}{2}\\ 1 & \frac{1}{2} & \frac{1}{2}\end{Bmatrix}\begin{Bmatrix}a'' & b'' & c''\\ c & \frac{5}{2} & \frac{5}{2}\\ 1 & \frac{5}{2} & \frac{5}{2}\end{Bmatrix}$$
$$\times\begin{Bmatrix}a'' & a' & 1\\ b & c & 1\end{Bmatrix}\begin{pmatrix}a' & a'' & 1\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}a' & b' & c'\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix}a'' & b'' & c''\\ 0 & 0 & 0\end{pmatrix}, \quad \text{(B10)}$$

$$\tilde{A}^{(r)}\equiv\sum_m(-1)^m\begin{pmatrix}\frac{5}{2} & \frac{5}{2} & r\\ -m & m & 0\end{pmatrix}A_m$$

and (B11)

$$\tilde{G}_k^{(r)}\equiv\sum_\sigma(-1)^\sigma\begin{pmatrix}\frac{1}{2} & \frac{1}{2} & r\\ -\sigma & \sigma & 0\end{pmatrix}\bar{G}_{k\sigma} .$$

To arrive at this result we multipled by

$$1=(-1)^{m'-\sigma'-(m-\sigma)}=(-1)^{m'+m+\sigma+\sigma'} , \quad \text{(B12)}$$

we used the symmetry of the 3-j symbols to write

$$\begin{pmatrix}\frac{5}{2} & \frac{5}{2} & b''\\ m & -m & 0\end{pmatrix}=(-1)^{b''+1}\begin{pmatrix}\frac{5}{2} & \frac{5}{2} & b''\\ -m & m & 0\end{pmatrix}$$

and (B13)

$$\begin{pmatrix}\frac{1}{2} & \frac{1}{2} & c'\\ \sigma' & -\sigma' & 0\end{pmatrix}=(-1)^{c'+1}\begin{pmatrix}\frac{1}{2} & \frac{1}{2} & c'\\ -\sigma' & \sigma' & 0\end{pmatrix}$$

in order to form the combinations $\tilde{A}^{(r)}$ and $\tilde{G}_k^{(r)}$ [Eqs. (B11)], and finally we noted $a'+b'+c'=$even to replace $(-1)^{a'+c'}$ by $(-1)^{b'}$.

In general

$$b',c'=0,1$$

and (B14)

$$b'',c''=0,1,\ldots,5 .$$

However, to lowest order in the magnetic field we want $r=1$ to appear once, and all the other $r=0$. This follows from the definition of the $\tilde{A}^{(r)}$ and $\tilde{G}_k(r)$ as irreducible tensors of rank r. They have the property that

$$\tilde{A}(r) \sim H^r$$
and (B15)
$$\tilde{G}_k(r) \sim H^r .$$

Therefore, to obtain the linear Hall constant we want $r=1$ to appear once. There are four possibilities. By evaluating the 3-j, 6-j, and 9-j symbols we find

$$\Gamma_{10,00}=\Gamma_{01,00}=-\frac{5}{2^2\times3^2\times7\sqrt{3\times7}}$$
and (B16)
$$\Gamma_{00,10}=\Gamma_{00,01}=\frac{\sqrt{5}}{2^2\times3^3\times7} .$$

By evaluating the $\tilde{A}^{(r)}$ and $\tilde{G}_k^{(r)}$ for $r=0,1$ and writing them in terms of the irreducible tensors defined by Eq. (4.11), we find

$$\tilde{A}^{(0)}=-\frac{i}{\sqrt{6}}A^{(0)} ,$$
$$\tilde{A}^{(1)}=\sqrt{2/(3\times5\times7)}\,iA^{(1)} ,$$
$$\tilde{G}_k^{(0)}=-\frac{i}{\sqrt{2}}\bar{G}_k^{(0)} , \qquad \text{(B17)}$$
and
$$\tilde{G}_k^{(1)}=\sqrt{2/3}\,i\bar{G}_k^{(1)} .$$

By placing these results in Eq. (B9) we find that the linear Hall constant due to spin contributions from type-II diagrams is proportional to

$$\sum_{m,m',\sigma,\sigma'} J_{m\sigma,m'\sigma'}A_m(\varepsilon''-\varepsilon'+\varepsilon)A_{m'}(\varepsilon'')\bar{G}_{k\sigma}(\varepsilon)\bar{G}_{k'\sigma'}(\varepsilon')$$
$$=\frac{1}{2^3\times3^3\times7^2}\sqrt{5/3}\{[A^0(\varepsilon'')A^1(\varepsilon''-\varepsilon'+\varepsilon)+A^1(\varepsilon'')A^0(\varepsilon''-\varepsilon'+\varepsilon)]$$
$$\times\bar{G}_k^0(\varepsilon)\bar{G}_{k'}^0(\varepsilon')-\tfrac{7}{3}A^0(\varepsilon'')A^0(\varepsilon''-\varepsilon'+\varepsilon)$$
$$\times[\bar{G}_k^0(\varepsilon)\bar{G}_{k'}^1(\varepsilon')+\bar{G}_k^1(\varepsilon)\bar{G}_{k'}^0(\varepsilon')]\}+O(H^3) . \qquad \text{(B18)}$$

This is how we arrived at Eq. (4.16).

APPENDIX C: WEAK COUPLING

In the limit of weak coupling the pseudo-f spectral function is given as[11]

$$A_m(\varepsilon)\approx\frac{\Gamma^*}{(\varepsilon-\varepsilon_{fm})^2+\Gamma^{*2}}$$
$$\equiv\frac{1}{\Gamma^*}\sin^2[\eta_m(\varepsilon)] , \qquad \text{(C1)}$$

where

$$\eta_m(\varepsilon)=\cot^{-1}\left[\frac{\varepsilon_{fm}-\varepsilon}{\Gamma^*}\right] ,$$
$$\Gamma^*\equiv\frac{\pi T_0}{N_f} ,$$
and
$$\varepsilon_{fm}=\varepsilon_f+\varepsilon_m .$$

The boson spectral function in weak coupling is[11,15]

$$B(\varepsilon)\approx\frac{\Gamma}{\pi\varepsilon^2}\sum_m f(\varepsilon_{fm}-\varepsilon)$$
$$=\frac{N_f\Gamma}{\pi\varepsilon^2}f(\varepsilon_f-\varepsilon)+O(H^2) , \qquad \text{(C2)}$$

and the $4f$ spectral function is relatively smooth in the range of integration about the Fermi surface, so that it can be moved outside the integral. Also the partition function is approximately given as $Z_{4f}\approx N_f e^{-\beta\varepsilon_f}$. Therefore, at temperatures high compared to T_0, i.e., in the limit of weak coupling, we find Eq. (4.24) is written as

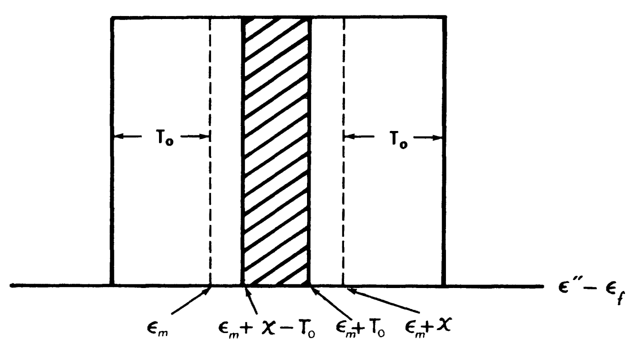

FIG. 3. The Lorentzians in Eq. (C3) modeled as rectangular functions. One function is centered about ε_{fm}, extends to $\varepsilon_{fm}\pm T_0$, and has a height of $\pi/2T_0$. The other is centered about $\varepsilon_{fm}+x$, where $x=\varepsilon'-\varepsilon$. Thus the area of each rectangular function is normalized to π in accordance with the definition for the spectral density $A_m(\varepsilon)$ (see Cox, Ref. 7). To obtain nonvanishing contributions to the integral [Eq. (C3)] x must lie in the range $-2T_0\le x\le 2T_0$.

$$I=\frac{\Gamma}{\pi}\int\frac{d\varepsilon}{2\pi}\left[-\frac{\partial f(\varepsilon)}{\partial\varepsilon}\right]\int\frac{d\varepsilon'}{\pi}f(\varepsilon')(1-e^{\beta(\varepsilon'-\varepsilon)})\int\frac{d\varepsilon''}{\pi}e^{-\beta(\varepsilon''-\varepsilon_f)}\frac{f(\varepsilon_f+\varepsilon'-\varepsilon'')}{(\varepsilon'-\varepsilon'')^2}$$
$$\times\frac{\partial}{\partial\varepsilon_m}\left[\frac{\Gamma^*}{(\varepsilon''-\varepsilon_{fm})^2+\Gamma^{*2}}\frac{\Gamma^*}{(\varepsilon''-\varepsilon'+\varepsilon-\varepsilon_{fm})^2+\Gamma^{*2}}\right]\Bigg|_{H=0}. \tag{C3}$$

The first point to note is that one cannot use the conventional approximation for the pseudo-f spectral function of letting Γ^* approach zero and replacing it by a δ function. This would make the integral zero. Second, the integral is large only when ε'' is close to the center of the Lorentzians, i.e., $\varepsilon''-\varepsilon_f\approx\Gamma^*$ *and* when the Lorentzians overlap, i.e., for $\varepsilon'-\varepsilon\approx\Gamma^*$.

It is not possible to find an analytic solution for Eq. (C3) by keeping the Lorentzians. Therefore we model them as rectangular functions of half-widths T_0 (which is approximately Γ^*) and height $\pi/2T_0$ (see Fig. 3):

$$A_m(\varepsilon'')=\frac{\pi}{2T_0}\{\Theta[\varepsilon''-(\varepsilon_{fm}-T_0)]-\Theta[\varepsilon''-(\varepsilon_{fm}+T_0)]\}. \tag{C4}$$

As we show, this produces very reasonable results in the limit of weak coupling.

By using rectangular functions for the pseudo-f spectral densities, we find

$$\frac{\partial}{\partial\varepsilon_m}[A_m(\varepsilon'',H)A_m(\varepsilon''-\varepsilon'+\varepsilon,H)]|_{H=0}=-\frac{\pi^2}{4T_0^2}\{[\Theta(x)-\Theta(x-2T_0)][\delta(y-x+T_0)-\delta(y-T_0)]$$
$$+[\Theta(x)-\Theta(x+2T_0)][\delta(y-x-T_0)-\delta(y+T_0)]\}, \tag{C5}$$

where

$$x\equiv\varepsilon'-\varepsilon$$

and

$$y\equiv\varepsilon''-\varepsilon_f.$$

When we place this in Eq. (C3) we find that the last integral is

$$I_3(\varepsilon,\varepsilon')\equiv\int\frac{d\varepsilon''}{\pi}e^{-\beta(\varepsilon''-\varepsilon_f)}\frac{f(\varepsilon_f+\varepsilon'-\varepsilon'')}{(\varepsilon'-\varepsilon'')^2}\frac{\partial}{\partial\varepsilon_m}[A_m(\varepsilon'',H)A_m(\varepsilon''-\varepsilon'+\varepsilon,H)]\Bigg|_{H=0}$$
$$=-\frac{\pi}{4T_0^2}\{[e^{-\beta x}g^+(\varepsilon)-g^-(\varepsilon')][\Theta(x)-\Theta(x-2T_0)]+[e^{-\beta x}g^-(\varepsilon)-g^+(\varepsilon')][\Theta(x)-\Theta(x+2T_0)]\}, \tag{C6}$$

where

$$g^{\pm}(\varepsilon)=\frac{e^{\pm\beta T_0}f(\varepsilon\pm T_0)}{[(\varepsilon-\varepsilon_f)\pm T_0]^2}. \tag{C7a}$$

As the range of integration in Eq. (C3) for the variable ε is limited to T (in units of k_B) by $[-\partial f(\varepsilon)/\partial\varepsilon]$, and both T and T_0 are much less than ε_f, the denominator can be replaced by ε_f. When we expand the Fermi function we find $g^{\pm}(\varepsilon)$ can be approximated as

$$g^{\pm}(\varepsilon)\approx\frac{e^{\pm\beta T_0}}{|\varepsilon_f|^2}\left[f(\varepsilon)\mp T_0\left[-\frac{\partial f(\varepsilon)}{\partial\varepsilon}\right]\right]. \tag{C7b}$$

Then the integral I_3 becomes

$$I_3(\varepsilon,\varepsilon')\approx-\frac{\pi}{4T_0^2}\left[\frac{1}{|\varepsilon_f|^2}[e^{-\beta x}f(\varepsilon)-f(\varepsilon')]Q(x)\right.$$
$$\left.+\frac{T_0}{|\varepsilon_f|^2}\left\{\beta[e^{-\beta x}f(\varepsilon)+f(\varepsilon')]-\left[e^{-\beta x}\left[-\frac{\partial f(\varepsilon)}{\partial\varepsilon}\right]+\left[-\frac{\partial f(\varepsilon')}{\partial\varepsilon'}\right]\right]\right\}P(x)\right], \tag{C6'}$$

where

$$Q(x)\equiv[\Theta(x)-\Theta(x-2T_0)]+[\Theta(x)-\Theta(x+2T_0)]$$

and (C8)

$$P(x)\equiv[\Theta(x)-\Theta(x-2T_0)]-[\Theta(x)-\Theta(x+2T_0)],$$

so that $Q(x)$ is an odd function of x, while $P(x)$ is even. The range of integration for $x=\varepsilon'-\varepsilon$ is limited by the rectangular functions to $-2T_0 \le x \le 2T_0$, while ε itself is limited by the derivative of the Fermi function to $-T \lesssim \varepsilon \lesssim T$. As x varies over a very narrow range, we transform the variables ε and ε' in Eq. (C3) to the variables

$$\varepsilon'-\varepsilon=x \ , \quad \varepsilon'+\varepsilon\equiv z \ , \tag{C9}$$

so that

$$\varepsilon'=\tfrac{1}{2}(x+z) \ ,$$

$$\varepsilon=-\tfrac{1}{2}(x-z) \ ,$$

and

$$d\varepsilon\, d\varepsilon'=\tfrac{1}{2}\, dx\, dz \ .$$

Then the integral Eq. (C3) is rewritten as

$$I=-\frac{\beta\Gamma}{16\pi^2 T_0^2|\varepsilon_f|^2}\int dx \int dz\, f(-\tfrac{1}{2}(x-z))f(\tfrac{1}{2}(x-z))f(\tfrac{1}{2}(x+z))(1-e^{\beta x}) \times\{[e^{-\beta x}f(-\tfrac{1}{2}(x-z))-f(\tfrac{1}{2}(x+z))]Q(x) +\beta T_0[e^{-\beta x}f^2(-\tfrac{1}{2}(x-z))+f^2(\tfrac{1}{2}(x+z))]P(x)\} \ . \tag{C10}$$

As the range of integration for x is much less than z at high temperatures, i.e., $T_0 \ll T$, we can expand the Fermi functions about $x=0$, and by keeping the leading terms we find

$$I\approx-\frac{\beta\Gamma}{16\pi^2 T_0^2|\varepsilon_f|^2}\int dx\int dz\, f^2(\tfrac{1}{2}z)f(-\tfrac{1}{2}z)\left[1-\frac{\beta x}{2}f(\tfrac{1}{2}z)\right] \times(-\beta x)\left[1+\frac{\beta x}{2}\right]\left[-\beta x\left[f^2(\tfrac{1}{2}z)+\frac{\beta x}{2}f(\tfrac{1}{2}z)[1+f(-\tfrac{1}{2}z)]\right]Q(x) +\beta T_0 f^2(\tfrac{1}{2}z)(2-\beta x)P(x)\right] \ . \tag{C11}$$

$Q(x)$ $[P(x)]$ is an odd (even) function of x, and the inteval for x is symmetric. Therefore, we pick up only odd (even) functions of x in the integrand from $Q(x)$ $[P(x)]$ and find after integrating over x,

$$I\approx-\frac{\beta^3 T_0^2\Gamma}{4\pi^2|\varepsilon_f|^2}\int du\, f^2(u)f(-u)[f^2(u)+f(u)f(-u)+f^2(u)f(-u)+\tfrac{4}{3}f^3(u)] \ , \tag{C12}$$

where $u=\beta z/2$. By evaluating the integrals over the Fermi functions we finally find in the limit of high temperatures $T \gg T_0$,

$$I\approx-\frac{13}{80\pi^2}\frac{\beta^3 T_0^2\Gamma}{|\varepsilon_f|^2} \ . \tag{C13}$$

APPENDIX D: STRONG COUPLING

In strong coupling, the pseudo-f spectral functions have only an exponential tail for $\varepsilon<E_0$; for $T=0$ K they are cut off at the ground-state energy E_0, i.e., at $T=0$ K,[8,11]

$$A_m(\varepsilon)=\frac{1}{\Gamma^*}\sin^2[\eta_m(\varepsilon)]\Theta(\varepsilon-E_0) \ , \tag{D1a}$$

where η_m is given by Eq. (C1). For small but finite temperatures $T \ll T_0$ we posit

$$A_m(\varepsilon)=\frac{1}{\Gamma^*}\sin^2[\eta_m(\varepsilon)]f(E_0-\varepsilon) \ , \tag{D1b}$$

that is, we replace the step function by the Fermi function, which at low temperature mimics a "rounded" step function.

The boson spectral function consists of a continuum part [see Eq. (C2)] and a singular part that gives rise to the Kondo resonance.[8,11] The latter is a strong function of temperature and it peaks near the ground-state energy E_0. It appears prominently for $T<T_0$; at $T=0$ K we can write it as

$$B^{\mathrm{sing}}(\varepsilon)=Z\pi\delta(\varepsilon-E_0) \ , \tag{D2}$$

where Z is the renormalization constant for the Kondo problem, $Z\approx\pi T_0/N_f\Gamma$. The continuum part of the boson spectral function is negligible compared to the singular [Eq. (D2)] in the region $\varepsilon\approx E_0$ where there are significant contributions to the integral I [see Eq. (4.24)].

Thus it will suffice to use only the singular part [Eq. (D2)].

The $4f$ spectral function has, in additon to a continuum, a part that becomes increasingly pronounced for $T<T_0$, i.e., the Kondo resonance. For $T=0$ K we can write

$$\rho^{4f}(\varepsilon)\approx\rho^{4f}_{\rm cont}(\varepsilon)+\frac{1}{N_f\Gamma}\sum_m \sin^2[\eta_m(\varepsilon+E_0)] \quad \text{(D3)}$$

where $\Gamma=\pi N(0)|V_k|^2$ is the hybridization width, and is related to the half-width of the Friedel-Anderson (charge) resonance. To lowest order in the magnetic field,

$$\frac{1}{N_f}\sum_m \sin^2\eta_m=\sin^2\eta_3+O(H^2)\ , \quad \text{(D3a)}$$

where $\eta_3\equiv\eta_m(H=0)$. Therefore, the Kondo resonance in the $4f$ spectral density of states does not have a term linear in the field, i.e., it is independent of field up to $O(H^2)$. Finally, the partition function as temperature approaches zero is

$$Z_{4f}(T)\approx e^{-\beta E_0}\ . \quad \text{(D4)}$$

Therefore, we find that in the limit of strong coupling, in particular at $T=0$ K, the integral I [Eq. (4.24)] is written as

$$I=\frac{1}{(\Gamma^*)^2}\rho_f^2(0)\int\frac{d\varepsilon}{2\pi}\left[-\frac{\partial f(\varepsilon)}{\partial\varepsilon}\right]\rho_f^{-1}(\varepsilon)\int\frac{d\varepsilon'}{\pi}f(\varepsilon')(1-e^{\beta(\varepsilon'-\varepsilon)})\rho_f^{-1}(\varepsilon')\int\frac{d\varepsilon''}{\pi}e^{-\beta(\varepsilon''-E_0)}Z\pi\delta(\varepsilon''-\varepsilon'-E_0)$$
$$\times\frac{\partial}{\partial\varepsilon_m}\left\{\sin^2[\eta_m(\varepsilon'')]f(E_0-\varepsilon'')\sin^2[\eta_m(\varepsilon''-\varepsilon'+\varepsilon)]f(E_0-\varepsilon''+\varepsilon'-\varepsilon)\right\}\Bigg|_{H=0}\ . \quad \text{(D5)}$$

By integrating over ε'' we find

$$I=\frac{Z\rho_f^2(0)}{2\pi^2\Gamma^{*2}}\frac{\partial}{\partial\varepsilon_m}\left\{\int d\varepsilon\left[-\frac{\partial f(\varepsilon)}{\partial\varepsilon}\right]f(-\varepsilon)\rho_f^{-1}(\varepsilon)\sin^2[\eta_m(\varepsilon+E_0)]\right.$$
$$\left.\times\int d\varepsilon'\,f(\varepsilon')f(-\varepsilon')(e^{-\beta\varepsilon'}-e^{-\beta\varepsilon})\rho_f^{-1}(\varepsilon')\sin^2[\eta_m(\varepsilon'+E_0)]\right\}\Bigg|_{H=0}$$
$$\equiv\frac{Z\rho_f^2(0)}{2\pi^2\Gamma^{*2}}(I_a-I_b)\ , \quad \text{(D6)}$$

where

$$I_a=\frac{\partial}{\partial\varepsilon_m}\left\{\int d\varepsilon\left[-\frac{\partial f(\varepsilon)}{\partial\varepsilon}\right]f(-\varepsilon)\rho_f^{-1}(\varepsilon)\sin^2[\eta_m(\varepsilon+E_0)]\right.$$
$$\left.\times\int d\varepsilon'\,f(\varepsilon')f(-\varepsilon')e^{-\beta\varepsilon'}\rho_f^{-1}(\varepsilon')\sin^2[\eta_m(\varepsilon'+E_0)]\right\}\Bigg|_{H=0} \quad \text{(D7)}$$

and

$$I_b=\frac{\partial}{\partial\varepsilon_m}\left\{\int d\varepsilon\left[-\frac{\partial f(\varepsilon)}{\partial\varepsilon}\right]f(-\varepsilon)e^{-\beta\varepsilon}\rho_f^{-1}(\varepsilon)\sin^2[\eta_m(\varepsilon+E_0)]\right.$$
$$\left.\times\int d\varepsilon'\,f(\varepsilon')f(-\varepsilon')\rho_f^{-1}(\varepsilon')\sin^2[\eta_m(\varepsilon'+E_0)]\right\}\Bigg|_{H=0}\ . \quad \text{(D8)}$$

From the definition of the phase shift η_m [Eq. (C1)],

$$\frac{\partial}{\partial\varepsilon_m}\sin^2[\eta_m(\varepsilon+E_0)]\Bigg|_{H=0}=-\frac{1}{\Gamma^*}\sin[2\eta_3(\varepsilon+E_0)]\sin^2[\eta_3(\varepsilon+E_0)]\ . \quad \text{(D9)}$$

Also, from the definition of the $4f$ density of states [Eq. (D3)] we find, after taking the derivative with respect to ε_m and setting $H=0$ in Eqs. (D7) and (D8), that

$$\rho_f^{-1}(\varepsilon)\sin^2[\eta_3(\varepsilon+E_0)]=\frac{\sin^2[\eta_3(\varepsilon+E_0)]}{\frac{1}{\Gamma}\sin^2[\eta_3(\varepsilon+E_0)]+\rho^{4f}_{\rm cont}(\varepsilon)}$$
$$\approx\begin{cases}\Gamma, & p_1T_0\le\varepsilon\le p_2T_0\\ 0, & \text{otherwise}\end{cases}\ . \quad \text{(D10)}$$

To arrive at this *approximation* we consider that the Lorentzian is negligible compared to the continuum part of ρ^{4f} when ε is several (p) half-widths Γ^* from its center which is at $\varepsilon = T_0$. Thus

$$p_{1,2}T_0 \equiv T_0 \mp p\Gamma^* = T_0\left[1 \mp \frac{p\pi}{N_f}\right] . \tag{D11}$$

Note that we must choose p such that p_1 is negative, so that there is a finite density at the Fermi surface. With this approximation we find that the integrals [Eqs. (D7) and (D8)] are written as

$$I_a = -\frac{\Gamma}{Z}\int_{p_1T_0}^{p_2T_0} d\varepsilon \left[-\frac{\partial f(\varepsilon)}{\partial\varepsilon}\right] f(-\varepsilon)\sin[2\eta_3(\varepsilon+E_0)]\int_{p_1T_0}^{p_2T_0} d\varepsilon' f^2(\varepsilon') + \Gamma\int_{p_1T_0}^{p_2T_0} d\varepsilon\left[-\frac{\partial f(\varepsilon)}{\partial\varepsilon}\right] f(-\varepsilon)\frac{\partial}{\partial\varepsilon_m}\int d\varepsilon' f^2(\varepsilon')\rho_f^{-1}(\varepsilon')\sin^2[\eta_m(\varepsilon'+E_0)]\bigg|_{H=0} , \tag{D7'}$$

and

$$I_b = -\frac{\Gamma}{Z}\left\{\int_{p_1T_0}^{p_2T_0} d\varepsilon\left[-\frac{\partial f(\varepsilon)}{\partial\varepsilon}\right] f(\varepsilon)\sin[2\eta_3(\varepsilon+E_0)]\int_{p_1T_0}^{p_2T_0} d\varepsilon'\frac{1}{\beta}\left[-\frac{\partial f(\varepsilon')}{\partial\varepsilon'}\right] + \int_{p_1T_0}^{p_2T_0} d\varepsilon\left[-\frac{\partial f(\varepsilon)}{\partial\varepsilon}\right] f(\varepsilon)\int_{p_1T_0}^{p_2T_0} d\varepsilon'\frac{1}{\beta}\left[-\frac{\partial f(\varepsilon')}{\partial\varepsilon'}\right]\sin[2\eta_3(\varepsilon'+E_0)]\right\} . \tag{D8'}$$

In all the integrals except one, we directly took the derivative of the Lorentzian. The one exception occurs when the integrand does not contain a derivative of the Fermi function; for this case one can shift variables so that the Fermi function depends on ε_m. If one adopts this approach one finds, for $T \ll T_0$ and for $p_1 < 0$,

$$I_m = \frac{\partial}{\partial\varepsilon_m}\int d\varepsilon' f^2(\varepsilon')\rho_f^{-1}(\varepsilon')\sin^2[\eta_m(\varepsilon'+E_0)]\bigg|_{H=0} = \Gamma\int_{p_1T_0}^{p_2T_0} d\varepsilon'\frac{\partial}{\partial\varepsilon_m} f^2(\varepsilon'+\varepsilon_m) = -\Gamma . \tag{D12}$$

One obtains the same result if one assumes $\rho_f^{-1}(\varepsilon)$ constant and removes it from the integrand, i.e.,

$$I_m = -\rho_f^{-1}(0)\int d\varepsilon' f^2(\varepsilon')\sin[2\eta_3(\varepsilon')]\frac{d\eta_3(\varepsilon')}{d\varepsilon'} , \tag{D13}$$

where we used

$$\frac{\partial\eta_m(\varepsilon')}{\partial\varepsilon_m} = -\frac{\partial\eta_3(\varepsilon')}{\partial\varepsilon'}$$

which follows from the definition [Eq. (C1)]. At $T = 0$ K this integral reduces to

$$I_m = -\rho_f^{-1}(0)\int_{-\infty}^{0} d\varepsilon'\sin[2\eta_3(\varepsilon')]\frac{d\eta_3(\varepsilon')}{d\varepsilon'} = -\rho_f^{-1}(0)\int_{-\infty}^{0} d\eta_3\sin 2\eta_3 = -\rho_f^{-1}(0)\sin^2[\eta_3(0)] = -\Gamma , \tag{D14}$$

where the last step follows from Eqs. (D3) when one recognizes that for $\varepsilon = 0$, $\rho_{\rm cont}^{4f}(0) \ll \Gamma^{-1}\sin^2[\eta_3(E_0)]$.

However, if we do not remove $\rho_f^{-1}(\varepsilon)$ from the integrand, and if we do not take the derivative of the Lorentzian we find for $T = 0$ K,

$$I_m = -\frac{1}{Z}\int_{p_1T_0}^{p_2T_0} d\varepsilon' f^2(\varepsilon')\sin[2\eta(\varepsilon')] = -\frac{1}{Z}\int_{p_1T_0}^{0} d\varepsilon'\sin[2\eta(\varepsilon')] = -\Gamma\ln\left[\frac{(|p_1|+1)^2+(\pi/N_f)^2}{1+(\pi/N_f)^2}\right] , \tag{D15}$$

where we took $p_1 < 0$. In this approach we obtain the same result *modulo* a factor of order 1, e.g, for large N_f and $|p_1| = 1$, we obtain

$$I_m = -\ln 4\,\Gamma = -1.38\Gamma . \tag{D15a}$$

Therefore, this one integral is somewhat difficult to evaluate, and we can say its value is $-\Gamma$ *modulo* a factor of order 1. For all the other integrands in Eqs. (D7) and (D8), a *derivative* of the Fermi function enters, thus we take the derivative of the Lorentzian and *not* the Fermi function.[16]

At zero temperature the integrals in I_b [Eq. (D8')] are zero, and for the integrals in I_a [Eq. (D7')] it suffices to set the derivative of the Fermi function equal to a δ function $\delta(\varepsilon)$. We find, at $T = 0$ K,

$$I_a = -\tfrac{1}{2}A\Gamma^2 - \frac{1}{2}\frac{p_1T_0}{Z}\Gamma\sin[2\eta_3(E_0)] = -\tfrac{1}{2}\Gamma^2\left[A + \frac{p_1N_f}{\pi}\sin[2\eta_3(E_0)]\right] , \tag{D16}$$

where we used $Z = \pi T_0/N_f\Gamma$, and A is of order 1 [see Eqs. (D12), (D14), and (D15)]. We also find that the integral I [see Eqs. (4.24) and (D6)] in the strong-coupling limit at $T=0$ K is

$$I=-\frac{\rho_f^2(0)}{4\pi^2 Z}\left[A+\frac{p_1 N_f}{\pi}\sin[2\eta_3(E_0)]\right]$$

$$=-\frac{\sin^4[\eta_3(0)]}{4\pi^2\Gamma\Gamma^*}\left[A+\frac{p_1 N_f}{\pi}\sin[2\eta_3(0)]\right], \quad \text{(D17)}$$

where we used Eqs. (D3) and (D3a) for $\rho_f(0)$, and equated the phase shift of the pseudo-f electron at E_0 to that of the $4f$ electron at the Fermi surface $\varepsilon=0$, i.e., we set

$$\eta_3^{\text{pseudo-}f}(E_0)=\eta_3^{4f}(0)\ . \quad \text{(D17a)}$$

This is reasonable, as the contribution of the continuum to the $4f$ density near the Fermi surface is negligible [see Eq. (D3)].

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