

## Size Dependence in the Disordered Kondo Problem

Ivar Martin, Yi Wan, and Philip Phillips

*Loomis Laboratory of Physics, University of Illinois at Urbana-Champaign, 1100 W. Green Street, Urbana, Illinois, 61801-3080*  
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We study here the role randomly placed nonmagnetic scatterers play on the Kondo effect. We show that spin-relaxation effects (with time  $\tau_s^0$ ) in the vertex corrections to the Kondo self-energy lead to an exact cancellation of the singular temperature dependence arising from the diffusion poles. For a thin film of thickness  $L$  and a mean-free path  $\ell$ , disorder provides a correction to the Kondo resistivity of the form  $\tau_s^0/(k_F L \ell^2) \ln T$  that explains the disorder-induced depression of the Kondo effect observed by Blachly and Giordano [Phys. Rev. B **51**, 12 537 (1995)]. [S0031-9007(96)02064-9]

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At low temperatures, the resistivity of a metal alloy acquires a logarithmic temperature dependence [1] in response to spin-flip scattering between local magnetic impurities and the conduction electrons. This behavior persists down to a temperature (the Kondo temperature  $T_K$ ) where the magnetic impurities and conduction electrons begin to condense into singlet states. The presence of the  $\ln T$  term in the resistivity signifies that spin-flip scattering between conduction electrons and localized magnetic centers has a singular frequency ( $\omega$ ) dependence. Magnetic impurities are not alone in this respect. It is well known that even nonmagnetic impurities can generate a singular ( $\ln \omega$  in  $d = 2$ ) frequency dependence in the conductivity [2,3]. In a sample containing both magnetic and nonmagnetic impurities, the question arises: Which singularity ultimately wins, or can the interplay between the singularities lead to a suppression of either localization or the Kondo effect? In this Letter, we resolve these questions.

The motivation for this study is twofold. First, while there have been numerous treatments of this problem [4–7], a clear consensus has not been reached. Most recently, Ohkawa, Fukuyama, and Yosida [6] showed that disorder results in a singularity of the form  $T^{d/2-2}$  in the conductivity. As a result, they conclude that static disorder can mask the Kondo resistivity as  $T \rightarrow 0$ . On the experimental side, Blachly and Giordano [8] recently measured the conductivity in a series of thin films containing magnetic as well as nonmagnetic impurities. They found no evidence for the  $T^{d/2-2}$  singularity but observed instead a suppression of the Kondo resistivity as the strength of the disorder increased and as the sample thickness decreased. Earlier experiments by Korn [9] also failed to observe the  $T^{d/2-2}$  singularity but observed instead an enhancement in the Kondo resistivity. The point of agreement between these experiments is that disorder couples nontrivially to the Kondo effect and ultimately modifies the coefficient of the  $\ln T$  dependence. Given the strong dimensional dependence of weak localization, disorder could eventually lead to a sample size dependence of the Kondo resistivity.

At the outset, we set aside the still controversial issue [Ref. [8(c)]] of the sample size dependence and focus on the seemingly straightforward problem of the role

weak localization plays in the Kondo effect. The new wrinkle we introduce in this problem is the feedback effect spin scattering has on weak localization. While it is standard to consider the direct influence of weak localization on the Kondo effect, the reverse effect has not been included [10]. Nonetheless, it is well known that to second order in the exchange interaction  $J$ , electron scattering by disordered Heisenberg spins introduces a cutoff of the diffusion pole in both the particle-hole (diffuson) and particle-particle (Cooperon) channels except for the  $S = 0$  particle-hole channel [11]. Within this approximation for the diffusion propagators, the fate of the  $T^{d/2-2}$  singularity rests on whether the  $S = 0$  particle-hole propagator contributes to the Kondo self-energy. We show explicitly it *does not*. With the singularity removed, we calculate the conductivity to lowest order in  $J$  and  $1/(k_F \ell)$ .

The starting point for our analysis is a model Hamiltonian  $H = H_0 + H_{sd}$  that contains both normal impurities

$$H_0 = \sum_{k\sigma} (\varepsilon_k - \varepsilon_F) a_{k\sigma}^\dagger a_{k\sigma} + \frac{v}{\Omega} \sum_{k,k',i} e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_i} a_{k\sigma}^\dagger a_{k'\sigma}$$

as well as magnetic scatterers

$$H_{sd} = -\frac{J}{\Omega} \sum_{R_n, k, k', \sigma, \sigma'} e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{R}_n} \boldsymbol{\sigma}_{\sigma, \sigma'} \cdot \mathbf{S}_n a_{k\sigma}^\dagger a_{k'\sigma'}$$

where  $v$  measures the strength of the scattering with the nonmagnetic disorder,  $R_n$  denotes the position of the impurities, magnetic or otherwise,  $\mathbf{S}_n$  is the spin operator for the magnetic impurity at site  $n$ , and  $\Omega$  is the volume. The two natural time scales in this problem are  $\tau_s^0$  and  $\tau_0$ , the magnetic and nonmagnetic scattering times. In terms of the density of states of the host metal,  $\rho_0$ , and the concentrations of magnetic and nonmagnetic scatterers,  $n_s$  and  $n_0$ , respectively, we have that  $\hbar/2\tau_s^0 = 3\pi n_s \rho_0 |J|^2/4$  and  $\hbar/2\tau_0 = \pi n_0 \rho_0 |v|^2$ . The total scattering rate is  $1/\tau = 1/\tau_s^0 + 1/\tau_0$ . To measure the strength of the nonmagnetic disorder, we define  $\lambda = \hbar/(2\pi \varepsilon_F \tau_0)$ . We assume that the concentration of localized spins is dilute so that long-range spin glass effects are irrelevant. Also, we work in the regime in which normal impurity scattering dominates,  $1/\tau_0 \gg 1/\tau_s^0$ .

To evaluate the conductivity above  $T_K$ , we must first calculate the Kondo self-energy. To include the dynamical effects of the localized spins, it is sufficient to calculate the self-energy to third order in the exchange interaction  $J$ . At this order, static disorder can be included by decorating the single and double spin-flip vertices with Cooperon and diffuson propagators [6,7]. In previous work [6,7], spin-independent Cooperons and diffusons of the form  $C(Q, \omega) = D(Q, \omega) \propto (DQ^2 - i\omega)^{-1}$  were used where

$$C_{\alpha\beta\gamma\delta} = \frac{\hbar^2}{8\pi\rho_0\tau^2(DQ^2 - i\omega + 2/\tau_s^0)} (\delta_{\alpha\beta}\delta_{\gamma\delta} - \boldsymbol{\sigma}_{\alpha\beta} \cdot \boldsymbol{\sigma}_{\gamma\delta}) + \frac{\hbar^2}{8\pi\rho_0\tau^2(DQ^2 - i\omega + 2/3\tau_s^0)} (3\delta_{\alpha\beta}\delta_{\gamma\delta} + \boldsymbol{\sigma}_{\alpha\beta} \cdot \boldsymbol{\sigma}_{\gamma\delta}) \quad (1)$$

and the diffuson becomes

$$D_{\alpha\beta\gamma\delta} = \frac{\hbar^2}{8\pi\rho_0\tau^2(DQ^2 - i\omega)} (\delta_{\alpha\beta}\delta_{\gamma\delta} + \boldsymbol{\sigma}_{\alpha\beta} \cdot \boldsymbol{\sigma}_{\gamma\delta}) + \frac{\hbar^2}{8\pi\rho_0\tau^2(DQ^2 - i\omega + 4/3\tau_s^0)} (3\delta_{\alpha\beta}\delta_{\gamma\delta} - \boldsymbol{\sigma}_{\alpha\beta} \cdot \boldsymbol{\sigma}_{\gamma\delta}), \quad (2)$$

where  $\alpha\beta$  and  $\gamma\delta$  are spin indices. These expressions were obtained by summing ladder diagrams with both normal and spin scattering treated in the first Born approximation. Two-particle self-energy corrections which may lead to  $O(J^3)$  corrections to the propagator lifetimes were not included [12]. We also neglected all other inelastic processes such as electron-electron and electron-phonon in-

$Q$  and  $\omega$  are the net momentum and energy transfer and  $D = 2\hbar\varepsilon_F\tau/dm$  is the diffusion constant. It is the diffusion pole that leads to the  $T^{d/2-2}$  divergence. However, this is inconsistent because  $C(Q, \omega)$  and  $D(Q, \omega)$  couple to electron lines of different spin. Such propagators are well known [11] to depend on spin, and hence we include explicitly the spin dependence here. If all scattering processes are treated in the first Born approximation, the Cooperon propagator [11] is transformed to

interactions, because in our regime of interest  $\hbar/\tau_s^0$  dominates. The two terms in each propagator correspond to singlet and triplet scattering, respectively.

The diagrams shown in Fig. 1 contain the dominant quantum corrections [6] to the Kondo self-energy at third order in the presence of disorder. The sum of all such diagrams is

$$\Sigma_{3q}(k, i\epsilon_n) = \frac{2}{\beta^2} \sum V_{\alpha\beta\nu\eta}^\pm(i\omega_\ell, i\omega_m) G(iz_{nm}, q) \left[ G(iz_{n\ell}, k + Q) + n_0|v|^2 \sum_{k'} G^2(i\epsilon_n, k') G(iz_{n\ell}, k' + Q) \right] \times [D_{\sigma\alpha\beta\gamma}(i\omega_\ell, Q) D_{\gamma\nu\eta\sigma}(i\omega_\ell, Q) + C_{\sigma\alpha\gamma\nu} C_{\beta\gamma\eta\sigma}], \quad (3)$$

where repeated indices,  $\pm$ , and  $q$  are summed over, the arguments of the Cooperons are the same as those of the diffusons,  $z_{nm} = \epsilon_n + \omega_m$ ,  $G(i\epsilon, q) = [i\epsilon + \epsilon_F - \hbar^2 q^2/2m + i(\hbar/2\tau)\text{sgn}(\epsilon)]^{-1}$ , the electron energies are the Matsubara frequencies  $\epsilon_n = (2n+1)\pi T$ ,  $\omega_\ell = 2l\pi T$ ,  $DQ^2 < \hbar/\tau_0$ , and  $(\epsilon_n + \omega_\ell)\omega_\ell < 0$ . We

have set  $k_B = 1$ . The factor of 2 arises from the two possible couplings of the diffusion propagators to the internal electron lines and the  $\pm$  from the two orientations of the pseudofermion loops. The pseudofermion part involves a trace over the components of the impurity spin operators and hence simplifies to

$$V_{\alpha\beta\nu\eta}^\pm(i\omega_l, i\omega_m) = \frac{1}{4} J^3 n_s \beta \left[ \frac{1}{i\omega_\ell} (\delta_{m0} - \delta_{\ell m}) (1 - \delta_{\ell 0}) + \frac{1}{i\omega_m} \delta_{\ell 0} (1 - \delta_{m0}) \pm \frac{\beta}{2} \delta_{m0} \delta_{\ell 0} \right] (\sigma_{\alpha\beta}^a \sigma_{\nu\eta}^a). \quad (4)$$

From the pseudofermion contribution, we see that the sum over the spin indices separates into two identical sums of the form  $D_{\sigma\alpha\beta\gamma} \sigma_{\alpha\beta}^a$  with repeated indices summed over. If we use the identity  $(\boldsymbol{\sigma}_{\nu\alpha} \cdot \boldsymbol{\sigma}_{\beta\gamma}) \sigma_{\alpha\beta}^a = -\sigma_{\nu\gamma}^a$ , we find immediately that the cancellation of the  $S=0$  diffuson  $D_{\nu\alpha\beta\gamma}^S \sigma_{\alpha\beta}^a \propto (\delta_{\nu\alpha}\delta_{\beta\gamma} + \boldsymbol{\sigma}_{\nu\alpha} \cdot \boldsymbol{\sigma}_{\beta\gamma}) \sigma_{\alpha\beta}^a = 0$  from the third order Kondo self-energy is exact. To any order in  $J$ , in the most divergent approximation, the cancellation of the  $S=0$  diffuson can be seen as follows. Within this scheme, each diffuson encircles a vertex that is exactly equal to the Abrikosov [13] vertex function  $\Gamma \propto \boldsymbol{\sigma} \cdot \mathbf{S}$ . When this function is now multiplied by  $D^{S=0}$  and summed over the spin indices, the cancellation to all orders follows immediately from the spin identity

given above. Note this cancellation relies on the spin algebra and hence is not tied to the approximations used to obtain  $D^{S=0}$ . The cancellation of the  $S=0$  component of the diffuson is fundamentally tied to the fact that the Kondo interaction does not conserve the electron's spin. Summing over the spin indices in the remaining propagators in the self-energy reduces the problem to one in which the diffuson and Cooperon are spin independent:  $\tilde{D} = \hbar^2/(2\pi\rho_0\tau^2)(DQ^2 - i\omega + 4/3\tau_s^0)^{-1}$  and  $\tilde{C} = \hbar^2/(4\pi\rho_0\tau^2)[(DQ^2 - i\omega + 2/\tau_s^0)^{-1} + (DQ^2 - i\omega + 2/3\tau_s^0)^{-1}]$ .

To calculate the resistivity, we evaluate the standard self-energy as well as the Cooperon weak-localization diagrams [6]. We do not include the diffuson singlet

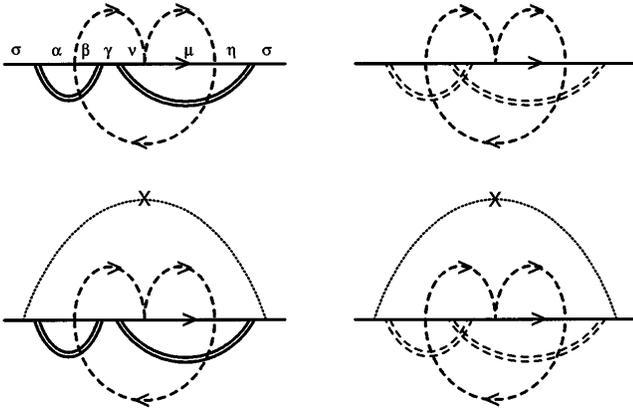


FIG. 1. Feynman diagrams contributing to the Kondo self-energy. The dashed lines correspond to Abrikosov pseudofermions and the double solid lines to diffusons and double dashed lines to the Cooperons. The Greek letters indicate the spin. The X indicates a single nonmagnetic impurity scattering event.

contribution because it is of higher order in  $1/(k_F \ell)$  than the Cooperon term. Because the results are rather lengthy, we present only the asymptotic behavior. For  $d = 2$  in the limit  $T \gg \hbar/\tau_s^0$ , we recover the inverse temperature dependence [6,7]

$$\frac{\hbar}{2\tau^C} = \frac{\hbar}{2\tau^D} \approx \frac{-\pi\hbar\rho_0\lambda J}{3\tau_0} \frac{\hbar}{\tau_s^0 T} \ll -\rho_0\lambda J \frac{\hbar}{\tau_0}, \quad (5)$$

where  $1/2\tau^{C,D} = \int d\epsilon (-\frac{\partial f}{\partial \epsilon}) [-\text{Im}\Sigma_{3q}^{C,D}(\epsilon + i0)]$ . The superscript refers to self-energy diagrams with Cooperons or diffusons. Without the cancellation theorem, the lower bound in temperature for the  $1/T$  behavior is set by  $\max[\hbar/\tau_\phi, T_K]$ , where  $\tau_\phi$  is the inelastic scattering time. We find here that by explicitly including spin scattering in the diffusion propagators, the algebraic behavior occurs when  $\hbar/(\tau_s^0 T) \ll 1$ . We will see later that as a result of this restriction, the contribution of the  $1/T$  term to the conductivity is negligible. In the opposite regime,  $T \ll \hbar/\tau_s^0$ , the relaxation times

$$\frac{\hbar}{2\tau^D} + \frac{\hbar}{2\tau^C} = -\left(\frac{5}{2} + \frac{3\ln 3}{4}\right)\rho_0\lambda J \frac{\hbar}{\tau_0} \ln \frac{\hbar}{T\tau_s^0} \quad (6)$$

are both logarithmic functions of temperature.

The final contribution to the relaxation time comes from the Cooperon weak-localization diagram. In two dimensions in the presence of isotropic spin-flip scattering, the weak-localization contribution is  $\Delta\sigma_{\text{loc}} = -e^2/(2\pi^2\hbar) \times \ln(\sqrt{3}\tau_{\text{es}}/\tau_0)$ , where  $\hbar/2\tau_{\text{es}} = 8\hbar/(3\tau_s^0)[1 - \rho_0 J \ln(\epsilon_F/T)]$ , where we have explicitly included the  $O(J^3)$  contribution to the spin-scattering lifetime. Inclusion of the third order correction to the spin-scattering time enhances the spin-flip scattering rate, thereby weakening the effects of localization. To see this more clearly, we expand the argument of the logarithm for temperatures well above the Kondo temperature:  $\Delta\sigma_{\text{loc}} = -e^2/2\pi^2\hbar \ln(3\sqrt{3}\tau_s^0/8\tau_0) - e^2/2\pi^2\hbar\rho_0 J \ln(\epsilon_F/T)$ . We see clearly that the Kondo interaction reduces the weak localization correction because  $J < 0$ .

We collect all the contributions discussed above to determine the conductivity. In the temperature range  $T_K \ll T < \hbar/\tau_s^0$ , Cooperon, diffuson, and weak-localization corrections are logarithmic in temperature. Combining the results from Eq. (5) with the weak-localization correction, we find that the magnitude of the logarithmic part of the conductivity

$$\Delta\sigma^T = \sigma_0 \frac{4\tau_0\rho_0 J}{\tau_s^0} \left(1 + 1.4\lambda \frac{\tau_s^0}{\tau_0}\right) \ln \frac{\epsilon_F}{T} \quad (7)$$

is enhanced by disorder. The first term in this expression arises from the unperturbed Kondo effect and the latter from the interplay with disorder. Inclusion of disorder in the self-energy always enhances the Kondo resistivity by increasing repetitive scattering at magnetic impurities.

For temperatures  $T \gg \hbar/\tau_s^0$ , the self-energy contribution to the relaxation time scales as  $1/T$ , whereas the weak-localization correction is proportional to  $\ln T$ . However, comparison of the magnitude of Eq. (5) and  $\Delta\sigma_{\text{loc}}$  reveals that the temperature-dependent weak-localization term dominates and the magnitude of the resultant logarithmic correction

$$\Delta\sigma^T = \sigma_0 \frac{4\tau_0\rho_0 J}{\tau_s^0} \left(1 - \frac{\lambda\tau_s^0}{4\tau_0}\right) \ln \frac{\epsilon_F}{T} \quad (8)$$

is suppressed by the disorder. The ratio  $\lambda/\tau_0$  scales as  $1/\ell^2$ , where  $\ell$  is the mean-free path. We see then that, in the dilute impurity regime, disorder suppresses the Kondo effect. The crossover from enhancement to suppression of the Kondo effect occurs because the magnitude and functional dependence of the quantum corrections to the self-energy are determined by the shortest of two length scales: the phase-breaking length,  $L_\phi = \sqrt{D\tau_s^0/\hbar}$  and the diffusion length,  $L_T = \sqrt{D/T}$ . The latter arises because coupling of diffusion propagators to internal electron lines in the self-energy leads to an effective electron-electron interaction.

Let us now apply our results to thin films with a thickness  $L$ . We will assume that  $\ell < L \ll L_\phi$ . Then we can treat the films as quasi-2D with respect to localization, but because  $\ell < L$  the electron gas is characterized by a three-dimensional density of states  $\rho_0 = 1/(2\pi)^2(2m/\hbar^2)^{3/2}\epsilon_F^{1/2}$  with a diffusion constant given by  $D = 2\hbar\epsilon_F\tau_0/3m$ . The summation on  $Q$  in the Cooperon and diffuson is restricted to small momentum transfers such that  $DQ^2 < 1/\tau_0$ . However, for thicknesses of the sample on the order of  $\ell$ , the smallest wave vector in the transverse direction does not satisfy this constraint. To rectify this problem, Volkov [14] showed that surface boundary conditions must be treated consistently. For thin films, his treatment shows that the boundaries always give rise to a strictly two-dimensional weak-localization correction and an explicit finite size dependence. To account for the former, the momentum integration in the Cooperon and diffuson must be restricted to the plane. The density of states that arises from converting the sum to an integral will be the two-dimensional density of states  $\rho_0^{2D} = \pi\rho_0/(k_F L)$ . Hence,

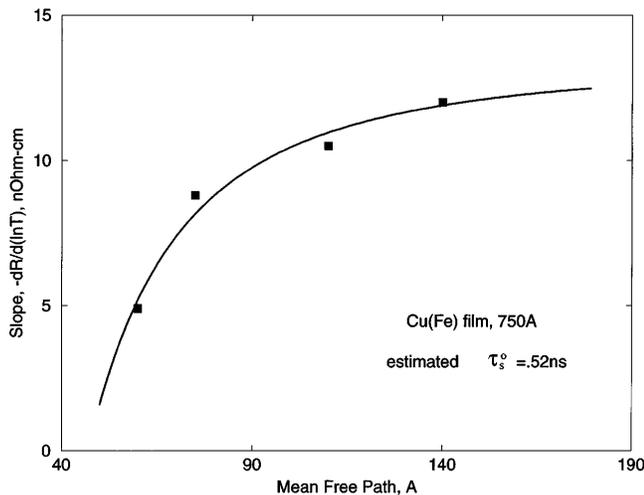


FIG. 2. Comparison of the theoretical prediction for the Kondo resistivity predicted from the second of Eq. (9) with the experimental data of Blachly and Giordano [8] Fig. 7. The horizontal axis measures the strength of the static disorder through the mean-free path.

the self-energy diagrams will generate a size dependence to the conductivity. The explicit finite-size weak-localization correction is [14]  $\Delta\sigma_{\text{loc}} = -e^2/(2\pi^2\hbar L) \times \ln\{\sqrt{3}\tau_{\text{es}}/\tau_0[\sinh(L/\ell)(\ell/L)]\}$ . The size dependence in the logarithm yields an effective size dependence in the spin-relaxation time. However, this will not affect the temperature dependence of the conductivity. The only size dependence that is coupled to the temperature is the  $1/L$  prefactor of the weak-localization correction.

We now combine these results in the low- and high-temperature limits discussed earlier. In the two limits, we obtain

$$\Delta\sigma^T = \begin{cases} \tilde{\sigma}\left(1 + \frac{2.3\hbar\tau_s^0}{\pi mk_F L \ell^2}\right) \ln \frac{\epsilon_F}{T}, T_K \ll T < \hbar\tau_s^0 \\ \tilde{\sigma}\left(1 - \frac{1.2\hbar\tau_s^0}{\pi mk_F L \ell^2}\right) \ln \frac{\epsilon_F}{T}, T_K, \hbar/\tau_s^0 \ll T \end{cases} \quad (9)$$

an explicit size and disorder correction that scales as  $1/(\ell^2 L)$  with  $\tilde{\sigma} = 4\sigma_0\tau_0\rho_0 J/\tau_s^0$ . The fact that only the coefficient of  $\ln T$  is modified is a direct consequence of the cancellation theorem.

In the concentrated impurity limit  $T < \hbar/\tau_s^0$ , increasing disorder enhances the resistivity. In Cu(Fe) alloys at impurity concentrations ranging from (0.3–2.1)%, Korn observed an enhancement in the Kondo resistivity that is consistent with the first equation above. However, in the dilute limit,  $T \gg \hbar/\tau_s^0$ , we predict a suppression of the Kondo effect as the disorder is increased and the size of the sample decreases. In the experiments of Blachly and Giordano [8],  $\hbar/\tau_s^0 \approx 0.1$  K, which is much less than the Kondo temperature for Cu(Fe). The second of Eqs. (9) should be valid. Figure 2 shows a comparison between the experimental data and the theoretical predictions. The best fit to the data was obtained with  $\tau_s^0 = 0.52$  ns, which is consistent with the experimental range of  $10^{-10}$  s. As

is evident, theory and experiment are in good agreement. Although electron-electron interactions could also give rise to  $\ln T$  corrections to the conductivity, no  $\ln T$  was observed [8] in the absence of magnetic impurities. Regarding the size dependence, we note that Ujsaghy *et al.* [15] have proposed a hindered spin-orbit [15] mechanism that also generates a size dependence. By comparing the magnitude of the corrections to the Kondo resistivity, we find that the disorder mechanism is expected to dominate when  $v_F\tau_s^0/k_F^2 > \ell^2\min(\lambda_0, \ell)$ , where  $\lambda_0$  is the hindered spin-orbit length [15]. For the Cu(Fe) samples [8], this corresponds to a mean-free path of  $\ell \approx 500$  Å, below which the contribution from disorder is expected to dominate the size dependence of the Kondo resistivity. In the other regime, the spin-orbit mechanism of Ujsaghy *et al.* [15] dominates. We conclude that disorder provides either an enhancement or a suppression correction to the Kondo resistivity of the form  $1/(\ell^2 L)$ .

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