

## Energy-resolved inelastic electron scattering off a magnetic impurity

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We study inelastic scattering of energetic electrons off a Kondo impurity. If the energy  $E$  of the incoming electron (measured from the Fermi level) exceeds significantly the Kondo temperature  $T_K$ , then the differential inelastic cross section  $\sigma(E, \omega)$ , i.e., the cross section characterizing scattering of an electron with a given energy transfer  $\omega$ , is well defined. We show that  $\sigma(E, \omega)$  factorizes into two parts. The  $E$  dependence of  $\sigma(E, \omega)$  is logarithmically weak and is due to the Kondo renormalization of the effective coupling. We are able to relate the  $\omega$  dependence to the spin-spin correlation function of the magnetic impurity. Using this relation, we demonstrate that in the absence of the magnetic field, the dynamics of the impurity spin causes the electron scattering to be inelastic at any temperature. At temperatures  $T$  low compared to the Kondo temperature  $T_K$ , the cross section is strongly asymmetric in  $\omega$  and has a well-pronounced maximum at  $\hbar\omega \sim T_K$ . At  $T \gg T_K$ , the dependence  $\sigma$  vs  $\omega$  has a maximum at  $\omega=0$ ; the width of the maximum exceeds  $T_K/\hbar$  and is determined by the Korringa relaxation time of the magnetic impurity. Quenching of the spin dynamics by an applied magnetic field results in a finite elastic component of the electron scattering cross section. The differential scattering cross section may be extracted from the measurements of relaxation of hot electrons injected in conductors containing localized spins.

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### I. INTRODUCTION

Scattering of an electron off a magnetic impurity embedded in a conductor is known to be anomalously strong.<sup>1</sup> The origin of the anomaly is rooted in the degeneracy of the localized spin states. This degeneracy, being removed by a weak exchange interaction with the itinerant electrons in a metal, gives rise to the strong scattering of electrons with low energy—the Kondo effect. Perturbation theory in the exchange interaction constant  $J$  is singular. The second-order contribution in  $J$  to the scattering amplitude diverges logarithmically<sup>2</sup> if the electron energy  $E$  (measured from the Fermi level) and temperature  $T$  are approaching zero. It is important to notice that the logarithmically divergent contribution to the amplitude corresponds to an elastic process. Indeed, this contribution comes from the change of state of *one* electron: states of all other itinerant electrons are the same in the beginning and end of the scattering process. Therefore, the energies of the electron before and after the scattering is unchanged.

The divergence noticed by Kondo is not unique to the second order of the perturbation theory. Its higher orders ( $n > 2$ ) also contain divergent terms of the type  $J^n \ln^{n-1}(D/\varepsilon)$ , where  $\varepsilon = \max(E, T)$ , and  $D$  is some ultraviolet energy cutoff, whose value depends on the specific model:  $D \gg \varepsilon$ . These leading logarithmic terms may be summed up by diagrammatic method<sup>3</sup> or by means of the “Poor man’s scaling”<sup>4</sup> renormalization group (RG), yielding for the scattering amplitude

$$A_{k,\sigma,S \rightarrow k',\sigma',S'} = \frac{1}{\ln(\varepsilon/T_K)} \mathbf{s}_{\sigma,\sigma'} \cdot \mathbf{S}_{s,s'}, \quad (1)$$

where  $\mathbf{s}_{\sigma,\sigma'}$  and  $\mathbf{S}_{s,s'}$  are the spin operators of the conduction electrons and the impurity, respectively. The so-called Kondo temperature is given in terms of the cutoff  $D$  and the exchange interaction  $J$  as  $T_K = De^{-1/(J\nu)}$ , where  $\nu$  is the density of states. Like the lowest-order perturbation theory result, the leading-logarithmic approximation Eq. (1) corresponds to purely elastic electron scattering.

The leading-logarithmic approximation is adequate at  $\varepsilon \gg T_K$ , but it fails at low temperatures. A convenient phenomenological description of the low-energy behavior of a single-channel Kondo model is given by Nozières’ effective Fermi liquid theory. In this theory, a scattering problem can be formulated, too. It is clearly seen,<sup>5</sup> however, that the scattering is not purely elastic at  $\varepsilon \ll T_K$ . At  $T=0$ , for example, the inelastic contribution to the electron scattering cross section scales as  $(E/T_K)^2$  and becomes comparable to the elastic part at  $E \sim T_K$ .

The Kondo effect is a crossover phenomenon, rather than a phase transition. The measurable characteristics, such as the contribution to the susceptibility or resistivity due to magnetic impurities depend smoothly on temperature. Similarly, the electron scattering off a magnetic impurity, which is deeply inelastic at  $\varepsilon \sim T_K$ , must have some inelastic component at any energy  $E$ . In this paper, we investigate in detail the inelastic scattering of a high-energy electron off a magnetic impurity.

A study of the energy-resolved, differential cross section,  $\sigma(E, \omega)$ , is interesting in its own right, but it can, in principle, also be measured, e.g. in a modification of the experiments of Pothier *et al.*<sup>6</sup> Further motivation to study  $\sigma(E, \omega)$  beyond perturbation theory comes from the recent theoretical work of Zaránd *et al.*<sup>7</sup> In Ref. 7, the energy dependence of the *total* scattering cross section,  $\sigma_{\text{tot}}(E) = \int d\omega \sigma(E, \omega)$ , was addressed. With the help of the optical theorem, the total cross section  $\sigma_{\text{tot}}(E)$  was compared with the elastic part of it. The conclusion reached in Ref. 7 regarding the energy domain  $E \gg T_K$  is striking: at  $T=0$ , the scattering is deeply inelastic: the elastic part turns out to be negligibly small. This seemingly contradicts the leading-logarithmic result for the scattering amplitude Eq. (1). The physical explanation of this phenomenon, however, remained unclear in Ref. 7 and motivates us to revisit the problem of inelastic scattering. The dependence of the differential cross section  $\sigma(E, \omega)$  on  $\omega$ , which we consider in this paper, clarifies the issue, as we are able to determine the distribution of energy losses in the inelastic electron scattering off a magnetic impurity.

The separation of the electron scattering cross section in the Kondo effect into elastic and inelastic parts at  $E \gg T_K$  was not addressed for decades, as it does not affect the routinely measured quantity, the resistivity. The anomalously fast electron energy relaxation in some mesoscopic metallic wires,<sup>6</sup> which was discovered in the last decade, prompted a search for relaxation mechanisms driven by impurities with internal degrees of freedom. A viable mechanism of energy relaxation was suggested in Ref. 8 and was associated with the electron-electron scattering mediated by exchange interaction of electrons with magnetic impurities. The removal of degeneracy of the localized spin states by the exchange interaction results in an anomaly of the electron-electron scattering cross section at small energy transfers;<sup>8</sup> the collision of two electrons with energies  $E, E' \gg T_K$  leads to a redistribution of the energies between the two particles,  $E, E' \rightarrow E - \omega, E' + \omega$ , and has cross section  $K(\omega, E, E') \propto J^4/\omega^2$  in the lowest-order perturbation theory.<sup>10</sup> The  $1/\omega^2$  dependence of  $K$  allowed the experimental observations<sup>6</sup> to be explained qualitatively. Later experiments<sup>12</sup> performed in a magnetic field sufficient for the Zeeman splitting of impurity energy levels did confirm the origin<sup>8</sup> of the inelastic electron-electron scattering, and indicated the irrelevance of more exotic mechanisms, which assumed a generic non-Fermi liquid behavior introduced by impurities.<sup>13</sup>

The existence of energy exchange between electrons mediated by their interaction with a magnetic impurity indicates the inelastic nature of the electron scattering off a magnetic impurity. Indeed, using the Fermi Golden rule, we find

$$\sigma(E, \omega) \propto \frac{J^4}{\omega^2} \int_{-\infty}^{\infty} dE' f(E') [1 - f(E' + \omega)] \propto \frac{J^4}{\omega} \quad (2)$$

at  $\omega \gg T$ . So already in the simplest perturbation theory, it becomes clear that there is an inelastic contribution to scattering. As long as  $E, \omega \gg T$ , temperature does not affect the inelastic cross section in this order. It is not clear, however, what the relation is between the inelastic cross section  $\sigma(E, \omega)$  and the leading-logarithmic result Eq. (1): On one

hand,  $\sigma(E, \omega) \propto J^4$  is parametrically smaller than the scattering cross section following from Eq. (1). On the other hand, the total inelastic cross section obtained from Eq. (2),  $\sigma_{\text{tot}}(E) = \int d\omega \sigma(E, \omega)$ , diverges at  $\omega \rightarrow 0$ , indicating the inapplicability of the lowest-order perturbation results at small energy transfers.

The lowest-order perturbation theory for  $K(\omega, E, E')$  can be controllably improved in two respects. First, at  $E, E' \gg T_K$  and  $|\omega| \ll E, E'$  the four constants  $J$ , entering as a product in the perturbative result, may be replaced<sup>8</sup> by the properly renormalized<sup>4</sup> quantities.<sup>14</sup> Second, the divergence at  $\omega \rightarrow 0$  is cutoff due to the dynamics of localized spin. An adequate theory may be developed for high temperatures,  $T \gg T_K$ , where the cutoff occurs due to the Korringa relaxation.<sup>8</sup> These improvements allow one to see that  $\sigma_{\text{tot}}(E)$  is finite, but they are insufficient to investigate the details of the  $\sigma(E, \omega)$  dependence.

In this paper, we concentrate on the differential cross section,  $\sigma(E, \omega)$ , of inelastic scattering of a highly excited electron with energy  $E \gg T_K$ . Despite the many-body nature of the Kondo effect, this quantity is well defined at  $\omega \ll E$ . We show in Sec. II that in the limit  $E \gg T_K$ , the differential cross section is related to the dissipative part of the impurity spin susceptibility,  $\chi''$ . From the low-frequency and high-frequency asymptotes of  $\chi''$ , we extract in Secs. III and IV the behavior of the differential cross section  $\sigma(E, \omega)$  in the absence and presence of a Zeeman energy, respectively. The analytical asymptotes thus obtained are complemented by results of the numerical renormalization group<sup>17</sup> (NRG), which allows us to access also the intermediate range of frequencies and magnetic fields. The connection between the result of Ref. 7 and the leading-logarithmic approximation for the scattering amplitude (1) describing only elastic scattering will be explained in detail. Finally, in Sec. V, we discuss possible hot-electron experiments in metallic mesoscopic wires and in a semiconductor quantum-dot setup in order to measure the differential scattering cross section  $\sigma(E, \omega)$ .

## II. RELATION BETWEEN INELASTIC SCATTERING CROSS SECTION AND SUSCEPTIBILITY

The relation between the scattering cross section of a “foreign” spin-carrying particle and the spin-spin correlation function of a magnetic medium is well known from the theory of neutron scattering.<sup>18</sup> Here, we derive a similar relation for scattering off a magnetic impurity of a high-energy electron belonging itself to the Fermi liquid hosting the magnetic impurity.

The exchange interaction between the impurity spin and spins of electrons forming the Fermi liquid,

$$H_{\text{int}} = J \sum_{\mathbf{k}, \mathbf{k}'} \mathbf{S} \cdot \mathbf{s}_{\alpha\alpha'} c_{\mathbf{k}\alpha}^\dagger c_{\mathbf{k}'\alpha'} \quad (3)$$

gives rise to the Kondo effect. Here,  $J$  is the constant of exchange interaction between the impurity spin and itinerant electrons with energies  $\epsilon_{\mathbf{k}\sigma}$  (measured from the Fermi level) confined to some energy band,  $|\epsilon_{\mathbf{k}\sigma}| < D$ . Here,  $\mathbf{s}_{\alpha\alpha'}$  is  $\frac{1}{2}$

times the vector of Pauli matrices. The Kondo problem allows for a logarithmic renormalization: the low-energy properties of the system described by the Hamiltonian (3) coincide with those for a Hamiltonian defined in a narrower band, say  $|\epsilon_{\mathbf{k}\sigma}| < E$ , upon the proper renormalization of the exchange constant,

$$J(E) = \frac{J(D)}{1 - \nu J(D) \ln(D/E)}, \quad J(D) = J, \quad (4)$$

where  $\nu$  is the density of states of itinerant electrons. The perturbative renormalization Eq. (4) is valid as long as the running energy [ $E$  in the case of Eq. (4)] significantly exceeds the Kondo temperature  $T_K$ . An important property of the logarithmic renormalization is that only exponentially wide energy intervals ( $\epsilon_1, \epsilon_2$ ), such that  $\nu J |\ln(\epsilon_1/\epsilon_2)| \sim 1$  contribute significantly to the renormalization. That allows us to “skip” some relatively narrow strip of energies, say,  $(E - \Delta E, E + \Delta E)$ , with  $\Delta E \ll E$ , in the renormalization process, yielding a Hamiltonian

$$\begin{aligned} H_{\text{int}} = & J(\tilde{D}) \sum_{|\epsilon_{\mathbf{k}\alpha}|, |\epsilon_{\mathbf{k}'\alpha'}| < \tilde{D}} \mathbf{S} \cdot \mathbf{s}_{\alpha\alpha'} c_{\mathbf{k}\alpha}^\dagger c_{\mathbf{k}'\alpha'} \\ & + J(E) \sum_{E - \Delta E < \epsilon_{\mathbf{k}\alpha}, \epsilon_{\mathbf{k}'\alpha'} < E + \Delta E} \mathbf{S} \cdot \mathbf{s}_{\alpha\alpha'} c_{\mathbf{k}\alpha}^\dagger c_{\mathbf{k}'\alpha'} \\ & + J(E) \sum_{\substack{E - \Delta E < \epsilon_{\mathbf{k}\alpha} < E + \Delta E, |\epsilon_{\mathbf{k}'\alpha'}| < \tilde{D}; \\ E - \Delta E < \epsilon_{\mathbf{k}'\alpha'} < E + \Delta E, |\epsilon_{\mathbf{k}\alpha}| < \tilde{D}}} \mathbf{S} \cdot \mathbf{s}_{\alpha\alpha'} c_{\mathbf{k}\alpha}^\dagger c_{\mathbf{k}'\alpha'}, \quad (5) \end{aligned}$$

with  $\tilde{D} \ll E - \Delta E$ . The renormalized exchange constants here may be expressed in terms of the Kondo temperature,  $\nu J(\epsilon) = 1/\ln(\epsilon/T_K)$ . There is no need to distinguish between  $J(E - \Delta E)$ ,  $J(E)$ , or  $J(E + \Delta E)$  as long as  $E \gg T_K$ .

If the scattering of an electron with initial energy  $E$  leaves it in the energy domain  $(E - \Delta E, E + \Delta E)$ , then the corresponding cross section, within the lowest-order perturbation theory in  $J(E)$ , can be evaluated with the help of the Hamiltonian (5). The first line of Eq. (5) plays the role of the Hamiltonian of a magnetic medium in the neutron scattering problem, and the second line describes the interaction of the energetic particle (we deal with an electron rather than with a neutron, though) with the medium. The remaining part of the Hamiltonian does not contribute to the scattering cross section in the lowest-order calculation.

Consider such a scattering of an energetic electron with energy  $E$  and spin  $\sigma$  in the initial and  $E - \omega$  and  $\sigma'$ , respectively, in the final state with  $\omega \ll E$  such that  $E - \omega \in (E - \Delta E, E + \Delta E)$ . The state of the remaining system before and after scattering may be characterized by the wave functions  $\Psi_i$  and  $\Psi_f$ , respectively. The initial and final state of the total system is then given by the product states for the initial state,

$$|i\rangle = |E, \sigma\rangle \otimes |\Psi_i\rangle, \quad (6)$$

for the final state,

$$|f\rangle = |E - \omega, \sigma'\rangle \otimes |\Psi_f\rangle.$$

The differential cross section of inelastic scattering  $\sigma_{\sigma'\sigma}(E, \omega)$  is determined by the probability  $P_{\sigma'\sigma}(E, \omega)d\omega$  of

scattering of an electron with initial energy  $E$  and spin  $\sigma$  into a state within interval of energies  $(E - \omega, E - \omega - d\omega)$  and spin  $\sigma'$ ,

$$P_{\sigma'\sigma}(E, \omega)d\omega = v_F \sigma_{\sigma'\sigma}(E, \omega)d\omega, \quad (7)$$

where  $v_F$  denotes the Fermi velocity. By energy conservation,  $\omega = \xi_f - \xi_i$ , where energies  $\xi_i, \xi_f$  are associated respectively with the functions  $\Psi_i$  and  $\Psi_f$  involving the states in the domain  $|\epsilon_{\mathbf{k}\sigma}| < \tilde{D}$ . In the absence of a magnetic field, energy  $E$  is the orbital energy in the initial state, and  $\omega$  is the change in the orbital energy resulting from scattering. In the presence of Zeeman splitting, the initial energy and the energy transfer include the orbital and Zeeman parts, e.g.,  $E = \epsilon_{\mathbf{k}} + \sigma g_e \mu_B B / 2$ .

The standard application of the lowest-order perturbation theory in the interaction of the energetic electron with the remaining system yields for the scattering probability

$$w_{f \leftarrow i} = |J(E) \mathbf{s}_{\sigma\sigma'} \langle \Psi_f | \mathbf{S} | \Psi_i \rangle|^2 2\pi\nu \delta(\xi_i - \xi_f + \omega),$$

where  $\nu$  is the density of states for the energetic ( $\epsilon \sim E$ ) electron. After the summation over the final states and proper thermal averaging over the initial states, we are able to relate  $w_{f \leftarrow i}$  with  $\sigma_{\sigma'\sigma}(E, \omega)$  and obtain the differential scattering cross section

$$\begin{aligned} \sigma_{\sigma'\sigma}(E, \omega) = & \frac{\nu}{4v_F} J^2(E) \\ & \times [\delta_{\sigma'\sigma} \mathcal{S}_{zz}(\omega) + \mathbf{s}_{\sigma'\sigma}^+ \mathcal{S}_{+-}(\omega) + \mathbf{s}_{\sigma'\sigma}^- \mathcal{S}_{-+}(\omega)], \quad (8) \end{aligned}$$

where  $\mathbf{s}_{\sigma'\sigma}^\pm = \mathbf{s}_{\sigma'\sigma}^x \pm i \mathbf{s}_{\sigma'\sigma}^y$ . As in the theory of neutron scattering,<sup>18</sup> the cross section involves a spin-spin correlation function. Here, it is the correlation function of the local magnetic impurity spin,

$$\begin{aligned} \mathcal{S}_{ab}(\omega) = & \int_{-\infty}^{\infty} dt e^{i\omega t} \langle S^a(t) S^b(0) \rangle \\ = & \sum_{\{|\Psi_i\rangle, |\Psi_f\rangle\}} \frac{e^{-\beta\xi_i}}{Z} \langle \Psi_i | S^a | \Psi_f \rangle \langle \Psi_f | S^b | \Psi_i \rangle 2\pi \delta(\xi_i - \xi_f + \omega). \quad (9) \end{aligned}$$

We thus reduced the scattering cross section to an expression where its dependence on the energy of the scattering hot electron  $E$  separates from the dependence on the energy loss  $\omega$ . The dependence on the energy loss is determined by the dynamics of the impurity spin characterized by the correlation function  $\mathcal{S}$ . The spin correlator is related to the dissipative part of the impurity susceptibility via the fluctuation-dissipation theorem,

$$(g\mu_B)^2 \mathcal{S}_{ab}(\omega) = \frac{2}{1 - e^{-\beta\omega}} \chi''_{ab}(\omega). \quad (10)$$

Here,  $\mu_B$  is the Bohr magneton, and  $g$  is the impurity  $g$  factor. The behavior of  $\chi''$  in various limits will be discussed in the following sections. The spin dynamics is thus included in a nonperturbative fashion. It will allow us to investigate

the behavior of the cross section at any energy transfer; at  $\omega \ll T_K$ , we apply effective Fermi liquid theory, and the region of intermediate energies,  $\omega \sim T_K$ , is covered with the help of NRG calculations.

However, it is important to note that the total scattering cross section is fixed by the sum rule for the spin correlation function,  $\mathcal{S}_{ab}(\omega)$ . Consider the total cross section obtained after averaging over the initial electronic spin configurations  $\sigma$ , summing over the final ones  $\sigma'$ , and integrating over the energy transfer  $\omega$ ,

$$\sigma_{\text{tot}}(E) = \frac{1}{2} \sum_{\sigma, \sigma'} \int_{-\infty}^{\infty} d\omega \sigma_{\sigma' \sigma}(E, \omega) = \frac{3\pi}{8} \frac{1}{\nu v_F} \frac{1}{\ln^2 \frac{E}{T_K}}. \quad (11)$$

We substituted the explicit form for the energy dependent exchange interaction,  $J(E) = 1/[\nu \ln(E/T_K)]$ . The total scattering cross section will be used throughout the rest of the paper as a convenient basic unit of measurement for the differential cross section discussed below.

As we are mainly interested in the dependence of the scattering probability on the energy transfer  $\omega$ , we will confine ourselves in the following to an analysis of the scattering cross section averaged over the initial electronic spin configurations  $\sigma$  and summed over the final ones  $\sigma'$ ,

$$\sigma(E, \omega) = \sigma_{\text{tot}}(E) \frac{2}{3\pi} \left[ \mathcal{S}_{zz}(\omega) + \frac{1}{2} [\mathcal{S}_{+-}(\omega) + \mathcal{S}_{-+}(\omega)] \right]. \quad (12)$$

Note that a Zeeman energy of electrons forming the Fermi sea was already incorporated in the definition of the energies  $E$  and  $\omega$ . The generalization of our results to spin-resolved scattering is straightforward.

### III. INELASTIC ELECTRON SCATTERING IN THE ABSENCE OF ZEEMAN SPLITTING

In the absence of a magnetic field, the expression for the scattering cross section (12) simplifies considerably since the impurity spin correlator is diagonal,  $\mathcal{S}(\omega) \equiv \mathcal{S}_{zz}(\omega) = \frac{1}{2} \mathcal{S}_{+-}(\omega)$ ,

$$\sigma(E, \omega) = \sigma_{\text{tot}}(E) \frac{2}{\pi} \mathcal{S}(\omega). \quad (13)$$

Let us first establish the relation between Eq. (13) and the well-known result of the leading-logarithmic approximation.<sup>3,4</sup> For that, we need to substitute in Eq. (13) the function  $\mathcal{S}(\omega)$  evaluated in the zeroth order in the exchange interaction  $J(\tilde{D})$ . In this order,  $\mathcal{S}^{(0)}(\omega) = (\pi/2) \delta(\omega)$ , which yields the well-known result<sup>3,4</sup> for the cross section,

$$\sigma^{(0)}(E, \omega) = \sigma_{\text{tot}}(E) \delta(\omega), \quad (14)$$

i.e., scattering is elastic in the leading-logarithmic approximation. The elasticity breaks down, however, if one accounts for  $J(\tilde{D}) \neq 0$ . Indeed, the exchange interaction  $J(\tilde{D})$  leads to some dynamics of the impurity spin. The delta-function in

Eq. (14) gets broadened, and spectral weight is transferred to finite energies  $\omega \neq 0$ . The shape of the broadened peak is related to the character of the spin dynamics, which is different in the limits of high,  $T \gg T_K$ , and low,  $T \ll T_K$ , temperatures. We study the shape of the peak in these limits below. However, note that the broadening does not affect the *total* cross section, which is fixed by the sum rule and remains the same as for the elastic scattering, Eq. (14), evaluated in the leading-logarithmic approximation.

#### A. Inelastic electron scattering at $T \gg T_K$

At  $T \gg T_K$ , the local spin exhibits relaxational dynamics. The Bloch equations for the impurity spin in the absence of a magnetic field,

$$\frac{\partial}{\partial t} \langle S^a \rangle = - \frac{1}{\tau_K} \langle S^a \rangle, \quad (15)$$

imply the following form for the imaginary part of the susceptibility,<sup>19</sup>  $\chi''_{ab}(\omega) = \delta_{ab} \chi''(\omega)$  with

$$\chi''(\omega) = \chi_0(T) \frac{\omega/\tau_K}{\omega^2 + (1/\tau_K)^2}. \quad (16)$$

It involves the static susceptibility, which is given by  $\chi_0(T) = (g\mu_B)^2/(4T)$ . The decay time  $\tau_K$  in the Bloch equations is the Korringa relaxation time,<sup>20</sup>  $1/\tau_K = \pi[\nu J(T)]^2 T$ . Inserting the scale dependent exchange interaction  $J(T)$ , the Korringa relaxation rate reads explicitly,

$$\frac{1}{\tau_K} = \frac{\pi T}{\ln^2 \frac{T}{T_K}}. \quad (17)$$

It is parametrically smaller than  $T$  at temperatures  $T \gg T_K$ .

Expression (16) adequately accounts for the behavior of  $\chi''$  at low frequencies,  $\omega \lesssim T$ , but fails at higher frequencies. For  $\omega \gg T$ , the susceptibility can be evaluated within the lowest-order perturbation theory in the exchange constant,<sup>21</sup>  $J(\tilde{D})$ ,

$$(g\mu_B)^{-2} \chi''(\omega) = \frac{\pi}{4} \frac{1}{\omega \ln^2 \frac{|\omega|}{T_K}}. \quad (18)$$

The additional logarithmic frequency dependence arises from the logarithmic enhancement of the exchange interaction due to the perturbative RG, which is now cutoff at a bandwidth  $\tilde{D} \sim \omega$ .

The resulting differential cross section,  $\sigma(E, \omega)$ , can be found with the help of Eq. (10). It is symmetric in  $\omega$  at small energy transfers. It shows a narrow peak at  $\omega = 0$  and falls off significantly within the region of energies  $|\omega| \lesssim T$

$$\sigma(E, \omega) = \sigma_{\text{tot}}(E) \delta_{\Gamma}(\omega), \quad (19)$$

where we introduced a ‘‘broadened delta function,’’ which is a Lorentzian with linewidth  $\Gamma = 1/\tau_K$ ,

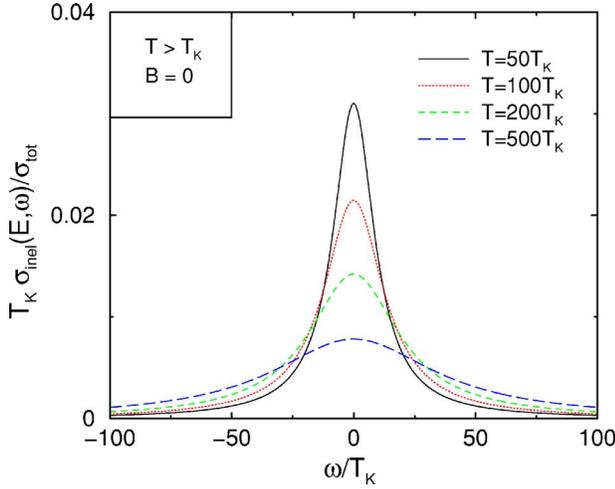


FIG. 1. (Color online) Differential cross section,  $\sigma(E, \omega)$ , at large temperatures,  $T \gg T_K$ , without Zeeman splitting,  $B=0$ , as given by Eq. (19). The Lorentzian peaks have a width given by the Korrington relaxation rate  $1/\tau_K$ , Eq. (17).

$$\delta_T(\omega) = \frac{1}{\pi} \frac{1/\tau_K}{\omega^2 + (1/\tau_K)^2}. \quad (20)$$

As  $1/\tau_K \ll T$ , see Eq. (17), almost the full weight of the total cross section is accounted for by Eqs. (19) and (20), see Fig. 1.

At higher energy transfers,  $|\omega| \gtrsim T$ , the cross section is asymmetric in  $\omega$ ,

$$\sigma(E, \omega) = \sigma_{\text{tot}}(E) \frac{1}{1 - e^{-\omega/T}} \frac{1}{\omega \ln^2(|\omega|/T_K)}. \quad (21)$$

The probability for the scattered electron to acquire energy ( $\omega < 0$ ) is exponentially suppressed. Although the contribution of Eq. (21) to the total cross section is parametrically small,  $\propto 1/\ln(T/T_K)$ , it is worth noting that its decay with  $\omega$  is remarkably slow.

The slow decay of  $\sigma(E, \omega)$  vs  $\omega$  is related to the dependence on the transferred energy of the cross section for inelastic electron-electron scattering mediated by a magnetic impurity.<sup>8</sup> The probability for such an inelastic scattering between two electrons with initial energies  $E$  and  $E'$  and final energies  $E - \omega$  and  $E' + \omega$  was calculated in Ref. 8; all of these four energies were assumed to be large compared to  $T_K$ . According to Ref. 8 [see also Eq. (9) of Ref. 9], the contribution  $K(\omega; E, E')$  of a single magnetic impurity to this probability in the limit of high energy,  $E \gg |\omega|$ , reads

$$K(\omega; E, E') = \frac{3\pi}{8\nu} \frac{1}{\ln^2 \frac{|E|}{T_K}} \frac{4}{\left( \ln \frac{|E'|}{T_K} + \ln \frac{|E' + \omega|}{T_K} \right)^2} \frac{1}{\omega^2}. \quad (22)$$

The differential cross section (21) can be obtained by integrating  $K(\omega; E, E')$  over the available phase space volume of one of the scattering electrons,

$$v_F \sigma(E, \omega) = \int dE' f(E') [1 - f(E' + \omega)] K(\omega; E, E'). \quad (23)$$

The Fermi functions in Eq. (23) confine the energy  $E'$  to an interval  $-\omega \lesssim E' \lesssim 0$ . This includes a regime where the arguments of the  $E'$ -dependent logarithmic factors are not meaningful anymore and should be replaced by temperature or the Korrington relaxation rate. After such a cutoff, integration over  $E'$  is easily performed, yielding  $\ln^{-2}|\omega|/T_K$  within logarithmic accuracy. This way, starting from the collision integral kernel of Ref. 8, one recovers Eq. (21).

### B. Inelastic electron scattering at $T \ll T_K$

When the temperature is below the Kondo temperature, the picture differs drastically from the zeroth order result (14). For  $T \ll T_K$ , the low-frequency behavior of the scattering cross section is beyond perturbation theory. Nevertheless, the cross section for small energy transfers,  $|\omega| \ll T_K$ , may be found with the help of the Shiba relation<sup>22</sup> for the susceptibility,

$$(g\mu_B)^2 \chi''(\omega) = 2\pi\omega [\chi_0(T=0)]^2. \quad (24)$$

The zero-temperature static susceptibility  $\chi_0(0)$  is used conventionally<sup>23</sup> to define the pre-exponential factor of the Kondo temperature,  $\chi_0(0) = [(g\mu_B)^2 W]/(4T_K)$ ; here  $W = 0.413\dots$  is Wilson's number. (We present a convenient derivation of the Shiba relation in Appendix A.) The corrections to the Shiba relation are of order  $O(\omega T^2/T_K^2, \omega^3/T_K^2)$  and are subleading. We, thus, obtain for the cross section at  $|\omega|, T \ll T_K$ ,

$$\sigma(E, \omega) = \sigma_{\text{tot}}(E) \frac{W^2}{2} \frac{1}{1 - e^{-\omega/T}} \frac{\omega}{T_K^2}. \quad (25)$$

The high-frequency limit,  $|\omega| \gg T_K$ , of the scattering cross section can still be obtained perturbatively and is given by Eq. (21).

Comparing the results of Eqs. (21) and (25), we see that for temperatures  $T \ll T_K$ , the differential cross section,  $\sigma(E, \omega)$ , peaks at energy transfers of the order of  $\omega \sim T_K$ . It then decreases linearly upon further decrease of  $\omega$ , until it crosses over (at  $|\omega| \lesssim T$ ) into the exponential tail for  $\omega < 0$ , see inset of Fig. 2. At zero temperature, the factor containing  $\exp(-\omega/T)$  in Eq. (25) becomes a step function which forbids any energy gain from the Kondo system,

$$\sigma(E, \omega) = \sigma_{\text{tot}}(E) \frac{W^2}{2} \Theta(\omega) \frac{\omega}{T_K^2}, \quad (26)$$

here  $\Theta(x) = 1$  if  $x > 0$  and 0 if  $x < 0$ .

The region between the asymptotes given in Eqs. (21) and (25) can be bridged by calculations performed with the NRG method. In this method, after the logarithmic discretization of the conduction band, one maps the Kondo Hamiltonian onto a semi-infinite chain with the impurity at the end. As a consequence of the logarithmic discretization, the hopping along the chain decreases exponentially,  $t_n \sim \Lambda^{-n/2}$ , where

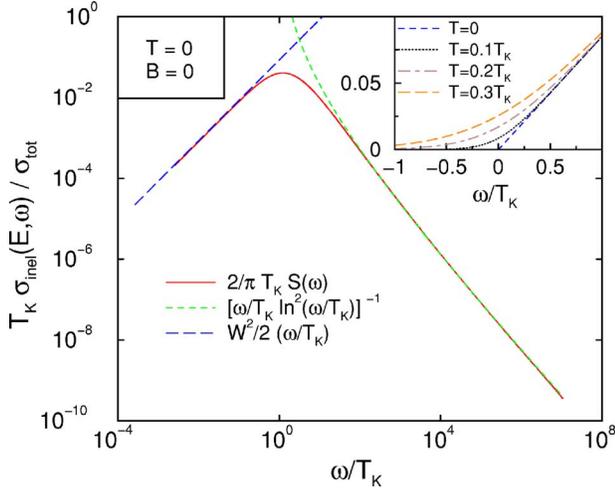


FIG. 2. (Color online) NRG result for  $\sigma(E, \omega)$  (solid line) on a logarithmic scale at  $T=0$  without Zeeman splitting,  $B=0$ . A maximum at finite  $\omega=T_K$  develops and scattering with small energy transfer  $\omega$  is suppressed. Whereas, the high-frequency tail is perturbatively accessible, see Eq. (21) (short-dashed line), the low-frequency tail, Eq. (25) (long-dashed line), is a property of the strong coupling fixed point described by Nozières' Fermi liquid theory. ( $W=0.413\dots$  is Wilson's number.) The inset shows the temperature correction according to Eq. (25); the contribution for negative  $\omega$  is exponentially small for temperatures  $0 < T \ll T_K$ .

$\Lambda > 1$  is the discretization parameter and  $n$  is the site index. (We have used  $\Lambda=2$  throughout the calculations presented in the paper.) The separation of energy scales provided by the exponential decay of the hopping rate allows us to diagonalize the Hamiltonian iteratively and keep the eigenstates with the lowest energy as the most relevant ones. Since we know the energy eigenvalues and eigenstates, we are able to calculate the impurity spin correlation function directly [see Eq. (9)] given that the Dirac delta function appearing in the Lehman representation must be broadened when performing a numerical calculation.<sup>24,25</sup> The result of the NRG calculation is shown in Fig. 2.

To summarize this section, we demonstrated that the dynamics of the impurity spin leads to inelastic electron scattering at all temperatures. The main contribution to the total scattering cross section comes from  $\omega \sim T_K$  or  $|\omega| \leq 1/\tau_K$  at  $T \ll T_K$  and  $T \gg T_K$ , respectively. The total scattering cross section is fixed by the sum rule for the impurity spin correlation function, see Eq. (11), and is thus determined by the effective exchange constant  $J(E)$  evaluated within the leading-logarithmic approximation.<sup>3</sup>

#### IV. ZEEMAN EFFECT IN THE ELECTRON SCATTERING

We now address the case when the degeneracy of the impurity spin is lifted by a magnetic field. The Zeeman splitting of the impurity spin is described by the Hamiltonian

$$H_{\text{Zeeman}} = -g\mu_B \mathbf{S}^z B. \quad (27)$$

In the presence of the Zeeman splitting, the scattering electron has to pay Zeeman energy in order to transfer spin to the

Kondo system. The resonance structure for electron scattering involving a spin flip will, therefore, differ from the one of non-spin-flip scattering. Evaluating the impurity spin correlator in zeroth order in  $J(\tilde{D})$ , we obtain for the scattering cross section (12) in the leading-logarithmic approximation,

$$\begin{aligned} \sigma^{(0)}(E, \omega) &= \sigma_{\text{tot}}(E) \frac{2}{1 + e^{-\beta\omega}} \\ &\times \frac{1}{3} \{ \delta(\omega) + \delta[\omega - \omega_Z(B)] + \delta[\omega + \omega_Z(B)] \}. \end{aligned} \quad (28)$$

The single delta function for  $B=0$ , Eq. (14), is now split into three contributions. In addition to a delta function at zero frequency, which is due to non-spin-flip scattering, there are two Zeeman satellites at  $\omega = \pm \omega_Z(B)$ . In the limit of low temperatures,  $T \ll B$ , the satellite at negative Zeeman energy corresponding to an energy gain of the scattering electron is exponentially small as it is clear from Eq. (28).

The Zeeman energy  $\omega_Z(B)$  depends on the renormalized  $g$  factor, which is different from its bare value  $g$  appearing in the Zeeman Hamiltonian (27). When we derived the effective interaction Hamiltonian (5), we integrated out a finite band of electronic degrees of freedom which lead to a renormalization of the exchange interaction  $J$ . The Zeeman term (27) is not invariant under this perturbative renormalization of the Kondo model. Similar to the exchange interaction  $J$ , the  $g$  factor is also renormalized when the band is reduced from  $D$  to  $\tilde{D}$ . As explained in Appendix B, the scale-dependent  $g$  factor in the leading-logarithmic order is given by

$$\frac{g(\tilde{D})}{g} = \left( 1 - \frac{1}{2 \ln \tilde{D}/T_K} \right). \quad (29)$$

To find the observable value of the  $g$  factor, one needs to set  $\tilde{D} = \max\{T, g\mu_B B\}$ . The position of the Zeeman resonances, to the leading-logarithmic order, is given by<sup>26</sup>

$$\omega_Z(B) = g \left( 1 - \frac{1}{2 \ln(\max\{T, g\mu_B B\}/T_K)} \right) \mu_B B. \quad (30)$$

Beyond the leading-logarithmic approximation, the dynamics of the local spin is characterized by a further redistribution of the spectral weight of the scattering cross section (28). However, a striking feature of the presence of a magnetic field is that a finite weight of the delta resonance at  $\omega = 0$  will still survive after accounting for the coupling of the impurity spin to the low-energy degrees of freedom of the Fermi sea. In other words, at any ratio  $T/T_K$ , a part of the scattering becomes elastic if a magnetic field  $B \neq 0$  is turned on. This can be best understood by considering the longitudinal spin correlation function in time. For  $B \neq 0$ , this correlation function will not fully decay with time but rather saturate at a value given by the finite expectation value of the impurity spin,  $\langle S^z(t) S^z(0) \rangle \rightarrow \langle S^z \rangle^2$  for  $t \rightarrow \infty$ . This finite saturation value leads to a finite weight of the delta function  $\delta(\omega)$  in its Fourier transform and in Eq. (8). Let us decompose  $\sigma(E, \omega)$  into the elastic and inelastic parts,

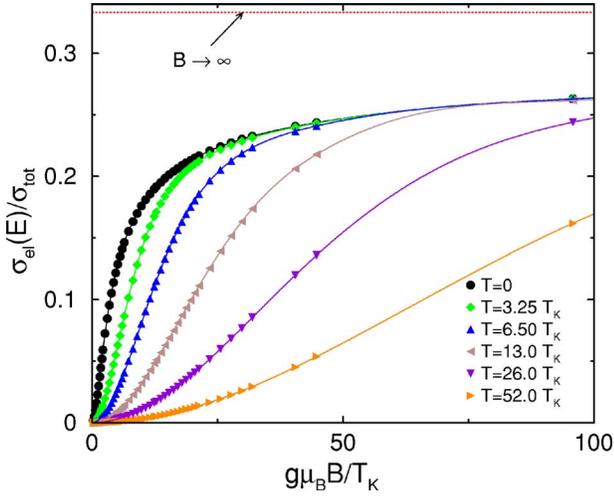


FIG. 3. (Color online) Weight of the elastic scattering cross section,  $\sigma_{el}(E) = \int d\omega \sigma_{el}(E, \omega)$ , see Eq. (32), determined by NRG. The weight increases as  $B^2$  for small magnetic fields and saturates logarithmically slowly to the limiting value for large  $B$ , see Eq. (43).

$$\sigma(E, \omega) = \sigma_{el}(E, \omega) + \sigma_{inel}(E, \omega). \quad (31)$$

The elastic part will be determined by the magnetization of the impurity spin

$$\sigma_{el}(E, \omega) = \sigma_{tot}(E) \frac{4}{3} \langle S^z \rangle^2 \delta(\omega). \quad (32)$$

Being a thermodynamic quantity,  $\langle S^z \rangle$  has a well-studied field and temperature dependence.<sup>23,27</sup> In the scaling regime,  $f(t, b) = \langle S^z \rangle$  is a function of  $t = T/T_K$  and  $b = g\mu_B B/T_K$ . The asymptote of  $f(t, b)$  at  $\max(t, b) \gg 1$  is with logarithmic accuracy given by

$$f(t, b) = \frac{1}{2} \left( 1 - \frac{1}{2 \ln[\max(t, b)]} \right) \times \tanh \left[ \frac{b}{2t} \left( 1 - \frac{1}{2 \ln[\max(t, b)]} \right) \right]. \quad (33)$$

Note that in the limit  $t=0, b \gg 1$ , Eq. (33) yields the ground-state value of  $\langle S^z \rangle$  in the perturbative regime. In the opposite limit of a weak field,  $b \ll 1 \ll t$ , spin polarization is small according to the Curie law,  $f \sim b/4t$ . In the developed Kondo regime,  $\max(t, b) \ll 1$ , the average spin is  $f(t, b) = (W/4)b$ .

The weight of the elastic scattering, Eq. (32), evaluated with NRG is shown in Fig. 3. In the limit of small magnetic fields, this weight increases as  $B^2$ . The saturation of the weight to its large-field limit,  $1/3$ , is remarkably slow due to the logarithmic correction to the magnetization,<sup>27</sup> see Eq. (33).

The inelastic part of the scattering cross section,  $\sigma_{inel}(E, \omega)$ , accounts for the remaining spectral weight. Note, however, that the total scattering cross section, i.e., the total spectral weight, is independent of the magnetic field: its value being fixed by the sum rule for the impurity spin correlator.

### A. Dissipative part of magnetic susceptibility

To analyze the inelastic scattering cross section in more detail for the two limiting cases  $T \gg T_K$  and  $T \ll T_K$ , we start from presenting the proper details regarding the frequency dependence of the dissipative parts of longitudinal and transversal impurity spin susceptibilities ( $\chi''_{zz}$  and  $\chi''_{+-}$ , respectively).

At  $T \gg T_K$ , one may treat the exchange interaction  $J(\tilde{D})$  perturbatively at any field  $B$ . The effect of  $B$  on  $\chi''$  is negligible as long as the Zeeman splitting,  $\omega_Z(B)$ , is smaller than the Korringa relaxation rate,  $1/\tau_K$ , see Eq. (17). At higher fields, the susceptibility becomes anisotropic,  $\chi''_{zz} \neq \frac{1}{2}\chi''_{+-}$ , and its frequency dependence acquires a well-resolved structure. The dissipative part of the susceptibility can be found from the Bloch equations.<sup>18</sup> The transversal part takes the form

$$\chi''_{+-}(\omega) = 2\chi_T \frac{\omega/T_2}{[\omega - \omega_Z(B)]^2 + (1/T_2)^2}, \quad (34)$$

where the static transversal differential susceptibility can be expressed with the help of Eq. (33) as  $\chi_T = (g\mu_B)f(t, b)/B$ . The longitudinal part reads

$$\chi''_{zz}(\omega) = \chi_L^D \frac{\omega/T_1}{\omega^2 + (1/T_1)^2}, \quad (35)$$

where  $\chi_L^D$  is given by

$$\chi_L^D = \frac{(g\mu_B)^2 \left( 1 - \frac{1}{\ln[\max\{T, g\mu_B B\}/T_K]} \right)}{4T \cosh^2 \frac{\omega_Z(B)}{2T}}. \quad (36)$$

The factor  $\chi_L^D$  can be understood as the contribution to the static susceptibility which originates from the response of the occupation factors of the two Zeeman levels to a varying magnetic field,  $\chi_L^D = g_{\text{eff}} \mu_B \partial \langle n_+ - n_- \rangle / \partial B$ ; here  $g_{\text{eff}}$ , see Eq. (29), is the appropriately renormalized  $g$  factor. Note that only in the limit  $\omega_Z(B) \lesssim T$ , when the renormalized  $g$  factor (29) is insensitive to the magnetic field,  $\chi_L^D$  does coincide with the full static longitudinal differential susceptibility  $\chi_L = g\mu_B \partial f(t, b) / \partial B$ .

In the case of a moderately high field,  $1/\tau_K \ll \omega_Z(B) \lesssim T$ , the relaxation times,  $T_1$  and  $T_2$ , equal each other<sup>18</sup> and are given by Eq. (17),  $T_1 = T_2 = \tau_K$ .

At even higher fields,  $\omega_Z(B) \gtrsim T$ , the peak structure in  $\chi''_{+-}(\omega)$  is still described by a Lorentzian form of Eq. (34), but the corresponding relaxation time is determined now by the Zeeman splitting rather than by temperature,<sup>19</sup>

$$\frac{1}{T_2} = \frac{\pi}{4} \frac{\omega_Z(B)}{\ln^2 \frac{\omega_Z(B)}{T_K}}. \quad (37)$$

The frequency dependence of the longitudinal susceptibility, however, requires additional discussion.

Generally, the susceptibility,  $\chi_{ij}(\omega)$ , describes the response of the magnetic impurity to a local magnetic field that oscillates with frequency  $\omega$ . At low frequencies, the variation of the dissipative part of the longitudinal component  $\chi''_{zz}(\omega)$

given by Eq. (35) can be understood in the framework of the Debye mechanism<sup>28</sup> of relaxational losses: At  $\omega=0$ , relaxation caused by the exchange interaction between the local magnetic moment and itinerant electrons establishes equilibrium Gibbs occupation factors for the two Zeeman-split levels. At finite, but small frequency  $\omega$ , the Zeeman splitting, which is caused by the sum of a constant and a slowly varying magnetic field, changes with time slowly, and the relaxation acts to adjust the occupation factors to the instant values of the Zeeman splitting. The adjustment occurs via the emission (or absorption) of particle-hole pairs with energy  $\varepsilon_{ph} \sim \omega_Z(B)$  by flips of the local spin. It is the time variation of the occupation factors of the Zeeman-split levels that leads to dissipation. In the limit  $\omega \rightarrow 0$ , the leading term in  $\chi''_{zz}(\omega)$ , according to Eq. (35), is

$$\chi''_{zz}(\omega)|_{\text{Debye}} = \chi_L^D T_1 \omega. \quad (38)$$

As was already mentioned, in the weak-field case,  $1/T_1$  is given by Eq. (17). In the limit,  $\omega_Z(B) \gg T$ , the time  $T_1$  was found<sup>19</sup> to be  $T_1 = T_2/2$  with  $T_2$  of Eq. (37). The contribution (38) to  $\chi''_{zz}$  from the Debye relaxational losses is valid at arbitrary ratio,  $\omega_Z(B)/T$ . Note, however, that despite the fact that Eq. (38) describes dissipation at low frequency, the Debye mechanism is associated with the emission of particle-hole pairs with a comparatively high energy  $\varepsilon_{ph} \sim \omega_Z(B)$ . In the limit,  $\omega_Z(B) \gg T$ , the Debye mechanism thus yields only an exponentially small contribution to dissipation,

$$\chi''_{zz}(\omega)|_{\text{Debye}} = \frac{2}{\pi} \frac{(g\mu_B)^2 \omega}{T} \frac{\ln^2 \frac{\omega_Z(B)}{T_K}}{\omega_Z(B)} \exp\left[-\frac{\omega_Z(B)}{T}\right]. \quad (39)$$

The exponential smallness of  $\chi_L^D$  comes from the small probability of the thermal occupation of the highly excited state, corresponding to the upper of the two Zeeman-split levels. Temporal variations in this exponentially small quantity leads to an exponentially small contribution to  $\chi''_{zz}(\omega)$ .

Under these conditions, a second contribution, originating from the low-energy part of the spectrum,  $|\varepsilon| \leq \max[\omega, T]$ , becomes important. The processes contributing here do not involve real impurity spin-flip processes (which are exponentially suppressed), but only virtual transitions. The starting point is the observation that the impurity magnetization locally polarizes the Fermi sea. If the Zeeman splitting of the impurity is slowly varied with a small frequency  $\omega$ , the magnetic polarization of the Fermi sea will adjust itself to the instantaneous adiabatic value of the impurity magnetization. Since the spectrum of the particle-hole pairs is continuous, this adjustment results in dissipation via the emission of pairs with small frequency  $\varepsilon_{ph} \sim \omega$ , which is in contrast to the Debye mechanism, where the emitted particle-hole pairs carry a large energy of the order of Zeeman splitting. As shown in Appendix A, this contribution to the susceptibility can be obtained by applying Nozières' Fermi liquid theory and is adequately accounted for by the generalized Shiba

relation, Eq. (A6). Evaluating  $d\langle S^z \rangle/dB$  with the help of Eq. (33) at  $T \ll g\mu_B B$ , we find for the dissipative part of the longitudinal susceptibility,

$$\chi''_{zz}(\omega) = \frac{\pi (g\mu_B)^2 \omega}{8} \frac{1}{\omega_Z^2(B) \ln^4 \frac{\omega_Z(B)}{T_K}}, \quad \omega \lesssim \omega_Z(B). \quad (40)$$

Comparing Eq. (40) with the result for the Debye mechanism, we see that the strong-field asymptote Eq. (39) for the latter mechanism is important only in a narrow interval of temperatures  $\omega_Z(B) \geq T \geq \omega_Z(B)/6$ , as for all practical purposes in  $\ln \ln(\omega_Z/B) \approx 1$ . Dispensing with that interval, we will use for the dissipative part of the longitudinal susceptibility, Eq. (35) with  $T_1 = \tau_K$  in the case of  $\omega_Z(B) \leq T$  and Eq. (40) in the case of  $\omega_Z(B) \geq T$ .

At low temperatures,  $T \ll T_K$ , there is little effect of the magnetic field on  $\chi''(\omega)$  for weak fields,  $g\mu_B B \ll T_K$ . In the strong-field regime,  $\omega_Z(B) \gg T_K \gg T$ , the main contribution to the transversal part of the dissipative susceptibility is given by Eq. (34) with the relaxation time  $T_2$  of Eq. (37). The longitudinal part is described by Eq. (40) at  $\omega \ll \omega_Z(B)$ . Equation (34) adequately describes the nonmonotonic behavior of  $\chi''_{+-}(\omega)$ , but fails at higher frequencies; similarly, the linear dependence in  $\chi''_{zz}(\omega)$  does not stretch beyond  $\pm \omega_Z(B)$ . In the limit,  $|\omega| \gg \omega_Z(B)$ , the magnetic field does not affect significantly the dissipation, and Eq. (18) is applicable.

## B. Elastic and inelastic components of electron scattering

The coupling of the impurity spin to the low-energy degrees of freedom of the Fermi seas will lead to a broadening and redistribution of the spectral weight of the three delta functions in Eq. (28).

### 1. High temperatures: $T \gg T_K$

At high temperature,  $T \gg T_K$ , and weak magnetic field,  $\omega_Z(B) \ll T$ , the spin polarization is weak, and the elastic component of the scattering is small. Using Eqs. (32) and (33), we find

$$\sigma_{\text{el}}(E, \omega) = \sigma_{\text{tot}}(E) \frac{4}{3} \left[ 1 - \frac{2}{\ln(T/T_K)} \right] \left[ \frac{g\mu_B B}{4T} \right]^2 \delta(\omega). \quad (41)$$

The major contribution to the scattering cross section comes from the inelastic processes. At fields satisfying the condition  $\omega_Z(B) \tau_K \gg 1$ , which still belongs to the domain of weak fields,  $\omega_Z(B) \ll T$ , the single maximum in the  $\omega$  dependence of the cross section, see Eq. (19), splits into three

$$\sigma_{\text{inel}}(E, \omega) \approx \sigma_{\text{tot}}(E) \frac{1}{3} \{ \delta_{\Gamma}(\omega) + \delta_{\Gamma}[\omega - \omega_Z(B)] + \delta_{\Gamma}[\omega + \omega_Z(B)] \}. \quad (42)$$

The broadened delta function was defined in Eq. (20) with a relaxation rate  $\Gamma$ , given by the inverse Korringa time,  $\Gamma = 1/\tau_K$ . (We neglected a small part of the spectral weight

which moved to the elastic component of the scattering cross section).

With the increase of the ratio  $\omega_Z(B)/T$ , the intensity of the elastic scattering increases, and in the strong-field limit, we find

$$\sigma_{\text{el}}(E, \omega) = \sigma_{\text{tot}}(E) \frac{1}{3} \left[ 1 - \frac{1}{\ln(g\mu_B B/T_K)} \right] \delta(\omega). \quad (43)$$

Simultaneously, the maximum of  $\sigma_{\text{inel}}(E, \omega)$  at negative  $\omega$  gets suppressed, and the structure at  $|\omega| \ll \omega_Z(B)$  broadens and becomes asymmetric. In the limit  $\omega_Z(B)/T \gg 1$ , only a single maximum at positive  $\omega$  remains in the inelastic cross section,

$$\begin{aligned} \sigma_{\text{inel}}(E, \omega) &= \sigma_{\text{tot}}(E) \frac{2}{3\pi} \frac{1}{1 - e^{-\omega/T}} \frac{1}{\omega_Z(B)} \\ &\times \frac{\omega/T_2}{[\omega - \omega_Z(B)]^2 + (1/T_2)^2}. \end{aligned} \quad (44)$$

Here the relaxation time  $T_2$  is defined by Eq. (37). This main contribution to the inelastic scattering is proportional to  $\chi''_{+-}(\omega)$  and comes from the spin-flip processes. The comparison of Eqs. (39) and (40) with Eq. (34) shows that at  $\omega_Z(B) \gg T_K$ , the effect of the dissipative part of longitudinal susceptibility is small starting from  $\omega_Z(B)/T \gtrsim 4$ . Under this condition,  $\chi''_{zz}(\omega)$  yields a contribution to  $\sigma(E, \omega)$ , which is small compared to Eq. (44).

The high-frequency tail,  $|\omega| \gg \max[T_K, g\mu_B B, T]$ , is unaffected by the Zeeman splitting and is still given by Eq. (21).

## 2. Low temperatures: $T \ll T_K$

We turn now to the opposite limit of small temperature,  $T \ll T_K$ . At weak magnetic field,  $g\mu_B B \lesssim T_K$ , the low-frequency behavior of the scattering cross section is beyond perturbation theory. In this regime, the electron scatters from a fully developed, many-body Kondo singlet. Here we can use the Shiba relation, Eq. (25), to access the low-frequency tail of the cross section. In the presence of a magnetic field, there are additional corrections to the Shiba relation of order  $O[\omega(g\mu_B B)^2/T_K^2]$  which are subleading and are neglected in the following. We get for the low-frequency part  $|\omega| \ll T_K$ ,

$$\sigma(E, \omega) = \sigma_{\text{tot}}(E) \frac{W^2}{2} \frac{1}{1 - e^{-\omega/T}} \left[ \frac{1}{6} \left( \frac{g\mu_B B}{T_K} \right)^2 \delta(\omega) + \frac{\omega}{T_K^2} \right], \quad (45)$$

where  $W$  is again Wilson's number.<sup>23</sup> The scattering cross section decreases linearly with frequency. At  $\omega \lesssim T$ , the linear decrease crosses over into an exponential tail which extends to negative frequencies. In Fig. 4, NRG results at  $T=0$  for the inelastic cross section at small magnetic fields are compared with the NRG data at  $B=0$ . In finite field, the slope in the linear low-frequency regime is reduced. The difference in slope is of order  $O(g\mu_B B/T_K)^2$ , a correction alluded to but neglected in Eq. (45). This difference, however, accounts for the reduction of the inelastic scattering weight. The weight of order  $O(g\mu_B B/T_K)^2$  is transferred from the inelastic to the elastic scattering contribution leading to a delta peak at

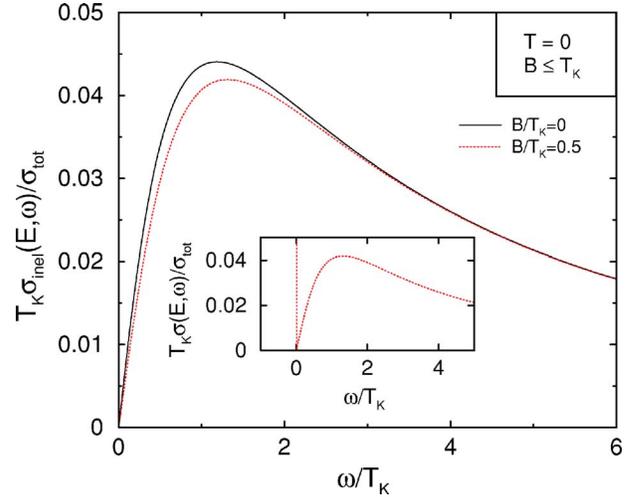


FIG. 4. (Color online) NRG result for  $\sigma(E, \omega)$  at  $T=0$  for magnetic fields  $g\mu_B B < T_K$ . The difference of the curves indicates the scattering weight which for  $B > 0$  is transferred from the inelastic to the elastic component leading to a delta-function peak at  $\omega=0$ , as sketched in the inset.

$\omega=0$ , as sketched in the inset of Fig. 4. In contrast to the case of high temperatures ( $T \gg T_K, g\mu_B B$ ), the elastic scattering contribution now does not sit on top of a large Lorentzian peak, but is rather located within the scattering pseudogap. Although its weight is small, here it is easily distinguishable from the background. The crossover from the linear dependence on  $\omega$  to the high-frequency behavior occurs at  $\omega \sim T_K$ , where the inelastic scattering cross section has a maximum. The high-frequency tail is still given by the perturbative expression (21).

When the magnetic field is increased above the Kondo temperature,  $g\mu_B B \gg T_K$ , the elastic and inelastic components of the scattering cross section are given by Eqs. (43) and (44), respectively. The elastic peak at  $\omega=0$  now exhausts almost the full spectral weight of the longitudinal correlator, i.e., it accounts for approximately 1/3 of the total scattering cross section, see Fig. 3. The remaining 2/3 of the total spectral weight are to be found in the extended structure of the Zeeman satellite (44) centered at  $\omega = \omega_Z(B)$ . The effect of Zeeman splitting on the cross section is confined to the region of energies  $|\omega| \lesssim \omega_Z(B)$ . At  $|\omega| \gg \max[T_K, g\mu_B B, T]$ , the behavior of  $\sigma(E, \omega)$  is again given by Eq. (21).

In Fig. 5, the inelastic cross section is shown in the limit of large magnetic fields,  $g\mu_B B \gg T_K$ , as given by Eq. (44). The inset compares the result with the NRG. The low-frequency and high-frequency asymptotes are reproduced in the numerical calculation fairly well. The deviation in the width of the Zeeman peak, however, demonstrates the limitation of the NRG method. Due to the logarithmic frequency resolution, the NRG tends to overbroaden any peak in the spectral function centered around a *nonzero* frequency.

## V. POSSIBLE EXPERIMENTS

As we have shown above, the differential scattering cross section of the magnetic impurity shows a rich structure in

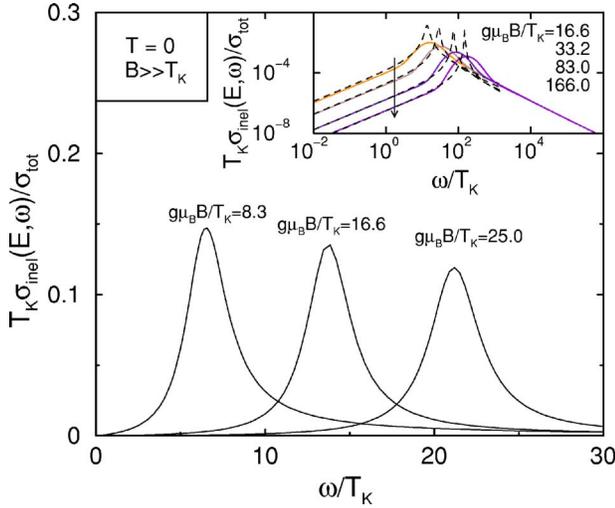


FIG. 5. (Color online) Inelastic scattering cross section for several magnetic field values,  $B \gg T_K$ , at  $T=0$  according to Eq. (44), which is applicable unless  $\omega \gg B$ . Note that the position of the resonance is shifted away from the Zeeman energy as described by Eq. (30). The inset shows the comparison of the analytical result (44) (dotted lines) with NRG calculation (colored lines). The low-frequency tail matches nicely. However, the NRG overestimates the width of the peak.

frequency space. In the following, we suggest two experiments that are sensitive to the dynamics of a Kondo impurity and from which, in principle, the energy-resolved scattering cross section can be extracted.

### A. Mesoscopic wires

Inelastic scattering off magnetic impurities has been identified to be at the origin of an anomalously large energy relaxation in mesoscopic metallic wires.<sup>6</sup> We propose a modification of the original experiment performed by Pothier *et al.*<sup>6</sup> that allows us, in principle, to access the scattering cross section considered in this paper. We assume that the wire is connected to the reservoirs on one end by an open contact and on the other via a tunnel junction, see Fig. 6. In the limit of small transparency of the tunnel junction, the wire is almost in equilibrium; only a small amount of energetic quasiparticles tunnel into the wire and relax their energy during scattering processes on magnetic impurities. In the lowest order in the transparency of the tunnel junction,

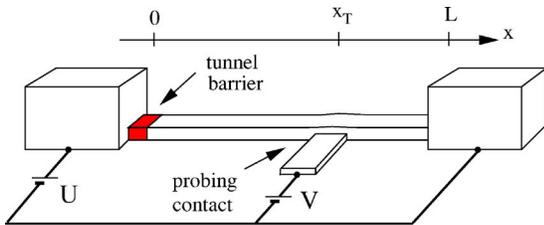


FIG. 6. (Color online) Experimental setup of Pothier *et al.*<sup>6</sup> with an additional tunnel barrier which limits the injection of hot electrons into the wire. The voltage drop across the wire is denoted by  $U$ . The voltage applied at the probing contact is  $V$ .

we can treat this relaxation mechanism in terms of the differential scattering cross section,  $\sigma(E, \omega)$ , of a test particle coming with energy  $E$  in an otherwise equilibrium system.

Consider a mesoscopic wire of length  $L$ . The equilibrium distribution in the right and left reservoir is given by a Fermi function,  $f_F(E)$  and  $f_F(E-eU)$ , respectively, where the energy  $E$  is measured with respect to the chemical potential of the right reservoir. The voltage drop across the wire is  $U$ . Within the wire, the distribution function,  $f(E; x, U)$ , will depend on the position across the wire,  $x \in [0, L]$ . It is determined by the relaxation mechanisms and carries information on the differential scattering cross section,  $\sigma(E, \omega)$ . This distribution function is probed by an additional tunnel contact that is attached to the wire at a certain position  $x_T \in [0, L]$  and connects it to a conductor with a sharp feature in the density of states. Measurement of a small tunneling current through this auxiliary contact as a function of voltage  $V$ , see Fig. 6, allows one<sup>6</sup> to probe the electron energy distribution. This way, the distribution function,  $f(E; x_T, U)$ , in the wire at some point  $x_T$  in the presence of a bias  $U$  applied across the wire was investigated.<sup>6,12</sup> The sharp feature in the electron density of states in the probe was due to its superconducting state<sup>6</sup> (the BCS anomaly) or due to the Coulomb interaction in a low-dimensional diffusive electron system<sup>12</sup> (zero-bias anomaly). In the following, we show that measurement of the derivative  $\partial f(E; x_T, U) / \partial U$  in a modified (compared to Ref. 6) setup of Fig. 6 allows one to access the inelastic scattering cross section,  $\sigma(E, \omega)$ .

The distribution function within the wire is governed by the diffusive Boltzmann equation<sup>29</sup>

$$-D \frac{\partial^2 f(E; x, U)}{\partial x^2} = I[f], \quad (46)$$

where  $D$  is the diffusion coefficient of the wire. The collision integral is local in space,

$$I[f] = c_{\text{imp}} \nu_F \int_{-\infty}^{\infty} d\omega \{ f(E) [1 - f(E - \omega)] \sigma(E, \omega) - [1 - f(E)] f(E - \omega) \sigma(E - \omega, -\omega) \}, \quad (47)$$

where  $c_{\text{imp}}$  is the impurity concentration within the wire, and  $\sigma(E, \omega)$  is the differential cross section of a single magnetic impurity; for notational convenience, the dependence of the distribution function  $f$  on  $x$  and  $U$  has been omitted. The boundary condition at the open contact to the right reservoir is simply  $f(E; x=L, U) = f_F(E)$ . The boundary condition at the tunnel contact, which connects the wire to the left reservoir, is determined by current conservation

$$g_T [f_F(E - eU) - f(E; x=0, U)] = -\nu D \frac{\partial f(E; x=0, U)}{\partial x}, \quad (48)$$

where  $g_T$  is the dimensionless conductance of the tunneling contact and  $\nu$  is the density of states of the wire.

In zeroth order in the collision integral, we obtain the solution

$$f^{(0)}(E;x,U) = f_F(E) \frac{L_0+x}{L_0+L} + f_F(E-eU) \frac{L-x}{L_0+L}, \quad (49)$$

where we introduced the length  $L_0$ ; the relation of  $L_0$  to the length of the wire  $L$  is determined by the ratio of conductances of the wire and the tunneling contact,  $L_0/L = g_w/g_T$ , with  $g_w = \nu D/L$ . In the limit of the large transparency of the tunneling contact,  $L_0/L \ll 1$ , the obtained solution reduces to the well-known formula for the distribution function of a diffusive wire with open contacts.<sup>29</sup> However, we are focusing on the other limit of a large tunneling barrier,  $L/L_0 \ll 1$ , where we get  $f^{(0)}(E;x,U) = f_F(E) + \delta f^{(0)}(E;x,U)$  with

$$\delta f^{(0)}(E;x,U) = [f_F(E-eU) - f_F(E)] \frac{L-x}{L_0} + O\left(\frac{L}{L_0}\right)^2. \quad (50)$$

The deviation of the energy distribution in the wire from the one in the right reservoir is of first order in the small parameter  $L/L_0$ .

In the following, we consider the correction to the distribution function in the lowest order in the collision integral and in the small parameter  $L/L_0$ . We get in leading order in  $L/L_0$

$$\begin{aligned} I[f^{(0)}] &= c_{\text{imp}} v_F \frac{L-x}{L_0} [f_F(E-eU) - f_F(E)] \\ &\times \int_{-\infty}^{\infty} d\omega \sigma(E,\omega) (1 - e^{-\beta\omega}) \\ &\times [f_F(E-\omega-eU) - f_F(E-\omega)]. \end{aligned} \quad (51)$$

Returning now to Eq. (46), we are able to find the correction to the distribution function. The energy dependence of  $\partial f(E;x,U)/\partial U$  within the interval  $0 < E < eU$  is caused by electron energy relaxation. At  $T=0$  it is given by

$$\frac{\partial f(E;x,U)}{\partial(eU)} = \frac{c_{\text{imp}} v_F}{DL_0} \left( -\frac{x^3}{6} + \frac{Lx^2}{2} - \frac{L^2x}{3} \right) \sigma(eU, eU-E). \quad (52)$$

The structure of the distribution function in this energy interval is directly related to the differential scattering cross section,  $\sigma(E,\omega)$ . The simple relation between  $\partial f(E;x,U)/\partial U$  and the cross section holds as long as the events of scattering off magnetic impurities occur rarely over the time limited by the diffusion of an electron across the wire. Note, however, that in addition to Eq. (52), there is a sharp contribution at the edge of the energy interval,  $E=eU$ , resulting from the zeroth order contribution (50) to the nonequilibrium distribution function. At finite temperature, this limits the experimental accessibility of  $\sigma(E,\omega)$  for  $\omega \lesssim T$ .

### B. Quantum dot in the Kondo regime

A second experimental possibility is very similar in spirit to the first one, but considers a quantum dot setup. The starting point is a semiconductor-based ballistic wire that has on its right-hand side contact with a large reservoir, see Fig. 7. On the other end, the wire is connected to a quantum dot in

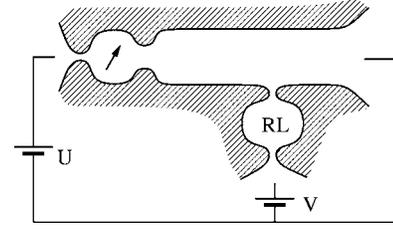


FIG. 7. Experimental quantum dot setup. A wire leads to a quantum dot in the Kondo regime (indicated by the arrow), which is in addition weakly connected to another reservoir at a voltage  $U$ . The resonance-level (RL) quantum dot acts as a probe.

the Kondo regime. In this regime, the spin of the dot forms a many-body ground state with the electrons in the wire. Electrons injected at a bias  $U$  into the wire through the quantum dot form a nonequilibrium distribution, which is probed via an auxiliary weak contact having potential  $V$ . The auxiliary contact consists of a second quantum dot, marked RL in Fig. 7, which is tuned to the resonant tunneling regime. In the case of a sharp resonance, the setup of Fig. 7 allows one to measure the electron energy distribution in the quantum wire. This nonequilibrium distribution, in turn, is sensitive to the inelastic transport through the Kondo dot and bears the signatures of the differential scattering cross section of the Kondo spin.

If the left reservoir is disconnected from the Kondo dot, the electrons within the ballistic wire have a equilibrium Fermi distribution,  $f^{(0)}(E) = f_F(E)$ . The injection of hot electrons from the left reservoir will lead to a nonequilibrium correction to the distribution function of the right movers within the wire,  $f(E) = f_F(E) + \delta f(E)$ . We obtain in the lowest order in the tunneling between the left lead and the dot,

$$\begin{aligned} v_F \delta f(E) &= v_F \int d\xi \sigma(\xi, \xi-E) [f_F(\xi-eU) (1-f_F(E)) \\ &- e^{-\beta(\xi-E)} f_F(E) [1-f_F(\xi-eU)], \end{aligned} \quad (53)$$

where we used already the detailed balance relation,  $\sigma(E,\omega)e^{-\beta\omega} = \sigma(E-\omega,-\omega)$ . After taking the derivative with respect to  $U$ , the above equation simplifies considerably at  $T=0$ , and we get

$$\frac{\partial f(E)}{\partial(eU)} = \sigma(eU, eU-E). \quad (54)$$

The measurement of this quantity with help of the auxiliary contact thus yields direct access to the differential inelastic scattering cross section of a Kondo system.

## VI. SUMMARY

We analyzed inelastic scattering of energetic electrons off a magnetic impurity. For such scattering, the dependence of the differential cross section,  $\sigma(E,\omega)$ , on energy  $E$  of the incoming electron is logarithmically weak at  $E \gg T_K$  and arises from the renormalization of the exchange coupling. In the leading-logarithmic approximation, the total cross section  $\sigma_{\text{tot}} = \int d\omega \sigma(E,\omega)$  is proportional to  $1/\ln^2(E/T_K)$ , in agree-

ment with Ref. 3. More interestingly, the electron scattering is inelastic, and the dependence of  $\sigma(E, \omega)$  on the energy transfer  $\omega$  is determined by the spin-spin correlation function of the impurity or, equivalently, by the dissipative part of the impurity spin susceptibility  $\chi''$ . In the absence of the magnetic field, the elastic component of scattering appears only in the order  $1/\ln^4(E/T_K)$ .

Our findings confirm and quantify the conclusion of Ref. 7 regarding the inelastic nature of Kondo scattering and also provide a clear physical picture of the mechanism of inelastic scattering. In the absence of the magnetic field, the inelastic scattering cross section is parametrically larger than the elastic one. The typical energy transfer  $|\omega|$  in an inelastic scattering event is, however, small compared to  $E$ . At high temperatures,  $T \gg T_K$ , the characteristic energy transfer is determined by the Korringa relaxation rate of the magnetic impurity, and at low temperatures, it is defined by the value of  $T_K$ . In the high-temperature limit, the cross section is maximal at  $\omega=0$ , and at  $T \ll T_K$ , it reaches its maximum at  $\omega \sim T_K$ . The decrease of the cross section in the domain  $\omega \gg T_K$  is remarkably slow,  $\sigma(E, \omega) \propto [\omega \ln^2(\omega/T_K)]^{-1}$ . The domain of intermediate energy transfers,  $\omega \sim T_K$ , is covered by NRG calculations. The numerical results fit well with the analytically evaluated asymptotes at  $\omega \ll T_K$  and  $\omega \gg T_K$ . In the presence of an external magnetic field, the Zeeman splitting of the magnetic impurity levels results in the appearance of an elastic component of electron scattering already in the leading logarithmic order (in  $E/T_K$ ).

Finally, we proposed possible hot-electron experiments with a metallic mesoscopic wire and with a semiconductor quantum-dot device which in principle allow one to access the differential scattering cross section of a localized magnetic moment.

### ACKNOWLEDGMENTS

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### APPENDIX A: DERIVATION OF SHIBA RELATION

Here, we provide a simple derivation of the Shiba relation,<sup>22</sup> using Nozières’ idea of a low-temperature Fermi liquid description of the Kondo problem.

Within Nozières’ theory, at  $T \ll T_K$ , the effect of a weak ( $g\mu_B B \ll T_K$ ) magnetic field applied to a Kondo impurity is described by a local-field Hamiltonian,

$$H_B = \frac{2\chi_0}{g\mu_B\nu} B \sum_{k,k',\sigma} s_{\sigma\sigma}^z \psi_{k\sigma}^\dagger \psi_{k'\sigma}. \quad (\text{A1})$$

Here,  $\nu$  is the density of states at the Fermi level,  $\chi_0 = [W(g\mu_B)^2]/(4T_K)$  is the linear susceptibility, summation over  $k$  and  $k'$  occurs within a shell of states  $\Delta k$  sufficiently

close to the Fermi level ( $\Delta k \sim T_K/v_F$  with  $v_F$  being the Fermi velocity), and field  $B$  is applied along the  $z$  axis. One may easily check that the action of the field described by the Hamiltonian (A1) indeed results in a local magnetization  $M = \chi_0 B$ . For that, one starts with the evaluation of the spin-dependent scattering phase  $\delta_\sigma$  off the local perturbation, Eq. (A1), using the Born approximation,

$$\delta_\sigma = \pi\sigma\nu \frac{\chi_0}{g\mu_B\nu} B, \quad \sigma = \pm 1. \quad (\text{A2})$$

Having the phase difference  $\delta_+ - \delta_-$ , we evaluate the magnetization using the Friedel sum rule,

$$M = \frac{g\mu_B}{2} \frac{\delta_+ - \delta_-}{\pi} = \chi_0 B. \quad (\text{A3})$$

Having the right form of the local perturbation, we now allow for a slow variation of the field,  $B = B_0 \cos(\omega t)$ , assuming that the frequency  $\omega \ll T_K$ . Next, we evaluate the energy absorption rate  $w$  caused by such time-dependent perturbation. Using the Fermi Golden rule, we arrive at

$$\begin{aligned} w &= \pi\omega \left[ \frac{\chi_0 B_0}{g\mu_B\nu} \right]^2 \nu^2 \int d\epsilon f(\epsilon) [f(\epsilon - \omega) - f(\epsilon + \omega)] \\ &= \pi\omega^2 \left[ \frac{\chi_0 B_0}{g\mu_B} \right]^2. \end{aligned} \quad (\text{A4})$$

In the last line, we discarded corrections of order  $O(e^{-T_K/T})$  arising from the boundaries of the energy integral. Recalling finally that  $w = \frac{1}{2}\omega\chi''(\omega)B_0^2$ , we arrive at the Shiba relation, Eq. (24).

Using the framework of the above derivation, it is straightforward to generalize the Shiba relation to the case of a weak, slowly varying field applied to the local moment on top of a time-independent field  $B$  of arbitrary strength. In the generalized relation,  $\chi_0$  is the static differential susceptibility, and the relation is applicable in the regime  $\omega, T \ll \max\{B, T_K\}$ .

We assume that the basis of the effective low-energy Hamiltonian has been chosen such that it incorporates already the effect of the time-independent local magnetic field  $B$ . Consider now a small perturbation to this effective Hamiltonian induced by a small change in the applied local magnetic field  $B + \delta B$ ,

$$H_{\delta B} = \frac{2}{g\mu_B\nu} \frac{\partial M}{\partial B} \delta B \sum_{k,k',\sigma} s_{\sigma\sigma}^z c_{k\sigma}^\dagger c_{k'\sigma}. \quad (\text{A5})$$

The summation over  $k$  and  $k'$  is bounded by  $|k|, |k'| \lesssim \max\{g\mu_B B, T_K\}/v_F$ . The prefactor can be determined in the same way as before. In contrast to the limit  $B=0$ , here the resulting phase shift yields information about the change in magnetization  $M(B + \delta B) - M(B) = (\partial M/\partial B)\delta B$ , where  $\partial M/\partial B$  is the differential susceptibility. The same arguments as above will yield the generalized Shiba relation,

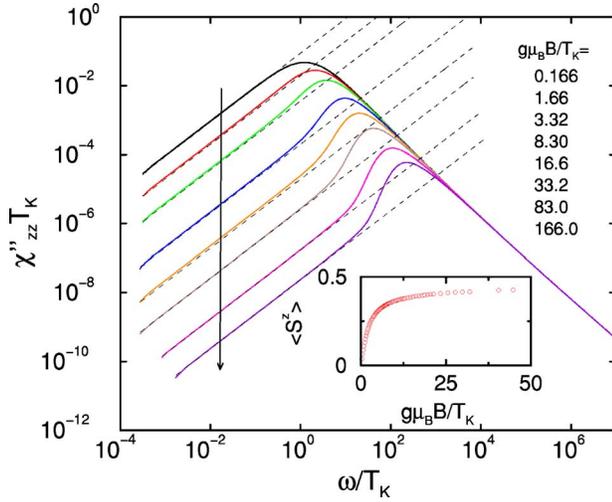


FIG. 8. (Color online) NRG comparison of the low-frequency asymptote of  $\chi''_{zz}$  with the prediction of the generalized Shiba relation, Eq. (A6) (dotted lines). The inset shows the numerically evaluated magnetization whose derivative enters Eq. (A6).

$$\chi''_{zz}(\omega) = 2\pi\omega \left[ \frac{\partial \langle S^z \rangle}{\partial B} \right]^2. \quad (\text{A6})$$

Here,  $\langle S^z \rangle$  is the equilibrium average spin value in the presence of field  $B$ . In the perturbative regime, the average is given in Eq. (33).

In Fig. 8, the prediction of the generalized Shiba relation (A6) is illustrated with the NRG result. The susceptibility,  $\chi''_{zz}$ , and the nonlinear static susceptibility,  $\chi_0 = g\mu_B \partial \langle S^z \rangle / \partial B$ , have been independently evaluated with the NRG. The dashed line in Fig. 8 is plotted with the help of Eq. (A6) and compares well with the low-frequency asymptote of  $\chi''_{zz}$ .

## APPENDIX B: RG EQUATION FOR THE IMPURITY $g$ FACTOR

We present a derivation of the two-loop RG equation for the impurity  $g$  factor of the Kondo model and, in particular, explain the different roles played by the impurity and conduction electron  $g$  factor in the renormalization process. To this end, we will use Abrikosov's pseudofermion representation<sup>3</sup> for the impurity spin,  $\mathbf{S} = f^\dagger \frac{1}{2} \boldsymbol{\sigma} f$ , where  $f^\dagger = (f^\dagger_\uparrow, f^\dagger_\downarrow)$  in a compact spinor notation and  $\boldsymbol{\sigma}$  is the vector of Pauli matrices. We will need the action of the Kondo model, which consists of three parts,  $\mathcal{S} = \mathcal{S}_s + \mathcal{S}_d + \mathcal{S}_K$ . The quadratic part of the Abrikosov pseudofermions reads

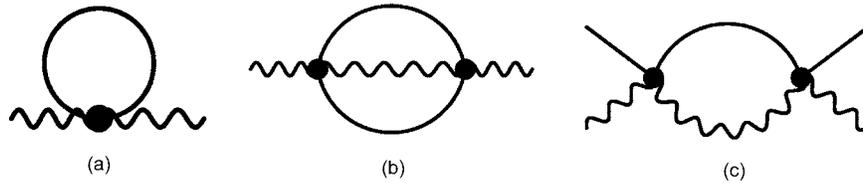


FIG. 9. (a) First-order Knight-shift diagram; (b) two-loop self-energy correction; (c) one-loop vertex correction. The wiggled line represents the propagator of the Abrikosov fermions and the solid line, the electron propagator. The dot signifies the Kondo interaction.

$$\mathcal{S}_d = \int_0^\beta d\tau f^\dagger(\tau) \left[ \partial_\tau - \lambda_0 - g\mu_B \frac{1}{2} \boldsymbol{\sigma}^a B_a \right] f(\tau), \quad (\text{B1})$$

where  $g$  is the impurity  $g$  factor and  $B^a$  is the magnetic field, which is taken to point in the  $z$  direction,  $B^a = B \delta_{az}$ . In order to enforce the Hilbert space constraint,  $f^\dagger f = 1$ , a chemical potential,  $\lambda_0 \rightarrow \infty$ , is introduced.<sup>3</sup> The Kondo interaction is given by

$$\mathcal{S}_K = \int_0^\beta d\tau \left( \Psi^\dagger(\tau) \frac{1}{2} \boldsymbol{\sigma}^a \Psi(\tau) \right) J_{ab} \left( f^\dagger(\tau) \frac{1}{2} \boldsymbol{\sigma}^b f(\tau) \right), \quad (\text{B2})$$

where the local electron operator at the impurity site is  $\Psi^\dagger = \int dk / 2\pi v_F (c_{k\uparrow}^\dagger, c_{k\downarrow}^\dagger)$ . We allow for different values of the exchange interaction in the direction orthogonal and perpendicular to the magnetic field,  $(J_{ab}) = \text{diag}\{J_\perp, J_\perp, J_\parallel\}$ . Finally, the quadratic part of the  $s$  electrons reads

$$\mathcal{S}_s = \int_0^\beta d\tau \int_{-D}^D \frac{dk}{2\pi v_F} c_{k\sigma}^\dagger(\tau) [\partial_\tau + k] c_{k\sigma}(\tau). \quad (\text{B3})$$

In the presence of a Zeeman energy for the  $s$  electrons, the Fermi sea of the spin-up and spin-down electrons are shifted with respect to each other giving rise to a finite Pauli magnetization. In Eq. (B3), we assumed that the band has already been symmetrized around the respective Fermi energies by integrating out a finite number of electronic degrees of freedom. This process results in a perturbative renormalization of the impurity  $g$  factor due to the so-called Knight shift. The first-order Knight-shift diagram is shown in Fig. 9(a). The  $g$  factor  $g$  appearing in (B1) is, therefore, understood to be already the Knight-shifted impurity  $g$  factor,

$$g = g_i - \frac{J_\parallel \nu}{2} g_e + O(J_\parallel \nu)^2, \quad (\text{B4})$$

where  $g_i$  and  $g_e$  are the bare impurity and electronic  $g$  factors, respectively, and the density of states is  $\nu = 1/(2\pi v_F)$ . As is clear from Eq. (B4), the electronic  $g_e$  can be absorbed in an effective impurity  $g$  factor. The Knight shift is, thus, only a perturbative phenomenon and, in particular, is not enhanced by logarithmic renormalizations. This is expected since the Pauli magnetization affects only electronic states far away from the Fermi edge deep inside the Fermi sea.

The field theory can be renormalized<sup>30</sup> with a wave function, impurity  $g$  factor, and Kondo-coupling renormalization (in addition to a counterterm absorbing a shift in the unphysical chemical potential  $\lambda_0$ ),

$$f = \sqrt{Z}f^R, \quad g = \frac{g^R}{Z}, \quad J_{ab} = \frac{J_{ab}^R}{Z}. \quad (\text{B5})$$

We compute the renormalization of the Kondo coupling to one-loop order and the renormalization of the wave function and  $g$  factor to two-loop order. The corresponding diagrams are shown in Figs. 9(b) and 9(c). The resulting RG equations for the Kondo vertex are the well-known poor man's scaling equations,<sup>4</sup>

$$\frac{d(J_{\perp}\nu)}{d \ln D} = -(J_{\perp}\nu)(J_{\parallel}\nu), \quad \frac{d(J_{\parallel}\nu)}{d \ln D} = -(J_{\perp}\nu)^2. \quad (\text{B6})$$

For the wave-function renormalization, we obtain

$$\frac{d \ln Z}{d \ln D} = \frac{1}{8}[(J_{\parallel}\nu)^2 + 2(J_{\perp}\nu)^2]. \quad (\text{B7})$$

Finally, the main result is the RG equation for the  $g$  factor,

$$\frac{dg}{d \ln D} = \frac{1}{2}g(J_{\perp}\nu)^2. \quad (\text{B8})$$

Solving this equation in the isotropic case,  $J_{\perp}=J_{\parallel}=J$ , and expanding the result in leading-logarithmic order, we get

$$g(D) = g_i \left[ 1 - \frac{1}{2 \ln \frac{D}{T_K}} + \left( 1 - \frac{g_e}{g_i} \right) \frac{J\nu}{2} \right], \quad (\text{B9})$$

where we already substituted the Knight-shifted  $g$  factor (B4). In the scaling limit,  $J \rightarrow 0$ , while  $T_K$  is held fixed, any dependence on the electronic  $g$  factor  $g_e$  vanishes, and we obtain the result cited in the body of the paper, Eq. (29). In particular, note that in the absence of a Knight shift,  $g_e=0$ , the perturbative correction to the  $g$  factor starts only in the second order in the exchange coupling  $J$  but, nevertheless, after renormalization group improvement leads to a correction which is of leading-logarithmic order. At zero temperature, the RG equation for the  $g$  factor coincides with the RG equation for the impurity magnetization, which was already determined in Ref. 31.

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