Theory of Inelastic Scattering from Magnetic Impurities

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We use the numerical renormalization group method to calculate the single-particle matrix elements $\mathcal{T}$ of the many-body T matrix of the conduction electrons scattered by a magnetic impurity at $T = 0$ temperature. Since $\mathcal{T}$ determines both the total and the elastic, spin-diagonal scattering cross sections, we are able to compute the full energy, spin, and magnetic field dependence of the inelastic scattering cross section $\sigma_{\rm inel}(\omega)$. We find an almost linear frequency dependence of $\sigma_{\rm inel}(\omega)$ below the Kondo temperature T_K, which crosses over to a ω^2 behavior only at extremely low energies. Our method can be generalized to other quantum impurity models.

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Quantum mechanical phase coherence in mesoscopic structures is destroyed by inelastic processes, where excitations such as spin waves, electron-hole excitations, phonons, etc., are created in the environment, leading to dephasing and loss of quantum coherence after a time $\sim\tau_\varphi$ [1]. In some weak localization measurements of the dephasing time τ_φ down to very low temperatures, a surprising saturation of τ_φ has been observed [2]. This unexpected saturation remained a puzzle for a long time until recently, when further experiments on mesoscopic quantum wires confirmed that the most likely candidates to produce this surprising behavior are magnetic impurities [3,4]. These magnetic impurities seem to be present even in samples of extreme purity and unavoidably lead to inelastic scattering and the dephasing.

Theoretical calculations also confirmed these expectations and showed that the experimental data can be quantitatively explained assuming weak inelastic scattering off Kondo impurities [5,6]. These calculations were performed in the weak coupling regime, i.e., at energies higher than the Kondo temperature, T_K. However, Nozières's theory implies that well below T_K the magnetic impurity spin is screened by the conduction electrons and acts as a strong but conventional potential scatterer, producing no inelastic scattering. Therefore the inelastic scattering rate from magnetic impurities must show a *peak* around T_K and then drop to zero well below T_K [7].

These observations motivate us to study the complete energy dependence of the inelastic scattering rate off a magnetic impurity. Here we focus on the simplest possible case of $T = 0$ temperature, where the inelastic scattering rate can be defined as follows: Assume that we have a single scattering impurity at the origin and we create an incoming flux of electrons with momentum $\mathbf{k}$, spin σ, and energy E above the Fermi energy far away from the origin. This incoming flux can be scattered off the impurity in two different ways: (i) Either the electrons scatter *elastically* (both energy and spin unchanged) with a scattering cross section $\sigma_{\rm el}(E)$ into an outgoing single-particle state, without perturbing the environment or (ii) they scatter off *inelastically* with a corresponding cross section $\sigma_{\rm inel}(E)$; i.e., and they leave behind some electron-hole or spin excitations.

In the present Letter, we show how the full energy and magnetic field dependence of $\sigma_{\rm inel}(E)$ can be determined. The basic idea is simple: The single-particle matrix elements of the many-body T matrix, $\langle \mathbf{k}\sigma|\hat{T}|\mathbf{k}'\sigma'\rangle$, determine the elastic cross section, but they are also related to the total scattering cross section $\sigma_{\rm tot} = \sigma_{\rm el} + \sigma_{\rm inel}$ through the optical theorem. Therefore, we have only to find a way to compute the $\langle \mathbf{k}\sigma|\hat{T}|\mathbf{k}'\sigma'\rangle$'s to obtain the inelastic scattering cross section as the difference of the total and elastic scattering cross sections:

$$\sigma^\sigma_{\rm inel} = \sigma^\sigma_{\rm total} - \sigma^\sigma_{\rm el}. \tag{1}$$

To determine $\langle \mathbf{k}\sigma|\hat{T}|\mathbf{k}'\sigma'\rangle$, we first relate them through *reduction formulas* to some local correlation functions [8], which we then calculate using the nonperturbative method of the numerical renormalization group (NRG) [9]. Note that we evaluate the $\hat{T}$ matrix elements for single electron states (which are not eigenstates of the Hamiltonian) rather than for quasiparticles; cf. [10]. As a consequence, we find ineleastic scattering at any finite energy (even at $T = 0$). Though here we focus exclusively on the case of zero temperature, where excitations are created from the vacuum state [11], our discussions carry over, with some modifications, to the case of finite temperatures, too [12].

To be specific, consider the Anderson model (AM), but our method is rather general and applies to practically any local quantum impurity problem. We write the Hamiltonian as $H = H_0 + H_{\rm int}$, where H_0 denotes the "free" quadratic part of the Hamiltonian,

$$H_0 = \sum_\sigma \epsilon_d d_\sigma^\dagger d_\sigma + \sum_{\sigma,\mathbf{k}} \xi(\mathbf{k}) c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma},$$

and $H_{\rm int}$ stands for the on-site Hubbard interaction and hybridization

$$H_{\rm int} = U n_\uparrow n_\downarrow + V \sum_{\sigma,\mathbf{k}} (c_{\mathbf{k}\sigma}^\dagger d_\sigma + \text{H.c.}), \qquad (2)$$

with $n_\sigma = d_\sigma^\dagger d_\sigma$. The operator $c_{\mathbf{k}\sigma}^\dagger$ creates an electron in a plane wave state with momentum $\mathbf{k}$, energy $\xi(\mathbf{k}) = \frac{\mathbf{k}^2}{2m} - \mu$, and spin σ, while d_σ is the annihilation operator of the d electron.

We proceed to define incoming and outgoing *scattering states* as well as the corresponding field operators and Hilbert spaces [8]. As the impurity is local, the interaction switches off far away and the "in" and "out" states are eigenstates of the full Hamiltonian with the asymptotic boundary condition of behaving as plane waves in the $t \to -\infty$ and $t \to \infty$ limits, respectively. The many-body S-matrix and the T-matrix elements are then simply defined in terms of the overlaps of the incoming and outgoing scattering states,

$$\langle b, \text{out} | a, \text{in} \rangle \equiv \langle b, \text{in} | \hat{S} | a, \text{in} \rangle, \qquad (3)$$

$$\hat{S} = 1 + i\hat{T}. \qquad (4)$$

In the interaction representation, the explicit form of the S matrix is given by the well-known expression $\hat{S} = T \exp\{-i \int_{-\infty}^{\infty} H_{\rm int}(t) dt\}$, where T is the time ordering operator.

We are primarily interested in scattering of single electron states $c_{\mathbf{k}\sigma}^\dagger |0\rangle$ off the impurity. As noted, these are eigenstates of H_0 and not of H, but as $H(t \to -\infty) \to H_0$ they can be used to label the full eigenstates $|a, \text{in}\rangle = |\mathbf{k}, \sigma\rangle$ by imposing the boundary condition, $|\mathbf{k}, \sigma\rangle \to c_{\mathbf{k}\sigma}^\dagger |0\rangle$ as $t \to -\infty$, with the single-particle scattering being described by matrix elements of the T matrix, $\langle \mathbf{k}, \sigma | \hat{T} | \mathbf{k}', \sigma' \rangle$. Separating the Dirac delta contribution due to energy conservation and defining the on-shell T matrix $\mathcal{T}$ via $\langle \mathbf{k}, \sigma | \hat{T} | \mathbf{k}', \sigma' \rangle = 2\pi\delta[\xi(\mathbf{k}) - \xi(\mathbf{k}')] \times \langle \mathbf{k}, \sigma | \mathcal{T} | \mathbf{k}', \sigma' \rangle$, we can express the latter through standard manipulations [8] as

$$\langle \mathbf{k}\sigma | \mathcal{T} | \mathbf{k}'\sigma' \rangle = -s G_0^{-1}(\xi, s\mathbf{k}) G_{s\sigma, s\sigma'}(\xi, s\mathbf{k}, s\mathbf{k}') G_0^{-1}(\xi, s\mathbf{k}'), \qquad (5)$$

where $s = \text{sgn}\xi$ distinguishes electronlike excitations from holelike excitations, $G_0^{-1} = i\frac{\partial}{\partial t} + \mu + \frac{1}{2m}\nabla^2$ denotes the inverse of the free Green function, and G is the time-ordered single-particle Green function. The meaning of Eq. (5) becomes more transparent in the diagrammatic language of Fig. 1: As indicated by the large, thin crosses there, one has to drop the contributions of the two external legs of all scattering diagrams to the single electron Green function, and the rest is just the on-shell single-particle matrix element of the many-body T matrix. In the particular case of the AM, $\mathcal{T}$ does not depend on the direction of incoming and outgoing momenta, and a simple Dyson equation relates it to the d level's time-ordered propagator (see Fig. 1)

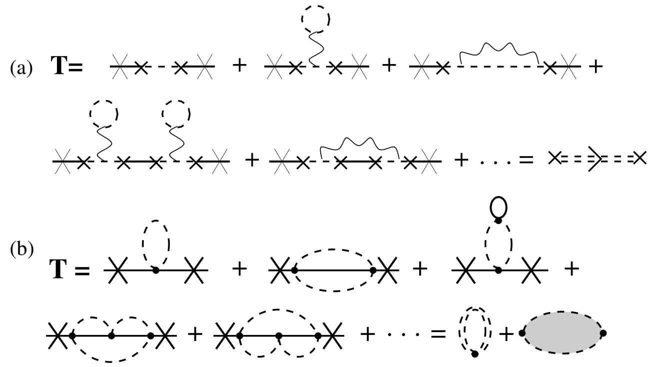

FIG. 1. (a) Diagrammatic derivation of Eq. (6). Dashed and continuous lines denote the bare propagators of the d level and the conduction electrons, small fat crosses stand for hybridization V, and wavy lines denote the on-site interaction U. (b) A diagrammatic representation of the T matrix in the Kondo problem. Dashed lines denote pseudofermion propagators and describe the evolution of the impurity spin, while continuous lines denote free conduction electron propagators. Filled circles stand for the exchange interaction J. The first term of the T matrix is simply proportional to the expectation value of the impurity spin, it is frequency independent, and vanishes at zero magnetic field. The second term can be identified as the composite fermions correlation function.

$$\mathcal{T}^{\sigma}(\omega) = -s V^2 G_d^{s;\sigma}(\omega), \qquad (6)$$

where $s = \text{sgn}\omega$, and we allowed for spin dependence due to the presence of an external magnetic field B [13].

According to the optical theorem, the spin-dependent total scattering cross section is given by the imaginary part of the diagonal matrix elements of the $\mathcal{T}$ matrix:

$$\sigma_{\rm total}^{\sigma} = \frac{2}{v_F} \text{Im} \langle \mathbf{p}\sigma | \mathcal{T} | \mathbf{p}\sigma \rangle, \qquad (7)$$

where v_F denotes the Fermi velocity. The elastic scattering cross section, on the other hand, is related to the square of $\mathcal{T}$:

$$\sigma_{\rm el}^{\sigma} = \frac{1}{v_F} \int \frac{d\mathbf{p}'}{(2\pi)^3} 2\pi\delta(\xi' - \xi) |\langle \mathbf{p}'\sigma | \mathcal{T} | \mathbf{p}\sigma \rangle|^2. \qquad (8)$$

Once these two cross sections are known, we can compute the inelastic cross section $\sigma_{\rm inel}$ through Eq. (1).

It is instructive to rewrite $\sigma_{\rm inel}$ in the case of the AM. For electrons we have

$$\sigma_{\rm inel}^{\sigma}(\omega > 0) = \frac{4\pi}{k_F^2} \left[-\frac{\Gamma}{2} \text{Im} G_d^{\sigma} - \left(\frac{\Gamma}{2}\right)^2 |G_d^{\sigma}|^2 \right], \qquad (9)$$

where $\Gamma = 2\pi V^2 \varrho_0$ denotes the width of the d level and

$\varrho_0 = k_F^2/2\pi^2 v_F$ is the conduction electrons's density of states for one spin direction. For $B = 0$, this expression reduces to

$$\sigma_{\rm inel}(\omega > 0) = \frac{2\pi}{k_F^2} \frac{\Gamma[-\Sigma''(\omega)]}{[\omega - \epsilon_d - \Sigma'(\omega)]^2 + [\Sigma''(\omega) - \frac{\Gamma}{2}]^2},$$

where Σ' and Σ'' denote, respectively, the real and imaginary parts of the d-propagator's self-energy. The analytical properties of the Green function imply that the above expression is always positive and vanishes only where Σ'' becomes zero. Furthermore, the Fermi liquid (FL) theory of Yamada and Yoshida tells us that $\Sigma'' \sim \omega^2$ as $\omega \to 0$ [14], and thus $\sigma_{\rm inel}$ vanishes as ω^2 at the Fermi energy. Note that at the same time $\sigma_{\rm total}$ approaches the unitary limit.

We demonstrate the power of the method outlined above by computing the inelastic scattering cross section for the Kondo Hamiltonian

$$H_K = \frac{J}{2} \sum_{\mathbf{k},\mathbf{k}'} \vec{S} \cdot (c^\dagger_{\mathbf{k}\sigma} \vec{\sigma}_{\sigma\sigma'} c^\dagger_{\mathbf{k}'\sigma'}). \tag{10}$$

This spin Hamiltonian captures the low-energy physics and the formation of the Kondo resonance in the AM, though for finite values of Γ/U differences are expected for intermediate energies, $T_K \ll \omega \sim U, \Gamma$. In the Kondo model (KM), the T matrix of Eq. (5) is simply related to the correlation function of the following composite fermion operator, $F_\sigma \equiv \sum_{\sigma',\mathbf{k}} \vec{S} \cdot \vec{\sigma}_{\sigma\sigma'} c_{\mathbf{k}\sigma'}$ [15], and the spectral function of F_σ, $\varrho_F(\omega)$ is thus directly proportional to the low-energy part of the spectral function of the d-level propagator in the AM. (For a diagrammatic proof, see Fig. 1.) The imaginary part of $\mathcal{T}$ can be determined by simply computing $\varrho_F(\omega)$ numerically, and then a Hilbert transform can be used to get the real part of $\mathcal{T}$ and thus the full T matrix. In all these calculations it is essential to have high quality data [16]. It is also crucial to determine the normalization factor of $\mathcal{T}$ correctly. This can be done by using the FL relation, $-{\rm Im} 2\pi\varrho_0 \mathcal{T}_d^\sigma(\omega = 0^+) = 2\sin^2\delta_\sigma$, with δ_σ the phase shift at the Fermi energy. We extracted the latter directly from the finite size NRG spectrum of the KM [9,17].

Our results for the case of $B = 0$ are shown in Fig. 2. Most of the scattering is inelastic at energies above the Kondo energy $|\omega| > T_K$. Decreasing the energy of the incoming electrons (holes), $\sigma_{\rm total}$ increases and, at energies below T_K, it finally saturates at a value $\sigma_0 = 4\pi/k_F^2$. This behavior must be contrasted to $\sigma_{\rm inel}$, which slowly increases as ω decreases, has a broad maximum around T_K, then suddenly drops and vanishes at the Fermi energy. On linear energy scales (see Fig. 3), $\sigma_{\rm inel}$ varies rather slowly above T_K, is very large even at $\omega \sim 20T_K$, and vanishes rather suddenly around $\omega \sim T_K$. For very small energies $\sigma_{\rm inel} \sim \omega^2$, in agreement with FL theory; however, this quadratic behavior appears only at very low energies, and $\sigma_{\rm inel}$ is almost linear for $0.1T_K < \omega < T_K$. At energies $\omega \gg T_K$ the inelastic rate is simply dominated by spin-flip scattering and is therefore expected to scale as $\sim 1/\ln^2(T_K/\omega)$, as we indeed find numerically. Note that the Nagaoka-Suhl approximation [18] is appropriate only for $\omega \gg T_K$ (see the inset of Fig. 2).

We also computed $\sigma_{\rm inel}$ in the presence of a local magnetic field B, directed downwards along the z axis (see Fig. 3). In this case there is a dramatic difference between the inelastic scattering properties of spin-up and

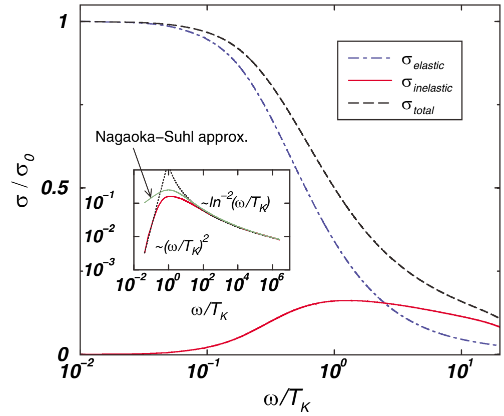

FIG. 2 (color online). Inelastic, elastic, and total scattering rates in units of $\sigma_0 = 4\pi/k_F^2$ at $T = 0$ and $B = 0$, as a function of the logarithm of the incoming electron's energy. Only the electronic contribution ($\omega > 0$) is plotted. $\sigma_{\rm inel}$ has only a very weak (logarithmic) energy dependence above T_K, scales approximately linearly with ω for $0.1T_K < \omega < T_K$, and scales as $\sim\omega^2$ for $\omega < 0.1T_K$. The inset shows the $\sim\omega^2$ and $\ln^{-2}(T_K/\omega)$ regimes for $\omega \ll T_K$ and $\omega \gg T_K$, respectively.

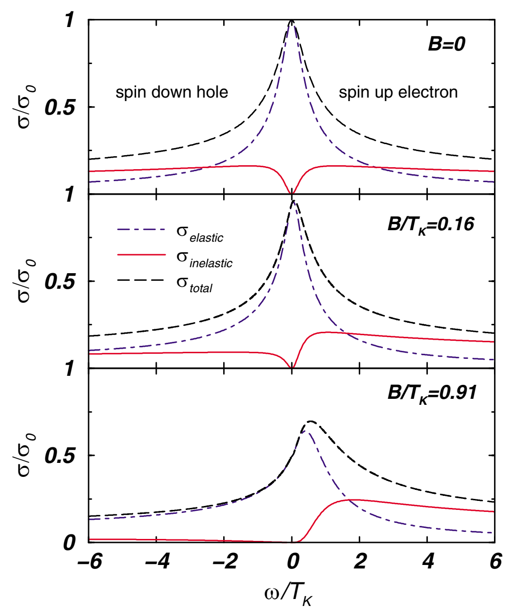

FIG. 3 (color online). Energy dependence of spin-dependent elastic and inelastic scattering rates in units of $\sigma_0 = 4\pi/k_F^2$, at $T = 0$ and in the presence of a local magnetic field B.

spin-down particles. Already a small field, $B \sim 0.1T_K$ results in a strong spin dependence of the inelastic scattering, but for $B \sim T_K$, this difference is even more dramatic. At this field the spin of the magnetic impurity is practically aligned with the external field and points downwards. Therefore an incoming spin-down particle (electron or hole) is unable to flip the impurity spin. More precisely, only higher order inelastic processes can result in a flip of the local impurity spin. This is, however, not true for spin-up particles: An incoming spin-up electron can exchange its spin with the magnetic impurity in a first order process, resulting in a maximum in $\sigma_{\rm inel}$ around $\omega \sim B$ for spin-up electrons and holes and a very broad inelastic background for $\omega > B$.

Though here we mostly focused on the simplest cases of the AM and the single channel spin $S = 1/2$ KM at $T = 0$ temperature, our formalism can be extended to other models and to finite temperatures as well [12]. In particular, while for some quantum impurity models no simple diagrammatic theory is available, the composite fermion's spectral function can be computed in any Kondo-type model to obtain the matrix elements of the T matrix, and the renormalization group flow of the eigenvalues of the S matrix can be studied in all these cases [12]. While usually a thorough numerical analysis is needed to understand the full behavior of $\sigma_{\rm inel}$, in some models simple analytical results can also be obtained. In the specific case of the two-channel KM, e.g., we know that the single-particle matrix elements of the S matrix identically vanish at the Fermi energy, $\omega = 0$ [19,20]. This implies that $\varrho_0 \mathcal{T}^{\rm 2CK}(\omega = 0) = i/\pi$ and leads to the rather surprising relation at the Fermi level, $\sigma_{\rm inel}^{\rm 2CK} = \sigma_{\rm el}^{\rm 2CK} = \sigma_{\rm tot}^{\rm 2CK}/2$: Though the S matrix vanishes identically, half of the scattering processes remain elastic. The nonvanishing $\sigma_{\rm inel}$ is characteristic of non-FL quantum impurity models. Application of any finite magnetic field drives the two-channel KM to a FL fixed point and gives rise to a vanishing $\sigma_{\rm inel}$ at the Fermi energy.

We have to emphasize that, though they must be related, the $\sigma_{\rm inel}$ we computed is *not* identical to τ_φ^{-1} measured in weak localization experiments [2], since the former contains spin-flip scattering processes as well as the creation of electron-hole pairs. While we computed only $\sigma_{\rm inel}(\omega, T = 0)$, we expect that $\sigma_{\rm inel}(\omega = 0, T)$ has a very similar form. In this sense, our finding that $\sigma_{\rm inel}$ is roughly linear with ω for $0.05T_K < \omega < 0.5T_K$ agrees qualitatively with the recent experimental results of Ref. [21].

In summary, we have shown how the full energy and magnetic field behavior of the $T = 0$ inelastic scattering rate can be computed by exploiting the reduction formulas and then using the powerful machinery of NRG to compute the single-particle matrix elements of the many-body T matrix. We have shown that the FL theory of Yamada and Yoshida directly implies a quadratically vanishing inelastic scattering rate at the Fermi energy in the specific case of the AM. Scattering properties of the KM have been computed by calculating the composite fermion's spectral function. Our numerical calculations show that the above-mentioned $\sigma_{\rm inel} \sim \omega^2$ regime appears only at energies well below T_K. In a magnetic field $B > T_K$ the inelastic scattering is very sensitive to the spin of the scattered single-particle excitation.

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