Universal dephasing rate due to diluted Kondo impurities

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We calculate the dephasing rate due to magnetic impurities in a weakly disordered metal as measured in a weak localization experiment. If the density \( n_S \) of magnetic impurities is sufficiently low, the dephasing rate \( 1/\tau_\phi \) is a universal function, \( 1/\tau_\phi = (n_S/\nu)f(T/T_K) \), where \( T_K \) is the Kondo temperature and \( \nu \) the density of states. We show that inelastic vertex corrections with a typical energy transfer \( \Delta E \) are suppressed by powers of \( 1/(\tau_\phi \Delta E) \propto n_S \). Therefore the dephasing rate can be calculated from the inelastic cross section proportional to \( \pi \nu \Im T - |\pi T|^2 \), where \( T \) is the \( T \)-matrix which is evaluated numerically exactly using the numerical renormalization group.

Dephasing, i.e. the loss of wave coherence, is a ubiquitous phenomenon in the quantum mechanics of complex systems. It is of relevance to any experiment where both interference and interactions play a role and is, therefore, of profound importance in all areas of nanoscopic and mesoscopic physics.

While the basic phenomenon of dephasing as such is of rather general nature, the concrete definition of a dephasing rate, and its experimental determination vary from context to context. In this Letter we consider the dephasing rate as determined by weak-localization (WL) measurements in metals [1]. In weakly disordered metals, the interference of electronic wave functions on time-reversed paths leads to a characteristic reduction (or enhancement in the presence of spin-orbit interactions) of the conductivity. The magnitude of this effect is controlled by the dephasing time \( \tau_\phi \)— the typical time-scale over which electrons get entangled with their environment (phonons, other electrons or dynamical impurities) thereby loosing the ability to interfere. Even small magnetic fields break time-reversal invariance thus prohibiting the interference of time-reversed paths. Fitting the magneto-resistivity to WL theory is a means to determine the dephasing rate \( 1/\tau_\phi \) with high precision.

Surprisingly, most of these experiments [2] show a saturation of the dephasing rate at the lowest accessible temperatures \( T \), while theoretically it is expected that in the limit \( T \to 0 \) all inelastic processes freeze out when the system approaches its (time-reversal invariant and unique) ground-state. This has lead to an intense discussion [3, 4, 5, 6] as to whether quantum fluctuations can induce dephasing at \( T = 0 \). While we believe that this latter scenario is theoretically excluded for electrons in a disordered metal, the presence of only a few parts-per-million (ppm) of dynamical impurities — realized by atomic two-level systems [6] or by magnetic impurities [7, 8, 9, 10] — may be an alternative cause of the saturation phenomenon. Indeed it has been shown experimentally that magnetic impurities lead to an apparent saturation of \( 1/\tau_\phi \) at least in some \( T \) range [4]. In contrast, some extremely pure Au and Ag samples with negligible concentration of impurities [10] show no saturation and seem to follow the predictions of Altshuler, Aronov and Khmelnitsky [11] for the dephasing induced by Coulomb interactions.

The effect of dynamic magnetic impurities on \( 1/\tau_\phi \) has first been considered by Ohkawa, Fukuyama and Yosida [12] (for the static case see Ref. [13]) using perturbation theory (generalized to renormalized perturbation theory in Refs. [8, 14]) which limits the range of applicability to temperatures \( T \gg T_K \) larger than the Kondo temperature, \( T_K \). For \( T \ll T_K \), a quadratic \( T \) dependence, \( 1/\tau_\phi \propto T^2 \) has been predicted [14] based on Fermi liquid arguments. In this paper we argue that the impact of static and diluted dynamic impurities can largely be treated separately. This separation enables us to combine a perturbative approach to the static disorder with a (numerically) exact treatment of the Kondo interaction. In this way, the effect of a small concentration, \( n_S \), of magnetic impurities on \( 1/\tau_\phi \) can be explored in the entire crossover range from \( T \gg T_K \) down to \( T \ll T_K \).

We consider the Hamiltonian \( H = H_0 + H_S \), where

\[
H_0 = \int d^d x c_\sigma^\dagger(x) \left[ \frac{\hbar^2}{2m} - \mu + V(x) \right] c_\sigma(x) \tag{1}
\]

describes electrons in a weak non-magnetic disorder potential \( V \), modeled for convenience by Gaussian white noise: \( \langle V(x)V(x') \rangle = \frac{1}{2\pi\nu} \delta(x-x') \) where \( \nu \) is the density of states (DOS), \( \tau = 1/\nu T \) the elastic scattering time and \( T \) the elastic mean free path. (None of our results is affected by the precise choice of band-structure or model of disorder.) The coupling of the electrons to a small concentration \( n_S \) of spin-1/2 impurities is described by the Kondo Hamiltonian

\[
H_S = J \sum_i \hat{S}_i c_\sigma^\dagger(x_i) \sigma_{\sigma\sigma'} c_{\sigma'}(x_i). \tag{2}
\]

To calculate physical quantities, we have (i) to average over \( V(x) \) and (ii) the positions \( x_i \) of the spins, taking into account (iii) the exchange coupling \( J \) to all orders. Two small parameters will help us in attacking this problem: The concentration of magnetic impurities \( n_S \) is tiny [more precisely \( n_S/\nu T_K \ll 1 \)] and also the ratio of electronic wave-length and elastic mean free path, \( 1/(k_F l) \), is small but finite.
We wish to explore the impact of dynamic impurity scattering on the WL corrections to the electric conductivity. Technically, this amounts to computing the impurity generated ‘self energy’ or ‘mass’ of the Cooperon describing the coherent propagation of an electron and a time-reversed hole in the disordered environment. As justified in detail below, we neglect mixed interaction/disorder diagrams. The problem therefore reduces to the solution of the Bethe-Salpeter equation depicted diagrammatically in Fig. 1(a). To linear order in \( \epsilon \), the two-particle irreducible vertex \( \Gamma \) shown in Fig. 1(b) can be separated into three distinct contributions: self-energy diagrams (the first two terms in Fig. 1(b)), an ‘elastic’ vertex correction with no energy transfer between upper and lower line, and an ‘inelastic’ vertex where interaction lines connect the two lines. We begin by focusing on the elastic contributions to the Cooperon self energy as inelastic contributions give vanishingly small corrections for small \( n_S \), see below.

Since self-energy and elastic vertex contributions conserve the energy of single electron lines, the solution of the reduced Bethe-Salpeter amounts to a straightforward summation of a geometric series. Setting the center-of-mass frequency \( \Omega \) (see Fig. 1) to 0, the Cooperon obtains \( C_0 = \text{bare Cooperon} \) in the absence of interactions and \( \Gamma \) the irreducible vertex obtained by adding self-energy, elastic- and inelastic vertex contributions. The crosses with attached dashed lines denote the averaging over impurity positions \( x_i \), the squares the interactions to arbitrary order in \( J \).

The WL correction to the conductivity is given by

\[
\begin{align*}
\epsilon + \Omega/2 & \quad \epsilon' - \Omega/2 \\
C & = \begin{array}{c}
\begin{array}{c}
\epsilon + \Omega/2 \\
\epsilon' - \Omega/2
\end{array}
\end{array} + \begin{array}{c}
\begin{array}{c}
\epsilon + \Omega/2 \\
\epsilon' - \Omega/2
\end{array} + \Gamma C
\end{array}
\end{align*}
\]

We begin by considering the lowest order expansion of the Bethe-Salpeter equation in the inelastic vertex (cf. Fig. 2(b)).

\[
\Delta \sigma_1 = \int d\epsilon \int d\Omega \tilde{\epsilon}(\epsilon, \Omega) \Gamma_{\text{in}}(\epsilon, \Omega) I_d(\epsilon, \Omega).
\]

Here, \( \tilde{\epsilon} \) denotes some thermal function restricting \( \epsilon \) and \( \Omega \) to values smaller than \( T \), \( \Gamma_{\text{in}} \) is the inelastic vertex and \( I_d(\epsilon, \Omega) \sim \left[ (1/\tau_{\varphi})^2 + \Omega^2 \right]^{d-1} \) results from momentum-integration over two Cooperons in \( d \) dimensions. For sufficiently small \( n_S \ll \nu T_K \) the typical energy \( \Delta E \sim \Omega \sim T \) exchanged at the inelastic vertex greatly exceeds the dephasing rate (see below) \( 1/\tau_{\varphi} \propto n_S \). Evaluating the integral \( \int \) for \( \Delta E \gg 1/\tau_{\varphi} \), we obtain

\[
\Delta \sigma_1 \sim \frac{1}{\Delta E \tau_{\varphi}} \left( \frac{n_S}{\nu T_K} \right)^{(d-1)/2} \ll 1.
\]

It is straightforward to verify that this estimate pertains to higher orders in the expansion in the inelastic vertex. The irrelevancy of the inelastic vertex for processes with typical energy transfer larger than \( 1/\tau_{\varphi} \) has been observed before by several authors (e.g. [11,14,17]). Semi-classically, vertex corrections describe the interference of two (time-reversed) electrons undergoing an interaction process (see Fig. 2(a)). Due to the transfer of a certain energy \( \Delta E \), the two electrons subsequently accumulate a phase difference, \( e^{i\Delta E t} \), where \( t \sim \tau_{\varphi} \). Therefore, vertex corrections with \( \Delta E > 1/\tau_{\varphi} \) (characteristic for our
problem) do not effectively contribute to WL. In contrast, Coulomb interactions in $d \leq 2$ are dominated by low-energy transfers and vertex corrections are required to regularize infrared singularities.  

We next turn to the discussion of the second family of corrections potentially altering our above results, correlated disorder-interaction processes as shown in Fig. 2(c). A preliminary indication as to the relevance of such contributions may be obtained by estimating the sample-to-sample fluctuations of the Kondo temperature, $T_K$,

$$
\left( \frac{\delta T_K}{T_K} \right)^2 = \frac{1}{\nu} \int_{T_K}^{E_F} d\omega \int_{T_K}^{E_F} d\omega' \frac{\langle \delta \nu(\omega) \delta \nu(\omega') \rangle_{T}}{\omega \omega'}.
$$

(7)

Substituting the results for the fluctuations of the local density of states $\delta \nu$ in weakly disordered $d$–dimensional metals, we obtain

$$
\left( \frac{\delta T_K}{T_K} \right)^2 \sim \begin{cases} 
\frac{1}{T(K_{FL} L_1 L_2)^2} & \text{in (quasi) } d = 1, \\
\frac{1}{k_F l (\nu)^2} & \text{in } d = 2, \\
\frac{1}{k_F l (\nu)^2} & \text{in } d = 3,
\end{cases}
$$

(8)

where $L_1^2$ is the cross-section of a quasi one-dimensional wire. We assume, henceforth, that $k_F l$ is sufficiently large, so that $\delta T_K \ll T_K$. While this condition seems restrictive in quasi-1d, it turns out to be always met in the WL regime, $\delta T_{\text{WL}} \ll \sigma_{\text{Drude}}$, realized in experiments (and assumed in this paper).

More formally, the role of correlations disorder/interactions may be explored in terms of the diagrams shown in Fig. 2(c). On the face of it, these diagrams are smaller by factors of $1/(k_F l)$ than the leading contributions considered above (as quantum interference maintained across the impurity limits the momentum exchanged to values $\lesssim l^{-1}$ much smaller than $k_F$). However, for very low $T$ the enhanced singularity caused by the presence of extra diffusion modes may over-compensate this phase space suppression factor. Using that for $T \ll T_K$, the bare interaction may be described by Fermi liquid theory, we find that only in one dimension the additional diagrams ($\propto T^{(d+2)/2} + T^2$) lead to contributions of anomalously strong singularity. Specifically, we obtain a correction to the dephasing rate, $1/\tau_{\varphi, c} \sim n_S T^{3/2}/[\nu T_K^2 \sqrt{k_F L_1 L_2}]$. Therefore, for

$$
T \lesssim \frac{1}{(k_F l L_1 L_2)^2} \frac{1}{\tau T_K} T_K \ll T_K
$$

(9)

the separation disorder/interactions used above becomes invalid in $d = 1$.

At very low $T$, yet another type of correction begins to play a role: The diluted Kondo impurities become indistinguishable from a conventional disordered Fermi liquid with short-range momentum-conserving interactions 20 and the dephasing rate is determined by Altshuler-Aronov-Khmelnitsky 11,20 type processes which, in our context, are encapsulated in the third family of diagrams shown in Fig. 2(d). Contributing only at order $n_S^2$ they generate corrections scaling as $T^2$ in $d = 1, 2, 3$, respectively. Evaluating the prefactors (again in Fermi liquid theory) we find that these contributions become sizeable at temperatures

$$
T \lesssim \begin{cases} 
\frac{1}{k_F l (\tau T_K)^2} \left( \frac{n_S}{\nu T_K} \right)^2 & d = 3, \\
\frac{1}{k_F l (\tau T_K)} \left( \frac{n_S}{\nu T_K} \right)^2 & d = 2, \\
\frac{1}{k_F l (\tau T_K)^{1/4}} \left( \frac{n_S}{\nu T_K} \right)^{1/4} & d = 1.
\end{cases}
$$

(10)

In all cases this crossover scale is well below $T_K$ and may arguably be neglected in all relevant experiments. Further corrections to $1/\tau_{\varphi}$ of order $n_S^2$ and higher arise from clusters of two and more magnetic impurities which are sufficiently close that the inter-impurity coupling dominates over the Kondo effect.

Fitting to $\Delta \sigma = 2\tau^2 \sigma_{\text{Drude}} \int d^3 q (qDq^2 + \tau_{\varphi}^{-1}(T))^{-1}$, we next relate our results to the $T$–dependent dephasing rates, $\tau_{\varphi}^{-1}(T)$ extracted from experiments. Comparison with the energy–resolved representation results in

$$
\frac{1}{\tau_{\varphi}(T)} = \begin{cases} 
\exp \left[ -\int \frac{d\nu f'(|\nu|) T_{\varphi}(\nu)}{2 T_{\varphi}(\nu)} \right] & d = 1, 3, \\
\exp \left[ -\int \frac{d\nu f'(|\nu|) T_{\varphi}(\nu)}{2 T_{\varphi}(\nu)} \right] & d = 2, \\
-\int \frac{d\nu f'(|\nu|) T_{\varphi}(\nu)}{2 T_{\varphi}(\nu)} & \omega_B \tau_{\varphi} \gg 1,
\end{cases}
$$

where the last line applies to the case where a strong magnetic field is present and the Cooperon can be expanded in $1/(\omega_B \tau_{\varphi})$. ($\omega_B$ is the "cyclotron" frequency of the Cooperon.)

Just two parameters enter the expression for $1/\tau_{\varphi}$: the Kondo temperature $T_K$ and the dimensionless density of magnetic impurities $n_S/|\nu T_K| \ll 1$. The $T$-matrix in Eq. 21 can be evaluated for arbitrary values of $T/T_K$ and $\epsilon/T_K$ using the numerical renormalization group generalized to the calculation of dynamical quantities in Refs. 22, 24). The result is shown in Fig. 3 where we define $T_{\varphi}^{(0)}$ and determine the Kondo temperature $T_K = T_{\varphi}^{(0)}$ from the $T = 0$ susceptibility $\chi = (g\mu_B)^2/(4T^2)$. For $T >> T_K$, we obtain (correcting factors 2 in 18 and 16 in 14) $1/\tau_{\varphi} \approx 3\pi n_S/\nu ln^2[T/T_{\varphi}]$ giving rise to a very weak $T$ dependence for $T \gtrsim T_K$. For $T \lesssim 0.3 T_K$ one observes a crossover regime where $1/\tau_{\varphi}$ varies almost linear in $T$ while at lowest $T$ one obtains the expected $T^2$ behavior. This low-temperature regime can also be calculated analytically using Fermi liquid theory 10, 21

$$
\frac{1}{\tau_{\varphi}(T)} \approx c_{FL} \frac{2 n_S}{\pi \nu} \left( \frac{T}{T_K} \right)^2 \pi^4 \frac{24}{24}
$$

(11)

with $c_{FL} \approx 0.927, 0.946, 0.969$ in $d = 1, 2, 3$ and $c_{FL} = 1$ for $\omega_B \tau_{\varphi} \gg 1$ (correcting prefactors in Ref. 14). Accidentally, the dependence of both the analytical and numerical results on $\omega_B \tau_{\varphi}$ (and on $d$) is very weak, implying
that the usual fits of the magnetoresistivity can be used to determine $1/\tau_\varphi$.

In the comparison to concrete experiments one needs to account for the interplay of dephasing due to magnetic impurities and due to Coulomb interactions [11]. Since the latter are controlled by infrared divergences in $d \leq 2$, the respective rates do not add. Instead one needs to solve, e.g. in quasi one-dimensional systems, the equation

$$\frac{1}{\tau_\varphi} = \kappa T \sqrt{\tau_\varphi} + \frac{1}{\tau_\varphi, S} \approx \left\{ \frac{(\kappa T)^{2/3} + 2/(3\tau_\varphi, S)}{1/\tau_\varphi, S + \kappa T \sqrt{\tau_\varphi, S}} \right\} \quad (12)$$

where the first term describes the self-consistently calculated effects of Coulomb interactions while $1/\tau_\varphi, S$ is the dephasing rate due to the magnetic impurities. The first (second) line holds when the Coulomb dephasing (Kondo dephasing) dominates.

In conclusion, we have shown that the dephasing rate due to diluted magnetic impurities can be calculated directly from the inelastic cross section [1] introduced in [17]. This result is valid for all types of diluted dynamical impurities as long as typical energy transfers remain larger than $1/\tau_\varphi$. In the case of Kondo impurities the dephasing rate depends on just two parameters, the Kondo temperature $T_K$ and the dimensionless density of magnetic impurities $n_S/(\nu T_K) \ll 1$. A measurement of $\tau_\varphi$ for spin-1/2 impurities along with an independent experimental determination of $T_K$ and $n_S$ would put our theory to a parameter–free test [up to fitting the Coulomb background, Eq. (12)]. An open question is how spin-orbit interactions and disorder influence the Kondo effect in systems with larger spins, e.g. Fe in Au [3].

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[1] B. L. Altshuler and A. G. Aronov, in Electron-Electron Interaction in Disordered Systems, edited by A. L. Efros and M. Pollak (North-Holland, Amsterdam, 1985)
[2] P. Mohanty, E. M. Q. Jariwala and R. A. Webb, Phys. Rev. Lett. 78, 336673669 (1997); P. Mohanty and R. A. Webb, Phys. Rev. B 55, R13452 (1997).
[3] D. S. Golubov and A. D. Zaikin, Phys. Rev. Lett. 81, 1074 (1998).
[4] I. L. Aleiner, B. L. Altshuler and M. E. Gershenson, Waves in Random Media 9, 201 (1999).
[5] J. v. Delft, J. Phys. Soc. Jpn., Suppl. A, 72, 24 (2003).
[6] A. Zawadowski, J. v. Delft and D.C. Ralph, Phys. Rev. Lett. 83, 2632 (1999).
[7] P. Mohanty, R. Webb, Phys. Rev. Lett. 84, 4481 (2000).
[8] C. Van Haesendonck, J. Vranken and Y. Bruynseraeae Phys. Rev. Lett. 58, 1968?1971 (1987).
[9] F. Schopier et al., Phys. Rev. Lett. 90, 056801 (2003).
[10] F. Pierre et al., Phys. Rev. B 68, 085413 (2003).
[11] B. L. Altshuler, A. G. Aronov and D. E. Khmelnitsky, J. Phys. C: Solid State Phys., 15, 7367-7386 (1982).
[12] F. J. Okhawa, H. Fukuyama and K. Yosida, J. Phys. Soc. Jpn. 52, 1701-1709 (1983); F. J. Okhawa, Prog. Th. Phys. Suppl. 84, 166 (1985).
[13] S. Hikami, A.I. Larkin, and Y. Nagaoka, Progr. Theor. Phys. 63, 707 (1980).
[14] M. G. Vavilov and L. I. Glazman, Phys. Rev. B 67, 115310 (2003); M. G. Vavilov, L. I. Glazman, A. I. Larkin, Phys. Rev. B 68, 075119 (2003).
[15] G. Zarand, L. Borda, J. v. Delft and N. Andrei, Phys. Rev. Lett. 93, 107204 (2004).
[16] More precisely, $\Delta E \approx T$ in the Fermi liquid regime $T \ll T_K$, $\Delta E \approx T/\ln^2[T/T_K]$ is given by the life-time of the spin. Comparing this with $1/\tau_\varphi \sim n_s/\nu$ at $T \sim T_K$, we obtain the criterion stated in the text.
[17] J. S. Meyer, V. I. Fal’ko, B.L. Altshuler, Nato Science Series II, Vol. 72, edited by I.V. Lerner et al. (Kluwer Academic Publishers, Dordrecht, 2002) cond-mat/0206024.
[18] S. Kettemann and E. R. Mucciolo, cond-mat/0508251.
[19] A. C. Hewson, The Kondo Problem to Heavy Fermions (Cambridge University Press, 1993).
[20] B. N. Narozhny, Gábor Zala and I. L. Aleiner, Phys. Rev. B 65, 180202(R) (2002).
[21] G. Frossati et al., Physica B84, 33 (1976).
[22] K. G. Wilson, Rev. Mod. Phys. 47, 773 (1975).
[23] T. A. Costi, A. C. Hewson and V. Zlatic, J. Phys.: Condens. Matter 6, 2519 (1994).
[24] W. Hofstetter, Phys. Rev. Lett. 85, 1508 (2000).
[25] In literature [13] a number of other definitions of $T_K$ are used. The perturbative $T_K$ is given by $0.4107 T_K^{(0)}$, the half width half maximum of the spectral function at $T = 0$ is $\approx 2.05 T_K^{(0)}$. At $T \approx 0.94 T_K^{(0)}$ the resistivity of diluted Kondo impurities in a dirty (clean) metal and the conductance through a quantum dot have half of their maximal value.
[26] correcting a factor 2 in [8].