Iron impurities in gold and silver (II): Comparison of transport measurements to numerical renormalization group calculations exploiting non-Abelian symmetries

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We consider iron impurities in the noble metals gold and silver and compare experimental data for the resistivity and decoherence rate to numerical renormalization group results. By exploiting non-Abelian symmetries we show improved numerical data for both quantities as compared to previous calculations [Costi et al., Phys. Rev. Lett. 102, 056802 (2009)]. In addition we also carry out finite-temperature calculations for the magnetoresistivity of fully screened Kondo models with \( S = \frac{1}{2}, 1 \) and \( \frac{3}{2} \), and compare the results with available measurements for iron in silver, finding excellent agreement between theory and experiment for the spin-\( \frac{3}{2} \) three-channel Kondo model. This lends additional support to the conclusion of Costi et al. that the latter model provides a good effective description of the Kondo physics of iron impurities in gold and silver.

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The magnetic alloys for which the Kondo effect was first observed, in the 1930s, were iron impurities in gold and silver\(^1,2\). They showed an anomalous rise in the resistivity with decreasing temperature, which Kondo explained in 1964 as being due to an antiferromagnetic exchange coupling between the localized magnetic impurity spins and the spins of the delocalized conduction electrons\(^3\). For his work, Kondo used a spin-\( \frac{1}{2} \), one-band model, which undoubtedly captures the essential physics correctly in a qualitative way.

However, detailed comparisons between theory and experiment have since shown that this model does not yield a quantitatively correct description of the Kondo physics of dilute Fe impurities in Au or Ag. Such a description must meet the challenge of quantitatively reproducing, using the Kondo temperature \( T_K \) as only fitting parameter, several independent sets of experimental measurements: the contributions by magnetic impurities (indicated by a subscript \( m \)) to the temperature- and field-dependence of the resistivity, \( \rho_m(T, B) \), and to the temperature-dependence of the decoherence rate, \( \gamma_m(T) \), extracted from weak (anti)localization measurements. The spin-\( \frac{1}{2} \), 1-band Kondo model does not meet this challenge: when comparing its predictions, obtained by the numerical renormalization group (NRG)\(^4,5\) to transport measurements on dilute Fe impurities in Ag wires, different Kondo scales were required for fitting the resistivity and decoherence rates\(^7,8\). In a recent publication (Ref. 9, involving most of the present authors, henceforth referred to as paper I), it was argued that the proper effective low-energy Kondo model for Fe in Au or Ag is, in fact, a fully screened, spin-\( \frac{3}{2} \) three-channel Kondo model. Paper I arrived at this conclusion by the following chain of arguments. Previous transport experiments\(^7,8\) had indicated that these systems are described by a fully screened Kondo model, i.e. a Kondo model in which the local spin, \( s \), is related to the number of conduction bands, \( n \), by \( s = n/2 \). As mentioned above, the choice \( n = 1 \) had already been ruled out in earlier work\(^7,8\). Based on density-functional theory calculations for Fe in Au and Ag, paper I suggested that the fully-screened Kondo models with \( n = 2 \) and \( n = 3 \) are the most likely candidates. \( \rho_{m}(T, 0) \) and \( \gamma_{m}(T) \) were then calculated using NRG, for \( n = 1, 2 \) and 3. Next, for both material systems (Fe in Au and Ag), the \( \rho_{m}(T, 0) \) curves were fitted to experimental data to obtain a Kondo temperature, \( T_{K}^{(n)} \), for each of the three models. Finally, using these \( T_{K}^{(n)} \)-values, the \( \gamma_{m}(T) \) curves, which constituted parameter-free predictions of the decoherence rate, were compared to corresponding measurements, with the conclusion that the choice \( n = 3 \) worked distinctly better than \( n = 2 \).

The goal of the present paper is to extend the analysis of paper I to the case of finite magnetic fields. Indeed, though experimental data for \( \rho_{m}(T, B \neq 0) \) had been available for Fe in Ag even at the time of writing of paper I, it had not been possible then to compare them to theoretical predictions for \( n = 3 \). The reason is that multichannel calculations present an enormous challenge for the NRG, as the numerical complexity grows exponentially with the number of channels. In paper I only abelian symmetries (charge conservation in each channel and total spin \( S_z \)) were exploited. For the purposes of paper I, this turned out to be sufficient, but for the abovementioned three-channel Kondo model the calculations were numerically extremely costly, and even at \( B = 0 \) just barely within the limits of feasibility. When the present authors attempted, in subsequent work (unpublished), to treat the more general case of a finite magnetic field using the same approach, the latter turned out to be inadequate, plagued by numerical convergence
issues. Therefore, further progress required enhancing the numerical efficiency by exploiting non-abelian symmetries.

Now, the effective fully screened symmetric three-channel Kondo model mentioned above has several non-abelian symmetries, including, in particular, an SU(3) channel symmetry. We took this observation as incentive to implement non-abelian symmetries in our code on a completely generic footing for tensor networks such as the NRG. Although the application of symmetries, abelian as well as non-abelian, together with their respective strong gain in numerical efficiency is well known in the literature, the treatment of non-abelian symmetries in NRG has been largely restricted to the symmetry of SU(2). The non-abelian symmetry SU(2), however, is simpler than the general case, since for \( n \geq 3 \) the SU(\( n \)) representation theory involves complications due to the presence of inner and outer multiplicities. A generic numerical framework for treating arbitrary non-abelian symmetries thus had been missing, and became available only very recently. More specifically, the model Hamiltonians studied here possess SU(2) particle-hole symmetry, SU(\( n \)) channel symmetry, and SU(2) spin symmetry for \( B = 0 \) or abelian \( S_2 \)-symmetry for \( B \neq 0 \). By exploiting these symmetries, we were able to drastically reduce the computational effort and generate fully converged numerical data, even for the highly challenging case of three channels. With a significantly more powerful NRG at our hands then, the following analysis serves two purposes. First, we present a thorough reanalysis of paper I with improved NRG data; the new numerical results do show discernible quantitative differences w. r. t. paper I, but these turn out to be minor. Second, we present a detailed analysis of the new numerical magnetoresistivity data and compare these to experimental results for Fe in Ag. The results of both analyses fully confirm the main conclusion of paper I: the effective microscopic model for dilute iron impurities in the noble metals gold and silver is given by a fully screened three-channel Kondo model.

The remainder of this paper is organized as follows: Sec. I describes the model, Sec. II describes NRG-related details. Sec. III provides a comparison of experimental and numerical magnetoresistance data, followed by a summary in Sec. IV.

I. MODEL

In order to calculate the magnetic-impurity-induced contributions to the resistivity \( \rho_m(T, B) \) and the decoherence rate \( \gamma_m(T) \) using NRG, we found it numerically convenient to start not from a pure Kondo model but from the following effective Anderson-type model:

\[
\hat{H} = \hat{H}_J + \sum_{\alpha=1}^{n} \sum_{k\sigma} \left( t(d^\dagger_{\alpha\sigma}c_{k\sigma} + \text{H.c.}) + \varepsilon_k c^\dagger_{k\sigma\alpha} c_{k\sigma\alpha} \right),
\]

(1)

which reduces to a Kondo-type model at low energies.

The index \( \alpha \) labels \( n \) degenerate local levels as well as \( n \) independent channels of conduction electrons, each forming a flat band of half-bandwidth \( D = 1 \) with constant density of states \( \nu \) per spin and channel. \( d^\dagger_{\alpha\sigma} \) is the annihilation operator of an impurity electron with spin \( \sigma \) in level \( \alpha \), whereas \( c_{k\sigma\alpha} \) annihilates a reservoir-electron in channel \( \alpha \) with wave number \( k \) and energy \( \varepsilon_k \). Levels and channels are tunnel-coupled diagonally, resulting in a width \( \Gamma = \pi \nu \hbar^2 \) for each level, with \( t \) being the hopping matrix element between impurity and reservoir. To favor a local spin of \( S = n/2 \), we add a Hund-type exchange term \( \hat{H}_J = -J^{(n)}_H \mathbf{S}^2_{\text{imp}} \) with \( J^{(n)}_H > 0 \), where \( \mathbf{S}^2_{\text{imp}} = \sum_{\alpha=1}^{n} \mathbf{S}_\alpha \) is the total impurity spin, \( \mathbf{S}_\alpha = \frac{1}{2} \sum_{\sigma\sigma'} d^\dagger_{\alpha\sigma} \tau_{\sigma\sigma'} d_{\alpha\sigma} \) is the spin of the electrons in level \( \alpha \) and \( \tau = (\tau_x, \tau_y, \tau_z) \) are Pauli spin matrices. To ensure particle-hole symmetry (which renders the numerics more efficient) we take \( \varepsilon_{\alpha\sigma} = 0 \) for the local level positions and do not include any further charging energy.

Using the Anderson model instead of the Kondo model for the numerical calculations has the advantage that an improved spectral function can be calculated using the self-energy. We then focus on an effective Kondo model by choosing the parameters such that the energies of the free orbital (FO) regime lie well above the bandwidth and the Kondo temperature well below the bandwidth. This shifts the numerically most expensive, yet irrelevant, FO-regime to an energy range which lies outside the range whose energies are finely resolved during the NRG-diagonalization. To be more precise, the energies of the FO states are split by roughly \( J^{(n)}_H S(S+1) \) and the energy difference between two FO-states that differ by spin \( \frac{1}{2} \) is therefore given by \( \Delta E = J^{(n)}_H [(S(S+1)-(S-\frac{1}{2})(S+\frac{1}{2})] = J^{(n)}_H (S+\frac{1}{2}) \). To separate the lowest FO-state from the others, we choose \( J^{(3)}_H = 57.14 \), so that \( \Delta E = 100 \) (all energies in units of half bandwidth). We set the level width to \( \Gamma = 25 \), and choose the Hund couplings as \( J^{(2)}_H = 112.8, J^{(1)}_H = 358.9 \) so that the Kondo temperatures, which are determined as HWHM of the spectral function, are equal with respect to bandwidth for all three cases, \( n \in \{1, 2, 3\} \), namely \( 10^{-3} D \). This choice of parameters allows the advantages of both the Kondo and the Anderson model to be exploited: on the one hand, pushing the FO regime to lie outside of the bandwidth, which is the numerical counterpart to a Schrieffer-Wolff transformation, reduces the numerical costs needed for treating the Anderson model to a level comparable to that of the Kondo model; on the other hand, the calculation of the spectral function using the improved self-energy can proceed as usual.

For the model in Eq. (1), the resistivity and decoherence rate due to magnetic impurities (relevant for weak
localization) can be calculated as follows:\textsuperscript{15,16},

\[
\rho_{m}^{\text{NRG}}(T, B) = \frac{\rho_{m}^{0}}{2\pi} \int d\omega f'(\omega) \sum_{\alpha\sigma} \text{Im}(G_{\alpha\sigma}^{R}(\omega)),
\]

(2)

\[
\gamma_{m}^{\text{NRG}}(T) = \left[ \int d\omega [-f'(\omega)] \sqrt{\gamma_{m}(\omega, T)} \right]^{2},
\]

(3)

\[
\gamma_{m}(\omega, T) = -\frac{\gamma_{m}^{0}}{2\pi} \sum_{\alpha\sigma} \text{Im}(G_{\alpha\sigma}^{R}(\omega)) + |G_{\alpha\sigma}(\omega)|^{2}.
\]

(4)

Here \(G_{\alpha\sigma}^{R}(\omega)\) is the fully-interacting retarded impurity Green’s function, \(f'(\omega)\) is the derivative of the Fermi function, \(\rho_{m}(0) = \rho_{m}^{0} = 2\tau\rho/\pi\hbar v_{0}\) and \(\gamma_{m}^{0} = 2/\pi\hbar v_{0}\), where \(\rho\) is the resistivity due to static disorder and \(\tau\) the corresponding elastic scattering time. For real materials with complex Fermi surfaces, both prefactors \(\rho_{m}^{0}\) and \(\gamma_{m}^{0}\) contain material-dependent (hence unknown) factors arising from integrals involving the true band structure of the conduction electrons.

II. NRG DETAILS

Within the NRG, the non-interacting bath in Eq. (1) is coarse grained using the dimensionless discretization parameter \(\Lambda > 1\), followed by the mapping onto the so-called Wilson chain in terms of the fermionic Wilson sites\textsuperscript{4–6} \(\hat{f}_{i'\alpha\sigma}\) with \(i' \in \{0, 1, \ldots\}\). Therefore, \(\hat{H} \cong \lim_{N \to \infty} \hat{H}_{N}\), where

\[
\hat{H}_{N} \cong \hat{H}_{\text{loc}} + \sum_{i' = 0}^{N-1} t_{i'} \sum_{\alpha = 1}^{n} \sum_{\sigma} \left( \hat{f}_{i'\alpha\sigma}^{\dagger} \hat{f}_{i'1,\alpha\sigma} + \text{H.c.} \right) \tag{5a}
\]

with

\[
\hat{H}_{\text{loc}} = \hat{H}_{J} + \sum_{\alpha = 1}^{n} \sum_{\sigma} \sqrt{4\pi} (d_{\alpha\sigma}^{b} \hat{f}_{0\alpha\sigma} + \text{H.c.}). \tag{5b}
\]

The impurity spin is coupled to a semi-infinite tight-binding chain with the exponentially decaying couplings \(t_{i'} \propto \Lambda^{-i'/2}\). For large enough \(\Lambda \gtrsim 2\), this ensures energy scale separation, and thus justifies the iterative diagonalization of the Hamiltonian in the representation of the Wilson chain.\textsuperscript{4–6} In particular, the energies of the Hamiltonian \(\hat{H}_{i}\) at intermediate iterations which include all terms \(i' < i\), are rescaled in units of \(\omega_{i}\), where

\[
\omega_{i} \equiv a\Lambda^{-i/2}.
\]

(6)

Here the constant \(a\) is chosen such that \(\lim_{i \to \infty} t_{i}/\omega_{i} = 1\).

An analytic expression for \(a\) in the presence of \(\gamma\)-shifts is given in Ref. 17.

To obtain the Green’s function \(G_{\alpha\sigma}^{R}(\omega)\), which determines \(\rho_{m}^{\text{NRG}}(T, B)\) and \(\gamma_{m}^{\text{NRG}}(T)\), we calculate the spectral function \(A_{\sigma}(\omega) = -\frac{\pi}{\nu} \text{Im}(G_{\alpha\sigma}(\omega))\) using its Lehmann representation:

\[
A_{\sigma}(\omega) = \sum_{a, b} e^{-\beta E_{ba}} + e^{-\beta E_{ba}} |\langle a|d_{\sigma}|b \rangle|^{2} \delta(\omega - E_{ba}), \tag{7}
\]

where \(E_{ba} = E_{b} - E_{a}\), with \(E_{a}\), \(E_{b}\) and \(|a\), \(|b\) being the eigenenergies and many-body eigenstates obtained by NRG in the full density matrix (FDM)-approach.\textsuperscript{18–21} Note that \(A_{\sigma}(\omega)\) and \(d_{\sigma}\) do not need to carry the index \(\alpha\), due to SU(\(n\)) channel symmetry.

For the calculation of \(\gamma_{m}(T)\) the knowledge of both the real and the imaginary part of \(G_{\alpha\sigma}(\omega)\) is necessary. The real part can be determined via the Kramers-Kronig relations from \(A_{\sigma}(\omega)\) after smoothing the discrete data. \(\rho_{m}^{\text{NRG}}(T, B)\), on the other hand, requires only the imaginary part of the Green’s function. This makes the application of the Kramers-Kronig relations and with it the broadening of the discrete data unnecessary and \(\rho_{m}^{\text{NRG}}(T, B)\) can therefore be directly calculated from the discrete data\textsuperscript{18}, thus avoiding possible broadening errors. Furthermore, due to particle-hole symmetry, it is sufficient to calculate \(A_{\sigma}(\omega)\) only for one spin \(\sigma\), since the spectral functions for opposite spins \(\sigma\) and \(\bar{\sigma}\) are symmetric with respect to each other: \(A_{\sigma}(\omega) = A_{\bar{\sigma}}(-\omega)\).

As mentioned in the introduction, when using Abelian symmetries the calculations described above are sufficient for \(n = 1\) and \(n = 2\), but a real challenge for \(n = 3\). In paper I this challenge was confronted by using a very particular truncation strategy, designed to reduce numerical costs: at early iterations, where the effects of truncation errors are largest, the truncation energy was chosen to lie between two well-separated energy multiplets, thus reducing the influence of the discarded states and drastically reducing the size of the matrix which has to be diagonalized at an NRG-iteration, with corresponding reductions in calculation times and memory requirements.

For the calculations presented here, we therefore use an improved code, which also exploits non-abelian symmetries.\textsuperscript{18} Here, the idea is to make use of the fact that degenerate states can be gathered into symmetry multiplets. By the Wigner-Eckart theorem, matrix elements including states from the same multiplet are then related via Clebsch Gordan coefficients. Thus, it is sufficient to keep track not of all individual states inside each multiplet, but only of entire multiplets, and to store only one reduced matrix element for each multiplet. This drastically reduces the size of the matrix which has to be diagonalized at an NRG-iteration, with corresponding reductions in calculation times and memory requirements.

Our model possesses the following non-abelian symmetries: SU(2) particle-hole symmetry, SU(2) spin symmetry (in the absence of magnetic field) and SU(\(n\)) channel symmetry. For many of our calculations, we need \(B \neq 0\),
FIG. 1: Eigenenergies of the \( n = 3 \) calculations from (a) paper I and (b) this work, for the lowest eigenstates (blue circles) and truncation energy (dashed red line) of NRG-iteration \( i = 1 \). This iteration includes the impurity and the first two Wilson sites \( f_0 \) and \( f_1 \), which by Eq. (5b) corresponds to \( H_1 \); it is the first iteration where truncation occurred. All energies \( E_s \) are given in units of \( \omega_1 \) [c.f. Eq. (6)]. In (a), each dark blue dot marks an eigenstate; in panel (b) each dark blue dot marks a multiplet, whose degeneracy is indicated by the length of the adjacent light blue lines. Dashed red lines indicate the truncation energy \( E_{\text{trunc}} \). The number of kept states at iteration \( i = 1 \) was 4840 in paper I [all shown in (a)] and 16384 in this work; this large number was achievable by grouping the states into 2688 degenerate symmetry multiplets ([b] shows only a small subset of these). The insets of (a) and (b) show, respectively, the full spectrum of states or multiplets at iteration \( i = 1 \). (The fine structure seen in the main panel in (b) is not resolved in the inset, since the latter uses a much coarser energy resolution on the vertical axis.) The spectra in (a) and (b) have different fine structure, because the model parameters were chosen differently in paper I and the present work, respectively: the former used \( J_{h}^{(3)} = 0.0229 \), \( \Gamma = 0.01 \), the latter \( J_{h}^{(3)} = 57.14 \), \( \Gamma = 25 \). As a result, the energy separation between degenerate multiplets at the truncation energy is different, namely \( O(t_1/\omega_1) \) in (a) versus \( O(J_{h}^{(3)}/\omega_1) \) in (b), where \( t_1 \) is the hopping matrix element between the first two sites of the Wilson chain [c.f. Eq. (5b)]. The different values of \( J_{h}^{(3)} \) and \( t_1 \) used in (a) and (b) are indicated by black lines in the plots.

in which case the SU(2) spin symmetry is reduced to an abelian symmetry using \( S_z \). Moreover, particle-hole symmetry and channel symmetry do not commute in general, yet their combination generates the larger symplectic symmetry \( \text{Sp}(2n) \) (Ref. 10). This symmetry, which encompasses both particle-hole and channel symmetry, fully exhausts the model’s symmetry; consequently no degeneracies remain between different \( \text{Sp}(2n) \) multiplets (a typical multiplet contains several hundreds up to several thousands of states). For the calculations presented in this work, using \( \text{SU}(n) \) (rather than \( \text{Sp}(2n) \)) turned out to be sufficient. Here we use \( \text{SU}(n) \) channel symmetry together with total charge for \( n \in \{2, 3\} \) and particle-hole symmetry for \( n = 1 \). The gain in numerical efficiency due to these symmetries is huge. For example, for \( n = 3 \), the largest \( \text{SU}(n) \) multiplets kept in our NRG calculations already reach dimensions of above 100. By exploiting these symmetries, calculation times as well as memory requirements are reduced by more than two orders of magnitude compared to those of paper I. As a consequence, the calculations presented here can be simply performed within a few hours on standard workstations.

We used an NRG-discretization parameter of \( \Lambda = 4 \). For \( n = 3 \), the computationally most challenging case, we used the following truncation scheme. For the diagonalization of \( H_0 \equiv H_{\text{loc}} \), all states were kept. For iteration \( i = 1 \), we used a truncation energy [given in rescaled units of \( \omega_{i=1} \), c.f. Eq. (6)] of \( E_{\text{trunc}} = 2J_1/D > 7 \). Fig. 1(b) shows a subset of the corresponding kept eigenenergies and multiplet degeneracies, while Fig. 1(a) shows corresponding information for the calculations from paper I. The inset of Fig. 1(b) shows that all Kondo-like states of the Anderson model have been retained. At iteration \( i = 2 \) we used \( E_{\text{trunc}} = 6 \) to reduce computational costs due to the extraordinary large density of states at that iteration; this choice of parameters corresponds to keeping \( \lesssim 10,000 \) multiplets (\( \lesssim 77,000 \) states). Finally, for iterations \( i \geq 3 \), we used \( E_{\text{trunc}} = 7 \). Using this scheme, a single NRG run for \( n = 3 \) required about 40 GB of RAM and took on the order of 10 hours of calculation time on an 8-core processor. The subsequent calculation of the spectral function required a similar amount of time and 55 GB memory. To minimize discretization artifacts, we use \( z \)-averaging with \( N_z = 2 \), thus \( z \in \{0,0.5\} \). The large number of kept multiplets then resulted in high numerical accuracy. In particular, the spectral functions calculated with and without using the improved self-energy, already agreed very well with each other, which clearly demonstrates fully converged numerical data. Having established this for a few representative cases, we proceeded to calculate the data presented below without using the improved self-energy.

III. COMPARISON WITH EXPERIMENT

To identify the microscopic model which describes the system of iron impurities in gold and silver correctly, we compare NRG-calculations for the resistivity \( \rho_{\text{NRG}}(T,B) \) and the decoherence rate \( \gamma_{\text{NRG}}(T) \) to experimental data, \( \rho_{\text{exp}}(T,B) \) and \( \gamma_{\text{exp}} \). In the following when referring to
both NRG and experiment, we omit the upper index and write $\rho_m(T, B)$ and $\gamma_m(T)$.] The data to be analysed stems from a detailed experimental study\cite{migration} performed in 2006 on quasi-one-dimensional wires. One AuFe-sample and two AgFe-samples were studied, to be denoted by AuFe3, AgFe2 and AgFe3, with impurity concentrations of 7 ± 0.7, 27 ± 3 and 67.5 ± 7 ppm, respectively. Low-field measurements of the temperature-dependence of the resistivity, performed at $B = 0.1$ T to suppress weak localization, are available for all three samples. We will denote this data by $\rho^\text{exp}_m(T, 0)$ [rather than $\rho^\text{exp}_m(T, 0.1T)$], and compare it to numerical results for $\rho^\text{NRG}_m(T, 0)$ computed at $B = 0$, since for the Kondo impurities considered here a field of 0.1T is very small on the scale set by the Kondo temperature. (To be precise, at $B = 0.1$ T we find $g\mu_B/k_B T_K \approx 0.08$ and 0.02 for AuFe and AgFe, respectively, using the $T_K$-values determined below.)

Moreover, experimental data is available for $\gamma^\text{exp}_m(T)$ from AgFe2 and AuFe3, and for $\rho^\text{exp}_m(T, B)$ from AgFe2.

The comparison between experiment and theory proceeds in three steps: (i) First, we compare measured data and NRG predictions for the resistivity at zero magnetic field $\rho_m(T, B = 0)$ to determine two fit parameters, $T_K^n$ and $\delta^n$, for each of the samples and each of the three models $n \in \{1, 2, 3\}$. After the fit parameters have been determined, we use $T_K^n$ and $\delta^n$ to make parameter-free predictions for (ii) the decoherence rate $\gamma_m(T)$ and (iii) the temperature-dependent magnetoresistivity $\rho_m(T, B)$, and compare these to experiment for those samples for which corresponding data is available. Here (i) and (ii) represent a thorough reanalysis of the experimental data of paper I using our new, improved numerical data, while (iii) involves experimental data not published previously, and new numerical data.

**Determination of fit parameters.** The experimental resistivity data to be discussed below (shown in Fig. 2) has several contributions of different physical origin:

$$\Delta \rho^\text{exp}(T, B) = \rho^\text{exp}_m(T, B) + \rho_\text{ph}(T) + \delta.$$  \hspace{1cm} (8)

Here $\rho^\text{exp}_m(T, B)$ is the resistivity due to magnetic impurities, $\rho_\text{ph}(T)$ is the resistivity due to phonon scattering, and $\delta$ is an unknown offset which does not depend on temperature or magnetic field. There are two further contributions to the resistivity: a classical contribution,\cite{migration} which scales as $B^2$, and a contribution due to electron-electron interactions,\cite{migration} which scales as $1/\sqrt{T}$. These have already been subtracted from the measured resistivity data shown in Figs. 2 and 4 using procedures described in Refs. 25,26, and hence are not displayed in Eq. (8).

To begin, we define the Kondo temperature $T_K^n$ associated with a given numerical resistivity curve $\rho^\text{NRG}_m(T, 0)$ by the condition

$$\rho^\text{NRG}_m(T_K^n, 0) = \frac{1}{2} \rho^\text{NRG}_m(0, 0).$$  \hspace{1cm} (9)

For the fitting process at $B = 0$, the normalized NRG-data $\rho^\text{NRG}_m(T, 0)/\rho^\text{NRG}_m(0, 0)$ are approximated by a fitting function $g_\mu(T/T_K^n)$ constructed from higher-order

| $n$ | AuFe3 $\pm$ | AgFe2 $\pm$ | AgFe3 $\pm$ |
|-----|-------------|-------------|-------------|
| 1   | 0.6 ± 0.1   | 2.5 ± 0.2   | 2.8 ± 0.2   |
| 2   | 1.0 ± 0.1   | 4.3 ± 0.3   | 4.7 ± 0.3   |
| 3   | 1.7 ± 0.1   | 7.4 ± 0.5   | 8.2 ± 0.5   |

**FIG. 2:** Similar figure as Fig. 3 of paper I, but using substantially improved numerical data. The figure shows low-field experimental data for the temperature-dependence of the resistivity, denoted by $\Delta \rho^\text{exp}(T, 0)$ but taken in a small field of 0.1 T to suppress weak localization (see text), and NRG-calculations for $n \in \{1, 2, 3\}$, performed at $B = 0$. The NRG-curves were fitted to the experimental data, using $T_K^n$ and $\delta^n$ as fitting parameters [see Eq. (10)] with the fitting range being indicated by arrows. For temperatures below the fitting range, the data are less reliable due to a long equilibration time, whereas for temperatures above the fitting range the phonon-contribution to $\Delta \rho^\text{exp}(T, B = 0)$ becomes relevant. For clarity, the curves for AgFe2 and AuFe3 have been shifted vertically by 0.25 and 0.75, respectively.

**TABLE I:** Values of parameters determined from fitting the experimental measurement. The values for $T_K^n$ and $\delta^n$ are extracted using the fitting procedure whose results are shown in Fig. 2. $\Delta \rho^\text{exp}(0, 0)$ is the measured value for the resistivity at zero magnetic field and the lowest temperature available. For the sake of completeness, we also show $\rho^\text{uni}(n, 0) = \Delta \rho^\text{exp}(0, 0) - \delta^n$, which, according to Eq. (10), corresponds to the unitary Kondo resistivity.
polynomials, where \( g_n(0) = 1 \) and \( T_K^{(n)} \) is fixed by scaling the temperature axis such that \( g_n(1) = \frac{1}{2} \). We then fit the experimental data to the form

\[
\Delta \rho_{\text{exp}}(T, 0) \approx \delta^{(n)} + |\Delta \rho_{\text{exp}}(0, 0) - \delta^{(n)}| g_n(T/T_K^{(n)}),
\]

using a \( \chi^2 \)-minimization with \( T_K^{(n)} \) and \( \delta^{(n)} \) as fit parameters. While a similar analysis was performed in paper I, the numerical data in the present paper are of improved quality, in that we can report fully converged data also for the numerically extremely challenging case of \( n = 3 \). The newly extracted values of \( T_K^{(n)} \) for the three samples are given in Table. I. For \( n \in \{1, 2\} \) they are slightly different from the ones of Ref. (9), yet within the given error bars (14 % and 0 % for AuFe3, 9 % and 5 % for AgFe, respectively) due to the fact that we used different fitting ranges to minimize the error arising from the phonon-contribution for larger \( T \) and because we use higher-order polynomials to approximate the NRG-data, which may be considered more accurate than the analytical expression used in Ref. (9). The difference in \( T_K \) is more substantial for \( n = 3 \) (31 % for AuFe3 and 51 % for AgFe) reflecting larger differences between the previous and our new, improved NRG results for \( n = 3 \). Experimental and fitted NRG-data are shown in Fig. 2.

Comparison of the decoherence rate \( \gamma_m(T) \). Using \( T_K^{(n)} \) for AgFe2 and AuFe3 as determined above, this allows us to make a parameter-free theoretical prediction of the decoherence rate. As shown in Fig. 3 for AgFe2 and AuFe3, the agreement is clearly best for \( n = 3 \) and becomes worse with decreasing \( n \), both for low and high temperatures. A quantitative measure for the agreement is given by the \( \chi^2 \)-values for \( n \in \{1, 2, 3\} \), which are displayed in each of the panels in Fig. 3. This conclusion is in accordance with Ref. (9), where the \( n = 3 \) case also agreed best with the experimental data, although \( T_K \) and \( \gamma_m(T) \) for \( n = 3 \) were significantly less accurate then.

Comparison of the resistivity \( \rho_m(T, B) \). Due to the above-mentioned implementation of non-Abelian symmetries in our NRG-code\(^{10}\), which drastically reduces computation time and memory requirements, it is possible to extend the analysis of \( \rho_m(T) \) of paper I to the whole two-dimensional parameter space of \( T \) and \( B \). Since the fitting procedure of \( \rho_m(T, B = 0) \) described above leaves no further free parameters, this comparison is an additional strong check of the validity of the \( n = 3 \) model. The experimental data of \( \rho_m(T, B) \) for the sample AgFe2 are shown together with the numerical data for \( n \in \{1, 2, 3\} \) in Fig. 4. [The values of \( \rho_m(T, B = 0) \) differ for \( n \in \{1, 2, 3\} \), due to the different \( \delta^{(n)} \)-values determined from Eq. (10)]. Again, the three-channel model reproduces the measured results best. Even though there are still slight deviations between theory and experiment at high magnetic field for the \( n = 3 \) curves at 0.1 K and 0.85 K, which might originate from very small temperature drifts, the overall agreement, combined with that for \( \gamma_m(T) \) (Fig. 3) and \( \rho_m(T, 0) \) (Fig. 2), is rather impressive. Thus, we conclude that the \( n = 3 \) model consistently re-

![FIG. 3: Similar figure as Fig. 4 of paper I, but using clearly improved numerical data. Panels (a), (b) and (c) show the normalized decoherence rate \( \gamma_m(T)/\gamma_m^{\text{max}} \) vs. \( T/T_K^{(n)} \) for \( n \in \{1, 2, 3\} \), respectively. The Kondo temperatures are determined from the fits of \( \rho_K^{\text{NRG}}(T, B = 0) \) to the experimental data according to Eq. (10). The \( \chi^2 \)-values indicated in the legends were obtained as the sum of the least squares between the experimental data and the linearly interpolated NRG-curves.](image)

produces all the transport data discussed above.

### IV. CONCLUSION

We have considered iron impurities in gold and silver and compared experimental data for the resistivity and decoherence rate to NRG results for a fully screened \( n \)-channel, spin-\( \frac{1}{2} \) Kondo model. Compared to previous work on this subject\(^5\), we showed improved numerical
FIG. 4: Experimental and theoretical results for $\rho_m(T,B)$, shown using solid or dashed curves, respectively. Left column: panels (a), (b) and (c) compare the experimental data for AgFe2 to NRG-calculations for $n \in \{1, 2, 3\}$, respectively. Right column: panels (d), (e) and (f) show the same data as in the left column, except that for clarity the curves for successive temperatures are shifted vertically by 0.15 to avoid them from overlapping, thus enabling a better comparison between experiment and theory for each temperature. $T_K^{(n)}$ and $\delta^{(n)}$ are already determined by the fitting procedure of Eq. (10), which allows a parameter-free theoretical prediction for $\rho_m(T,B)$. The $\chi^2$-values indicated in panels (d-f) were calculated using a set of 1000 uniformly-spaced field values in the range $B \in [0.07349, 3.05000]$T. The experimental data clearly show best agreement with theory for $n = 3$, which supports the conclusion from the examination of $\gamma_m$. For $T = 0.030$ K and $T = 0.10$ K, the signal to noise ratio is much lower than for the other curves since the measurement current had to be reduced to stay in thermal equilibrium; therefore, in the left panel the experimental data for these two temperatures have been smoothed for better visibility. For the largest temperature, $T = 10$ K, the phonon contribution has been subtracted from the experimental data for comparison to theory. For the purpose of this subtraction, the phonon-contribution was assumed to be $B$-independent and taken to correspond to the difference of $\Delta \rho(T = 10K, B = 0)/\Delta \rho(0,0)$ between experiment and theory (see Fig. 2).
data for both quantities at finite temperature, and extended our analysis to the resistivity at finite magnetic field by comparing the numerical calculations with as yet unpublished experimental data. In contrast to previous attempts to explain the experimental results with models with less channels which were inconsistent or yielded several different values for the Kondo temperature, depending on which set of measurements was used to extract $T_K$. We showed that all examined quantities can be described consistently with a single value of $T_K$. The excellent agreement between experiment and theory for $n = 3$ shows that both systems are well described by a spin-3/2 three-channel Kondo model.

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