Electron spin resonance in Kondo systems

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We calculate the dynamical spin response of Kondo impurity and Kondo lattice systems within a semiphenomenological Fermi liquid description, at low temperatures $T < T_K$, the Kondo temperature, and low magnetic fields $B \ll k_B T_K/g\mu_B$. Fermi liquid parameters are determined by comparison (i) with microscopic theory (numerical renormalization group) for the impurity model and (ii) with experiment for the lattice model. We find in the impurity case that the true impurity spin resonance has a width of the order of $T_K$ and disappears altogether if the $g$-factors of impurity spin and conduction electron spin are equal. However, there is an impurity-induced resonance contribution at the conduction electron resonance. The latter is broadened by spin lattice relaxation and is usually unobservable. In contrast, for the Anderson lattice in the Kondo regime we find a sharp ESR resonance line only slightly shifted from the local resonance and broadened by spin lattice relaxation, the latter significantly reduced by both the effects of heavy fermion physics and ferromagnetic fluctuations. We conjecture that our findings explain the sharp ESR-lines recently observed in several heavy fermion compounds.

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I. INTRODUCTION

The Kondo effect is arguably the best-studied many-body effect in condensed matter physics\textsuperscript{1}. In its initial form\textsuperscript{2}, it involves a local “impurity” spin in a $d$- or $f$-orbital, antiferromagnetically coupled to the spins of a conduction band in a dilute magnetic alloy. At temperatures $T$ below the dynamically generated energy scale $T_K$, the Kondo temperature, this interaction causes a local spin $1/2$ to be fully screened. This behavior should be noticeable in the $T$-dependence of the spin dynamics of the system, as probed by electron spin resonance (ESR). In fact, the local spin resonance in dilute Kondo compounds at $T \gg T_K$ had been observed even before the Kondo effect was understood. Afterward there were a number of systematic experimental investigations and perturbative calculations for the ESR at $T \gg T_K$ in dilute Kondo systems\textsuperscript{3}.

At low temperatures $T \ll T_K$, on the other hand, neutron scattering studies revealed the existence of a broad spin excitation peak of width $T_K$, interpreted as the Kondo bound state\textsuperscript{4}. Within the isotropic $s$-$d$ exchange (Kondo) model the total spin is conserved. Therefore, in the limit of equal $g$-factors of local moments and conduction electron spins one expects a single spin resonance line at all temperatures, only broadened by spin lattice relaxation. As we shall show below, in this limit the weight of the broad local spin resonance tends to zero.

In several recent experiments\textsuperscript{5-8}, low-temperature ESR has been observed in some heavy-fermion metals, in particular YRh$_2$Si$_2$ (YRS)\textsuperscript{8}. The phase diagram of YRS has a magnetic-field induced quantum critical point and is a model system for the study of quantum criticality in the Kondo lattice. Consequently, the observation of a narrow ESR resonance in this compound aroused great interest, especially since it was commonly believed that heavy-fermion ESR would be unobservable due to an enormous intrinsic linewidth $\Delta B$ of order $k_B T_K/g\mu_B$. Here $T_K$ is the lattice coherence (“Kondo”) temperature for the onset of heavy-fermion behavior and $g\mu_B$ is the gyromagnetic ratio for the resonance. These were the first observations of ESR in Kondo lattice systems at $T < T_K$.

In YRS, the observed narrow dysonian ESR line shape was originally interpreted\textsuperscript{9} as indicating that the resonance was due to local spins at the Yb sites. Therefore, initially the authors speculated that the appearance of a narrow ESR line might indicate the suppression of the Kondo effect near the quantum critical point, since, as explained above, carrying over Kondo impurity physics to the Kondo lattice one might expect the local spins to be screened by the Kondo effect, giving rise only to a broad spin excitation peak, too wide to be observed in ESR experiments. However, a closer look\textsuperscript{8} revealed that itinerant (heavy) electron ESR could give rise to a similar line shape since the carrier diffusion in YRS is quite slow. Thus, whether the resonance was that of localized or itinerant spins remains an open question.

Now, a common feature of the compounds in which ESR has been observed appears to be the existence of ferromagnetic fluctuations\textsuperscript{10}. These findings challenge our understanding of heavy fermion compounds: How does a sharp electron spin resonance emerge despite Kondo screening and spin lattice relaxation, and why is this process influenced by ferromagnetic fluctuations? We shall address these questions in the framework of Fermi liquid theory, taking the relevant parameters from numerical studies and experiment.
II. ANDERSON IMPURITY MODEL IN THE KONDO SCREENED REGIME

In the Kondo regime an impurity spin is screened by the conduction electron spins at (or near) the impurity. The dynamics of the impurity spin is governed by the energy scale of the corresponding many-body resonance, the Kondo temperature $T_K$. Nonetheless the conduction electrons in the vicinity of the impurity show the influence of the Kondo screened state in their dynamical behavior. In the Anderson model, the local spin is that of a localized $f$ electron. We assume that the Zeeman splittings $\omega_f$ and $\omega_c$ induced by a magnetic field acting on the local and conduction electron spins are small compared to the Kondo temperature $T_K$. Then the Kondo screened state is only weakly perturbed by the magnetic field. At temperatures $T \ll T_K$, the spin resonance behavior of the impurity may then be described by Fermi liquid theory.\footnote{11} We start from the bare Anderson model Hamiltonian

$$
H = H_c + \sum_{k, \sigma} c_{k \sigma} c_{k \sigma}^\dagger + \sum_{\sigma} \epsilon_{f \sigma} n_{f \sigma} + U n_{f \uparrow} n_{f \downarrow} + V \sum_{k, \sigma} (f_{\sigma}^+ c_{k \sigma} + h.c.),
$$

where $H_c$ is the conduction electron Hamiltonian and $c_{k \sigma}, f_{\sigma}^+$ are creation operators of the conduction electrons in momentum and spin eigenstates ($k, \sigma$), and of electrons in the local $f$ level, respectively. The operator $n_{f \sigma} = f_{\sigma}^+ f_{\sigma}$ counts the number of electrons on the local level, and $\epsilon_{f \sigma} = \epsilon_f - \omega_f / 2, \sigma = \pm 1$.

The effect of the interaction $U$ is to renormalize the parameters $\epsilon_{f \sigma}, U, V$ to $\tilde{\epsilon}_{f \sigma}, \tilde{U}, \tilde{V}$ in the renormalized Fermi liquid type low energy Hamiltonian, Eq. (1) with the renormalized parameters that may be calculated using the numerical renormalization group (NRG) method.\footnote{12} To keep the algebra simple, we assume particle-hole symmetry in the following. Then $\tilde{\epsilon}_{f \sigma} = -(\tilde{U} + \omega_f) / 2$. The hybridization of the local level with the conduction band leads to an $f$-level broadening $\tilde{U} = \pi \tilde{V}^2 N_0 \sim T_K$ with $N_0 = 1 / \tilde{W}$ the local conduction electron density of states (DOS) at the Fermi level (in the model with flat DOS, $W$ is the bandwidth). The initially rather large bare level width is renormalized down to the very narrow width of the Kondo resonance. The NRG calculation shows that $U = \pi \tilde{U}$ and $\tilde{V}^2$ is $O(T_K / T_F)$, where $T_F$ is the Fermi temperature of the conduction electrons.

In the framework of Fermi liquid theory, the interaction has two major consequences: (i) it gives rise to a molecular field renormalizing the collective response of the system (ii) it leads to a finite lifetime of quasiparticles. However, the quasiparticle relaxation rate is limited by the available phase space and vanishes quadratically as the excitation energy goes to zero. Therefore, at temperatures $T \ll T_K$ the Landau quasiparticles are well-defined. The quasiparticle decay contributes to the spin relaxation rate. As we shall show, the local moment relaxation is governed by rapid spin flips on the frequency scale of $T_K$, occurring as part of the many body resonance. Then at temperatures $T \ll T_K$ we may neglect the additional relaxation caused by the quasiparticle decay.

We now consider the effects of the molecular field caused by the Fermi liquid interaction $\tilde{U}$. We treat the interaction term in the Hamiltonian in mean field approximation: $\tilde{U} n_{f \uparrow} n_{f \downarrow} \approx \frac{1}{2} \tilde{U} (\langle n_f \rangle n_f - \langle n_f \rangle m_f + \text{const})$, where we defined the density and spin density operators $n_f = n_{f \uparrow} + n_{f \downarrow}$ and $m_f = n_{f \uparrow} - n_{f \downarrow}$. In the case of particle-hole symmetry, when $\langle n_f \rangle = 1$, the density term is cancelled by the single-particle energy. The spin-density term gives rise to an effective magnetic field so that $\tilde{\epsilon}_{f \sigma} + \frac{1}{2} \tilde{U} \langle n_f \rangle - \sigma \langle m_f \rangle = -\sigma \omega_f$, which amounts to a doubling of the Zeeman energy. Here we have used that the spin polarization is given by $m = \langle m_f \rangle = \chi_{f \downarrow} - \chi_{f \uparrow} = \chi_{f \uparrow} + \chi_{f \downarrow} - (\omega_f / \pi \tilde{T})$, with $\chi_{f \sigma} = 0$ the static susceptibility of the local spin and $\tilde{U} = \pi \tilde{T}$, as obtained from NRG calculations. Then the local electron Green’s function, including the coupling to the conduction electrons, is given by

$$
G_{f \sigma}(i\omega_n) = [i\omega_n + \sigma \omega_f + i\tilde{T} \text{sign}(\omega_n)]^{-1}
$$

The local spectral function is given by $A_{f \sigma}(\omega) = \text{Im} G_{f \sigma}(\omega + i0) = \tilde{\Gamma} / (\omega - \omega_f)^2 + \tilde{T}^2$, describing the Kondo resonance. We see that in a magnetic field the resonance is shifted from its zero field position $\omega = 0$ to the spin dependent position $\omega = -\sigma \omega_f$, which is a double the Zeeman shift.

We use the definitions $\omega_f = g_f \mu_B B, \omega_c = g_c \mu_B B$ and take $\chi_{f \uparrow \uparrow}, \chi_{f \uparrow \downarrow}, \chi_{f \downarrow \uparrow}, \chi_{f \downarrow \downarrow}$, etc. to be response functions of spin 1/2 operators. The dynamical conduction electron susceptibility $\chi_{ee}$ is characterized by a resonance peak broadened by spin-lattice relaxation. We follow Barnes and Zitkova-Wilcox and model the spin-lattice relaxation mechanism by a local random magnetic field $h_i$, that fluctuates in both direction and magnitude. Then the conduction electron Hamiltonian is

$$
H_c = \sum_{k, \sigma} c_{k \sigma} c_{k \sigma}^\dagger + \sum_{k, \sigma} \sum_{k', \sigma'} \sum_i h_i \cdot \hat{c}_{k \sigma}^\dagger \hat{c}_{k' \sigma'} e^{i(k-k') \cdot \mathbf{R}_i}
$$

The random field components are assumed to be Gaussian correlated, with $\langle h_i \rangle = 0$ and $\langle h^m_i h^n_j \rangle = \delta_{ij} \delta_{mn} \hbar^2$. In Born approximation the average conduction electron Green’s function is then given by

$$
G_{\epsilon_k}(k, i\omega_n) = [i\omega_n - \epsilon_k + \omega_c / 2 + i\gamma \text{sign}(\omega_n)]^{-1},
$$

where $\gamma = \pi N_0 \hbar^2$.

The impurity induced component of the dynamical transverse susceptibility $\chi_{\text{imp}}^\perp(\Omega)$, where $\Omega$ is the frequency of an a.c. electromagnetic field polarized transverse to the static magnetic field, is a sum of three contributions, from the conduction electrons (cc), the local
electrons (ff) and the mixed response of conduction electrons to a spin polarization of the local electrons or vice versa (cf):

\[
\chi_{\text{imp}}^+(\Omega) = \frac{2\mu_B^2|g_f|^2\chi_{ff}^+(\Omega) + 2g_e g_f \chi_{cf}^+(\Omega)}{\pi \Gamma} (1 + \pi) \Omega + \chi_{\text{bulk}}^-(\Omega) \}
\] (5)

The partial susceptibilities may be calculated using standard many body techniques, see the Appendix. One finds resonances at the two frequencies \(\omega_f\) and \(\omega_c\). They have very different widths: the local electron spin resonance is broadened by \(\Gamma\), whereas the bulk and the impurity induced conduction electron resonances are broadened by \(4\gamma\). The results are given in the Appendix, Eqs. (A1-A3). Assuming that \(\Gamma \gg 4\gamma\), it makes sense to consider the behavior at higher frequencies \(\Omega \gg (\omega_f,\omega_c,\gamma)\) (regime I) and low frequencies (regime II) separately. In regime I one finds:

\[
\chi_{\text{imp}}^-(\Omega) = \frac{2\mu_B^2(g_f - g_e)^2}{\pi \Gamma} (1 - \frac{i\Gamma}{\Omega + i\Gamma}) \Omega - \omega_f + i\Gamma
\] (6)

Neutron scattering data on diluted magnetic alloys show a broad resonance in \(\chi_{\text{imp}}^-(\Omega)\) of width \(\Gamma\), in accordance with the above result. Note that this broad vanishes in the case of equal g-factors, as a consequence of the conservation of magnetization in that case (leaving aside spin lattice relaxation for the moment). The result in regime II is:

\[
\chi_{\text{imp}}^+(\Omega) = \frac{2\mu_B^2(g_f - g_e)^2}{\pi \Gamma} \left( \frac{\omega_c g_c}{\Omega - \omega_c + 4i\gamma} + \frac{\omega_c}{\Omega - \omega_c + 4i\gamma} \right)
\] (7)

The last term carries vanishing spectral weight. The second term on the r.h.s. represents an impurity induced enhancement \((3g_f > 2g_e)\) or reduction of the bulk conduction electron spin resonance. This contribution vanishes if \(g_f = \frac{2}{3}g_e\). The static susceptibility takes the form

\[
\chi_{\text{imp}}^+(0) = \frac{2\mu_B^2 g_f^2}{\pi \Gamma}\]

To summarize, the impurity induced component of the total dynamical spin susceptibility of a Kondo ion is characterized by a broad excitation peak of width \(\Gamma \simeq T_K\) at \(\Omega = \omega_f\) and a narrow peak or dip of width \(4\gamma\) at \(\Omega = \omega_c\), where \(\gamma\) is the conduction electron relaxation rate. The relative weights of the two components depend sensitively on the ratio of g-factors. This structure is not easily detected in an ESR experiment. The narrow resonance line has the same position and width as the bulk ESR line. Its weight per atom is, however, enhanced by the large factor \(T_F/T_K\), which comes from the renormalized susceptibility scale prefactor \(\propto 1/\Gamma\). Therefore, the ESR response of a diluted magnetic alloy with a concentration of Kondo ions \(c > T_K/T_F\) will be dominated by the impurity contribution determined in the above Eqs. (6,7).

III. ANDERSON LATTICE MODEL IN THE KONDO SCREENED REGIME.

The Hamiltonian of the simplest Anderson lattice model, assuming momentum independent hybridization and an isotropic conduction band with flat density of states is given by

\[
H = H_c + \sum_{i,\sigma} \epsilon_{f\sigma} f_{\sigma i}^+ f_{\sigma i} + U \sum_i n_{fi}^+ n_{fi}
\]

\[
+ V \sum_{i,k,\sigma} (\epsilon_I(k) f_{\sigma i}^+ c_{k\sigma} + h.c.)
\]

Here \(H_c\) and \(\epsilon_{f\sigma}, V, U\) have been introduced in Sec. II and the \(\mathbf{R_i}\) are lattice site vectors. The single particle Green’s functions are given by Dyson’s equation

\[
\left( i\omega_n - \epsilon_{f\sigma} - \sum_{\sigma} \epsilon_{f\sigma}(i\omega_n, \mathbf{k}) \right) G = 1,
\]

where \(G = (G_{\sigma f}^{kk}, G_{\sigma f}^{kk}, G_{\sigma f}^{kk})\).

We assume Fermi liquid theory to hold. Then the self energy \(\Sigma_{f\sigma}(\omega, \mathbf{k})\) has a power series expansion in \(\omega\) at the Fermi surface, and its imaginary part is small \(\propto \omega^2\), and may be neglected in lowest order. One may use \(\omega - \epsilon_{f\sigma} - \Sigma_{f\sigma}(\omega, \mathbf{k}) = z_{\sigma}^{-1}[\epsilon_{f\sigma} - \epsilon_{f\sigma} - \Sigma_{f\sigma}(0, \mathbf{k})]\), with the quasiparticle weight factors \(z_{\sigma} = [1 - \partial \Sigma_{f\sigma}(\omega, \mathbf{k})/\partial \omega]^{-1}\) and the renormalized energy \(\epsilon_{f\sigma} = z_{\sigma} \epsilon_{d\sigma} + \Sigma_{f\sigma}(0, \mathbf{k})\). The conduction electron self-energy may be approximated by \(\Sigma_{cs}(\omega + i0, \mathbf{k}) = -i\gamma\), where \(\gamma\) is the spin-lattice relaxation rate defined earlier. Then for low energies one has a quasiparticle description, with \(G^{f\sigma}_{kk} = z_{\sigma} \tilde{G}^{f\sigma}_{kk}\). The renormalized hybridization amplitude \(V\) may be approximated \(V = z_{f\sigma}(\mathbf{k})^2\). The full matrix of quasiparticle Green’s functions is given by

\[
\left( \tilde{G}^{f\sigma}_{kk} \tilde{G}^{f\sigma}_{kk} \tilde{G}^{f\sigma}_{kk} \right) = \frac{1}{\text{det}} \left( \omega - \epsilon_{k\sigma} + i\gamma \tilde{V} \omega - \epsilon_{f\sigma} \right)
\] (10)

where \(\text{det} = (\omega - \epsilon_{f\sigma})(\omega - \epsilon_{k\sigma} + i\gamma) - V^2 = (\omega - \epsilon_{k\sigma}^+)(\omega - \epsilon_{k\sigma}^-)\). The complex energy eigenvalues are given by

\[
\epsilon_{k\sigma}^\pm = \frac{1}{2}(\epsilon_{f\sigma} + \epsilon_{k\sigma} - i\gamma) \pm \sqrt{\left[\frac{1}{4}(\epsilon_{f\sigma} - \epsilon_{k\sigma} + i\gamma)^2 + V^2 \right] - \epsilon_{f\sigma}^-}
\] (11)

where \(\epsilon_{k\sigma}^\pm = \text{Re} \epsilon_{k\sigma}^\pm\) and \(\gamma_{k\sigma}^\pm = -\text{Im} \epsilon_{k\sigma}^\pm\). We denote \(\gamma_{k\sigma}^+ > 0\). There are two energy bands separated by an (indirect) gap \((\epsilon_{k\sigma}^\min, \epsilon_{k\sigma}^\max)\) (denote the minimum or maximum of the conduction band):

\[
\Delta_{g\sigma} = \epsilon_{k\sigma}^\min - \epsilon_{k\sigma}^\max + \sqrt{(\epsilon_{f\sigma} - \epsilon_{k\sigma}^\max)^2 + 4V^2} + \sqrt{(\epsilon_{f\sigma} - \epsilon_{k\sigma}^\min)^2 + 4V^2} \gg \omega_{f,c}.
\]

We assume that the renormalized f-level \(\epsilon_{f\sigma}\) is inside the conduction band, close to the Fermi level, and consider
the case of almost half-filling, i.e. \( n \lesssim 2 \) electrons per lattice site. Then only the lower band is occupied in the ground state. We assume an isotropic band structure for simplicity. Then near the Fermi level at \( k = k_F \), the quasiparticle energy (we drop the spin dependence) has the form

\[
e_{k} - e_{k_F} = \frac{1}{2} (k - k_F) v_F \left[ 1 + \frac{(\tilde{e}_f - e_{k_F})}{\sqrt{(\tilde{e}_f - e_{k_F})^2 + 4V^2}} \right] \lesssim (k - k_F)^2 v_F^* ,
\]

where the renormalized Fermi velocity is defined by \( v_F^* = v_F \sqrt{2/\tilde{e}_f - e_{k_F}}^2 = v_F (m/m^*) \lesssim v_F z V^2/(\epsilon_{k_F})^2 \), and we used the fact that \( \epsilon_{k_F} \gg \tilde{e}_f \). Note that \( e_{k_F} \) is the bare conduction band energy at \( k = k_F \), which is far above the true Fermi energy. When \( z \ll 1 \), the Fermi velocity is renormalized to very low values and one has a “heavy fermion liquid” (effective mass \( m^* \gg m \)). The effective Fermi temperature of the heavy quasiparticles is given by \( T_F = \frac{1}{2} k_F v_F^* \ll T_F \).

To first order in \( \gamma \) the level widths are given by

\[
\gamma_{\pm}^{k_\sigma} = \frac{1}{2} \left[ 1 + \frac{\tilde{e}_f - e_{k_\sigma}}{e_{k_F} - e_{k_\sigma}} \right].
\]

We note that the hybridization induced width \( \Gamma \) of the \( f \)-electron energy level in the impurity problem is now absorbed in the electronic band structure: the coherent superposition of contributions from all lattice sites to \( \Sigma_{\alpha}(\omega + i0,k) \) removes the large constant \( i\Gamma \). The remaining imaginary part of the self-energy at finite temperatures may be approximated by a constant \( \Gamma_{FL} = c T^2/T_F \). We shall comment on the effect of quasiparticle scattering on the ESR-width at the end. Using partial fraction decomposition, we get the retarded Green function

\[
\tilde{G}_{f\sigma}^{ff}(\omega + i0) = \frac{a_{f\sigma}^{+\pm}}{\omega - \epsilon_{k_\sigma}^+} + \frac{a_{f\sigma}^{\pm-}}{\omega - \epsilon_{k_\sigma}^-}.
\]

and similar expressions for \( \tilde{G}_{f\sigma}^{cc} \) and \( \tilde{G}_{k_\sigma}^{cc} \), where, with \( \epsilon_{k_\sigma} = \epsilon_{k_\sigma}^+ - \epsilon_{k_\sigma}^- \),

\[
a_{f\sigma}^{\pm\pm} = \pm (\epsilon_{k_\sigma}^+ - \epsilon_{k_\sigma})/u_{k_\sigma}, \\
a_{f\sigma}^{\pm-} = \pm (\epsilon_{k_\sigma}^- - \epsilon_{f_\sigma})/u_{k_\sigma}, \\
a_{cc}^{\pm\pm} = \pm (\epsilon_{k_\sigma}^+ - \epsilon_{f_\sigma})/u_{k_\sigma}, \\
a_{cc}^{\pm-} = \pm V/u_{k_\sigma}.
\]

For sufficiently small spin-lattice relaxation, \( \gamma \ll (\tilde{V}, \tilde{e}_{f_\sigma}) \), we may neglect the imaginary parts in the weight factors \( a_{f\sigma}^{\pm\pm} \ldots \) and replace \( \epsilon_{k_\sigma}^+ \) by \( \epsilon_{k_\sigma}^- \).

The quasiparticles interact via the Fermi liquid interaction. For ESR, the relevant component of the Fermi liquid interaction is the isotropic spin-antisymmetric part described by the Landau parameter \( F_0^a \). An important contribution to \( F_0^a \) comes from the renormalized value \( \tilde{U} \) of the bare interaction \( U \), \( F_0^a = -2 N_0 \tilde{U} \), similar to the single impurity case discussed in Sec. II. For the lattice case, exact numerical results on \( \tilde{U} \) are not available. We note however, that the onsite repulsion \( U \) is likely to be screened down to a positive value of order \( N_0^{-1} \), which would lead to a ferromagnetic Landau parameter \( 0 > F_0^a \approx -1 \). Additional contributions to \( F_0^a \) may be generated by nonlocal interactions like the RKKY interaction, which may be ferro- or antiferromagnetic. We emphasize that this Fermi liquid interaction always leads to a ferromagnetic contribution to the fluctuation spectrum, which may be more or less important depending upon the other contributions.

Following the way in which the interaction was included in the impurity model, we may express the fully screened \( f \)-electron susceptibility in terms of the unscreened one

\[
\chi_{ff}^{\pm}(i\Omega_m) = \chi_{f\sigma}^{\pm}(i\Omega_m)/(1 - \tilde{U} \chi_{f\sigma}^{\pm}(i\Omega_m)),
\]

where

\[
\chi_{f\sigma}^{\pm}(i\Omega_m) = -\gamma \sum_{\omega_n} \sum_k \tilde{G}_{k,\sigma}^{ff}(i\omega_n + i\Omega_m) \tilde{G}_{k,\sigma}^{ff}(i\omega_n)
\]

The one-to-one correspondence of quasiparticles and bare particles, on which Landau’s Fermi liquid theory rests, allows to calculate the spin susceptibility from the quasi-particle Green’s functions defined above, without taking the incoherent parts into account. Here the subscript \( H \) indicates that the Zeeman energy \( \omega_f \) is replaced everywhere by

\[
\tilde{\omega}_f = \omega_f [1 + \tilde{U} \chi_{f\sigma}^{\pm}(0)] = \omega_f [1 - \tilde{U} \chi_{f\sigma}^{\pm}(0)]^{-1}
\]

Using the representation of \( \tilde{G}_{k,\sigma}^{ff} \) in terms of eigenstates, the summation in Eq. (17) on \( \omega_n \) and \( k \) may be done. In the case that only the lower band is occupied, the low frequency response is given by, see the Appendix, Eq. (A4):

\[
\chi^{\pm}(\Omega + i0) = \frac{\chi^{\pm}(0)(-\omega_r + i\gamma_r)}{\Omega - \omega_r + i\gamma_r},
\]

where \( \chi^{\pm}(0) \) is defined in the Appendix, Eq. (A5). The mean field shift largely cancels out of the resonance frequency

\[
\omega_r = \frac{1}{2} \omega_f \left[ 1 - \frac{(\tilde{e}_f - e_{k_F})}{\sqrt{(\tilde{e}_f - e_{k_F})^2 + 4V^2}} \right] \approx \omega_f (1 - m/m^*)
\]

The linewidth, however, is reduced by the exchange interaction, provided the interaction is ferromagnetic.

\[
\gamma_r = \gamma \left[ 1 + \frac{\tilde{e}_f - e_{k_F}}{\sqrt{(\tilde{e}_f - e_{k_F})^2 + 4V^2}} \right] [1 - \tilde{U} \chi_{f\sigma}^{\pm}(0)] \\
\approx 2 \gamma \frac{m}{m^*} [1 - \tilde{U} \chi_{f\sigma}^{\pm}(0)] \ll \gamma.
\]
It is seen that the main narrowing mechanism is provided by the hybridization through the renormalized amplitude $\tilde{V}$, which gives the small factor $m/m^*$. In simple terms, the quasiparticles at the Fermi surface have mainly $f$-character, with only a small admixture (fraction $m/m^*$) of conduction electron component. Since only the conduction electrons feel the spin lattice relaxation, the total spin relaxation is a fraction $m/m^*$ of the spin lattice relaxation. Vertex corrections to the spin-lattice relaxation are likely to increase $\gamma_r$ somewhat as they do in the impurity case, Appendix Eq. (A1), where $2\gamma$ becomes $4\gamma$.

In order to discuss the temperature and magnetic field dependence of the linewidth it is necessary to incorporate quasiparticle scattering effects and inelastic contributions to the spin-lattice relaxation. In the case that the $g$-factors are sufficiently different, the contribution to the linewidth from quasiparticle scattering will vary with temperature as $T^2/T_F^2$ and with magnetic field $H$ as $H^2/T_F^2$. In the case of equal $g$-factors the latter contribution will be cancelled by vertex corrections. Additional temperature dependence may arise from coupling to phonons.

IV. CONCLUSION

This paper is motivated by the recent observations of electron spin resonance at low temperature in some heavy-fermion compounds. We have calculated the dynamical susceptibility, which describes the resonance, at low temperature in the fully screened Kondo regime for both a single Kondo impurity spin as well as for the Kondo lattice, described here by the Anderson lattice model.

We have not addressed the behavior of the susceptibilities at temperatures in the neighborhood of the Kondo temperature, where linewidths are expected to be very large due to rapid spin fluctuations in that temperature range. Rather, we deal with the very low temperature regime, where a Kondo impurity is fully screened and where the heavy-electron Fermi liquid has formed in the Anderson lattice.

For the realistic case in which the $g$-factors of $f$-electrons and conduction electrons are different, we find for the single impurity that structure persists at both the $f$-electron and conduction electron resonance frequencies. The impurity resonance continues to have a large width, or decreases the amplitude depending on the ratio of $g$-factors.

The situation is quite different for the lattice case. Here, the hybridization of the $f$ and conduction electrons and Fermi-liquid interaction lead to modifications of the susceptibility that can lead to substantial line narrowing and hence the possibility of experimental observation. We find a sharp ESR line near the underlying local $f$ electron resonance. The line is substantially narrowed by a factor of the mass ratio $m/m^*$ and by the effect of the Fermi liquid interaction $F_{\alpha}^0$ provided it is negative (ferromagnetic).

We note that the ESR has been only been seen in heavy fermion compounds for which there is independent evidence for ferromagnetic fluctuations. We suggest that our analysis accounts for this observation.

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APPENDIX

1. Anderson impurity model in the Kondo screened regime: Green’s function approach to $\chi^+(\Omega)$

As derived in the main text, Eq. (2), the Green’s functions of conduction electrons and local electrons, including the Fermi-liquid interaction, are given by

$$G_{f\sigma}(i\omega_n) = [i\omega_n + \sigma\omega_f + i\Gamma\text{sign} (\omega_n)]^{-1},$$

$$G_{e\sigma}(k, i\omega_n) = [i\omega_n - \xi_k + \sigma\omega_e/2 + i\gamma\text{sign} (\omega_n)]^{-1}.$$  

The dynamical transverse susceptibility $\chi^+(\Omega)$, where $\Omega$ is the frequency of an a.c. electromagnetic field polarized transverse to the static magnetic field, is given by

$$\chi^+(\Omega) = \mu_B^2 [g_e^2 \chi_{ee}^+(\Omega) + g_f^2 \chi_{ff}^+(\Omega) + 2g_eg_f \chi_{ef}^+(\Omega)].$$

The partial susceptibilities are obtained by evaluating Feynman bubble diagrams dressed by vertex corrections of the ladder type referring to the Fermi liquid interaction (local electrons) and the spin-orbit interaction (impurity correlation lines for the conduction electrons).

The local susceptibility in the absence of vertex corrections is obtained as

$$\chi_{ff,H}^+(i\Omega_m) = -T \sum_{\omega_n} G_{f\uparrow}(i\omega_n + i\Omega_m)G_{f\uparrow}(i\omega_n)$$

$$= \frac{2}{\pi |\Omega_m - 2\omega_f|}.$$  

The vertex corrections are obtained from the Bethe-Salpeter equation

$$\Lambda(i\Omega_m) = 1 + U \chi_{ff,H}^+(i\Omega_m)\Lambda(i\Omega_m) = \frac{\Omega - 2\omega_f + 2i\Gamma}{\Omega - \omega_f + i\Gamma}.$$
where we used $\tilde{U} = \pi \tilde{T}$. Then

$$\chi_{ff}^{\pm}(i\Omega_m) = \chi_{ff,H}^{\pm}(i\Omega_m) \Lambda(i\Omega_m) = \frac{2}{\pi} \frac{-\omega_f + i\tilde{T}}{\Omega_m - \omega_f + i\tilde{T}}.$$

The conduction electron susceptibility consists of four contributions

$$\chi_{cc}^{\pm}(i\Omega_m) = \chi_{cc}^{bulk}(i\Omega_m) + \sum_{i=1}^{\text{3}} \chi_{cc}^{(i)}(i\Omega_m)$$

The bulk contribution has the form $\chi_{cc}^{bulk}(i\Omega_m) = N N_0 \chi_{cc}^{0}(\Omega + i0) \Phi(i\omega_n + i\Omega_m)$, where $N$ is the number of atoms in the system and $N_0 \chi_{cc}^{0}(\Omega + i0) = -T \sum_{k,m} G_{c\uparrow}(k, i\omega_n + i\Omega_m) G_{c\uparrow}(k, i\omega_n) = N_0 (-\omega_c + 2i\gamma)/(\Omega - \omega_c + 2i\gamma)$, where $N_0$ is the conduction electron density of states at the Fermi level. The vertex function $\Phi(i\omega_n, i\Omega_m)$ is found as solution to the equation:

$$\Phi(i\omega_n, i\Omega_m) = 1 - \hbar^2 \sum_{k} G_{c\uparrow}^0(k, i\omega_n + i\Omega_m) G_{c\uparrow}^0(k, i\omega_n) \Phi(i\omega_n, i\Omega_m)$$

as

$$\Phi(i\omega_n, i\Omega_m) = \theta(-\omega_n) \theta(\omega_n + \Omega_m) \frac{i\Omega_m - \omega_c + 2i\gamma}{i\Omega_m - \omega_c + 4i\gamma} + [1 - \theta(-\omega_n) \theta(\omega_n + \Omega_m)]$$

Note that the minus sign in front of $\hbar^2$ is generated by the Pauli matrices that appear in $H_c$, Eq. (3) of the main text (in the case of potential scattering there would be no sign change): $\sum_{i,\alpha,\delta} \sigma_i^{\alpha \delta} \sigma_i^{\beta \gamma} G_{cc}^{0} G_{cc}^{0} = -G_{c\uparrow} G_{c\uparrow}$. As a consequence, the vertex corrections double the linewidth: $2\gamma \rightarrow 4\gamma$. In the case of potential scattering the vertex corrections cancel the self-energy induced linewidth, so that potential scattering does not contribute to the spin relaxation, as expected. Combining the above results we find

$$\chi_{cc}^{bulk}(\Omega + i0) = N N_0 \frac{-\omega_c + 4i\gamma}{\Omega - \omega_c + 4i\gamma}. \quad (A.1)$$

The remaining contributions are obtained from

$$\chi_{cc}^{(1)}(i\Omega_m) = -\hbar^2 V^2 \sum_{\omega_n} \sum_{k} \left\{ [G_{c\uparrow}^{0}(k, i\omega_n + i\Omega_m)]^2 G_{c\uparrow}^{0}(k, i\omega_n) G_{f\uparrow}(i\omega_n + i\Omega_m) \right.\right.$$

$$+ \left. G_{c\uparrow}^{0}(k, i\omega_n + i\Omega_m) G_{c\uparrow}^{0}(k, i\omega_n) G_{f\uparrow}(i\omega_n) \right\};$$

$$\chi_{cc}^{(2)}(i\Omega_m) = -T \sum_{\omega_n} \left[ V^2 \sum_{k} G_{c\uparrow}^{0}(k, i\omega_n + i\Omega_m) G_{c\uparrow}^{0}(k, i\omega_n) \Phi(i\omega_n, i\Omega_m) \right]^2 G_{f\uparrow}(i\omega_n + i\Omega_m) G_{f\uparrow}(i\omega_n),$$

$$\chi_{cc}^{(3)}(i\Omega_m) = \left[ V^2 T \sum_{\omega_n} \sum_{k} G_{c\uparrow}^{0}(k, i\omega_n + i\Omega_m) G_{c\uparrow}^{0}(k, i\omega_n) \Phi(i\omega_n, i\Omega_m) G_{f\uparrow}(i\omega_n + i\Omega_m) G_{f\uparrow}(i\omega_n) \right]^2 \times [-\tilde{U} \Lambda(i\Omega_m)].$$

Using

$$\sum_{k} [G_{c\uparrow}^{0}(k, i\omega_n + i\Omega_m)]^2 G_{c\uparrow}^{0}(k, i\omega_n) = N_0 \frac{2\pi i}{(i\Omega_m - \omega_c + 2i\gamma)^2} = -\sum_{k} G_{c\uparrow}^{0}(k, i\omega_n + i\Omega_m) [G_{c\uparrow}^{0}(k, i\omega_n)]^2$$

and the identity

$$G_{f\uparrow}(i\omega_n + i\Omega_m) - G_{f\uparrow}^{\uparrow}(i\omega_n) = -(i\Omega_m - 2\omega_f + 2i\tilde{T}) G_{f\uparrow}(i\omega_n + i\Omega_m) G_{f\uparrow}(i\omega_n)$$

as well as

$$\Pi(i\Omega_m) = T \sum_{-\Omega_m < \omega_n < 0} G_{f\uparrow}(i\omega_n + i\Omega_m) G_{f\uparrow}(i\omega_n) = \frac{1}{\pi \tilde{T}} \frac{i\Omega_m}{i\Omega_m - 2\omega_f + 2i\tilde{T}}.$$
we get
\[
\chi^{(1)}_{cc}(i\Omega_m) = \frac{2}{\pi \Gamma (\Omega - 2\omega_f + 2i\Gamma)}
\]
\[
\chi^{(2)}_{cc}(i\Omega_m) = \frac{2}{\pi \Gamma (i\Omega_m - \omega_c + 4i\gamma)^2} \frac{\Omega}{\Omega - 2\omega_f + 2i\Gamma}
\]
\[
\chi^{(3)}_{cc}(i\Omega_m) = -\frac{2}{\pi \Gamma (i\Omega_m - \omega_c + 4i\gamma)^2 (\Omega - 2\omega_f + 2i\Gamma)(\Omega - 2\omega_f + 2i\Gamma)}
\]

Adding the three contributions we find
\[
\sum_{i=1}^{3} \chi^{(i)}_{cc}(i\Omega_m) = \frac{2}{\pi \Gamma (i\Omega_m - \omega_c + 4i\gamma)^2} \frac{i\Gamma}{\Omega - \omega_f + i\Gamma}
\]  \hspace{1cm} (A.2)

The mixed susceptibility may be calculated from the bubble diagram beginning with a conduction electron particle-hole line and ending with a local electron p-h line, dressed by vertex corrections at both ends:
\[
\chi^{\pm}_{cc}(\Omega_m) = -T \sum_{\omega_n, k} G^0_{cc}(k, i\omega_n + i\Omega_m) G^0_{cc}(k, i\omega_n) \Phi(i\omega_n, i\Omega_m)V^2 G_{f1}(i\omega_n + i\Omega_m) G_{f1}(i\omega_n) \Lambda(i\Omega_m)
\]
\[
= \frac{2}{\pi \Gamma} \frac{-i\Gamma}{i\Omega_m - \omega_c + 4i\gamma i\Omega_m - 2\omega_f + 2i\Gamma}
\]  \hspace{1cm} (A.3)

After analytical continuation to the real frequency axis and combining the contributions the total impurity susceptibility is obtained as given in the main text, Eqs. (6,7).

2. **Anderson lattice model in the Kondo screened regime: Green’s function approach to \(\chi^{\pm}(\Omega)\).**

As derived in the main text Eq. (10), the matrix of quasispinor Green’s functions is given by
\[
\begin{pmatrix}
\tilde{G}_{f f}^{cf} & \tilde{G}_{f c}^{cf} \\
\tilde{G}_{c f}^{cf} & \tilde{G}_{c c}^{cf}
\end{pmatrix} = \frac{1}{\text{det} \begin{pmatrix} \omega - \epsilon_{f\sigma} + i\gamma & \tilde{V} \\ \tilde{V} & \omega - \epsilon_{c\sigma} \end{pmatrix}} 
\]
where \text{det} = \(\omega - \epsilon_{f\sigma} + i\gamma - \tilde{V}^2 = (\omega - \epsilon_{c\sigma})(\omega - \epsilon_{c\sigma})\). The complex energy eigenvalues are given by
\[
\epsilon^{\pm}_{c\sigma} = \frac{1}{2}(\epsilon_{f\sigma} + \epsilon_{c\sigma} - i\gamma) \pm \frac{1}{4}(\epsilon_{f\sigma} - \epsilon_{c\sigma} + i\gamma)^2 + \tilde{V}^2 
\]
\[
= \epsilon^{\pm}_{f\sigma} + i\gamma^{\pm}_{c\sigma},
\]
where, expanding to leading order in \(\gamma\), as well as in \(\omega_f, \omega_c\),
\[
\epsilon^{\pm}_{c\sigma} = \text{Re} \epsilon^{\pm}_{c\sigma} \approx \frac{1}{2}(\epsilon_{f\sigma} + \epsilon_{c\sigma}) \pm \frac{1}{4}(\epsilon_{f\sigma} - \epsilon_{c\sigma})^2 + \tilde{V}^2 
\]
\[
= \epsilon^{\pm}_{f\sigma} - \frac{1}{2} \omega^{\pm}_{c\sigma}
\]
and
\[
\gamma^{\pm}_{c\sigma} = -\text{Im} \epsilon^{\pm}_{c\sigma} \approx \frac{1}{2} \gamma \left[ 1 \pm \frac{\epsilon_{f\sigma} - \epsilon_{c\sigma}}{\epsilon_{c\sigma} - \epsilon_{c\sigma}} \right] \approx \gamma^{\pm}_{c\sigma} - \frac{1}{2} \eta^{\pm}_{c\sigma},
\]

with
\[
\epsilon^{\pm}_{f\sigma} = \frac{1}{2}(\epsilon_{f\sigma} + \epsilon_{c\sigma}) \pm \frac{1}{2} \sqrt{(\epsilon_{f\sigma} - \epsilon_{c\sigma})^2 + 4\tilde{V}^2}
\]
\[
\omega^{\pm}_{c\sigma} = \frac{1}{2}(\omega_c + \omega_c) \pm \frac{1}{2} \sqrt{(\epsilon_{f\sigma} - \epsilon_{c\sigma})^2 + 4\tilde{V}^2}
\]
\[
\gamma^{\pm}_{c\sigma} = \frac{1}{2} \gamma \left[ 1 \pm \frac{\epsilon_{f\sigma} - \epsilon_{c\sigma}}{\sqrt{(\epsilon_{f\sigma} - \epsilon_{c\sigma})^2 + 4\tilde{V}^2}} \right] \approx \gamma^{\pm}_{c\sigma} - \frac{1}{2} \eta^{\pm}_{c\sigma} 
\]
\[
\eta^{\pm}_{c\sigma} = \frac{1}{2} \gamma \left[ \frac{\epsilon_{f\sigma} - \epsilon_{c\sigma}}{\sqrt{(\epsilon_{f\sigma} - \epsilon_{c\sigma})^2 + 4\tilde{V}^2}} \right] \approx \gamma^{\pm}_{c\sigma} - \frac{1}{2} \eta^{\pm}_{c\sigma}
\]

The susceptibility is, as in the case of the impurity, given by the sum of three contributions: \(ff\), \(cc\) and \((cf, fc)\):
\[
\chi^{\pm}(\Omega) = \rho_B^2 [g_c^2 \chi^{\pm}_{cc}(\Omega) + g_f^2 \chi^{\pm}_{ff}(\Omega) + 2g_c g_f \chi^{\pm}_{cf}(\Omega)].
\]
Here the \(ff\)-susceptibility is screened by the Fermi liquid interaction
\[
\chi^{\pm}_{ff}(i\Omega_m) = \chi^{\pm}_{ff,H}(i\Omega_m) \Lambda(i\Omega_m),
\]
with
\[
\Lambda(i\Omega_m) = 1/[1 - \tilde{U} \chi^{\pm}_{ff,H}(i\Omega_m)]
\]
where
\[
\chi^{\pm}_{ff,H}(i\Omega_m) = -T \sum_{\omega_n, k} \tilde{G}_{f f}^{cf}(i\omega_n + i\Omega_m) \tilde{G}_{c f}^{cf}(i\omega_n)
\]
Similarly, 
\[
\chi_{cf}^{\pm}(i\Omega_m) = \chi_{cf,H}^{\pm}(i\Omega_m)\Lambda(i\Omega_m),
\]
where
\[
ch_{cf,H}(i\Omega_m) = -T \sum_{\omega_n,k} \tilde{G}_{cf,k}^{\pm}(i\omega_n + i\Omega_m) G_{cf,k}^{\mp}(i\omega_n)
\]
and
\[
\chi_{cc,H}^{\pm}(i\Omega_m) = \chi_{cc,H}^{\pm}(i\Omega_m) + U[\chi_{cd,H}^{\pm}(i\Omega_m)]^2\Lambda(i\Omega_m),
\]
where
\[
\chi_{cc,H}^{\pm}(i\Omega_m) = -T \sum_{\omega_n,k} G_{cc,k}^{\pm}(i\omega_n + i\Omega_m) G_{cc,k}^{\mp}(i\omega_n)
\]
Using the representation of the Green’s functions in terms of the eigenstates \(\nu = \pm\), and the fact that low energy excitations are only possible close to the Fermi energy, which we assume to lie in the lower band (\(\nu = -\)), only the (-)-components contribute to \(\chi_{ij,H}(i\Omega_m)\):
\[
\chi_{f,H}^{\pm}(\Omega + i0) = -\sum_k a_{k_{f,-}} f(\begin{pmatrix} \hat{\varsigma}_{k_{f}}^- & \omega_{k_{f}}^- i\gamma_{k_{f}}^- \end{pmatrix}) - \hat{\varsigma}_{k_{f}}^- + i0,
\]
where in the arguments of the Fermi function \(f(\epsilon)\), the complex-valued energy \(\tilde{\varsigma}_{k_{f}}^\pm\) appears. Employing \(\tilde{\varsigma}_{k_{f}}^\pm - \tilde{\varsigma}_{k_{f}}^- \simeq \omega_{k_{f}}^- - 2i\gamma_{k_{f}}^-\), and \(\sum_k [f(\varsigma_{k_{f}}^-) - f(\varsigma_{k_{f}}^\pm)] \simeq \sum_k (\partial f/\partial \varsigma_{k_{f}}^-)(-\omega_{k_{f}}^- + 2i\gamma_{k_{f}}^-) = N_0(\omega_{k_{f}}^- - 2i\gamma_{k_{f}}^-)\), we get
\[
\chi_{f,H}^{\pm}(\Omega + i0) = N_0 a_{k_{f},-} a_{k_{f},-}^- \frac{-\omega_{k_{f}}^- + 2i\gamma_{k_{f}}^-}{\Omega - \omega_{k_{f}}^- + 2i\gamma_{k_{f}}^-}
\]
and hence
\[
\chi_{f,H}^{\pm}(0) = N_0 a_{k_{f},-} a_{k_{f},-}^-\frac{-\omega_{k_{f}}^- + 2i\gamma_{k_{f}}^-}{1 - \tilde{U} \chi_{f,H}^{\pm}(0)}.
\]
Equivalent expressions hold for the \(ff\) and \(cf\) components. The vertex function follows as
\[
\Lambda(\Omega + i0) = \frac{-\omega_{k_{f}}^- + 2i\gamma_{k_{f}}^-}{\Omega - \omega_{k_{f}}^- + 2i\gamma_{k_{f}}^-}
\]
and the renormalized \(ff\)-susceptibility takes the form
\[
\chi_{f}^{\pm}(\Omega + i0) = \chi_{f}^{\pm}(0) - \omega_{\nu}^- + i\gamma_{\nu}^- \Omega - \omega_{\nu}^- + i\gamma_{\nu}^- \frac{-\omega_{\nu}^- + 2i\gamma_{\nu}^-}{1 - \tilde{U} \chi_{f,H}^{\pm}(0)}
\]
and \(\chi_{f}^{\pm}(0) = \chi_{f,H}^{\pm}(0)/[1 - \tilde{U} \chi_{f,H}^{\pm}(0)]\) as discussed in the main text, Eqs. (20,21). The total susceptibility consists of two resonance terms:

\[
\chi_{f,H}^{\pm}(\Omega + i0) = \chi_{r}^{\pm}(0) - \omega_{\nu}^- + i\gamma_{\nu}^- + g^2 - \omega_{\nu}^- + 2i\gamma_{\nu}^- \frac{-\omega_{\nu}^- + 2i\gamma_{\nu}^-}{\Omega - \omega_{\nu}^- + 2i\gamma_{\nu}^-} \{ \chi_{cc,H}^{\pm}(0) + U[\chi_{cf,H}^{\pm}(0)]^2 \}
\]
where \(\chi_{r}^{\pm}(0) = g^2 \chi_{f}^{\pm}(0) + 2g_{cf} \chi_{cf}^{\pm}(0)\). In the case that \(\gamma_{\nu} \gg \gamma_{f},\) the resonance part simplifies to
\[
\chi_{f}^{\pm}(\Omega + i0) = \chi_{f}^{\pm}(0) - \omega_{\nu}^- + i\gamma_{\nu}^- \Omega - \omega_{\nu}^- + i\gamma_{\nu}^- \frac{-\omega_{\nu}^- + 2i\gamma_{\nu}^-}{\Omega - \omega_{\nu}^- + 2i\gamma_{\nu}^-} \{ \chi_{cc,H}^{\pm}(0) + U[\chi_{cf,H}^{\pm}(0)]^2 \}
\]

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