Kondo Destruction in RKKY-Coupled Kondo Lattice and Multi-Impurity Systems

Ammar Nejati,[1] Katinka Ballmann,[1] and Johann Kroha[1,2,*]

[1]Physikalisches Institut and Bethe Center for Theoretical Physics, Universität Bonn, Nussallee 12, D-53115 Bonn, Germany

[2]Center for Correlated Matter, Zhejiang University, Hangzhou, Zhejiang 310058, China

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In a Kondo lattice, the spin exchange coupling between a local spin and the conduction electrons acquires nonlocal contributions due to conduction electron scattering from surrounding local spins and the subsequent RKKY interaction. It leads to a hitherto unrecognized interference of Kondo screening and the RKKY interaction beyond the Doniach scenario. We develop a renormalization group theory for the RKKY-modified Kondo vertex. The Kondo temperature $T_K(y)$ is suppressed in a universal way, controlled by the dimensionless RKKY coupling parameter y. Complete spin screening ceases to exist beyond a critical RKKY strength y_c even in the absence of magnetic ordering. At this breakdown point, $T_K(y)$ remains nonzero and is not defined for larger RKKY couplings $y > y_c$. The results are in quantitative agreement with STM spectroscopy experiments on tunable two-impurity Kondo systems. The possible implications for quantum critical scenarios in heavy-fermion systems are discussed.

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The concept of fermionic quasiparticles existing even in strongly interacting many-body systems is fundamental for a wealth of phenomena summarized under the term Fermi liquid physics. In heavy-fermion systems [1], quasiparticles with a large effective mass are formed by the Kondo effect [2]. The conditions under which these heavy quasiparticles disintegrate near a quantum phase transition (QPT) have been an important, intensively debated, and still open issue for many years [1].

The heavy Fermi liquid, like any other Fermi liquid, may undergo a spin density-wave (SDW) instability, leading to critical fluctuations of the magnetic order parameter but leaving the heavy quasiparticles intact. This scenario is well described by the pioneering works of Hertz, Moriya, and Millis [3–5]. However, early on Doniach pointed out [6] that the Kondo spin screening of the local moments should eventually cease and give way to magnetic order, when the RKKY coupling energy between the local moments [7–9] becomes larger than the characteristic energy scale for Kondo singlet formation, the Kondo temperature T_K. It is generally believed that the Kondo destruction is driven by the critical fluctuations near a QPT. Several mechanisms have been proposed, invoking different types of fluctuations, including critical fluctuations of the local magnetization coupling to the fermionic quasiparticles (local quantum criticality) [10,11] and Fermi surface fluctuations self-consistently generated by the Kondo destruction [12]. Most recently, a scenario of critical quasiparticles with diverging effective mass and a singular interaction, induced by critical antiferromagnetic fluctuations, has been put forward [13–15]. Intriguing in its generality, it does, however, not invoke Kondo physics.

Here, we show that the heavy-electron quasiparticles can be destroyed by the RKKY interaction even without critical fluctuations. This occurs because of a hitherto unrecognized feedback effect: in a Kondo lattice or multi-impurity system, the RKKY interaction, parametrized by a dimensionless coupling y, reduces the Kondo screening energy scale $T_K(y)$. This reduction implies an increase of the local spin susceptibility at low temperatures T, $\chi_f(T=0) \sim 1/T_K(y)$, which in turn increases the effective RKKY coupling. We derive this effect and analyze it by a renormalization group (RG) treatment. In particular, we calculate the temperature scale for Kondo singlet formation in a Kondo lattice, $T_K(y)$. It is suppressed with increasing y in a universal way. Beyond a critical RKKY coupling y_c, complete Kondo singlet formation ceases to exist. However, at this breakdown point $T_K(y_c)$ remains finite, and the suppression with respect to the single-impurity Kondo scale takes a universal value, $T_K(y_c)/T_K(0) = 1/e$, where $e = 2.718\ldots$ is Euler's constant. These findings are consistent with conformal field theory results [16,17] and in quantitative agreement with STM spectroscopy experiments on tunable, RKKY-coupled two-impurity Kondo systems [18,19].

The present results directly apply to cases where long-range order does not play a role, that is, two-impurity Kondo systems [18–20], compounds where the magnetic ordering does not occur at the Kondo breakdown point [21], and temperatures sufficiently above the Néel temperature [22]. They will set the stage for a complete theory of heavy-fermion quantum criticality by including critical order-parameter fluctuations either of the incompletely screened magnetic moments or of an impending SDW instability.

The model.—We consider the Kondo lattice model

$$H = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + J_0 \sum_i \mathbf{S}_i \cdot \mathbf{s}_i, \tag{1}$$

where $c_{\mathbf{k}\sigma}$, $c^\dagger_{\mathbf{k}\sigma}$ denote the conduction (c) electron operators with dispersion $\varepsilon_{\mathbf{k}}$. $\mathbf{S}_i$ are the local spin operators at the lattice sites $\mathbf{x}_i$, exchange coupled to the conduction electron spins $\mathbf{s}_i = \sum_{\sigma,\sigma'} c^\dagger_{i\sigma}\boldsymbol{\sigma}_{\sigma\sigma'}c_{i\sigma'}$ via an on-site, antiferromagnetic coupling $J_0 > 0$. The local spins will henceforth be termed f spins, as they are typically realized in heavy fermion systems by the rare-earth $4f$ electrons. We will use the pseudofermion representation of the f spins, $\mathbf{S}_i = 1/2\sum_{\tau,\tau'} f^\dagger_{i\tau}\boldsymbol{\sigma}_{\tau\tau'}f_{i\tau'}$ with $\boldsymbol{\sigma}$ the vector of Pauli matrices and $f_{i\sigma}$, $f^\dagger_{i\sigma'}$ fermionic operators obeying the constraint $\hat{Q} = \sum_\sigma f^\dagger_{i\sigma}f_{i\sigma} = 1$. It is crucial that the coupling between different f spins is not a direct exchange interaction, but mediated by the conduction band [7–9] and generated in second order by the same spin coupling J_0 that also creates the Kondo effect. The essential difference can be seen from the example of a two-impurity Kondo system $\mathbf{S}_1, \mathbf{S}_2$: with a direct impurity-impurity coupling $K\mathbf{S}_1 \cdot \mathbf{S}_2$, and for a specific particle-hole symmetry [16], this model can exhibit a dimer singlet phase where the dimer is decoupled from the conduction electrons (scattering phase shift at the Fermi energy $\phi_{\text{dimer}} = 0$). As a function of K, this dimer singlet phase is then separated from the Kondo singlet phase (scattering phase shift $\phi_{\text{Kondo}} = \pi/2$) by a quantum critical point (QCP) [16,23], see also Ref. [17]. By contrast, when the interimpurity coupling is controlled by the RKKY interaction only, i.e., generated by J_0, a decoupled dimer singlet and, hence, a second-order QCP is not possible. Instead, we find below that the Kondo singlet formation at $T = 0$ breaks down at a critical strength of the RKKY coupling, however without a diverging local impurity susceptibility, that is, with a discontinuous jump of $T_K(y)$. The profound implications of this behavior will be discussed below.

RKKY-coupled c-f vertex and renormalization group.—We develop an analytical renormalization group for RKKY-coupled Kondo multi-impurity and lattice systems, taking the proper renormalizations of all appearing vertices into account. The RKKY vertex $\hat{\Gamma}_{ff}$ coupling two f spins has no logarithmic RG flow, since the recoil (momentum integration) of the itinerant conduction electrons prevents an infrared singularity of the RKKY interaction. $\hat{\Gamma}_{ff}$ thus remains in the weak coupling regime. The formation of the strong-coupling Kondo singlet, which is the origin of the heavy-Fermion state, is signalled by a RG divergence of the spin-scattering vertex operator $\hat{\Gamma}_{cf}$ between c electrons and an f spin. In the case of multiple Kondo sites, this vertex acquires nonlocal contributions in addition to the local coupling J at a site i, because a c electron can scatter from a distant Kondo site $j \neq i$, and the spin flip at that site is transferred to the f spin at site i via the RKKY interaction. In this way, $\hat{\Gamma}_{ff}$ will influence the RG flow of $\hat{\Gamma}_{cf}$, even though it is not renormalized itself. The corresponding diagrams are shown in Fig. 1(a). As seen from the figure, such a nonlocal scattering process necessarily involves the exact, local dynamical f-spin susceptibility $\chi_f(i\Omega)$ on site j. The resulting c-f vertex $\hat{\Gamma}_{cf}$ has the structure of a nonlocal Heisenberg coupling in spin space. The exchange diagram, $\gamma^{(x)}_{\text{RKKY}}$ in Fig. 1(a), contributes only a subleading logarithmic term as compared to $\gamma^{(d)}_{\text{RKKY}}$ [24]. In particular, it does not alter the universal $T_K(y)$ suppression derived below and can, therefore, be neglected. To leading (linear) order in the RKKY coupling, $\hat{\Gamma}_{cf}$ thus reads (in Matsubara representation)

$$\begin{aligned}\hat{\Gamma}_{cf} &= [J\delta_{ij} + \gamma^{(d)}_{\text{RKKY}}(\mathbf{r}_{ij}, i\Omega)]\mathbf{S}_i \cdot \mathbf{s}_j \\ &= [J\delta_{ij} + 2JJ_0^2(1-\delta_{ij})\chi_c(\mathbf{r}_{ij}, i\Omega)\tilde{\chi}_f(i\Omega)]\mathbf{S}_i \cdot \mathbf{s}_j, \quad (2)\end{aligned}$$

where $\mathbf{r}_{ij} = \mathbf{x}_i - \mathbf{x}_j$ is the distance vector between the sites i and j, and Ω is the energy transferred in the scattering process. $\chi_c(\mathbf{r}_{ij}, i\Omega)$ is the c electron density correlation function between sites i and j [bubble of solid lines in Fig. 1(a)] and $\tilde{\chi}_f(i\Omega) \coloneqq \chi_f(i\Omega)/(g_L\mu_B)^2$ with g_L the Landé factor and μ_B the Bohr magneton. Note that Eq. (2) contains the running coupling J at site i, which will be renormalized under the RG, while at the site j, where the c electron scatters, the bare coupling J_0 appears, since all vertex renormalizations on that site are already included in the exact susceptibility χ_f. Higher order terms, as for instance generated by the RG [see below, Fig. 1(b)], lead to nonlocality of the incoming and outgoing coordinates of the scattering c electrons, $\mathbf{x}_j$, $\mathbf{x}_{j'}$, but the f-spin coordinate $\mathbf{x}_i$ remains strictly local, since the pseudofermion propagator $G_f(i\nu) = 1/i\nu$ is local [26]. For this reason, speaking

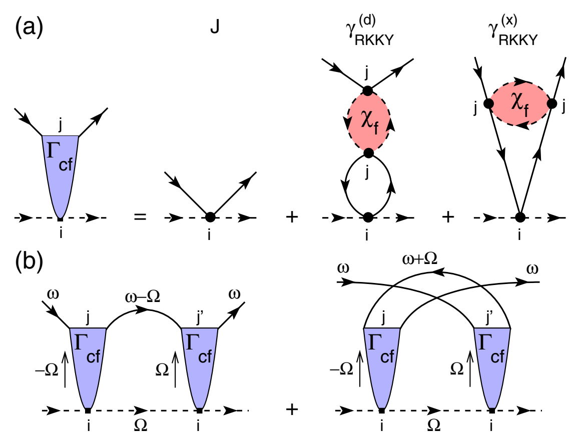

FIG. 1. (a) f-spin–c-electron vertex $\hat{\Gamma}_{cf}$, composed of the on-site vertex J at site i and the RKKY-induced contributions from surrounding sites $j \neq i$ to leading order in the RKKY coupling: $\gamma^{(d)}_{\text{RKKY}}$ (direct term) and $\gamma^{(x)}_{\text{RKKY}}$ (exchange term). (b) One-loop diagrams for the perturbative RG. Solid lines: electron Green's functions G_c. Dashed lines: pseudofermion propagators G_f of the local f spins. The red bubbles represent the full f-spin susceptibility at sites j.

of Kondo singlet formation on a single Kondo site is well defined even in a Kondo lattice, and so is the local susceptibility χ_f of a single f spin. The corresponding Kondo scale T_K on a site j is observable, e.g., as the Kondo resonance width measured by STM spectroscopy on one Kondo ion of the Kondo lattice. The temperature dependence of the single-site f-spin susceptibility is known from the Bethe ansatz solution [27] in terms of the Kondo scale T_K. It has a $T = 0$ value $\chi_f(0) \propto 1/T_K$ and crosses over to the $1/T$ behavior of a free spin for $T > T_K$. These features can be modeled in the retarded or advanced, local, dynamical f-spin susceptibility $\chi_f(\Omega \pm i0)$ as

$$\chi_f(\Omega \pm i0) = \frac{(g_L\mu_B)^2 W}{\pi T_K \sqrt{1+(\Omega/T_K)^2}}\left(1 \pm \frac{2i}{\pi}\operatorname{arsinh}\frac{\Omega}{T_K}\right), \tag{3}$$

where W is the Wilson ratio, and the imaginary part is implied by the Kramers-Kronig relation.

We now derive the one-loop RG equation for the c-f vertex $\hat{\Gamma}_{cf}$, including RKKY-induced, nonlocal contributions. The one-loop spin vertex function is shown diagrammatically in Fig. 1(b). Using Eq. (2), the sum of these two diagrams is up to linear order in the RKKY coupling

$$\begin{aligned} Y(\mathbf{r}_{ij}, i\omega) = -JT\sum_{i\Omega}&[J\delta_{ij} + \gamma^{(d)}_{\mathrm{RKKY}}(\mathbf{r}_{ij}, i\Omega) \\ &+ \gamma^{(d)}_{\mathrm{RKKY}}(\mathbf{r}_{ij}, -i\Omega)] \times [G_c(\mathbf{r}_{ij}, i\omega - i\Omega) \\ &- G_c(\mathbf{r}_{ij}, i\omega + i\Omega)]G_f(i\Omega). \end{aligned} \tag{4}$$

Here, ω is the energy of the incoming conduction electrons, $G_c(\mathbf{r}_{ij}, i\omega + i\Omega)$ is the single-particle c electron propagator from the incoming to the outgoing site. For example, for an isotropic system, $G_c(\mathbf{r}, \omega \pm i0) = -\pi N(\omega) e^{\pm ik(\varepsilon_F+\omega)r}/k(\varepsilon_F + \omega)r$ with the bare density of states $N(\omega)$, and $k(\varepsilon_F + \omega)$ the modulus of the momentum corresponding to the energy ω.

For the low-energy physics, the vertex renormalization for c electrons at the Fermi surface is required. This means setting the energy $i\omega \to \omega = 0 + i0$ and Fourier transforming the total vertex $Y(\mathbf{r}_{ij}, i\omega)$ with respect to the incoming and outgoing c electron coordinates $\mathbf{x}_j$, $\mathbf{x}_i$, and taking its Fourier component for momenta at the Fermi surface $\mathbf{k}_F$, see Ref. [24]. Note that at the Fermi energy $Y(\mathbf{k}_F, 0)$ is real, even though the RKKY-induced, dynamical vertex $\gamma^{(d)}_{\mathrm{RKKY}}(\pm i\Omega)$ appearing in Eq. (4) is complex valued [24]. This ensures the total vertex operator of the renormalized Hamiltonian is Hermitian. By analytic continuation, the Matsubara summation in Eq. (4) becomes an integration over the intermediate c electron energy from the lower and upper band cutoff D to the Fermi energy ($\Omega = 0$). The coupling constant renormalization is then obtained in the standard way by requiring that $Y(\mathbf{k}_F, 0)$ be invariant under an infinitesimal reduction of the running band cutoff D. Note that the band cutoff appears in both the intermediate electron propagator G_c and in χ_c. However, differentiation of the latter does not contribute to the logarithmic RG flow. This leads to the one-loop RG equation [24]

$$\frac{dg}{d\ln D} = -2g^2\left(1 - yg_0^2\frac{D_0}{T_K}\frac{1}{\sqrt{1+(D/T_K)^2}}\right), \tag{5}$$

where we have introduced the dimensionless couplings $g = N(0)J$, $g_0 = N(0)J_0$, and D_0 is the bare band cutoff. The first term on the right-hand side of Eq. (5) is the on-site contribution to the differential coupling renormalization (the β function), while the second term represents the RKKY contribution. It is seen that χ_f, as in Eq. (3), induces a soft cutoff on the scale T_K and the characteristic $1/T_K$ dependence to the RG flow of this contribution, where T_K is the Kondo scale on the surrounding Kondo sites. The dimensionless coefficient

$$y = -\frac{8W}{\pi^2}\mathrm{Im}\sum_{j\neq i}\frac{e^{-i\mathbf{k}_F\mathbf{r}_{ij}}}{N(0)^2}G^R_c(\mathbf{r}_{ij}, \Omega=0)\chi_c(\mathbf{r}_{ij}, \Omega=0) \tag{6}$$

arises from the Fourier transform $Y(\mathbf{k}_F, 0)$ and parametrizes the RKKY coupling strength. The summation in Eq. (6) runs over all positions $j \neq i$ of Kondo sites in the system. It is important to note that y is generically positive [24], even though the RKKY correlations $\chi_c(\mathbf{r}_{ij}, 0)$ may be ferro- or antiferromagnetic. For instance, for an isotropic and dense system with lattice constant a ($k_F a \ll 1$), the summation in Eq. (6) can be approximated by an integral, and with the substitution $x = 2k_F|\mathbf{r}_{ij}|$, y can be expressed as

$$y \approx \frac{2W}{(k_F a)^3}\int_{k_F a}^{\infty} dx(1-\cos x)\frac{x\cos x - \sin x}{x^4} > 0. \tag{7}$$

As a consequence, the RKKY correlations reduce the g renormalization in Eq. (5), irrespective of the sign of $\chi_c(\mathbf{r}_{ij}, 0)$, as one would physically expect.

Universal suppression of the Kondo scale.—The RG (5) can be integrated analytically [24]. The Kondo scale for singlet formation on site i is defined as the running cutoff value where the c-f coupling g diverges. By equivalence of all Kondo sites, this is equal to the Kondo scale T_K on the surrounding sites $j \neq i$, which appears as a parameter in the β function on the right-hand side of Eq. (5). This implies an implicit equation for the Kondo scale $T_K = T_K(y)$ in a Kondo lattice, and that it depends on the RKKY parameter y

$$\frac{T_K(y)}{T_K(0)} = \exp\left(-y\alpha g_0^2\frac{D_0}{T_K(y)}\right). \tag{8}$$

Here, $T_K(0) = D_0 \exp(-1/2g_0)$ is the single-ion Kondo scale without RKKY coupling, and $\alpha = \ln(\sqrt{2}+1)$. By the rescaling, $u = T_K(y)/(y\alpha g_0^2 D_0)$, $y_c = T_K(0)/(\alpha e g_0^2 D_0)$, Eq. (8) takes the universal form (e is Euler's constant),

$$\frac{y}{e y_c} u = e^{-1/u}. \tag{9}$$

Its solution can be expressed in terms of the Lambert W function [28] as $u(y) = -1/W(-y/ey_c)$. The inset of Fig. 2 visualizes solving Eq. (9) graphically. It shows that Eq. (9) has solutions only for $y \le y_c$. This means that y_c marks a Kondo breakdown point beyond which the RG does not scale to strong coupling; i.e., a Kondo singlet is not formed for $y > y_c$ even at the lowest energies. Using the above definitions, the RKKY-induced suppression of the Kondo lattice temperature reads $T_K(y)/T_K(0) = u(y)y/(ey_c) = -y/[ey_c W(-y/ey_c)]$. It is shown in Fig. 2. In particular, at the breakdown point it vanishes discontinuously and takes the finite, universal value (see the inset of Fig. 2)

$$\frac{T_K(y_c)}{T_K(0)} = \frac{1}{e} \approx 0.368. \tag{10}$$

We emphasize that the RKKY parameter y depends on details of the conduction band structure, including band renormalizations caused by the Kondo effect (coupling to the heavy-fermion band). It also depends on the spatial arrangement of Kondo sites. Subleading contributions to Γ_{cf} may modify the form of the cutoff function in the RG (5) and thus the nonuniversal parameter α. However, all this does not affect the universal dependence of $T_K(y)$ on y given by Eq. (9).

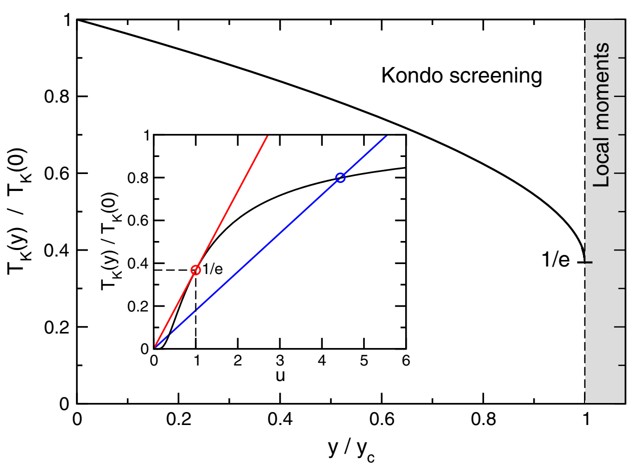

FIG. 2. Universal dependence of $T_K(y)/T_K(0)$ on the normalized RKKY parameter y/y_c, solution of Eq. (9). The inset visualizes the solution of Eq. (9) graphically. Black, solid curve: right-hand side of Eq. (9). Blue line: left-hand side for $y < y_c$. Red line: left-hand side for $y = y_c$ (where the red line and black curve touch). It proves that there is a critical coupling y_c beyond which Eq. (9) has no solution, and $T_K(y_c)/T_K(0) = 1/e$.

The critical RKKY parameter, as defined before Eq. (9), can be expressed solely in terms of the single-ion Kondo scale

$$y_c = \frac{4}{\alpha e} \tau_K (\ln \tau_K)^2 \tag{11}$$

with $\tau_K = T_K(0)/D_0$. Note that [via $T_K(0) = D_0 \exp(-1/2g_0)$ and $N(0) = 1/(2D_0)$] this is equivalent to Doniach's breakdown criterion [6] $N(0) y_c J_0^2 = T_K(0)$ up to a factor of $O(1)$. However, the present theory goes beyond the Doniach scenario in that it predicts the behavior of $T_K(y)$.

Comparison with experiments.—The present theory applies directly to two-impurity Kondo systems and can be compared to corresponding STM experiments [18,19]. In Ref. [18], the Kondo scale has been extracted as the line width of the (hybridization-split) Kondo-Fano resonance. In this experimental setup, the RKKY parameter y is proportional to the overlap of tip and surface c electron wave functions and, thus, depends exponentially on the tip-surface separation z, $y = y_c \exp[-(z - z_0)/\xi]$. Identifying the experimentally observed breakdown point $z = z_0$ with the Kondo breakdown point, the only adjustable parameters are a scale factor ξ of the z coordinate and $T_K(0)$, which is the resonance width at large separation, $z = 300$ pm. The agreement between theory and experiment is striking, as shown in Fig. 3. In particular, at the breakdown point $T_K(y_c)/T_K(0)$ coincides accurately with the prediction (10) without any adjustable parameter. In the STM experiment of Ref. [19], the strongest observed suppression ratio is $T_K(y)/T_K(0) = 46\text{K}/110\text{K} \approx 0.42$, again in excellent agreement with the strongest theoretical suppression of $1/e$, considering that in Ref. [19] the RKKY coupling y

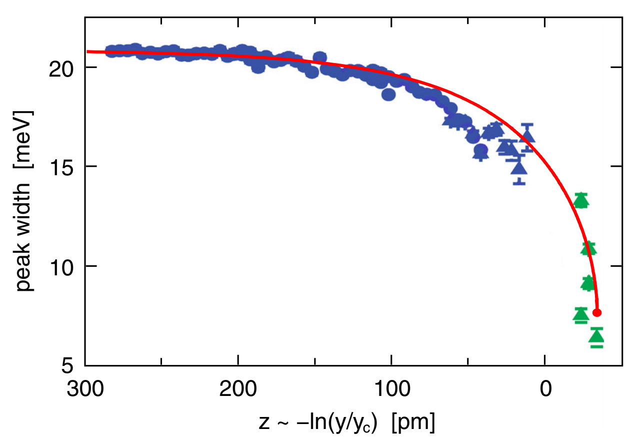

FIG. 3. Comparison of the theory (9) (red curve) with STM spectroscopy experiments on a tunable two-impurity Kondo system [18] (data points). The data points represent the Kondo scale T_K as extracted from the STM spectra by fitting a split Fano line shape of width T_K to the experimental spectra. Blue points: STM tunneling regime. Green points: contact regime. See Ref. [18] for experimental details.

cannot be varied continuously. The detailed analysis of that experiment will be published elsewhere [29].

Discussion and conclusion.—We have derived a perturbative renormalization group theory for the interference of Kondo singlet formation and RKKY interaction in Kondo lattice and multi-impurity systems, assuming that magnetic ordering is suppressed, e.g., by frustration. The equivalence of the c-f vertices on all Kondo sites is reminiscent of a dynamical mean-field theory treatment; however, it goes beyond the latter in taking the nonlocal RKKY contributions into account. Equations (8) or (9) represent a mathematical definition of the energy scale for Kondo singlet formation in a Kondo lattice, i.e., of the Kondo lattice temperature $T_K(y)$. The theory predicts a universal suppression of $T_K(y)$ and a breakdown of complete Kondo screening at a critical RKKY parameter $y = y_c$. At the breakdown point, the Kondo scale takes a finite, universal value $T_K(y_c)/T_K(0) = 1/e \approx 0.368$, and vanishes discontinuously for $y > y_c$. In the Anderson lattice, by contrast to the Kondo lattice, the locality of the f spin no longer strictly holds, but our approach should still be valid in this case. The parameter-free, quantitative agreement of this behavior with different spectroscopic experiments [18,19] strongly supports that the present theory captures the essential physics of the Kondo-RKKY interplay.

The results may have profound relevance for heavy-fermion magnetic QPTs. In an unfrustrated lattice, the partially screened local moments existing for $y > y_c$ must undergo a second-order magnetic ordering transition at sufficiently low temperature. This will also imply a power law divergence of the c electron correlation χ_c in Eq. (2). We have checked the effect of such a magnetic instability, induced either by the ordering of remanent local moments or by a c electron SDW instability: the breakdown ratio $T_K(y_c)/T_K(0)$ will be altered, but must remain nonzero. The reason is that the inflection point of the exponential function on the right-hand side of Eq. (9) (see Fig. 2) is not changed by such a divergence and, therefore, the solution ceases to exist at a finite value of $T_K(y_c)$. This points to an important conjecture about a possible, new quantum critical scenario with Kondo destruction: the Kondo spectral weight may vanish continuously at the QCP, while the Kondo scale $T_K(y)$ (resonance width) remains finite, both as observed experimentally in Ref. [18]. Such a scenario may reconcile apparently contradictory experimental results in that it may fulfill dynamical scaling, even though $T_K(y_c)$ is finite at the QCP. The present theory sets the stage for constructing a complete theory of magnetic ordering and RKKY-induced Kondo destruction.

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*kroha@physik.uni-bonn.de

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