Disorder-Driven Non-Fermi-Liquid Behavior in Kondo Alloys

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We show how a model of disordered Anderson lattices can account for many non-Fermi-liquid features observed in some Kondo alloys. Because of the exponential nature of the Kondo temperature scale T_K, even moderate disorder leads to a rather broad distribution of Kondo temperatures, inducing strong *effective* disorder seen by the conduction electrons. Spins with very low T_K's remain unquenched and dominate the low-temperature properties. This single underlying mechanism leads to logarithmic divergences in thermodynamic quantities and a linear temperature dependence of the resistivity. [S0031-9007(96)02090-X]

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Non-Fermi-liquid (NFL) behavior in metals represents one of the key unresolved issues in condensed matter physics. There exists by now a large class of nonmagnetic metallic *f*-electron materials which do not behave as Fermi liquids at low temperatures [1–8]. In some of them the proximity to a $T = 0$ quantum critical point appears to be the origin of the anomalous behavior [6,8,9]. However, in several other cases NFL behavior occurs only when the system has been sufficiently alloyed so that it is not close to any phase boundary. This is the case of the alloys $UCu_{5-x}Pd_x$ [1,2], $M_{1-x}U_xPd_3$ ($M =$ Sc, Y [3,7], $La_{1-x}Ce_xCu_{2.2}Si_2$ [4], $Ce_{1-x}Th_xRhSb$ [5], and $U_{1-x}Th_xPd_2Al_3$ [7]. In all of these systems the specific heat varies as $C(T)/T \approx a \ln(T_0/T)$ and the resistivity is linear with a large zero-temperature intercept $\rho(T) \approx \rho_0(1 - T/T_1)$. The magnetic susceptibility has been often fitted by a logarithm or a weak power law.

Some attempts have been made to explain the anomalous low-temperature properties based on exotic one-impurity mechanisms, such as the quadrupolar Kondo model [10]. Inconsistencies with the predictions of the model for the resistivity ($\approx\sqrt{T}$) and in an applied magnetic field in some of these systems, however, invite the consideration of other mechanisms for NFL behavior [11].

Quite generally, the *large residual resistivity* of these systems together with their alloy nature immediately suggests that disorder could be significant. In an important recent study [2], the strong broadening of the copper NMR line of $UCu_{5-x}Pd_x$ ($x = 1$ and 1.5) has provided an independent indication of the essential role played by disorder in at least one of these compounds. These results suggested the presence of strong spatial fluctuations in the characteristic Kondo temperature T_K of the local moments [12]. Indeed, by using a model distribution function $P(T_K)$ and well-known single-impurity results, they were then able to quantitatively describe the low-temperature thermodynamic properties (specific heat and magnetic susceptibility) as well as the NMR linewidths. The proposed picture implicitly assumes independent local moments, which is usually sufficient for understanding the thermodynamics of most heavy fermion compounds. Of course, in the context of transport in concentrated Kondo systems, such an assumption appears to be unjustified, since it cannot be reconciled with the well-established coherence effects at low temperatures.

The central question addressed in this Letter is whether disorder effects can explain not only the thermodynamics, but also *the anomalous transport* in these systems. We will formulate a theory appropriate for *concentrated* magnetic impurities, which can describe the coherence effects in the clean limit. We will show that correlation effects strongly enhance any extrinsic disorder, generating an extremely broad distribution of Kondo temperatures. This leads to the destruction of coherence and, for sufficient disorder, to the breakdown of Fermi-liquid behavior. The low-temperature properties can be viewed as resulting from a *dilute gas* of localized elementary excitations: those Kondo spins that remain unquenched. This picture of dirty Kondo lattices, similar in spirit to the original Landau description of simple metals, provides a unified theoretical underpinning for one possible route to marginal Fermi-liquid behavior.

We start with a disordered nondegenerate infinite-*U* Anderson lattice model

$$H = \sum_{\sigma} \epsilon(\boldsymbol{k}) c_{\sigma}^{\dagger} c_{\sigma} + \sum_{j\sigma} E_j^f f_{j\sigma}^{\dagger} f_{j\sigma} + \sum_{j\sigma} V_j (c_{j\sigma}^{\dagger} f_{j\sigma} + \text{H.c.}), \qquad (1)$$

where c_{σ} destroys a conduction electron with momentum $\boldsymbol{k}$ and spin σ from a broad uncorrelated band with dispersion $\epsilon(\boldsymbol{k})$ and half bandwidth D, and $f_{j\sigma}$ destroys an *f* electron at site j with spin σ. The infinite-*U* constraint

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at each f orbital is assumed ($n_j^f \leq 1$). The on-site energies E_j^f and the hybridization matrix elements V_j are assumed to be distributed according to some distribution functions $P_1(E_f)$ and $P_2(V)$. In the Kondo limit, the local Kondo temperature is given by $T_{Kj} = D\exp(E_j^f/2\rho_0 V_j^2)$ ($\rho_0 \approx \frac{1}{2D}$) and will be correspondingly distributed. Because of the strong scattering off the f sites, disorder in f parameters is dominant, and we will thus neglect other types of disorder in the c band.

To analyze the properties of our model, we focus on the dynamical self-consistent theory of strong correlations and disorder [13,14]. The problem can then be reduced to an ensemble of one-impurity problems in a self-consistently generated self-averaging bath of conduction electrons. The equations simplify considerably in the case of a semicircular conduction electron density of states, where the ensemble of impurity problems is governed by the action

$$S_j^{\mathrm{imp}} = \sum_{\omega_n} (f_{j\sigma}^\dagger[-i\omega_n + E_j^f + \Delta_j(i\omega_n)]f_{j\sigma}), \qquad (2)$$

where the infinite-U constraint is implied and

$$\Delta_j(\omega) = \frac{V_j^2}{\omega + \mu - t^2\overline{G}_c(\omega)}. \qquad (3)$$

Here t is the hopping parameter, μ the chemical potential, and $\overline{G}_c(\omega)$ is the disorder-averaged local conduction electron Green's function. The latter is determined self-consistently by

$$\overline{G}_c(\omega) = \left\langle \frac{1}{\omega + \mu - t^2\overline{G}_c(\omega) - \Phi_j(\omega)} \right\rangle^{\mathrm{av}}, \qquad (4)$$

where

$$\Phi_j(\omega) = \frac{V_j^2}{\omega - E_j^f - \Sigma_{fj}^{\mathrm{imp}}(\omega)}. \qquad (5)$$

Here $\langle\cdots\rangle^{\mathrm{av}}$ denotes the average over disorder and $\Sigma_{fj}^{\mathrm{imp}}(\omega)$ is the f electron self-energy derived from the impurity model of Eq. (2). In the absence of disorder, these equations reduce to the dynamical mean-field theory of the Anderson lattice [14], while for $U = 0$ they are equivalent to the CPA treatment of disorder [15] for the *conduction electrons* [16]. In general, the theory is exact in the limit of large coordination. Once $\overline{G}_c(\omega)$ has been determined, the conduction electron self-energy $\Sigma_c(\omega)$ can be obtained from

$$\overline{G}_c(\omega) = \int d\epsilon \, \frac{\rho_0(\epsilon)}{\omega + \mu - \epsilon - \Sigma_c(\omega)}, \qquad (6)$$

where $\rho_0(\epsilon) = \sqrt{1 - (\epsilon/2t)^2}/\pi t$.

Let us analyze the qualitative behavior of $\Phi_j(\omega)$. From the Fermi-liquid analysis of the impurity problem, it is well known that $\Sigma_{fj}^{\mathrm{imp}}(\omega = 0)$ is a real quantity at $T = 0$ [17]. Therefore, one can write

$$\Phi_j(\omega = 0) = -\frac{V_j^2}{E_j^f + \mathrm{Re}[\Sigma_{fj}^{\mathrm{imp}}(0)]}. \qquad (7)$$

$\Phi_j(0)$ measures the scattering strength at site j at the Fermi level. In the clean limit, $\Phi_j(\omega)$ will be the same at every site and Eqs. (4) and (6) give $\Sigma_c(\omega) = \Phi(\omega)$. In this case $\Sigma_c(\omega = 0)$ is a real quantity, reflecting the coherent nature of the dc transport at zero temperature.

By contrast, when the system is disordered, a distribution of scattering strengths Φ_j is generated, strongly affecting the transport properties. By applying the large-N mean field theory to the impurity problems at zero temperature, we have solved the self-consistent problem defined by Eqs. (2)–(5). The resulting scattering rates as a function of the width of the E_f distribution (for a fixed uniform value of V) are shown in Fig. 1. Similar results are obtained for a distribution of V values holding E_f fixed. For the residual resistivities reported for the NFL alloys, e.g., $UCu_{5-x}Pd_x$ [1], one can estimate $D\tau \approx 3-5$. Because of the strong f-shell correlations, rather large scattering rates can be generated by a small disorder strength in f parameters [see Fig. 1 and Eq. (7)]. Comparable amounts of disorder, in the absence of correlations, cannot produce these large resistivities.

Thus with sufficient disorder, scattering off the f sites becomes incoherent and the resistivity assumes a monotonically decreasing temperature dependence, resembling the single-impurity result. The actual scattering rate, however, requires the solution of the full set of Eqs. (2)–(5). If $P(T_K)$ is broad enough, the low-temperature dependence can be nontrivial. To analyze that, it is useful to rewrite the above equations in terms of the impurity T matrix $T_j^{\mathrm{imp}}(\omega) \equiv V_j^2 G_{fj}(\omega)$, where $G_{fj}(\omega)$ is the f Green's function computed from the action in Eq. (2). We find (for $\mu = 0$)

$$\overline{G}_c(\omega) = \frac{1}{\omega - t^2\overline{G}_c(\omega)} + \frac{\langle T_j^{\mathrm{imp}}(\omega)\rangle^{\mathrm{av}}}{[\omega - t^2\overline{G}_c(\omega)]^2}, \qquad (8)$$

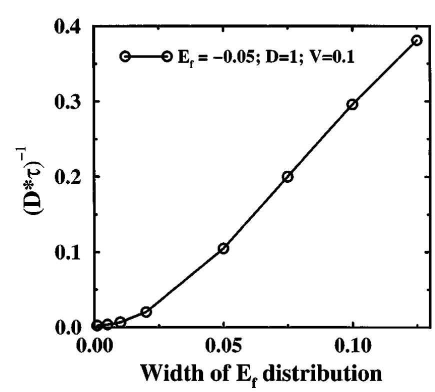

FIG. 1. Scattering rate as a function of the width of the E_f distribution. The parameters used are shown in the figure. The strong correlations in the f shell produce an enhanced effective disorder.

and, from Eq. (6),

$$\Sigma_c(\omega) = \frac{\langle T_j^{\rm imp}(\omega)\rangle^{\rm av}}{\overline{G}_c(\omega)[\omega - t^2\overline{G}_c(\omega)]}. \quad (9)$$

We now raise the temperature slightly from 0 to T and denote corresponding variations by δ_T. Then

$$\delta_T\Sigma_c(\omega) = \frac{1 - t^2G_c^2(\omega)}{G_c^2(\omega)}\bigg|_{T=0}\delta_T G_c(\omega); \quad (10a)$$

$$A(\omega)\delta_T G_c(\omega) - \int d\omega' B(\omega,\omega')\delta_T G_c(\omega') = \langle\delta_T T_j^{\rm imp}(\omega)\rangle^{\rm av}\bigg|_{G_c^0}, \quad (10b)$$

where

$$A(\omega) = \left\{t^2 + [\omega - t^2G_c(\omega)][\omega - 3t^2G_c(\omega)] - \frac{t^2\langle[T_j^{\rm imp}(\omega)]^2\rangle^{\rm av}}{[\omega - t^2G_c(\omega)]^2}\right\}\bigg|_{T=0}; \quad (11a)$$

$$B(\omega,\omega') = \left\langle\frac{[T_j^{\rm imp}(\omega)]^2}{V_j^2}\,\frac{\delta\Sigma_{fj}^{\rm imp}(\omega)}{\delta G_c(\omega')}\right\rangle^{\rm av}\bigg|_{T=0}. \quad (11b)$$

Here the temperature dependence of the self-energy is expressed in terms of the temperature dependence of the disorder-averaged T matrix. In general, the self-consistency condition couples different frequencies, as seen in the integral equation (10b). However, the *leading low-temperature behavior* is determined only by the $\omega = 0$ component of the averaged T matrix, so in the following we concentrate on this object.

Figure 2 shows the result of averaging the imaginary part of the single impurity T matrix over the distribution of Kondo temperatures deduced from the experiments of Ref. [2]. For the single impurity dependence, we used a simple scaling form with the correct asymptotic behavior at high and low temperatures. The dependence is linear at low temperatures.

It is easy to understand the origin of the linear behavior and why it does not depend on the detailed shape of $P(T_K)$. We will focus on the imaginary part of the impurity T matrix since it gives the dominant contribution. It has the following scaling form:

$$T''_{\rm imp}(T) = \frac{\sin^2\delta_0}{\pi\rho_0}\,t\left(\frac{T}{T_K}\right), \quad (12)$$

where δ_0 is the phase shift at $T = 0$. The function $t(x)$ has the following asymptotics:

$$t(x) \approx \begin{cases} 1 - \alpha x^2, & x \ll 1, \\ \beta/[\ln(x)]^2, & x \gg 1, \end{cases} \quad (13)$$

where α and β are universal numbers. It follows that

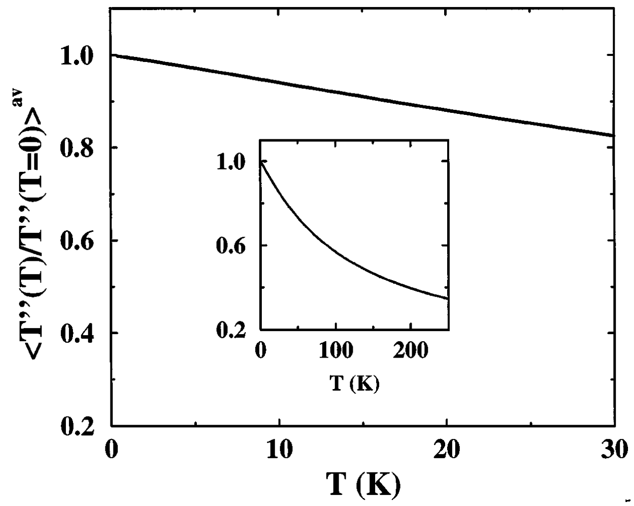

FIG. 2. Temperature dependence of the imaginary part of the single impurity T matrix averaged over the disorder distribution appropriate for $UCu_{3.5}Pd_{1.5}$, as determined experimentally in Ref. [2]. The inset shows the same quantity over a wider temperature range.

$$\delta_T T''_{\rm imp} = -\frac{\sin^2\delta_0}{\pi\rho_0}\left[1 - t\left(\frac{T}{T_K}\right)\right] \equiv -\frac{\sin^2\delta_0}{\pi\rho_0}F(T/T_K). \quad (14)$$

Now, *for a fixed temperature T and as a function of* T_K

$$F(T/T_K) \approx \begin{cases} \dfrac{\alpha T^2}{T_K^2}, & T_K \gg T, \\ 1 - \dfrac{\beta}{[\ln(T/T_K)]^2}, & T_K \ll T. \end{cases} \quad (15)$$

$F(T/T_K)$ is strongly peaked at $T_K \approx 0$, decays as $1/T_K^2$, and has a width of order T (see Fig. 3). For low T, it can be written in terms of a delta function of T_K, hence

$$\delta_T T''_{\rm imp} \approx -\frac{a\sin^2\delta_0}{\pi\rho_0}T\delta(T_K), \quad (16)$$

where $a = \int dx F(1/x)$. When inserted into Eqs. (10), this yields

$$\delta_T\Sigma_c \approx -\frac{iaP(0)}{\pi\rho_0 A_0}T. \quad (17)$$

Therefore, the low-temperature dependence probes only $P(T_K)$ at low values of T_K, as is clear from Fig. 3. In that region, $P(T_K)$ can be taken to be a constant and the temperature can be scaled out of the average, yielding the negative linear term [18]. As long as the distribution of Kondo temperatures is wide enough so that $P(0)$ is appreciable, there will be a sizable linear range. For sufficiently weak disorder, $P(0)$ is zero or negligible and Fermi-liquid behavior is recovered.

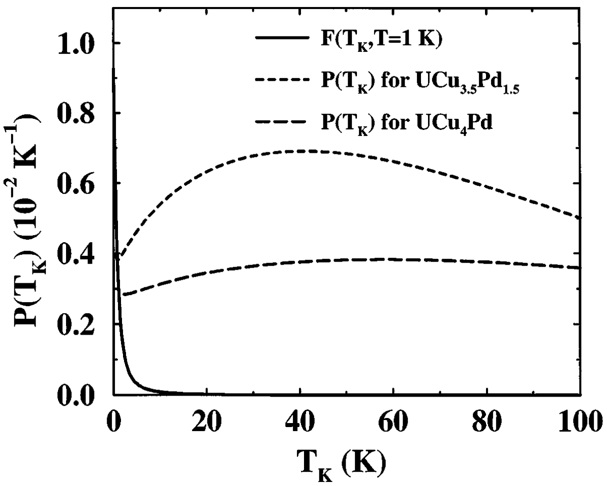

FIG. 3. Comparison of the experimentally determined distribution of Kondo temperatures of the alloys $UCu_{5-x}Pd_x$ ($x = 1, 1.5$) (from Ref. [2]) with the function $F(T_K, T)$ defined in the text (see also [18]). The function $F(T_K, T)$ probes only the $T_K = 0$ value of the distributions at low T.

Physically, it is clear what is happening. As the temperature is raised, *a few diluted* spins with $T_K < T$ are unquenched and cease to contribute to the resistivity. The linear term essentially counts the number of liberated spins. Since this number is small at low temperatures, they form a dilute system of removed scatterers, whose effect is additive (or rather, subtractive), rendering our treatment of disorder essentially exact. Thus even though the zero-temperature resistivity is a functional of the whole distribution $P(T_K)$, the low-temperature linear behavior is a much more robust feature which depends only on the low T_K tail $P(0)$.

Within the dynamical mean field theory it is possible to show that the picture of independent f sites of Ref. [2] is justified for thermodynamic quantities. An argument similar to the ones above then gives $\chi(T) \sim \ln(T_2/T)$ and $C_V(T)/T \sim \ln(T_0/T)$. Again in this case, the NFL behavior is due to the presence of very-low-T_K spins.

It is important to comment on the potential limitations of this approach. In particular, we note that the dynamical mean field approach cannot describe the effects of the RKKY interactions. One could imagine that pairs of local moments with very low T_K could well condense into RKKY singlets, affecting the temperature dependence. However, if $P(T_K)$ is very broad, the fraction of low-T_K spins is very small, and they will be, in general, very far apart, rendering the RKKY interaction less effective.

In summary, we have analyzed the effects of disorder in concentrated Kondo alloys with the dynamical mean field theory. We find that sufficient disorder can lead to considerable modifications of low-temperature properties, leading to the breakdown of conventional Fermi liquid behavior, consistent with some Kondo alloys. The NFL features are traced back to a single unifying mechanism: the presence of very-low-T_K spins which remain unquenched at any finite temperature.

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[15] E. N. Economou, *Green's Functions in Quantum Physics* (Springer-Verlag, Berlin, 1983), p. 141.
[16] The central approximation in the treatment of disorder is to ignore the spatial fluctuations of the *conduction* electrons, but *not* of the localized f electrons. In Kondo lattices, this is a good approximation, since the conduction electron bandwidth is the largest energy scale in the problem and so the conduction electrons are not close to Anderson localization, where we can expect our approach to break down. In contrast, the f-electron fluctuations are included and are, in fact, at the origin of most anomalies.
[17] See, e.g., A. C. Hewson, *The Kondo Problem to Heavy Fermions* (Cambridge University Press, Cambridge, England, 1993), Sec. 5.
[18] Actually, $P(T_K)$ from Ref. [2] diverges weakly as $[T_K \ln^2(T_K/D)]^{-1}$ as $T_K \longrightarrow 0$. However, the upturn sets in only at $T_K \approx 0.8$ K ($x = 1.5$) and $T_K \approx 2.4$ K ($x = 1.5$), which can hardly be distinguished on the scale of Fig. 3, has a very small weight, and does not affect our conclusions down to these low temperatures.