Disorder-driven non-Fermi liquid behavior in Kondo alloys

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We demonstrate that a model of disordered Anderson lattices can account for many non-Fermi liquid features observed in a number of Kondo alloys. Due to the exponential nature of the Kondo temperature scale, even moderate disorder leads to a rather broad distribution of Kondo temperatures, inducing strong effective disorder seen by the conduction electrons. Spins with very small Kondo temperatures remain unquenched and dominate the low temperature properties. The model predicts logarithmic divergences in thermodynamic quantities at low temperatures. We also find a linear temperature dependence of the resistivity, a feature that remained a stumbling block in previous theoretical attempts. We argue that for realistic amounts of disorder, such marginal Fermi liquid behavior is a very robust feature of disordered Kondo alloys.

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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 non-magnetic metallic f-electron materials which do not behave as Fermi liquids at low temperatures [1-8]. In some of them, the proximity to a quantum critical point appears to be the origin of the anomalous behavior [8]. However, in several other cases, NFL behavior only occurs when the system has been sufficiently alloyed so that it is not close to any phase boundary. This is the case of the alloys UCu5-xPdx [1,2], M1-xUxPd3 (M = Sc,Y) [3,4], La1-xCe2Cu2Si2 [5], Ce1-xThxRhSb [6], U1-xThxPd2Al3 [7]. In all of these systems the specific heat varies as C(T)/T ≈ a ln(T0/T) and the resistivity is linear with a large zero temperature intercept ρ(T) ≈ ρ0(1 − T/T0). 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 (∝ T) and in an applied magnetic field in some of these systems, however, invite the consideration of other mechanisms for NFL behavior.

Quite generally, the large residual resistivity of these systems together with their alloy nature immediately suggest that disorder could be significant. In an important recent study [3], the strong broadening of the copper NMR line of UCu5-xPdx (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 TK of the local moments [11]. Indeed, by using a model distribution function P(TK) 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 will 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 clear theoretical underpinning for one route towards marginal Fermi liquid behavior.

We start with a disordered non-degenerate infinite-U Anderson lattice model

\[
H = \sum_{k\sigma} \epsilon(k)c_{k\sigma}^\dagger c_{k\sigma} + \sum_{\beta\sigma} E^{f}_{\beta} f_{\beta\sigma}^\dagger f_{\beta\sigma} + \sum_{j\sigma} V_{j}(c_{j\sigma}^\dagger f_{j\sigma} + H.c.),
\]

where, c_{k\sigma} destroys a conduction electron with moment-
tum $k$ and spin $\sigma$ from a broad uncorrelated band with dispersion $\epsilon(k)$ and half bandwidth $D$ and $f_{j\sigma}$ destroys an f-electron at site $j$ with spin $\sigma$. The infinite-U constraint at each f-orbital is assumed ($n_f^j \leq 1$). The on-site energies $E_f^j$ 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 $T_{Kj} = D \exp(E_f^j/(2\rho_0 V_j^2))$ ($\rho_0 \approx 4\pi$) 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 correlation and disorder [3]. 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 spherical conduction density of states, where the ensemble of impurity problems is governed by the action

$$S_{imp}^{j} = \sum_{\omega_n} \left[ f_{j\sigma}^\dagger \left( -i\omega_n + E_f^j + \Delta_j(i\omega_n) \right) f_{j\sigma} \right],$$

(2)

where the infinite-U constraint is implied and

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

(3)

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

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

(4)

where

$$\Phi_j(\omega) = \frac{V_j^2}{\omega - E_f^j - \Sigma_{imp}^{j}(\omega)}.$$  

(5)

Here $\langle \ldots \rangle^{av}$ denotes the average over disorder and $\Sigma_{imp}^{j}(\omega)$ is the f-electron self-energy derived from the impurity model of Eq. (3). In absence of disorder, these equations reduce to the dynamical mean-field theory of the Anderson lattice [13], while for $U = 0$ they are equivalent to the CPA treatment of disorder [14] for the conduction electrons [13]. 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

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

(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 $\Sigma_{imp}^{j}(\omega = 0)$ is a real quantity at $T = 0$ [14]. Therefore, one can write

$$\Phi_j(\omega = 0) = -\frac{V_j^2}{E_f^j + \text{Re}[\Sigma_{imp}^{j}(0)]},$$  

(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 (5) 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 $\Phi_j$ 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. (3–5). 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$_x$ [4], one can estimate $D \tau \approx 3$–$5$. Due to 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. 1). 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 dependence on temperature, 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 non-trivial. To analyze that, it is useful...
to rewrite the above equations in terms of the impurity T-matrix $T_{\text{imp}}^j(\omega) \equiv V_j^2 G_{IJ}(\omega)$, where $G_{IJ}(\omega)$ is the f-Green’s function computed from the action in Eq. (2).

We find

$$G_c(\omega) = \frac{1}{\omega - t^2 G_c(\omega)} + \frac{(T_{\text{imp}}^j(\omega))^\alpha}{(\omega - t^2 G_c(\omega))^2}$$

(8)

and, from Eq. (5),

$$\Sigma_c(\omega) = \frac{(T_{\text{imp}}^j(\omega))^\alpha}{G_c(\omega)(\omega - t^2 G_c(\omega))}.$$  

(9)

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

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

(10a)

$$A(\omega) \delta_T G_c(\omega) = \int d\omega' B(\omega, \omega') \delta_T G_c(\omega')$$

$$= \left( \delta_T T_{\text{imp}}^j(\omega)^\alpha \right)_{G_c};$$  

(10b)

where

$$A(\omega) = \left\{ t^2 + \left[ \omega - t^2 G_c(\omega) \right] \left[ \omega - 3t^2 G_c(\omega) \right] \right. \right.$$  

$$- \frac{t^2 \left[ (T_{\text{imp}}^j(\omega))^\alpha \right]^\alpha}{(\omega - t^2 G_c(\omega))^2} \bigg|_{T=0};$$  

(11a)

$$B(\omega, \omega') = \left\{ \frac{(T_{\text{imp}}^j(\omega))^\alpha \delta G_c(\omega)}{V_j} \left. \frac{\delta G_c(\omega')}{G_c(\omega')} \right|^\alpha \bigg|_{T=0}.$$  

(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.

Fig. 2 shows the result of averaging the imaginary part 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 the curve. We will focus on the imaginary part of the impurity T-matrix since it gives the dominant contribution. It has the following scaling form

$$T''_{\text{imp}}(T) = \frac{\sin^2 \theta_0}{\pi \rho_0} t\left( \frac{T}{T_K} \right),$$  

(12)

where $\theta_0$ is the phase shift at $T = 0$. The function $t(x)$ has the following asymptotics

\[ t(x) = \begin{cases} 1 - \frac{x^2}{\ln(x)^2} & x \ll 1 \\ 1 - \frac{x}{T_K} & x \gg 1 \end{cases}, \]

(13)

where $\alpha$ and $\beta$ are universal numbers. It follows that

$$\delta_T T''_{\text{imp}} = -\frac{\sin^2 \theta_0}{\pi \rho_0} \left[ 1 - t\left( \frac{T}{T_K} \right) \right] \equiv -\frac{\sin^2 \theta_0}{\pi \rho_0} F(T/T_K),$$  

(14)

where

\[ F(T/T_K) \approx \begin{cases} \frac{\alpha T^2}{T_K} & T_K \gg T \\ 1 - \frac{t(\beta)}{\ln(T/K)^2} & T_K \ll T \end{cases}, \]

(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 $T$. For low $T$, it can be written in terms of a delta function of $T_K$, hence

$$\delta_T T''_{\text{imp}} = -\frac{a \sin^2 \theta_0}{\pi \rho_0} T \delta(T_K),$$  

(16)

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

$$\delta_T \Sigma_c \approx -\frac{ia P(0)}{\pi \rho_0 A_0} T.$$  

(17)

Therefore, the low temperature dependence only probes the $P(T_K)$ distribution 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. 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.
physically, it is clear what is happening. As the temperature is raised, a few diluted spins with \( T_K < T \) are quenched and cease to contribute to the resistivity. The linear term essentially counts the number of isolated f-sites of Ref. [2] 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 \( P(T_K, T) \), 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 \( \chi(T) \sim \ln(T_0/T) \) 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 investigated the effects of disorder in concentrated Kondo alloys, by solving dynamical mean field equations of disordered correlated electrons. We find that disorder effects can lead to considerable modifications of low temperature properties, leading to the breakdown of conventional Fermi liquid behavior, consistent with some Kondo alloys. Essentially, disorder fluctuations lead to the absence of a characteristic energy scale associated with a conventional Fermi liquid.

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