Localization effects in disordered Kondo lattices

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Abstract

We investigate the role of localization effects in the Kondo disorder mechanism for non-Fermi liquid behavior in disordered Kondo lattices. We find that the distribution of Kondo temperatures is strongly affected by fluctuations of the conduction electron density of states, a feature neglected in the previous treatment. For moderate disorder, the self-consistent distribution of Kondo temperatures flows to a universal log-normal form, *irrespective* of the form of the bare disorder distribution. For sufficient disorder, the system enters a Griffiths phase with diverging thermodynamic responses.

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The question of the origin of Non-Fermi liquid (NFL) behavior in metals remains unsolved. The issue has become particularly intriguing in the case of f-electron materials, where it has elicited such diverse explanations as the proximity to a quantum critical point, exotic impurity models or disorder-driven mechanisms [1]. The present authors have emphasized the possibility of explaining the singular behavior of these systems by considering that disorder leads to a wide distribution of Kondo temperatures [2–4]. In a series of previous papers [4], we demonstrated that such disorder effects can explain not only the thermodynamics, but also the anomalous transport in these systems. In this case, very low T_K spins remain unquenched at low temperatures and lead to the anomalous NFL behavior. The model has been most thoroughly investigated in the alloys $\mathrm{UCu}_{5-x}\mathrm{Pd}_x$ [5,3,6], where its predictions have been quite successful in explaining the available data.

We formulated a theory appropriate for concentrated magnetic impurities, able to describe the coherence effects in the clean limit. We showed that correlation effects strongly enhance any extrinsic disorder, generating a broad distribution of Kondo temperatures. The approach used was based on the dynamical mean field theory (DMFT) of correlations and disorder [7]. However, the DMFT is unable to accomodate localization effects, in that it treats conduction electron disorder "on the average", at the CPA level. Therefore, an outstanding issue that needs to be addressed is the role of fluctuations in the local conduction electron density of states. Indeed, local Kondo temperatures are given by $T_K = De^{-1/\rho J}$ and fluctuations of the conduction electron density of states ρ should be at least equally important in determining the distribution of Kondo temperatures. The goal of the present study is to incorporate such Anderson localization effects into our DMFT.

Our approach has been used before to study the Mott-Anderson transition in a disordered Hubbard model [8]. In it, the correlation aspects of the problem are taken into account in a DMFT fashion, but we also allow for *spatial variations* of the DMFT order parameter in order to accommodate Anderson localization effects. Such approach has been dubbed "statistical mean field theory" (SMFT) [8].

We concentrate on the disordered Anderson lattice model given by the Hamiltonian

$$H = \sum_{ij\sigma}(-t_{ij} + \varepsilon_i\delta_{ij})c^\dagger_{i,\sigma}c_{j,\sigma} + \sum_{j\sigma} E^f_j f^\dagger_{j\sigma} f_{j\sigma} + \sum_{j\sigma} V_j(c^\dagger_{j\sigma} f_{j\sigma} + \text{H.c.}) + U\sum_i f^\dagger_{i,\uparrow}f_{i,\uparrow}f^\dagger_{i,\downarrow}f_{i,\downarrow}, \quad (1)$$

where, in principle, we allow for random c- and f-site energies (ϵ_i and E^f_j) and hybridization matrix elements V_j.

The SMFT is considerably simplified when formulated on a Bethe lattice of coordination z (cf. Ref. [9]). We are then led to solve a set of stochastic equations by sampling. The equations for the disordered Anderson lattice read [8]

$$G^{(i)(-1)}_{cj}(\omega) = \omega - \epsilon_j - \sum_{k=1}^{z-1} t^2_{jk} G^{(j)}_{ck}(\omega) - \frac{V_j^2}{\omega - E^f_j - \Sigma_{fj}(\omega)}; \quad (2a)$$

$$S^{(j)}_{\text{eff}} = \sum_\sigma \int_o^\beta d\tau \int_o^\beta d\tau' f^\dagger_{j,\sigma}(\tau)\left[\delta(\tau-\tau')\left(\partial_\tau + E^f_j\right) + \Delta_j(\tau-\tau')\right] f_{j,\sigma}(\tau')$$
$$+ U\sum_\sigma \int_o^\beta d\tau f^\dagger_{i,\uparrow}(\tau)f_{i,\uparrow}(\tau)f^\dagger_{i,\downarrow}(\tau)f_{i,\downarrow}(\tau); \quad (2b)$$

$$\Delta_j(\omega) = \frac{V_j^2}{\omega - \epsilon_j - \sum_{k=1}^{z-1} t^2_{jk} G^{(j)}_{ck}(\omega)}. \quad (2c)$$

Here, $G^{(i)}_{cj}(\omega)$ is the c-electron Green's function on site j with the nearest neighbor site i removed and $\Sigma_{fj}(\omega)$ is the f-electron self-energy calculated from the effective action (2b) [8]. We calculate the self-energy with the large-N mean-field theory at $T = 0$ and $U \to \infty$ [10].

We briefly summarize our results. We will only discuss the effect of f-disorder (E_f and V). We have found that the inclusion of localization effects can significantly enhance the width of the distribution of Kondo temperatures as compared with the CPA results previously obtained [4]. This effect is depicted in Fig. (1), where $P(T_K)$ obtained by the present method is compared with $P(T_K)$ obtained within the dynamical mean field theory [4].

Furthermore, irrespective of the bare distribution of physical parameters, the self-consistent $P(T_K)$ *flows to a universal log-normal distribution*, for weak to intermediate disorder. This is illustrated in Fig. (2), where a bare uniform distribution of V's was used.

Finally, for a range of disorder strengths, we have found a Griffiths phase characterized by non-Fermi liquid behavior with diverging magnetic susceptibility and linear specific heat coefficient. This is shown if Fig. (3).

In summary, we have explored the effect of fluctuations in the conduction electron density of states (localization effects) in the distribution of Kondo temperatures in the Kondo disorder model. These were shown to play a role that is at least as important as the fluctuation of Kondo coupling constants considered before.

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FIGURES

FIG. 1. Comparison between $P(T_K)$ with (full line) and without (dashed line) localization effects. The latter shows an enhanced standard deviation σ. This is for a uniform V-distribution with $< V >= 0.45$ and width $W_V = 0.1$, $\mu = -0.1$, $E_f = -1$, in units of t and $z = 3$.

FIG. 2. Universal form of the distribution of T_K's with localization effects. The bare distribution of V's is constant, but the self-consistent $P(T_K)$ is log-normal. Same parameters as in Fig. (1).

FIG. 3. Inverse $T = 0$ magnetic susceptibility $\chi(0)$ within the SMFT for various disorder strengths. Above a threshold disorder ($W_V \sim 0.2$), $\chi(0) \to \infty$. Same parameters as in Fig. (1).