

Localization-Induced Griffiths Phase of Disordered Anderson Lattices

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(Received 13 March 2000)

We demonstrate that local density of states fluctuations in disordered Anderson lattice models universally lead to the emergence of non-Fermi liquid (NFL) behavior. The NFL regime appears at moderate disorder ($W = W_c$) and is characterized by *power-law* anomalies, e.g., $C/T \sim 1/T^{(1-\alpha)}$, where the exponent α varies continuously with disorder, as in other Griffiths phases. This Griffiths phase is *not* associated with the proximity to any magnetic ordering, but reflects the approach to a disorder-driven metal-insulator transition (MIT). Remarkably, the MIT takes place only at *much* larger disorder $W_{\text{MIT}} \sim 12W_c$, resulting in an extraordinarily robust NFL metallic phase.

DOI: 10.1103/PhysRevLett.86.264

PACS numbers: 71.10.Hf, 71.27.+a, 72.15.Rn, 75.20.Hr

The nature of the non-Fermi-liquid (NFL) behavior observed in several heavy fermion compounds remains largely unresolved [1]. In the cleaner systems, the proximity to a quantum critical point seems to be at the origin of many of the observed properties [2,3]. Exotic impurity models cannot be discarded [4], though their behavior in concentrated systems remains ill understood [5].

In other compounds, nonstoichiometry has prompted the investigation of disorder-based mechanisms. A *phenomenological* “Kondo disorder” model (KDM), describing a broad distribution of Kondo temperatures T_K , has been successfully applied to several of these systems [6,7]. Alternatively, the formation of large clusters of magnetically ordered material within the disordered phase has also been proposed [8]. Both scenarios lead to a wide distribution of energy scales, giving rise to similar thermodynamic anomalies and NMR response [7]. In addition, the predictions of the KDM prove to be consistent with a number of other experiments, including optical conductivity [9], magnetoresistance [10], and dynamic neutron scattering [6,11] measurements.

Despite these successes, a number of basic questions remain unresolved, including the following: (1) What is the *microscopic* origin of the ubiquitous power-law (or logarithmic) anomalies? (2) Can a model calculation be done, which can produce these power laws in a universal fashion? (3) Are these properties tied to the proximity to a quantum phase transition, and if so, which one? (4) How robust is the anomalous behavior with respect to the variation of materials parameters?

Within our model, all these questions find clear-cut and physically transparent answers: (i) The anomalies can be ascribed to a *power-law* distribution of T_K 's, whose exponent varies continuously with disorder strength. The resulting NFL behavior, e.g., $\gamma = C/T \sim 1/T^{(1-\alpha)}$, $\alpha < 1$ sets in for relatively weak randomness, *irrespective* of the detailed model for disorder. This should be contrasted with the KDM [6,7], where the occurrence of NFL behavior requires fine-tuning. (ii) We find universal behavior

reflecting the *nonlocal*, many-body processes associated with Anderson localization effects in the presence of strong electron correlations. (iii) For stronger disorder, the NFL metallic behavior persists over a surprisingly large interval before a disorder-driven metal-insulator transition (MIT) is reached. This novel Griffiths phase is a manifestation of quantum critical behavior associated with the approach to a disorder-driven metal-insulator transition and does not require the proximity of any magnetically ordered phase.

We consider a disordered infinite- U Anderson lattice Hamiltonian

$$H = \sum_{i,j\sigma} (-t_{ij} + \varepsilon_i \delta_{ij}) c_{i\sigma}^\dagger c_{j\sigma} + \sum_{j\sigma} E_{fj} f_{j\sigma}^\dagger f_{j\sigma} + \sum_{j\sigma} V_j (c_{j\sigma}^\dagger f_{j\sigma} + \text{H.c.}), \quad (1)$$

in usual notation. The infinite- U constraint at each f orbital is assumed ($n_j^f = \sum_{\sigma} f_{j\sigma}^\dagger f_{j\sigma} \leq 1$). We have studied different types of disorder, including randomness in the conduction electron site energies ε_i , the f -electron energies E_{fj} , as well as the hybridization V_j . Within our approach, we find that most of our conclusions remain valid for *any* specific form of disorder, indicating robust and universal behavior.

We treat the above Hamiltonian within the recently proposed statistical dynamical mean field theory [12]. This approach reduces to the usual dynamical mean-field theory in the limit $z \rightarrow \infty$ (with $t_{jk} \sim t/\sqrt{z}$) [6,13,14], but unlike the latter, it incorporates Anderson localization effects. As a result, the spectral function of the local bath “seen” by each impurity has strong spatial fluctuations and contains information coming from sites which are many lattice parameters away. Physically, the fluctuations of the conduction electron wave functions lead to the distribution of Kondo temperatures, which in turn creates a *renormalized* effective disorder seen by the conduction electrons. This nonlocal feedback mechanism results in

the universal form of all the relevant distribution functions that we find.

The simplest model for incorporating localization effects is obtained by focusing on a Bethe lattice of coordination z (with nearest neighbor hopping t , used as a unit of energy). The resulting set of self-consistent stochastic equations is governed by the local actions [12,15]

$$S_{\text{eff}}^{(j)} = \int_0^\beta d\tau \sum_\sigma f_{j,\sigma}^\dagger(\tau) (\partial_\tau + E_{fj}) f_{j,\sigma}(\tau) + \int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma f_{j,\sigma}^\dagger(\tau) \Delta_j(\tau - \tau') f_{j,\sigma}(\tau'); \quad (2)$$

$$\Delta_j(\omega) = \frac{V_j^2}{\omega - \varepsilon_j - \sum_{k=1}^{z-1} t_{jk}^2 G_{ck}^{(j)}(\omega)}. \quad (3)$$

Here $G_{ck}^{(j)}(\omega)$ is the local c -electron Green's function on site k with the nearest neighbor site j removed. It is determined recursively from [12,15]

$$G_{cj}^{(i(-1))}(\omega) = \omega - \varepsilon_j - \sum_{k=1}^{z-1} t_{jk}^2 G_{ck}^{(j)}(\omega) - \Phi_j(\omega), \quad (4)$$

$$\Phi_j(\omega) = \frac{V_j^2}{\omega - E_{fj} - \Sigma_{fj}(\omega)}. \quad (5)$$

The local self-energy $\Sigma_{fj}(\omega)$ is obtained from the solution of the effective action (2) [12,15,16]. In order to solve the impurity problems, we have used the large- N mean-field theory at $T = 0$ [17]. We have solved Eqs. (2)–(5) numerically by sampling. In implementing this procedure, we have carried out large-scale simulations for $z = 3$, with ensembles containing up to $N_s = 200$ sites, and frequency meshes containing up to $N_{\text{omega}} = 8000$ frequencies. The numerical integrations needed to solve the impurity problems have been done by a combination of spline interpolations and adaptive quadrature routines. These careful numerics have made it possible to obtain Kondo temperatures spanning 15 orders of magnitude, which was crucial in order to examine the long tails of the relevant distribution functions.

One of the greatest advantages of our approach is its ability to focus on full distribution functions, which is essential for characterizing any Griffiths phase. Some typical results are presented in Fig. 1, where we show the evolution of the distribution of local Kondo temperatures as a function of disorder, from which one computes the overall response of the lattice system (see the discussion in the first reference of [6]). We find that [Fig. 1(a)] the distribution has a universal log-normal form for weak disorder. We have verified that such a log-normal behavior is obtained *irrespective* of the type and shape of the bare disorder distribution, as long as it is not too large.

As the disorder is increased, the distribution $P(T_K)$ no longer retains its log-normal form. Instead, a long tail

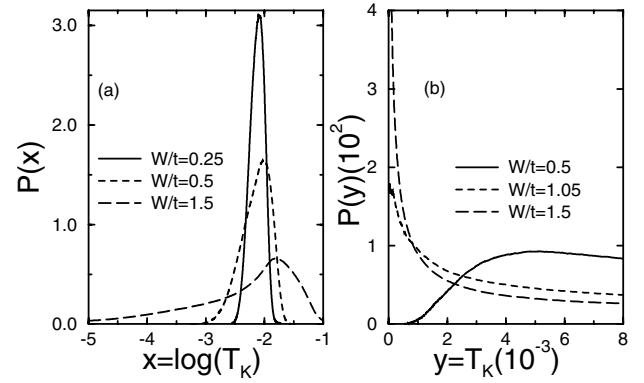


FIG. 1. (a) Distribution of $\log(T_K)$ for various values of disorder strength W/t . (b) Distribution of T_K showing the emergence of NFL behavior. Here ε_i 's are distributed uniformly with width W , and we have used $z = 3$, $E_f = -1$, $V = 0.5$, and $\mu = -0.5$, in units of t .

emerges on the low- T_K side, with a power-law asymptotic form [Fig. 1(b)]

$$P(T_K) \sim T_K^{-(\alpha-1)}. \quad (6)$$

The exponent α varies continuously with disorder, as seen on a plot of $\log[P(\log(T_K))]$ in Fig. 2.

Note that the value $\alpha = 1$ [Figs. 1(b) and 2], with $P(T_K) \sim \text{const}$, corresponds to the condition for *marginal* Fermi liquid behavior observed in some Kondo alloys [6,7], with logarithmically divergent magnetic susceptibility $\chi(T)$ and specific heat coefficient γ . This divergent behavior becomes more singular as the disorder is increased past this marginal case. For example, if we use the simple Wilson interpolation formula for $\chi(T)$ [18]

$$\chi(T) \sim \int_0^\Lambda \frac{T_K^{(\alpha-1)}}{T + aT_K} dT_K \sim \frac{1}{T^{(1-\alpha)}}. \quad (7)$$

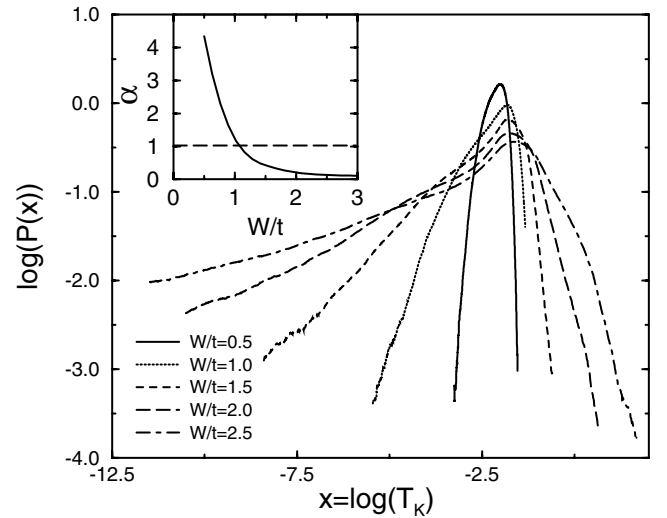


FIG. 2. Power-law asymptotics of $P(\log(T_K))$ as the disorder increases. The linear behavior for small $\log(T_K)$ implies a power-law dependence of $P(T_K)$. Inset: The exponent α of Eq. (6). Same parameters as in Fig. 1.

We thus have power-law divergences with exponents which vary continuously with the disorder strength. If we take $t \sim 10^4$ K, this should be observed below a few tens of Kelvin. Such generic behavior has been fitted to some NFL compounds [19]. Besides, $\chi(0)$ will diverge at a critical disorder strength ($W_c \approx 1$ in Fig. 2)

$$\begin{aligned} \chi(0) &\sim \int \frac{P(T_K)}{T_K} dT_K \sim \int_0^\Lambda T_K^{(\alpha-2)} dT_K \\ &\sim \frac{1}{\alpha-1} \sim \frac{1}{W_c - W}, \end{aligned} \quad (8)$$

with a similar result for γ . Note, however, that other higher order correlation functions, such as the nonlinear susceptibility $\chi_3(0)$, which probes higher negative moments of the distribution [$\chi_3(0) \sim 1/T_K^3$], will begin to diverge at different critical values of disorder,

$$\chi_3(0) \sim \frac{1}{\alpha-3} \sim \frac{1}{W_{c3} - W}, \quad (9)$$

where $W_{c3} \approx 0.66$ for the parameters of Fig. 2.

This general behavior is characteristic of Griffiths phases [20] and should not be confused with a true phase transition. The system should be viewed as a *disordered metal with embedded clusters of Anderson insulators*. It is precisely these poor conducting regions, with depleted densities of states, which give rise to imperfectly quenched spins and the corresponding singular thermodynamic properties.

We should also stress that the main mechanism that dominates the Griffiths phase is qualitatively different from the one in the KDM. There, T_K fluctuations were simply caused by the distribution of *local* parameters (V_j, E_{jj}) and the conduction electron density of states (DOS) does not fluctuate. By contrast, in the present treatment, fluctuations in the latter are dominant. To illustrate this, all the results we present are obtained for a model with conduction band disorder *only*, although similar results follow for any form of disorder. We stress that, in a KDM treatment of this case, T_K fluctuations are severely limited. Here, however, T_K fluctuations are enhanced by the fluctuations in the local conduction DOS, reflecting the localization effects and the approach to a disorder-driven MIT.

To confirm this picture, we examine the localization properties of the conduction electrons. We focus on the *typical* DOS $\rho_{\text{typ}} = \exp\{\langle \ln \rho_j \rangle\}$; $\rho_j = (1/\pi)\text{Im}G_{c,j}(\omega = 0)$, as shown in Fig. 3. This quantity vanishes at any disorder-driven MIT [12], and thus can serve as an order parameter for localization. Remarkably, we find a strong decrease of this quantity upon entering the Griffiths phase ($W/t \approx 1$), reflecting the strongly enhanced conduction electron scattering due to Kondo disorder. Yet, the actual localization transition, where the typical DOS vanishes, occurs only at much larger disorder ($W/t \approx 12$). This results in a very extended NFL metallic region, where the thermodynamics is singular, and the conduction electrons are almost, but not completely, localized.

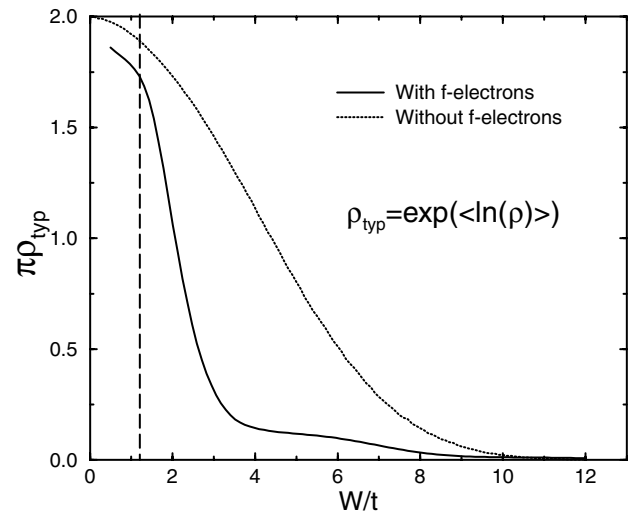


FIG. 3. Localization properties of the conduction electrons as monitored by the typical DOS as a function of disorder. The same quantity in the absence of Kondo spins is shown for comparison. The vertical dashed line indicates the boundary of the NFL phase. Same parameters as in Fig. 1.

This dramatic effect has a simple physical origin. Consider the distribution of the effective scattering potentials of the conduction electrons $\Phi_j(\omega = 0)$ [see Eq. (5)] introduced by the f sites. Note that [6] $\Phi_j(\omega = 0) = -Z_j V^2 / \tilde{\epsilon}_{fj}$, where Z_j is the quasiparticle weight and $\tilde{\epsilon}_{fj}$ the (renormalized) energy of the Kondo resonance at site j . For sufficient disorder, the Kondo resonances are randomly shifted up or down in energy, giving rise to Φ_j 's that can be random in magnitude but also in *sign*. The resulting distribution for the inverse quantity Φ_j^{-1} is shown in Fig. 4 and

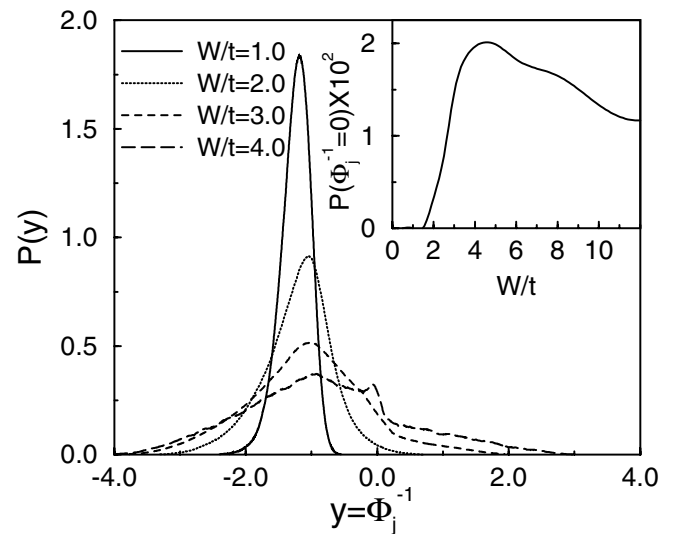


FIG. 4. Distribution function for the quantity $\Phi_j^{-1}(0)$ as a function of disorder. The inset shows the behavior of the concentration of the strong scattering Kondo centers [$\Phi_j^{-1}(0) = 0$], which reaches a maximum just after the NFL phase is entered. Same parameters as in Fig. 1.

is found to broaden with disorder. For $W/t \approx 1.5$, a *finite density* of $\Phi_j^{-1} = 0+$ (i.e., $\Phi_j = +\infty$) sites emerges. This is crucial, since the corresponding f sites act as unitary scatterers (US's), characterized by a maximally allowed scattering phase shift ($\delta = \pi/2$) for the conduction electrons. If all the f sites were US's, the system would be a Kondo insulator. The presence of a finite fraction of US's should be viewed as the emergence of *droplets* of a Kondo insulator within the heavy metal. Interestingly, at stronger disorder ($W/t > 4$) the distribution of $\Phi_j^{-1}(0)$ continues to broaden, leading to a *decrease* in the number of US's. This is illustrated by plotting $P(\Phi_j^{-1} = 0)$ in the inset of Fig. 4. In this regime, while the bare disorder increases, the *effective disorder* produced by the f sites is reduced, stabilizing the almost localized metallic phase. This mechanism may be at the origin of the puzzling behavior of materials such as SmB_6 [21], where the low temperature resistivity remains anomalously large yet finite over a broad range of parameters.

Finally, we note that a similar NFL phase was identified in a study of the Mott-Anderson transition in the disordered Hubbard model [12]. We have reexamined this system, and concluded that the NFL behavior should be attributed to a related Griffiths phase rather than a separate thermodynamic phase of the system. Despite the similarities, several features prove dramatically different. For Hubbard models, the emergence of NFL behavior does not have a dramatic effect on the conduction electrons and no US's emerge. This observation may explain the strong correlation between thermodynamic and transport anomalies in Kondo alloys, but not in doped semiconductors. In the latter materials, the thermodynamics is still singular close to the MIT, while transport remains more conventional [22].

It would be of particular interest if it could be tested experimentally whether these localization effects are responsible for the observed NFL behavior of disordered heavy fermion systems. A scanning tunneling microscopy study might be able to detect the predicted insulator droplets. In order to distinguish this from the magnetic Griffiths phase scenario [8], a systematic study of systems with comparable amounts of disorder but different magnetic character would be useful. Besides, since the present theory relies very little on intersite magnetic correlations, a determination of the typical size of the relevant magnetic clusters could also serve as a test.

In summary, we have investigated and solved a microscopic model for disordered Anderson lattices that displays an unprecedented sensitivity to disorder, leading to localization-induced non-Fermi-liquid behavior. Our results demonstrate that a well defined Griffiths phase can exist, which is not restricted to the vicinity of any magnetic or-

dering and yet seems to be consistent with most puzzling features of disordered heavy fermion systems and Kondo alloys.

We acknowledge useful discussions with M. C. Aronson, D. L. Cox, G. Kotliar, D. E. MacLaughlin, A. J. Millis, and G. Zarand. This work was supported by FAPESP and CNPq (E. M.), NSF Grant No. DMR-9974311 and the Alfred P. Sloan Foundation (V. D.).

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