Nonperturbative Scaling Theory of Free Magnetic Moment Phases in Disordered Metals

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The crossover between a free magnetic moment phase and a Kondo phase in low-dimensional disordered metals with dilute magnetic impurities is studied. We perform a finite-size scaling analysis of the distribution of the Kondo temperature obtained from a numerical renormalization group calculation of the local magnetic susceptibility for a fixed disorder realization and from the solution of the self-consistent Nagaoka-Suhl equation. We find a sizable fraction of free (unscreened) magnetic moments when the exchange coupling falls below a critical value J_c. Between the free moment phase due to Anderson localization and the Kondo-screened phase we find a phase where free moments occur due to the appearance of random local pseudogaps at the Fermi energy whose width and power scale with the elastic scattering rate $1/\tau$.

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The Kondo problem is of central importance for understanding low-temperature anomalies in low-dimensional disordered metals [1–7] such as the saturation of the dephasing rate [8] and the non-Fermi-liquid behavior of certain magnetic alloys [1,9]. For a clean metal, the screening of a spin-1/2 magnetic impurity is governed by a single energy scale, the Kondo temperature T_K. Thermodynamic observables and transport properties obey universal functions which scale with T_K. Thus, in a metal where nonmagnetic disorder is also present, two fundamental questions naturally arise: (i) Is the T_K modified by nonmagnetic disorder? (ii) Is the one-parameter scaling behavior still valid? It is well known [1,3,5] that magnetic moments can remain unscreened when conduction electrons are localized. However, in weakly disordered two-dimensional systems, the localization length is macroscopically large and is not expected to influence the screening of magnetic moments for experimentally relevant values of exchange coupling J. Another way of quenching of the Kondo effect is the existence of a *global pseudogap* at the Fermi energy E_F, namely, $\nu(E) \sim (E - E_F)^\alpha$, where $\alpha > 0$ [10]. In clean metals, the pseudogap quenches the Kondo screening when J falls below a critical value $J_c(\alpha)$. So far, only a few values of α have been realized experimentally: $\alpha = 1$ in graphene and in d-wave superconductors and $\alpha = 2$ in p-wave superconductors. In this Letter we examine the quantum phase diagram of magnetic moments diluted in two-dimensional disordered metals using a modified version of the numerical renormalization group (NRG) method. We find a free moment phase which we attribute to the random occurrence of *local pseudogaps*. The existence of free moments is confirmed directly with the NRG by the Curie-like behavior of the local magnetic susceptibility at low temperatures at particular sites for a given disorder realization. Finite-size scaling is performed to demonstrate the robustness of our finding. Furthermore, the distribution of T_Ks obtained from the NRG is found to agree well with earlier results based on the solution of the Nagaoka-Suhl equation [3].

We consider the Kondo Hamiltonian of a magnetic impurity diluted in a disordered metal,

$$H_{\rm sd} = \sum_{n\sigma} E_n c^\dagger_{n\sigma} c_{n\sigma} + \frac{1}{2}\sum_{n,n'} J_{nn'}[S^+ c^\dagger_{n\downarrow} c_{n'\uparrow} + S^- c^\dagger_{n\uparrow} c_{n'\downarrow} + S_z(c^\dagger_{n\uparrow} c_{n'\uparrow} - c^\dagger_{n\downarrow} c_{n'\downarrow})]. \quad (1)$$

Here, E_n are eigenenergies of noninteracting disordered electrons, described by the Anderson tight-binding model,

$$H_V = -t\sum_{\langle ij\rangle,\sigma} (c^\dagger_{i\sigma} c_{j\sigma} + \text{H.c.}) + \sum_{i=1,\sigma}^{N} V_i c^\dagger_{i\sigma} c_{i\sigma}, \quad (2)$$

with band width D, nearest-neighbor hopping amplitude t, and random site potentials V_i, drawn from a flat box distribution of width W centered at zero. We consider square lattices of length L with $N = L^2$ sites and periodic boundary conditions. The exchange coupling matrix elements are then given by $J_{nn'} = J\psi^*_n(\mathbf{r})\psi_{n'}(\mathbf{r})$, with $\psi_n(\mathbf{r})$ being the amplitude of the single-electron eigenfunction at the position $\mathbf{r}$ of the magnetic impurity. Energies are given in units of t.

Finite-size scaling.—We obtain all eigenenergies and eigenfunctions of H_V by using state-of-the-art numerical diagonalization techniques for a large set of realizations of the disorder V [11]. The T_K is then obtained from the solution of the one-loop-Nagaoka-Suhl equation (NSE) [12],

$$1 = \frac{J}{2N}\sum_{n=1}^{N} \frac{L^2|\psi_n(\mathbf{r})|^2}{E_n - E_F} \tanh\left(\frac{E_n - E_F}{2T_K}\right). \quad (3)$$

E_F is located between energy levels. Numerical solution of Eq. (3) yields a distribution of T_K with strong deviations from Gaussian behavior even for weak disorder [3].

Figure 1 shows for $W = 3$ that a double-peak structure found previously [3] persists as the lattice size is increased from 900 to 4900 sites. This structure evolves into a power-law divergence in the strong-disorder limit [3]. In order to verify that these features are not an artifact of the one-loop approximation, we perform a comparative analysis with the nonperturbative NRG method for different system sizes and disorder strengths for a given disorder realization.

NRG for disordered systems.—In order to apply the NRG method to disordered systems, we use as a basis set the eigenfunctions and eigenenergies of the tight-binding model, Eq. (2), as obtained by the numerical exact diagonalization. We perform the Wilson logarithmic discretization of the conduction band and replace the interval of eigenenergies between $(D/2)\Lambda^{-n-1}$ and $(D/2)\Lambda^{-n}$, $n = 0, 1, 2, \ldots, N_c$, by one energy level equal to the average of eigenenergies in this interval. N_c is determined by the condition that in the interval $[-\Lambda^{-N_c-1}D/2,\ \Lambda^{-N_c-1}D/2]$, there is no energy level. Solving Eq. (3) for the logarithmically discretized spectrum at particular sites with the NRG, we found that the T_K saturates for values of the NRG discretization parameter below $\Lambda = 1.5$. Thus, fixing this value for Λ is sufficient for a statistical analysis of the T_K, as we confirmed by repeating the statistical analysis with $\Lambda = 1.3$ for one sample, finding almost undistinguishable results with a margin of less than one per cent. Next, by the tridiagonalization procedure, we numerically map this model onto a discrete Wilson chain. Then, we use an iterative diagonalization, keeping 1500 states after each iteration [13]. We calculate the local magnetic susceptibility $\chi_{\mathrm{loc}}(T)$, which is proportional to the local correlation function of the impurity spin, by differentiating the magnetic moment of the impurity with respect to a magnetic field that acts only at the impurity [14]. The local susceptibility is found to have a smooth temperature dependence (see Fig. 3) which can be used to define T_K: $T\chi_{\mathrm{loc}}(T)$ crosses over from the free spin value $1/4$ to a decay linear in T as the temperature is lowered below the T_K. For a clean flat band system, $\chi_{\mathrm{loc}}(T)$ coincides with the impurity susceptibility χ_{imp}, which is obtained as the difference between the susceptibility of the electronic system with and without the impurity. Wilson defined the T_K as the crossover temperature where $T_K\chi_{\mathrm{imp}}(T_K) = 0.07$ [13,15]. For disordered systems, we find that $T\chi_{\mathrm{imp}}(T)$ can strongly deviate from the scaling curve of the clean system [16]. It turns out, however, that this is an artifact of the definition of χ_{imp}: The susceptibility of the conduction electrons fluctuates widely and can result in negative values of χ_{imp} [17]. In Fig. 2, we show the distribution of T_Ks when T_K using Wilson's criterion $T_K\chi_{\mathrm{loc}}(T_K) = 0.07$. The data were extracted from a single sample of size $L = 70$ using two distinct sets of disorder and exchange coupling amplitudes: $W = 2$, $J = 0.3D$ [Fig. 2(a)], and $W = 3$, $J = 0.35D$ [Fig. 2(b)]. For comparison, we plot the distribution of T_K obtained from the solution of the one-loop NSE, where we accounted for the known higher-loop correction by rescaling T_K with $0.7\sqrt{J/D}$. The agreement is remarkable and demonstrates that the double-peak structure is not an artifact of the one-loop approximation. In Fig. 3(a), we plot the local impurity spin susceptibility, multiplied by temperature T, for the site with maximal T_K for a given realization of the disorder. In order to check that the modified version of the NRG is well suited for disordered systems, we also plot in Fig. 3(a) results obtained with the continuous-time quantum Monte Carlo method (CTQMC) [18] (dots) for the same site using the complete set of eigenstates of H_V. For temperatures close to T_K both methods agree well. The small deviations seen at larger temperatures can be attributed to the fact that the average of the wave function amplitudes in each Wilson discretization interval results in stronger suppression of fluctuations at higher energies. A full statistical analysis with the CTQMC method will be presented elsewhere. We note that the local density of states (LDOS), shown in the inset, has most of its weight in the lower half of the band, close to the Fermi energy. In contrast, in Fig. 3(b) we show the impurity susceptibility times T for a site where the magnetic impurity remains unscreened for $J/D < 0.35$. Note that $T\chi_{\mathrm{loc}}$ changes only weakly with temperature. For $T \ll \Delta$ it approaches its free value $1/4$ (not shown). The corre-

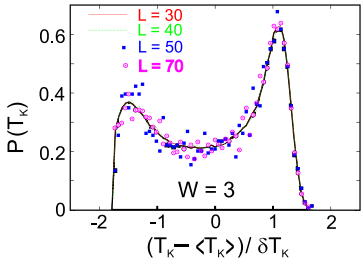

FIG. 1 (color online). Distribution of T_Ks obtained from the NSE [Eq. (3)] for electrons in square lattices with disorder strength $W = 3$. Data were obtained using all lattice sites and 1 ($L = 50$, 70), 5 ($L = 40$), and 100 ($L = 30$) samples, with $J/D = 0.35$.

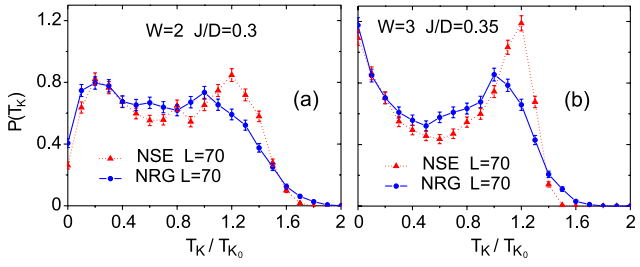

FIG. 2 (color online). The distribution of T_Ks obtained with the NRG for lattice size $L = 70$. (a) $W = 2$, $J/D = 0.3$, scaled with $T_{K_0} = 0.57De^{-D/J}$ (T_K in 1-loop approximation for a flat band of width D). (b) $W = 3$, $J/D = 0.35$ for one realization of the disorder potential. For comparison we plot the distribution obtained from NSE (higher-loop corrections are accounted for by rescaling T_K with $0.7\sqrt{J/D}$). The error bars denote the statistical error.

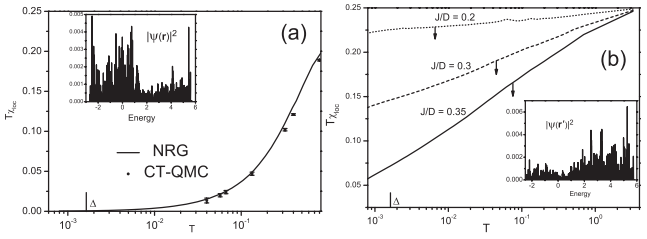

FIG. 3. Local spin susceptibility as function of temperature T for exchange coupling $J/D = 0.35$, disorder amplitude $W = 2$, and lattice size $L = 70$, obtained with NRG (lines) and CTQMC (dots) methods [17,18]. At a site (a) where T_K is maximal, (b) where the magnetic impurity remains free. Arrows indicate $T_{K_0}(J/D)$. Insets: The absolute square of eigenfunction amplitudes as a function of energy E ($E = 0$ denotes the Fermi energy). The mark indicates the mean level spacing Δ.

sponding LDOS (inset) shows that weight is shifted towards the upper half of the band, away from the Fermi energy (which is set at quarter filling), and that there is a minimum in the LDOS at the Fermi energy, resembling a *local pseudogap*.

Free moment phase.—Next, we use the NRG to analyze the impurity sites where the renormalization of the magnetic susceptibility remains too small to define a finite T_K. On such sites a magnetic moment remains free down to the lowest temperatures, the spin susceptibility χ_{loc} diverges, and $T\chi_{loc}(T)$ approaches a finite value. We employed this criterion to identify free magnetic moments and compare in Fig. 4 their fraction with that derived from the condition that Eq. (3) has no finite T_K solution. We see that the fraction of free moments obtained from NSE is smaller than the one from the NRG. This can be attributed to the fact that higher-loop corrections tend to lower T_K. Thus, the criterion that the NSE has no solution gives a lower bound for the fraction of free magnetic moments. This corresponds to $T_K \to 0$ in Eq. (3). Therefore, free moments exist when the effective LDOS, as defined by

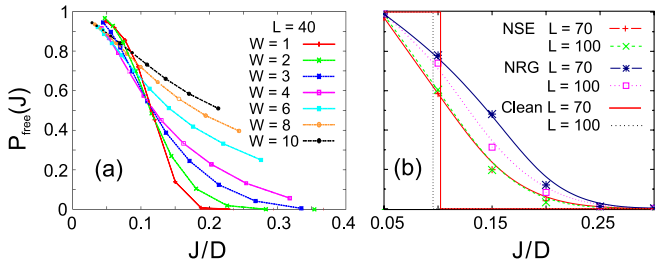

FIG. 4 (color online). Fraction of free moments as a function of exchange coupling J obtained (a) from the condition that the NSE has no solution and (b) from temperature dependence of local spin susceptibility calculated with the NRG for disorder $W = 2$, as compared with the result from NSE. The fraction of free moments in a clean sample (step functions) are plotted for comparison. The lines are guides to the eye.

$$\rho_{\text{eff}} = \frac{1}{2N}\sum_{n=1}^{N}\frac{L^2|\psi_n(\mathbf{r})|^2}{|E_n - E_F|}, \tag{4}$$

is smaller than the inverse exchange coupling $1/J$. For a fixed disorder realization this yields a lower bound for the critical exchange coupling J_c below which the magnetic impurity remains free. For clean systems with flat bands ρ_{eff} diverges logarithmically with the number of states N. Then, $J_c/D \sim 1/\ln N$. Since $T_K \sim D\exp(-D/J)$, the condition for free moments is $\Delta > cT_K$ ($c \gg 1$ depends on E_F). Since Δ vanishes in the thermodynamic limit, there are no free moments for any finite J in a clean metal. Can one conclude the same when nonmagnetic disorder is present? The answer is no for two reasons. First, in disordered systems of dimension $d \leq 2$, all eigenstates are localized in the absence of spin-orbit interaction or a strong magnetic field, with a finite local gap of order $\Delta_c = 1/(\nu\xi^d)$ at the Fermi energy (ν average density of states, ξ average localization length). Therefore, there are with certainty free moments when $\Delta_c \gg T_K$, or, equivalently, $J \ll J_c^A \sim D/\ln N_c$, where $N_c = D/\Delta_c$. In weakly disordered two-dimensional electron systems, $\xi(g) = g\exp(\pi g)$ in the absence of magnetic fields ($g = E_F\tau$ and at quarter filling $g = 96/(\pi W^2)$). Equation (4) yields,

$$J_c^A = D\{\ln[2\xi(W)^2] + C\}^{-1}, \tag{5}$$

where $C \approx 0.58$. This expression provides a lower bound for J_c, since both the localization length and the local effective DOS are widely distributed. In Fig. 5, we show the distribution of ρ_{eff} for moderate disorder. Remarkably, the point where the distribution drops sharply to zero, $\rho_{\text{eff}_{\min}}$, hardly depends on L. In the inset of Fig. 5, we plot $J_c = 1/\rho_{\text{eff}_{\min}}$ as function of disorder for various

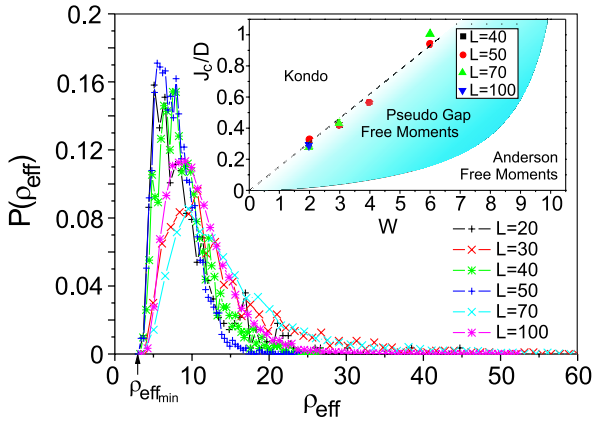

FIG. 5 (color online). Distribution of ρ_{eff} for $W = 2$ and lattice sizes L. Inset: Quantum phase diagram in (J, W) plane. Data points: $J_c = 1/\rho_{\text{eff}_{\min}}$ as function of W, obtained numerically for several L. Dashed line: guide to the eye. Full line: Critical exchange coupling due to Anderson localization, J_c^A, Eq. (5). For $J > J_c$, all magnetic moments are screened (Kondo). For $J < J_c^A$, magnetic moments remain free due to Anderson localization (Anderson free moments). For $J_c^A < J < J_c$, magnetic moments remain free due to *local pseudogaps*.

values of L, together with $J_c^{\mathrm{A}}(W)$ obtained from Eq. (5). This quantum phase diagram in the (J, W) plane shows a free magnetic moment phase due to Anderson localization for $J < J_c^{\mathrm{A}}$ and a Kondo-screened phase for $J > J_c(W)$. For intermediate couplings, $J_c^{\mathrm{A}} < J < J_c(W)$, we also find free magnetic moments for all lattice sizes considered. It is well known that a free moment phase exists when there is a pseudogap around the Fermi energy [10]. Indeed, as seen in Fig. 3(b), there is a dip in the LDOS at sites where the magnetic moment remains unscreened. In weakly disordered metals, the LDOS is correlated over a macroscopic energy interval of order of the elastic scattering rate $1/\tau$ [19]. Although these correlations are only of order $1/g$ and the LDOS can fluctuate in energy, they can cause dips in the LDOS within a range of order $1/\tau$. From the numerical results for $J_c(W)$ (inset of Fig. 5) and from the fact that a pseudogap with an exponent α yields $J_c = \alpha D$, we infer the exponent of the local pseudogaps in 2D metals. The critical exchange coupling increases with disorder strength W as $J_c \sim W \sim \sqrt{\pi\hbar/(96\epsilon_F\tau)}$. For Fe impurities in thin Ag films, where $\langle T_K \rangle \sim 4$ K [20] and $J/D \sim 0.1$, the paramagnetic moment phase extends to $\epsilon_F\tau \approx 25$. Thus, for diffusion constants $D_e < 25\ \mathrm{cm}^2/\mathrm{s}$ free magnetic moments contribute to the dephasing at $T \ll \langle T_K \rangle$ [3]. The anomalous dephasing reported in Ref. [20] in Ag wires where $D_e > 100\ \mathrm{cm}^2/\mathrm{s}$ may indicate the lowering of the exchange coupling J/D below 0.05 at interstitial sites or at the surface with a corresponding shift of the free moment quantum phase boundary.

In summary, a nonperturbative finite-size scaling of Kondo impurities in two-dimensional disordered electron systems is performed. Between the free moment phase due to Anderson localization and the Kondo-screened phase, we find a phase where free moments occur due to random local pseudogaps at the Fermi energy. The pseudogap width and exponent scale with the elastic scattering rate $1/\tau$. Experimentally, a local probe such as STM could be used to detect this *pseudogap free moment* phase directly.

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