Stabilization of local moments in gapless Fermi systems

Carlos Gonzalez-Buxton and Kevin Ingersent*
Department of Physics, University of Florida, P.O. Box 118440, Gainesville, Florida 32611-8440

(Received 26 July 1996; revised manuscript received 20 September 1996)

Renormalization-group methods are applied to the Anderson model for a localized level coupled to a Fermi system in which the density of states varies like $|\epsilon|^r$ near the Fermi energy ($\epsilon=0$). This model with $r=1$ or 2 may describe magnetic impurities in unconventional superconductors and certain semiconductors. The pseudogap suppresses mixed valence in favor of local-moment behavior. However, it also reduces the exchange coupling on entry to the local-moment regime, thereby narrowing the range of parameters within which the impurity spin becomes Kondo screened.
[S0163-1829(96)51946-6]

There exists a class of ''gapless'' Fermi systems which exhibit a pseudogap in the effective density of states $\rho(\epsilon)$ at the Fermi level, taken to be $\epsilon=0$. For instance, the valence and conduction bands of certain semiconductors — including $\mathrm{Pb}_{1-x}\mathrm{Sn}_x\mathrm{Te}$ at a critical composition,[1] and PbTe-SnTe heterojunctions[2] — touch in such a way that, for small $|\epsilon|$, $\rho(\epsilon)$ is proportional to $|\epsilon|^{d-1}$ in d spatial dimensions. The quasiparticle density of states in an unconventional superconductor can vary like $|\epsilon|$ or $|\epsilon|^2$ near line or point nodes in the gap.[3] Heavy-fermion and cuprate superconductors are candidates for this behavior. Electrons in a strong magnetic field[4] and exotic phases of the Hubbard model[5] are also predicted to exhibit a linear pseudogap in two dimensions. Finally, the single-particle density of states in the one-dimensional Luttinger model varies like $|\epsilon|^{2\alpha}$, where α varies continuously with the strength of the bulk interactions.[6]

Recently there has been considerable interest[7–12] in the behavior of magnetic impurities in gapless systems having a power-law density of states, $\rho(\epsilon)=\rho_0|\epsilon|^r$. This scenario may be relevant[8] for Ni-doping experiments[13] on $\mathrm{YBa}_2\mathrm{Cu}_3\mathrm{O}_{7-\delta}$. Poor man's scaling for the spin-$\frac{1}{2}$ (impurity degeneracy $N=2$) Kondo model[7] and large-N treatments[7,8] indicate that a Kondo effect (i.e., quenching of a local magnetic moment at low temperatures T) takes place only if the antiferromagnetic electron-impurity exchange $\rho_0 J$ exceeds a critical value, $\rho_0 J_c \approx r$; otherwise, the impurity decouples from the band. A large-N study of magnetic impurities in gapless superconductors[9] yields similar results, except that for $r\leqslant 1$ or $N=2$, any finite impurity concentration drives J_c to zero. Numerical renormalization-group calculations for the $N=2$ case, both at[10] and near[11] particle-hole symmetry, show that $J_c\to\infty$ for all $r>\frac{1}{2}$, while for $r<\frac{1}{2}$ the strong-coupling limit exhibits anomalous properties, including a nonzero moment. Away from this symmetry, a finite value of J_c is recovered; for $J>J_c$ the impurity spin is screened at $T=0$, but an electron phase shift of π suggests that the impurity contribution to the resistivity vanishes, instead of taking its maximal possible value as it does in the conventional Kondo effect.[11]

The Kondo model presupposes the existence of a local moment, i.e., an impurity level having an average occupancy $\langle n_d\rangle\approx 1$. This paper reports the systematic exploration of local-moment formation in gapless systems. Poor man's scaling[14] is applied to the Anderson impurity model,[15] in which mixed-valence ($0<\langle n_d\rangle<1$) and empty-impurity ($\langle n_d\rangle\approx 0$) regimes compete with local-moment behavior. Concentrating on the case of a localized level which lies within a power-law pseudogap, we show that the reduction in the density of states near the Fermi level has three main effects, each of which grows more pronounced as r increases: (1) The mixed-valence region of parameter space shrinks, and for $r\geqslant 1$ disappears altogether. (2) The local-moment regime expands. (3) The value of the Kondo J on entry to the local-moment regime is reduced. Since the threshold J for a Kondo effect rises with r (see above), these results imply — at least in the cases of greatest interest, $r=1$ and 2 — that over a large region of phase space, the low-temperature state has an uncompensated local moment. This should be contrasted with systems having a regular density of states, in which an Anderson impurity is always quenched at zero temperature. Our perturbative results are supported by numerical renormalization-group calculations of $\langle n_d\rangle$ and the magnetic susceptibility.

We start with the Anderson model,[15] in the form

$$H=\sum_{\sigma=\uparrow,\downarrow}\int_{-D}^{D}d\epsilon\,\epsilon c_{\epsilon\sigma}^{\dagger}c_{\epsilon\sigma}+\varepsilon_d n_d+U n_{d\uparrow}n_{d\downarrow}+\sum_{\sigma=\uparrow,\downarrow}\int_{-D}^{D}d\epsilon\sqrt{\rho(\epsilon)}\,t(c_{\epsilon\sigma}^{\dagger}d_{\sigma}+\text{H.c.}). \tag{1}$$

The noninteracting conduction band is taken to be isotropic in momentum space and to extend over an energy range $\pm D$ about the Fermi energy ($\epsilon=0$), while the operators $c_{\epsilon\sigma}$ obey $\{c_{\epsilon\sigma}^{\dagger},c_{\epsilon'\sigma'}\}=\delta(\epsilon-\epsilon')\,\delta_{\sigma,\sigma'}$. The impurity is described by its energy ε_d, and the Coulomb repulsion when it is doubly occupied, $U>0$. We have assumed purely local hybridization between the band and the impurity, and take t to be positive. In the cases of interest, t and $|\varepsilon_d|$ are smaller than U and D.

Pure power-law density of states. We first consider the density of states introduced in Ref. 7:

$$\rho(\epsilon)=\begin{cases}\rho_0|\epsilon/D|^r, & |\epsilon|\leqslant D;\\ 0, & \text{otherwise.}\end{cases} \tag{2}$$

Here, r can take any non-negative value, with $r=0$ representing a constant density of states. (We will later examine a more realistic case, in which the power-law variation is restricted to the vicinity of the Fermi level.)

In order to understand the behavior of Eq. (1) at low temperatures T, we apply poor man's scaling.[14] In this approach, electronic states with energies $|\epsilon|\gg T$ are progressively integrated out, yielding an effective description of the problem in terms of fewer degrees of freedom. Consider first an incremental reduction of the bandwidth from D to $D'\equiv D(1+\delta\ln D)<D$. The aim is to represent the same physical system by an effective Hamiltonian of the form of Eq. (1) and a density of states given by Eq. (2), but with D replaced by D' in both equations. This requires the couplings entering Eq. (1) to be adjusted to account for the states which have been eliminated. Provided that δD, ε_d, and t remain small compared to D, these renormalizations can be computed within perturbation theory. The band reduction can then be iterated, leading to differential equations for the couplings as functions of the effective bandwidth.

In previous implementations of poor man's scaling for the Anderson model with a constant density of states,[16,17] it was found that eliminating all states with energies $D'<|\epsilon|\leqslant D$ produces a leading correction

$$\delta\varepsilon_d=-\rho(D)t^2\,\delta\ln D=-(\Gamma/\pi)\,\delta\ln D, \tag{3}$$

where $\Gamma=\pi\rho_0 t^2$. The corrections to U and t enter at higher order in small couplings, and can be neglected.

For a power-law density of states, an additional correction is required because the coupling entering Eq. (1) is not t, but $\sqrt{\rho(\epsilon)}t\equiv\sqrt{\Gamma|\epsilon/D|^r}$. Replacing D by D' in Eq. (2) increases $\rho(\epsilon)$ by a factor of $(D/D')^r$. Γ must be reduced by the same factor so that the physical coupling remains unaffected by the change of variable, i.e., we require $\Gamma|\epsilon/D|^r=(\Gamma+\delta\Gamma)|\epsilon/D'|^r$, which gives

$$\delta\Gamma=r\Gamma\,\delta\ln D. \tag{4}$$

The novel behaviors of an Anderson impurity in gapless systems all stem from this correction to Γ, which has no counterpart for a constant density of states.

Equations (3) and (4) can be integrated to give the effective couplings $\varepsilon_d(D)$ and $\Gamma(D)$ at an arbitrary D in terms of the initial bandwidth D_0 and the bare couplings $\varepsilon_d^0\equiv\varepsilon_d(D_0)$ and $\Gamma_0\equiv\Gamma(D_0)$:

$$\Gamma(D)=\Gamma_0\cdot(D/D_0)^r, \tag{5}$$

$$\varepsilon_d(D)=\varepsilon_d^0+\frac{\Gamma_0}{\pi r}[u^r-(D/D_0)^r]\quad(r>0). \tag{6}$$

[The quantity $u\equiv\min(1,U/D_0)$ appears because, strictly speaking, Eq. (3) applies only in the range $D\lesssim U$; the scaling of ε_d is negligible for $D\gtrsim U$.] For a constant density of states, by contrast, only ε_d renormalizes:[17]

$$\varepsilon_d(D)=\varepsilon_d^0+(\Gamma_0/\pi)\ln(uD_0/D)\quad(r=0). \tag{7}$$

Note that U does not renormalize significantly for any r.

It is instructive to consider the behavior implied by Eqs. (5)–(7) as the bandwidth D is progressively reduced. For $D_0\geqslant D\gtrsim U$, all four impurity configurations are active, and the impurity susceptibility $\chi_{\rm imp}$ satisfies[18] $T\chi_{\rm imp}\approx 1/8$. Once $D\lesssim U$, the doubly occupied impurity becomes frozen out, and the system enters the *valence-fluctuation* regime. Real charge fluctuations between the remaining impurity states yield $T\chi_{\rm imp}=1/6$, and ε_d begins to scale according to Eq. (6) or Eq. (7).

Scaling can continue until either Γ/D or $|\varepsilon_d|/D$ grows to of order unity. At this point perturbation theory breaks down, and there is a crossover to one of three regimes in which real charge fluctuations are frozen out:

(1) *Local-moment* regime. If ε_d/D reaches -1, the impurity acquires a spin, and $T\chi_{\rm imp}$ rises to $\approx 1/4$. The scale $D_{\rm LM}$ for this crossover satisfies $D_{\rm LM}\equiv-\varepsilon_d(D_{\rm LM})$.

(2) *Empty-impurity* regime. If, instead, ε_d/D becomes equal to $+1$, the localized level is completely depopulated and $T\chi_{\rm imp}$ drops rapidly to zero.

(3) *Mixed-valence* regime. Finally, Γ/D may become of order unity, at a bandwidth $D_{\rm MV}\equiv\Gamma(D_{\rm MV})$. In this case, $T\chi_{\rm imp}\to 0$, but even at $D=0$ the value of $\langle n_d\rangle$ departs significantly from both 0 and 1.

There are a number of notable differences between the scaling behavior for $r=0$ and for $r>0$. First, a pseudogap markedly inhibits the renormalization of the impurity energy. Consider, for example, the maximum possible shift in ε_d. From Eq. (6), $\varepsilon_d(0)-\varepsilon_d^0=(\Gamma_0u^r)/(\pi r)$, whereas for $r=0$ this quantity is unbounded. For $r\geqslant\frac{1}{2}$ (say) and $\Gamma_0\ll|\varepsilon_d^0|$, it is a reasonable approximation to neglect the renormalization of ε_d altogether.

Second, as r increases from zero, the crossover scale for the mixed-valence regime is pushed down:

$$D_{\rm MV}=\begin{cases}\Gamma_0\cdot(\Gamma_0/D_0)^{r/(1-r)}, & 0\leqslant r<1;\\ 0, & r\geqslant 1.\end{cases} \tag{8}$$

For $r\geqslant 1$, the ratio Γ/D always *decreases* under scaling, which completely rules out mixed-valence behavior; instead, the system must eventually enter either the local-moment regime or the empty-impurity regime.

The depression of the mixed-valence scale $D_{\rm MV}$ and the weakened renormalization of ε_d both tend to widen the region of parameter space exhibiting local-moment behavior. To quantify this trend, let ε_{d*}^0 be the greatest (least negative) bare impurity energy which flows to the local-moment regime. This energy is given implicitly by the equation $D_{\rm MV}=D_{\rm LM}$. Using Eqs. (6) and (8),

$$\varepsilon_{d*}^0=\left(\frac{1}{\pi r}-1\right)D_{\rm MV}-\frac{\Gamma_0u^r}{\pi r}. \tag{9}$$

The plot of $\varepsilon_{d*}^0/\Gamma_0$ in Fig. 1 clearly shows the expansion of the local-moment region with increasing r. (In reality, ε_{d*}^0 describes not a sharp boundary between the mixed-valence and local-moment regimes, but rather a narrow crossover region in which both $-E$ and Γ become large.)

At the point where the system enters the local-moment regime, the Anderson model can be mapped via a Schrieffer-Wolff transformation[19] onto the Kondo model with an effective exchange coupling

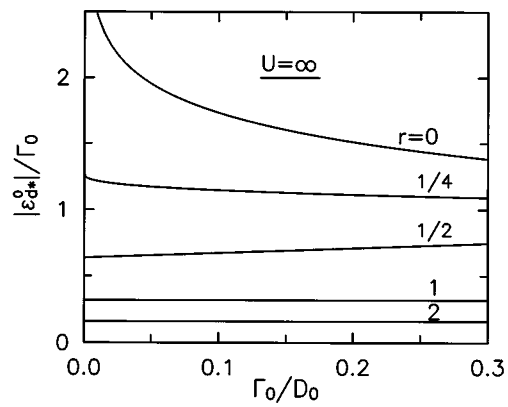

FIG. 1. Boundary of the local-moment regime, $|\varepsilon^0_{d*}|$ vs Γ_0, for different values of r. Any bare impurity energy $\varepsilon^0_d < \varepsilon^0_{d*}$ eventually leads to local-moment behavior.

$$\rho_0 J = \left[\frac{2\Gamma_0}{\pi D_{\rm LM}} + \frac{2\Gamma_0}{\pi(U - D_{\rm LM})} \right] \left(\frac{D_{\rm LM}}{D_0} \right)^r . \tag{10}$$

For given impurity parameters (ε^0_d, U, and Γ_0), the Kondo J for $r>0$ is reduced compared to that for a regular density of states, due both to the depression of Γ and to the weaker renormalization of ε_d. A lower bound on the reduction factor, obtained by neglecting the renormalization of ε_d, is $|\varepsilon^0_d/D_0|^r$. This effect is illustrated in Fig. 2, which plots $\rho_0 J$ as a function of ε^0_d, for $U=\infty$, $\Gamma_0 = 0.1 D_0$, and several values of r. For $r<1$, $\rho_0 J$ rises to reach $2/\pi$ (the dashed line in Fig. 2) at $\varepsilon^0_d = \varepsilon^0_{d*}$, the boundary of the local-moment region; whereas for $r>1$, $\rho_0 J$ decreases instead. Note that only for the $r=0$ and $r=1/4$ curves is the condition $\rho_0 J \gtrsim r$ for the existence of a Kondo effect satisfied over any great range of ε^0_d. This observation extends to other values of Γ_0 and U.

Poor man's scaling neglects higher-order corrections which conceivably could accumulate to become important at low energies. However, the scaling picture presented above is supported by nonperturbative renormalization-group calculations, similar to those for the Kondo model reported in Ref. 11. All the data presented here were computed for $U=\infty$ and $\Gamma_0 = 0.1 D_0$.

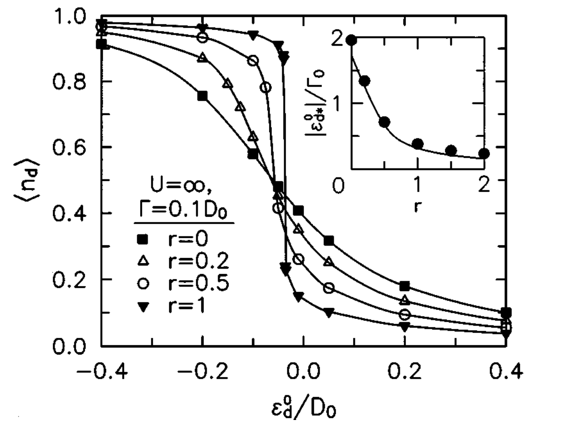

FIG. 3. Average impurity occupation $\langle n_d \rangle$ at temperature $T=10^{-6} D_0$, plotted vs ε^0_d for different values of r. The lines are provided as a guide to the eye. Inset: Comparison of the scaling prediction (solid line) and numerical data (circles) for the boundary of the local-moment regime, $|\varepsilon^0_{d*}|$ vs r.

Figure 3 plots the low-temperature impurity occupancy as a function of ε^0_d. The range of ε^0_d satisfying an operational definition of mixed valence ($0.25 \leqslant \langle n_d \rangle \leqslant 0.75$) narrows dramatically as r increases. The inset compares the boundary of the local-moment regime obtained using this criterion with the scaling result in Eq. (9). The alternative definitions of ε^0_{d*} are qualitatively equivalent, although there is a small shift between the two data sets.

Figure 4 shows numerical results for the impurity susceptibility. Three curves are plotted for $r=0.2$: For $\varepsilon^0_d = -0.1 D_0$, $T\chi_{\rm imp}$ falls monotonically (with decreasing temperature) from its valence-fluctuation value of 1/6, i.e., the system flows to mixed valence, a conclusion that is confirmed by the low-temperature value $\langle n_d \rangle = 0.63$. The curve for $\varepsilon^0_d = -0.3 D_0$ rises monotonically, indicating that the local-moment regime is entered, and furthermore that the effective exchange J falls short of the critical value J_c necessary for a Kondo effect, so the impurity moment decouples from the conduction band as $T \to 0$. The rise and subsequent fall of the $\varepsilon^0_d = -0.18 D_0$ curve (for which $\lim_{T\to 0} \langle n_d \rangle = 0.85$) shows that in this case $J > J_c$, meaning a Kondo effect does take place.

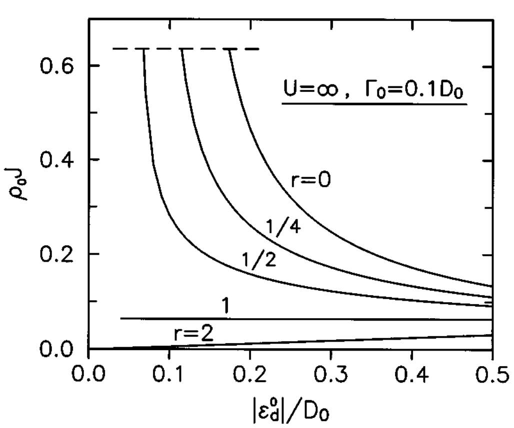

FIG. 2. Kondo coupling $\rho_0 J$ on entry to the local-moment regime, plotted vs $|\varepsilon^0_d|$ for different values of r.

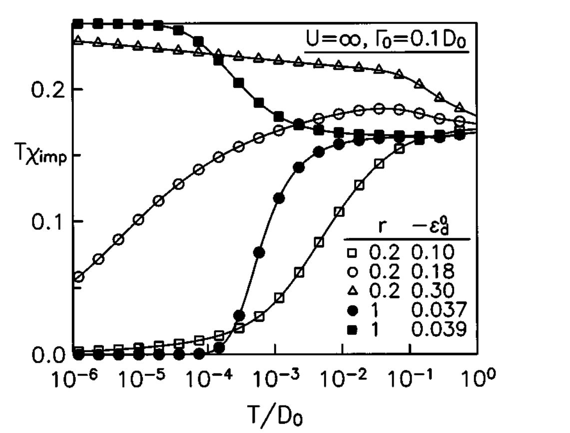

FIG. 4. Impurity susceptibility $T\chi_{\rm imp}$ vs T/D_0, for two different power-law densities of states defined in Eq. (2).

The two curves for $r=1$ show that for $\varepsilon_d^0=-0.037$, the system flows to the empty-impurity regime, whereas for $\varepsilon_d^0=-0.039$ it exhibits an unscreened local moment. Thus, the mixed-valence and Kondo-quenched regimes have essentially vanished, as predicted above.

Restricted power-law density of states: In most gapless systems, the power-law variation of the density of states does not extend over the entire band in the manner assumed in Eq. (2). We therefore repeat the preceding analysis for a density of states which rolls over to a constant outside a pseudogap of width Δ, i.e., $\rho(\epsilon)=\rho_0|\epsilon/\Delta|^r$ for $|\epsilon|<\Delta$, but $\rho(\epsilon)=\rho_0$ for $\Delta<|\epsilon|\leq D$.

At energies much greater than Δ, scaling should proceed very much as for a constant density of states. It is quite possible for the system to pass out of the valence-fluctuation regime before the pseudogap can have any real effect. However, we are more interested in values of ε_d^0 and Γ_0 which are sufficiently small that the bandwidth can be scaled into the range $D<\Delta$, where Eqs. (3) and (4) must apply. The subsequent renormalization of Γ and ε_d is identical to that for a system having a pure power-law density of states, but with a bare bandwidth Δ and a bare impurity energy $\varepsilon_d(\Delta)$ given by Eq. (7). The qualitative effects of the pseudogap should therefore be the same as those found above, although the magnitude of these effects will certainly decrease as the width of the pseudogap becomes smaller. The local-moment regime will still expand, and the Kondo J will be reduced relative to the case $r=0$ by a factor of at least $|\varepsilon_d(\Delta)/\Delta|^r$.

Finally, we note a parallel between our results and findings that an Anderson impurity in a Luttinger liquid has an expanded local-moment regime.[20] This similarity appears surprising, since in an interacting one-dimensional electron gas, independent fermionic excitations are replaced by collective bosonic modes.[6] It seems, though, that bulk interactions affect the valence-fluctuation regime of the impurity only by generating a power-law spectrum of one-electron states which hybridize with the localized level. The similarity with the noninteracting case does not extend into the local-moment regime: there is no threshold value of J required to achieve a Kondo effect in a Luttinger liquid.[21]

In summary, we have investigated local-moment formation in Fermi systems having a density of states which vanishes as $|\epsilon|^r$ near the Fermi energy. The pseudogap strongly suppresses hybridization between conduction electrons and an impurity level, and weakens the renormalization of the impurity energy. These effects in turn expand the range of bare impurity parameters that lead to localization of a spin at the impurity site, but reduce the value of the Kondo exchange coupling of this spin to the band, thereby decreasing the likelihood that the moment will be Kondo screened at low temperatures.

We thank P. Hirschfeld for useful comments. Portions of this work were carried out while one of us (K.I.) was visiting the Institute for Theoretical Physics, Santa Barbara. This research was supported in part by NSF Grants No. DMR93-16587 and PHY94-07194.

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*Affiliated with the National High Magnetic Field Laboratory, Tallahassee, Florida.

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