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On Magnetic Impurities in Gapless Fermi Systems

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Abstract

In ordinary metals, antiferromagnetic exchange between conduction electrons and a magnetic impurity leads to screening of the impurity spin below the Kondo temperature, T_K. In systems such as semimetals, small-gap semiconductors and unconventional superconductors, a reduction in available conduction states near the chemical potential can greatly depress T_K. The behavior of an Anderson impurity in a model with a power-law density of states, $N(\epsilon) \sim |\epsilon|^r$, $r > 0$, for $|\epsilon| < \Delta$, where $\Delta \ll D$, is studied using the non-crossing approximation. The transition from the Kondo singlet to the magnetic ground state can be seen in the behavior of the impurity magnetic susceptibility χ. The product $T\chi$ saturates at a finite value at low temperature for coupling smaller than the critical one. For sufficiently large coupling $T\chi \to 0$, as $T \to 0$, indicating complete screening of the impurity spin.

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Introduction. In a number of Fermi systems the density of states $N(\epsilon)$ vanishes at the Fermi surface E_F and varies linearly or quadratically for $|\epsilon|/D \equiv |E - E_F|/D \ll 1$, where D is the energy scale associated with the conduction electron bandwidth. This situation may arise e.g. in heavy-fermion or cuprate superconductors and anisotropic heavy fermion semiconductors. [1] Also exotic phases of the Hubbard model may possess $N(\epsilon) \sim |\epsilon|$ in two dimensions. [2]

In normal metals dilute impurities coupled antiferromagnetically to the conduction band lead to low-temperature reduction of the Curie term in the impurity magnetic susceptibility and an increase in the resistivity. This is known as a Kondo effect. The formation of the spin-singlet state favored by the antiferromagnetic coupling depends on the availability of electronic states at low energies.

Earlier studies by poor-man's scaling and large-N method, where N is impurity orbital degeneracy, showed that the Kondo effect survives if the coupling between electrons and the impurity J is larger than a critical value J_c. [3] In a gapless system with $N(\epsilon) \sim |\epsilon|^r$, J_c scales linearly with r for $r \ll 1$. A large-N approach to magnetic impurities in superconductors [4,5] leads to similar results for J_c. However, for $r \leq 1$ or $N = 2$, any finite impurity concentration was found to result in $J_c = 0$. Numerical renormalization group calculations [6,7] and third-order scaling [8] show that the Kondo effect does not occur for $r > 1/2$ in the particle-hole symmetric problem. Breaking this symmetry e.g. by potential scattering or band asymmetry helps the screening of the impurity moment. The critical coupling J_c was found to be strongly dependent on the magnitude of the potential scattering term. [6] Earlier calculations for the case of a full gap, $N(\epsilon) = 0$ for $|\epsilon| < \Delta \ll D$, also found finite J_c away from particle-hole symmetry. [9,10]

In this work the SU(N) Anderson model is studied in the non-crossing approximation (NCA). In the limit of large Coulomb repulsion U on the impurity site and for temperatures $T \ll U$, the model has the form,

$$H = \sum_{k,m} \epsilon_k c^\dagger_{km} c_{km} + E_f \sum_m f^\dagger_m f_m + V \sum_{k,m} (c^\dagger_{km} f_m b^+ + h.c.) + \lambda(\sum_m f^\dagger_m f_m + b^+ b - 1) \ , \quad (1)$$

where E_f is the position of the bare impurity level, f and b are the impurity fermion and the slave boson operators, respectively. The last term in the Hamiltonian follows from the restriction of the Hilbert space to a singly occupied impurity site, $\sum_m f^\dagger_m f_m + b^+ b = 1$, $m = 1, ..., N$. The self-energies of the slave boson and the impurity fermion Green's functions are given by

$$\Sigma_0(\omega + i0^+) = NV^2 \int_{-\infty}^{\infty} d\epsilon f(\epsilon) N(\epsilon) G_m(\omega + \epsilon + i0^+) \ , \tag{2}$$

and

$$\Sigma_m(\omega + i0^+) = V^2 \int_{-\infty}^{\infty} d\epsilon (1 - f(\epsilon)) N(\epsilon) G_0(\omega - \epsilon + i0^+) \ . \tag{3}$$

The density of states of the conduction band is assumed to be of the form $N(\epsilon) = C|\epsilon/\Delta|^r \exp(-(\epsilon/D)^2)$ for $0 < |\epsilon| < \Delta/D$, and $C\exp(-(\epsilon/D)^2)$ otherwise, and C is a normalization constant. The exponential part of $N(\epsilon)$ does not influence the low-energy physics in any important way, while it is convenient in solving the integral equations (2) and (3).

Numerical results. Here we focus on the non-degenerate case, $N = 2$. Results for static spin susceptibility are shown in Figure 1 for $\Delta/D = 10^{-5}$, $E_f/D = -0.67$, and $r = 1$ and $r = 2$. For larger $\Gamma \equiv \pi N_0 V^2$, $T\chi$ decreases to zero at low temperature, which is associated with the screening of the impurity spin. For Γ smaller than a certain critical coupling Γ_c, $T\chi$ remains finite, as $T \to 0$, indicating that impurity is not screened. The critical coupling for the data sets presented in Fig. 1 is $\Gamma_c/D \simeq 0.108$ for $r = 1$ and $\Gamma_c/D \simeq 0.115$ for $r = 2$. Qualitatively similar behavior of the impurity susceptibility was found by numerical renormalization group calculations. [6,7]

The transition from the spin-singlet ground state to unscreened moment is also reflected in the impurity density of states. The Abrikosov-Suhl resonance approaches the Fermi level when $\Gamma \to \Gamma_c$. For $\Gamma < \Gamma_c$ the resonance falls below E_F as illustrated in Figure 2. Analogous behavior of $N_f(\omega)$ was noted earlier by Ogura and Saso [11] for the case of a full gap ($r = \infty$).

Preliminary analysis of the dependence of the critical coupling on Δ in the limit $\Gamma \ll -E_f$, and $\Delta/D \ll 1$, indicates scaling $\Gamma_c \sim D/\ln(D/\Delta)$, independent of r, at least for $r \geq 1$. This can be expected on the basis of the large-N mean-field results in the Kondo limit, [4] where it was found that the critical exchange coupling is $J_c \simeq 2D/\ln(2D/\Delta)$ for $\Delta \ll D$ in a model with $N(\epsilon) = const$ outside the pseudogap region.

A more detailed study, including results for $N > 2$, will be presented in a separate publication.

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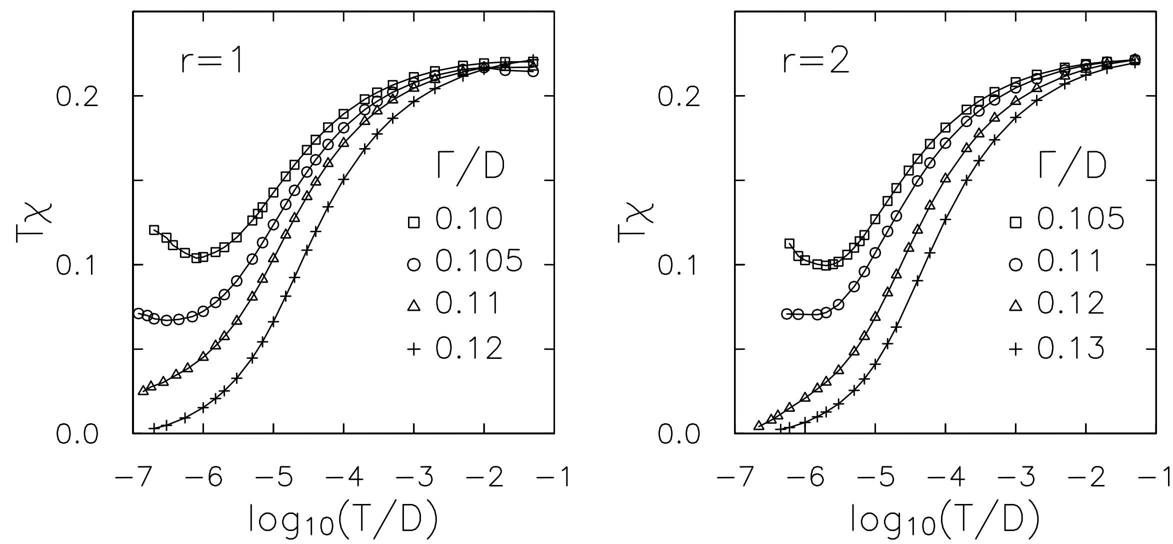
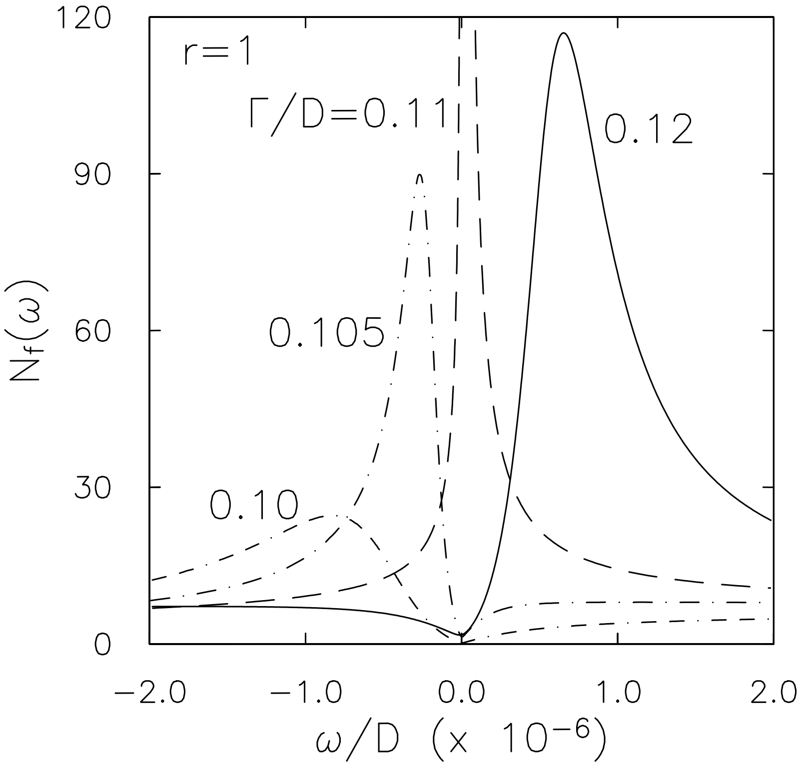
FIGURES

FIG. 1. Impurity spin susceptibility $T\chi$ as a function of $\log(T/D)$ for $r = 1$ and $r = 2$. The magnitude of the pseudogap is $\Delta/D = 10^{-5}$ and the bare impurity level is $E_f/D = -0.67$.

FIG. 2. The low-energy part of the impurity density of states $N_f(\omega)$ for $r = 1$ and the same data set as in Figure 1, evaluated at $T/D = 2 \times 10^{-7}, 1.2 \times 10^{-7}, 1.4 \times 10^{-7}$, and 2×10^{-7} for $\Gamma/D = 0.10, 0.105, 0.11,$ and 0.12, respectively.


r=1
Γ/D
0.10
0.105
0.11
0.12
Tχ
0.0
0.1
0.2
−7 −6 −5 −4 −3 −2 −1
log10(T/D)
r=2
Γ/D
0.105
0.11
0.12
0.13
Tχ
0.0
0.1
0.2
−7 −6 −5 −4 −3 −2 −1
log10(T/D)



r=1
Γ/D=0.11
0.12
0.105
0.10
$N_f(\omega)$
ω/D (x 10^{-6})
120
90
60
30
0
−2.0
−1.0
0.0
1.0
2.0