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ON MAGNETIC IMPURITIES IN GAPLESS FERMI SYSTEMS

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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, $\rho(\epsilon) \propto |\epsilon|^r$, $r > 0$, for $|\epsilon| < \Delta$, where Δ is small compared to the bandwidth, 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 $T\chi \rightarrow 0$, as $T \rightarrow 0$, indicating a complete screening of the impurity spin.

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1. Introduction

In a number of Fermi systems the density of states $\rho(\epsilon)$ vanishes at the Fermi surface E_{F} and varies linearly or quadratically for $|\epsilon|/D \equiv |E-E_{\mathrm{F}}|/D \ll 1$, 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 $\rho(\epsilon) \propto |\epsilon|$ in two dimensions [2].

In normal metals dilute impurities coupled antiferromagnetically to the conduction band lead to a 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 $\rho(\epsilon) \propto |\epsilon|^r$, 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, $\rho(\epsilon) = 0$ for $|\epsilon| < \Delta \ll D$, also found a finite J_c away from the 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 following form:

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

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, $\sum_m f^\dagger_m f_m + b^+ b = 1,\ m = 1, \ldots, N$. The self-energies of the slave boson and the impurity fermion Green's functions are given by

$$\Sigma_0(\omega + \mathrm{i}0^+) = NV^2 \int_{-\infty}^{\infty} \mathrm{d}\epsilon f(\epsilon) \rho(\epsilon) G_m(\omega + \epsilon + \mathrm{i}0^+) \tag{2}$$

and

$$\Sigma_m(\omega + \mathrm{i}0^+) = V^2 \int_{-\infty}^{\infty} \mathrm{d}\epsilon (1 - f(\epsilon)) \rho(\epsilon) G_0(\omega - \epsilon + \mathrm{i}0^+). \tag{3}$$

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

2. Numerical results

Here we focus on the non-degenerate case, $N = 2$. Results for static spin susceptibility are shown in Fig. 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, Tχ 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 $r = 2$. A 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 the unscreened moment is also reflected in the impurity density of states. The Abrikosov–Suhl resonance

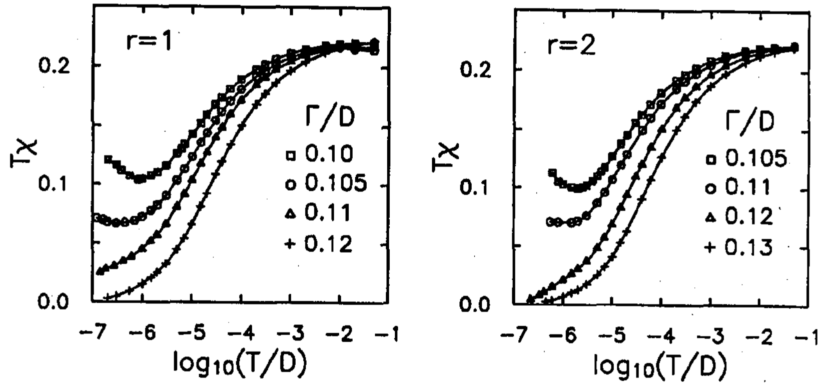

Fig. 1. Impurity spin susceptibility $T\chi$ as a function of $\log(T/D)$ for $r = 1$ and $r = 2$. The magnitude of the pseudogap is $\Delta/D = 10^{-5}$ and the bare impurity level is $E_f/D = -0.67$.

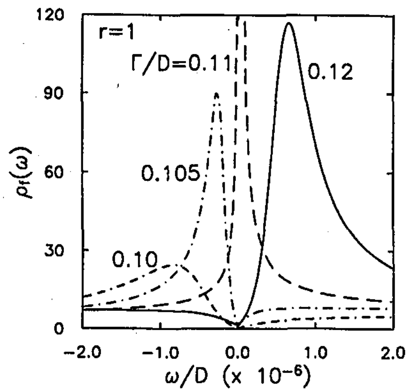

Fig. 2. The low-energy part of the impurity density of states $\rho_f(\omega)$ for $r = 1$ and the same data set as in Fig. 1, evaluated at $T/D = 2 \times 10^{-7}$, 1.2×10^{-7}, 1.4×10^{-7}, and 2×10^{-7} for $\Gamma/D = 0.10$, 0.105, 0.11, and 0.12, respectively.

approaches the Fermi level when $\Gamma \to \Gamma_c$. For $\Gamma < \Gamma_c$ the resonance falls below E_F as illustrated in Fig. 2. The analogous behavior of $N_f(\omega)$ was noted earlier by Ogura and Saso [11] for the case of a full gap ($r = \infty$).

A 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 $\Gamma_c \propto D/\ln(D/\Delta)$, 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 $\rho(\epsilon) = \text{const}$ outside the pseudogap region.

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

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