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Anderson Impurity in a Correlated Conduction Band

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We investigate the physics of a magnetic impurity with spin $1/2$ in a correlated metallic host. Describing the band by a Hubbard Hamiltonian, the problem is analyzed using dynamical mean-field theory in combination with Wilson's nonperturbative numerical renormalization group. We present results for the single-particle density of states and the dynamical spin susceptibility at zero temperature. New spectral features (side peaks) are found which should be observable experimentally. In addition, we find a general enhancement of the Kondo scale due to correlations. Nevertheless, in the metallic phase, the Kondo scale always vanishes exponentially in the limit of small hybridization.

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The Anderson model [1] has been successfully applied in the past to describe the physics of a magnetic impurity embedded in a conducting host. Extensive theoretical studies of this particular many-body problem led to considerable insight as well as progress in the development of new methods [2]. The most thoroughly analyzed case is that of an impurity in a noninteracting conduction band with a constant density of states. Several properties have been established by Wilson's numerical renormalization group (NRG) [3,4] and by the Bethe ansatz [5]. Most importantly, a new many-body energy scale T_K (the Kondo temperature) arises, which is exponentially small in the limit of vanishing hybridization. In addition, it has been demonstrated [6] that below this temperature the system can always be understood as a "local Fermi liquid" with strongly renormalized quasiparticles. The single-particle spectrum was shown to exhibit a generic three peak structure consisting of two atomic levels and a quasiparticle resonance of width T_K. Based on this model, a number of experimental results for dilute impurities in metals have been explained successfully, including measurements of the resistivity, the magnetic susceptibility, and the specific heat. For a review, see Ref. [7].

It has become clear, however, that the single impurity Anderson model is somewhat too simplified and that qualitatively different types of physical behavior are possible when a more general Hamiltonian is considered. One very important characteristic of real materials is the interaction among the conduction electrons. This aspect is usually neglected, mostly for technical reasons, i.e., to simplify the investigation. If taken into account, we expect, at least, a renormalization of the model parameters. Our work will focus on the question whether, in addition, qualitatively new physics is possible. An experimental realization frequently cited in this context is the cuprate system $Nd_{2-x}Ce_xCuO_4$ [8], a concentrated impurity system, where the energy scale of low temperature heavy fermion behavior is apparently incompatible with the standard Kondo picture.

Models with a single impurity embedded in a correlated host were studied already within several approaches. Perturbative calculations in a slave boson representation by Khaliullin and Fulde [9] yielded a renormalization of the effective Kondo coupling. Very similar results were obtained by Tornow *et al.* [10] within a noncrossing approximation. Furthermore, in the limit of high dimensions and using a variational treatment, Davidovich and Zevin [11] found a qualitative change of the behavior of the Kondo temperature T_K. According to these authors, above some intermediate value of the conduction band interaction, T_K is no longer exponentially small at vanishing exchange coupling. In our work, we will discuss this issue in detail. Finally, in the case of one dimension, Phillips and Sandler [12] and also Schiller and Ingersent [13] represented the interacting host as a Luttinger liquid, which makes a renormalization group treatment possible. Among other results, they found that in some region of parameter space an unquenched local moment may survive down to the lowest temperatures.

These studies already indicate the competition of several effects: (i) The conduction band correlations may change the density of states (DOS) of the conduction band. (ii) A repulsive on-site interaction will reduce the hybridization of the impurity level. (iii) The conduction electrons will become increasingly polarized, thus enhancing the effective spin coupling of the impurity moment. In the following, using Wilson's nonperturbative NRG, we will analyze which one of these factors dominates.

Our Hamiltonian consists of a spin-$1/2$ impurity embedded in an interacting host (see also Fig. 1) represented by a one-band Hubbard model [14]:

$$H = -\sum_{ij\sigma}(t_{ij} - \epsilon_c\delta_{ij})c_{i\sigma}^{\dagger}c_{j\sigma} + U_B\sum_i n_{i\uparrow}n_{i\downarrow} + V\sum_{\sigma}(f_{\sigma}^{\dagger}c_{0\sigma} + \text{H.c.}) + Un_{f\uparrow}n_{f\downarrow} + \epsilon_f n_f\,. \tag{1}$$

Note that the impurity hybridizes with a single conduction band orbital, which in the following will be denoted as the $i = 0$ Hubbard site.

We will be interested in the case of half filling, which—assuming a bipartite lattice and next-neighbor hopping

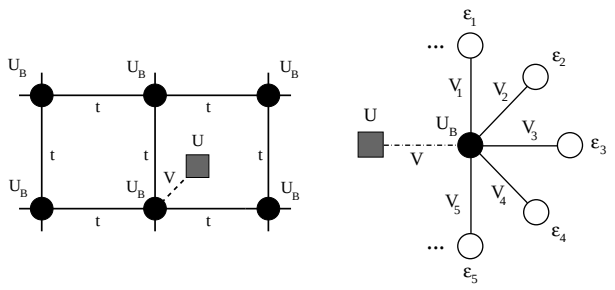

FIG. 1. Anderson impurity (square) coupled to one site of a correlated lattice (circles). The hybridization is taken to be purely local. Right: effective two-impurity model with noninteracting band orbitals (empty circles) of energy ϵ_i and hybridization V_i.

($t_{ij} = t$) only—is equivalent to $\epsilon_c = -U_B/2$ and $\epsilon_f = -U/2$. The calculations in our paper are restricted to the paramagnetic phase of the host. A controlled approach [15,16] to correlated lattice problems is possible in the limit of large coordination number $Z \to \infty$, scaling the hopping matrix elements as $t = (t^*/\sqrt{Z})$. In our treatment we will use the Bethe lattice and take the noninteracting half bandwidth $D = 2t^* = 1$ as the unit of energy. It should be emphasized, however, that the choice of the lattice is merely motivated by calculational convenience and should have no qualitative effect on the results [17].

It was pointed out in [11] that integrating out all the band fermions except those on the $i = 0$ Hubbard site (the so-called "cavity method") yields an effective action which has the same retarded part $S_{\text{eff,ret}} = -\int\int d\tau\, d\tau'\, c^\dagger_{0\sigma} \mathcal{G}_0^{-1}(\tau - \tau') c_{0\sigma}(\tau')$ as the pure Hubbard model. As a result, the system can be described as a two-impurity model (see Fig. 1) with an effective noninteracting bath defined by a hybridization function $\Delta_c(\omega) = \pi \sum_p |V_p|^2 \delta(\omega - \epsilon_p)$. In our calculation we will therefore follow a two-step procedure: First, we solve the Hubbard model in dimension $d \to \infty$ using Wilson's numerical renormalization group [2,4] as in [17]. In the paramagnetic phase considered here this leads to a Mott transition at a critical interaction strength $U_B^c \approx 2.92$. Correlations strongly influence the structure of the DOS; close to the transition point an effective narrow band [18] is formed by the quasiparticle resonance.

In the next step, we add the f impurity. The combined system is then again treated using NRG, this time without the self-consistency loop [the modification of the effective bath due to the impurity is $\mathcal{O}(1/N)$ and can therefore be neglected in the thermodynamic limit]. The band correlations enter via the previously determined DOS and the c-site interaction U_B. In our calculations we have confined ourselves to the metallic regime $U_B < 2.92$ and zero temperature.

First, we present results for the single-particle spectra $\rho_{f(c)}(\omega) = -\frac{1}{\pi}$, $\text{Im}G_{f(c)}(\omega)$ of the impurity f and the Hubbard site $i = 0$. Considering ρ_f (Fig. 2a), we obtain

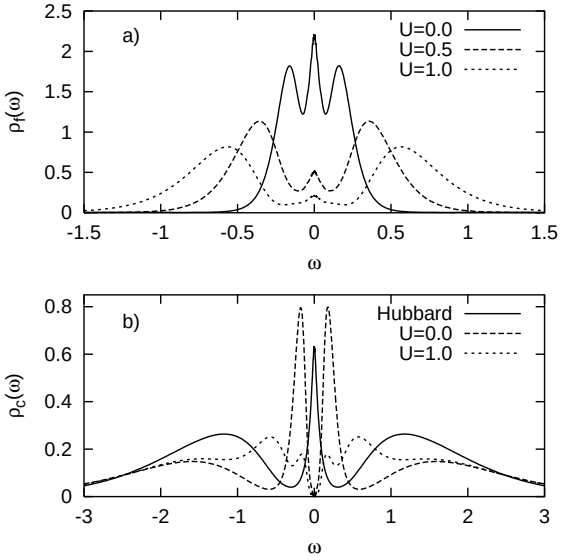

FIG. 2. Spectral densities ρ_f (a) and ρ_c (b) at zero temperature, $\Delta = 0.1$ and $U_B = 2.6$. For comparison, we also show the c spectral density at vanishing hybridization Δ, equivalent to the DOS of the Hubbard model.

a three peak structure in the spectrum already for $U = 0$ and small hybridization $\Delta = \frac{\pi V^2}{2D}$. This may be attributed to a narrowing of the effective band, leading to resonances at finite energy [18]. Upon increasing U, these peaks are reduced and weight is shifted to the atomic levels which for large interaction can be found at $\omega \approx \pm U/2$. In addition, the height of the quasiparticle peak is significantly reduced. Luttinger's theorem [19] which states that $\rho_f(0)$ is pinned at its $U = 0$ value is therefore found to be not valid in the case of an interacting conduction band.

Furthermore, we notice that the width of the quasiparticle resonance is almost independent of U, in contrast to the situation with $U_B = 0$. This already indicates a strong enhancement of the Kondo scale due to band correlations, as will be discussed in more detail below.

The corresponding results for ρ_c are shown in Fig. 2b. For any finite Δ a hybridization gap is formed. This is already the case at $U = 0$ and $U_B = 0$ (not shown here) and persists for finite interactions, indicating that the system is a Fermi liquid (a nonvanishing self-energy at $\omega = 0$ would smear out the gap). The Fermi liquid picture is independently supported by the fact that the fixed point of the NRG and its leading irrelevant eigenoperators are unchanged compared to the noninteracting case; see also [20].

A quantity which is more easily accessible experimentally is the (longitudinal) dynamic susceptibility, defined as the response of the impurity spin to a local magnetic field

$$\chi(\omega) = i \int_0^\infty dt\, e^{i\omega t} \langle [S_f^z(t), S_f^z(0)] \rangle . \qquad (2)$$

Within the NRG formalism it is convenient [21] to calculate the imaginary part $\chi''(\omega)$ directly and to obtain the

real part $\chi'(\omega)$ via Kramers-Kronig transformation. In particular, the static susceptibility is then given by $\chi_0 = \chi'(0)$. In the following we will focus on the spin relaxation function:

$$S(\omega) = \frac{\chi''(\omega)}{\pi\omega}. \tag{3}$$

In a first step, we consider its behavior with increasing band correlations for fixed Δ, U (see Fig. 3a).

In this plot we employed a normalization of $\chi''(\omega)$ suggested by the Shiba relation [22,23]

$$\lim_{\omega\to 0} \frac{\chi''(\omega)}{\pi\omega} = 2\chi_0^2 \tag{4}$$

derived for $U_B = 0$ [23]. For the noninteracting band this relation is indeed satisfied (with an error of less than 10% due to the NRG procedure). With increasing U_B systematic deviations arise, indicating that the general proof [23] based on Ward identities breaks down for an interacting conduction band. The line shape of $\chi''(\omega)$ also depends on U_B. For a weakly correlated band we obtain a single elastic peak, while close to the metal-insulator transition (MIT) at $U_B^c = 2.92$ two additional inelastic side peaks arise. They indicate that in this case the Kondo singlet is formed at an energy scale which lies outside the effective band. The width of the remaining elastic peak is determined by the effective bandwidth of the Hubbard model.

An increase of the impurity interaction U (Fig. 3b) leads to a suppression of the elastic peak and to a shift of the inelastic peaks (corresponding to a slight reduction of the singlet binding energy).

For the real part $\chi'(\omega)$, some typical results are shown in Fig. 4: Already at a weak band interaction U_B (when the Hubbard DOS is well approximated by the noninteracting one) the static susceptibility χ_0 is strongly reduced.

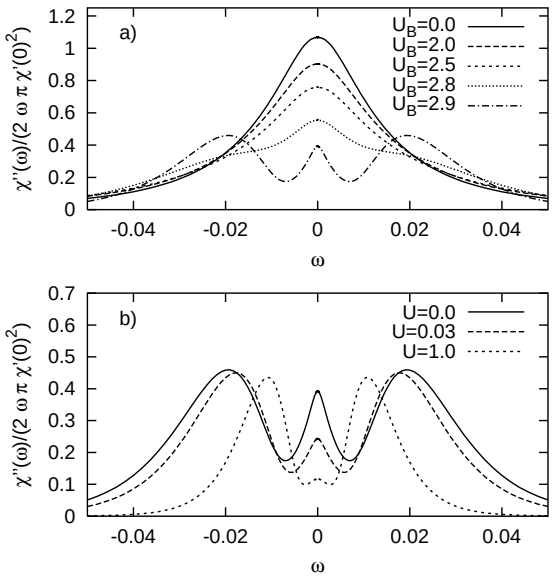

FIG. 3. Local spin relaxation function for fixed $U = 0$ (a) and $U_B = 2.9$ (b). In both cases, the hybridization has the value $\Delta = 0.01$. Note that due to the normalization a value of 1 at $\omega = 0$ would be consistent with the Shiba relation.

Of particular interest is the hybridization dependence of the low energy scale, the Kondo temperature T_K, at intermediate to strong band interaction. While there is agreement on the fact that a small U_B enhances the effective Kondo coupling [9–11,20] but still leads to an exponentially vanishing T_K at small hybridization Δ, it was found in Ref. [11] that above an intermediate U_B the Kondo temperature varies linearly in Δ. We will now consider this issue in detail.

We define T_K to be equal to the binding energy of the local singlet, which is given by the position of the maximum in $\chi''(\omega)$. Note that this definition also applies to the case of a noninteracting impurity ($U = 0$). With increasing Δ we observe a crossover from an exponential to a power law behavior $T_K \sim \Delta$. The crossover point depends on U_B and is proportional to the effective bandwidth D_{eff}. For very small Δ, the Kondo temperature always varies as $\ln T_K \sim -U/\Delta$. In contrast to Ref. [11] we therefore find an exponentially small T_K at any U_B, as long as the host is metallic. The discrepancy may be due to the approximate variational method used in Ref. [11].

At a finite band interaction, U_B can lead to a nonmonotonic behavior of T_K; see Fig. 5. The increase at small U_B can be attributed to the local interaction on the site $i = 0$ while the decrease close to the MIT is due to band narrowing. As $U_B \to U_{\text{MIT}}$, the Kondo scale approaches a finite limiting value, indicating that even in the paramagnetic insulator the local impurity is screened. We can understand this by considering the effective hybridization "seen" by the f impurity

$$\Delta_f = \frac{V^2}{\omega + i0^+ - \Delta_c(\omega^+)}. \tag{5}$$

In the insulating host $\Delta_c = 0$ and therefore

$$\Delta_f(\omega) \sim V^2\delta(\omega). \tag{6}$$

In this case, the impurity couples exclusively to the $i = 0$ site, the singlet is purely local, and no Kondo many-particle physics is possible.

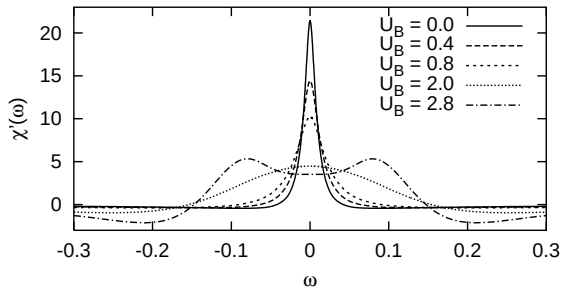

FIG. 4. Real part of the dynamic susceptibility at $\Delta = 0.1$ and $U = 1.0$.

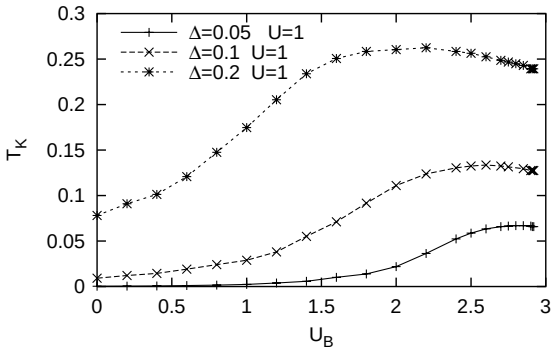

FIG. 5. Kondo temperature as a function of the band interaction.

In conclusion, we analyzed a model describing an Anderson impurity in a correlated band. The limit of large coordination numbers made a treatment within the dynamical mean-field theory possible. Using the nonperturbative numerical renormalization group, we solved the corresponding effective two-impurity model and obtained the one particle spectra and the dynamic susceptibility. We found that the system is always a Fermi liquid as long as the host is metallic. Band correlations lead to a strongly enhanced Kondo scale, indicating that the dominant effect of U_B is to increase the spin polarization of the conduction electrons. Nevertheless, T_K remains exponentially small as a function of hybridization. This is consistent with a Fermi liquid picture of the Hubbard host where the Kondo screening of the impurity is due to fermionic quasiparticles instead of bare electrons. In the spectral quantities, a change of the line shape and the formation of side peaks is observed close to the Mott transition. This is explained by a narrowing of the effective conduction band.

Of course it would be desirable to compare our results with experiments on systems that can actually be considered as dilute. One possibility might be to perform ESR measurements on rare earth systems, where impurities can be introduced into a correlated host in a controlled way. Here the main experimental signal [the absorption $\chi''(\omega)$] could be directly related to our model calculations.

In future calculations we will study the effects of finite temperature, different fillings, and antiferromagnetic order on our findings. We will also extend our analysis to thermodynamic and transport properties.

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