Impurity bands in Kondo insulators

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Kondo insulators like $Ce_3Bi_4Pt_3$ and CeNiSn are compounds with small-band-gap semiconductor properties. Nonmagnetic impurities, so-called Kondo holes, break the translational invariance and hence the coherence of the ground state. Isolated impurities give rise to a bound state in the gap, which pins the Fermi level and has magnetic properties (Curie susceptibility and Schottky anomaly in the specific heat). A finite concentration of Kondo holes gives rise to an impurity band inside the gap of the f-electron density of states, whose height and width are proportional to $\sqrt{c}$ for small concentrations. The specific heat is proportional to T at very low temperatures and the susceptibility is Pauli-like at low T. The correlations within the f band are introduced via a self-energy, evaluated to second-order perturbation in U. We use the $(1/d)$-expansion method of Schweitzer and Czycholl to leading order in which the $\mathbf{k}$ integrations are properly carried out, but the $\mathbf{k}$ dependence of the self-energy is neglected. The main effect of U is to narrow the gap, as well as the impurity band.

I. INTRODUCTION

The unusual low-temperature properties of heavy-electron systems have received much attention in recent years, in particular the development of *coherence* in stoichiometric compounds.[1,2] The coherence manifests itself most dramatically in low-temperature resistivity and magnetoresistivity, but also in the f-electron density of states (DOS). At high temperatures (compared with the Kondo temperature T_K), the properties of a metallic system are similar to that of dilute-impurity systems.[3] The scattering of the electrons is said to be *incoherent*, i.e., independent from site to site, giving rise to a large resistivity. At low T and for low energies, on the other hand, as a consequence of the translational invariance of the lattice, there is effectively no scattering (Bloch theorem) and the resistivity is then ideally zero for a heavy-fermion metal.

The effects of coherence are most pronounced in so-called Kondo insulators, which have small-band-gap semiconductor properties. As a consequence of the coherence, a hybridization gap opens at the Fermi level. In contrast, in the metallic situation, the Fermi level does not lie in the gap and the gap is smeared to a pseudogap by spin fluctuations via the f-electron self-energy. The Kondo insulators SmS, SmB_6, and TmSe were already an exciting topic about ten years ago.[4] The more recent discovery of several Ce, Yb, and U Kondo insulators, e.g., CeNiSn,[5] $Ce_3Bi_4Pt_3$,[6] YbB_{12},[7] and UNiSn,[8] has renewed and enhanced the interest in this subject. All systems seem to be nonmagnetic (i.e., van Vleck–dominated susceptibility) at low T, except TmSe and UNiSn, for which antiferromagnetic long-range order has been reported. In UNiSn the antiferromagnetic transition is accompanied by an insulator-metal transition, so that the system is semiconducting only at higher temperatures. In view of the small energy-band gaps involved, the properties of these compounds strongly depend on strains in the crystal and impurities.

The formation of the coherent state in the Kondo lattice can also be studied by introducing disorder into the system.[9] Alloying studies of mixed-valence and heavy-fermion compounds have been a subject of great experimental interest.[9] Here we focus our attention on the dilute limit of nonmagnetic impurities (Kondo holes) in a heavy-fermion lattice. Kondo holes are experimentally realized by substituting, for instance, a Ce ion in a stoichiometric Ce compound by a La or Th or a U ion in a U–heavy-fermion system by a Th impurity. Adding impurities to a Kondo lattice breaks the translational invariance and gradually destroys the coherence of the heavy-fermion ground state.

In recent publications[10,11] we reported a simple microscopic theory of the Kondo hole for both the metallic and insulating situations. We considered an Anderson lattice without orbital degeneracy, with on-site hybridization and a nearest-neighbor tight-binding dispersion for the conduction states on a simple cubic lattice. The Kondo hole is a missing f electron at a given site, and it is introduced by a very large local f-level energy, which prevents the occupation of the f level. The correlations within the f band are introduced via a self-energy, evaluated to second-order perturbation in U. We used the $(1/d)$-expansion method of Schweitzer and Czycholl[12] to leading order (mean field for $d=\infty$) in which the $\mathbf{k}$ integrations are properly carried out, but the $\mathbf{k}$ dependence of the self-energy is neglected. Although a second-order perturbation in U limits our results to small-U values, while in actual heavy-fermion system correlations are large, we do not expect large-U values to introduce further qualitative changes in the f DOS. We studied the effects of the scattering off the Kondo hole in the local density of f states in the neighborhood of the nonmagnetic impurity. The f DOS at the Kondo hole is, of course, zero. In the case of a Kondo insulator, a bound state (δ function) develops in the energy gap. The spectral weight

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of the bound state decreases rapidly with increasing distance from the impurity. In the metallic case we obtain a resonance of finite width in the pseudogap of the lattice, which again is localized in the neighborhood of the Kondo hole. These states only appear in the coherent phase and disappear in the continuum at higher temperatures.

In this paper we discuss some further properties of isolated Kondo holes in metallic and insulating environments and extend the theory to a finite concentration of Kondo holes in Kondo insulators. The localized bound state caused by an isolated hole in the gap of a Kondo insulator has remarkable magnetic properties. Although originating from a missing f electron, it gives rise to a Curie-like susceptibility. A small magnetic field magnetically polarizes the localized state. This effective spin could in principle be experimentally detected by electron paramagnetic resonance. In practice, however, the inhomogeneous broadening of this line will make difficult its observation. Because of slightly different surroundings, the resonance energies of the defects will have a distribution, whose width has to be of the order of 0.1 K to be observable. The Kondo holes are also going to affect the infrared-absorption spectrum of Kondo insulators, in particular at low frequencies. These effects are less pronounced in the metallic case, where the bound state acquires a width through the self-energy and the position of the resonance is not at the Fermi level.

When the concentration of Kondo holes is increased, an impurity band forms in the gap. The effect of adding nonmagnetic impurities is then gradually to smear the hybridization gap in the Kondo insulator. For a low density of Kondo holes, the width and height of this band depend nonanalytically on the impurity concentration. The Fermi level is pinned within this band. As a consequence of this finite bandwidth, there is a small low-temperature regime with a specific heat proportional to T. The γ coefficient is strongly enhanced. The susceptibility no longer diverges as $T\rightarrow 0$, as for the isolated Kondo hole, but follows a Curie-Weiss-like behavior with an antiferromagnetic Weiss temperature.

The remainder of the paper is organized as follows. In Sec. II we introduce the equations leading to the Kondo-hole bound state and the impurity band for a Kondo insulator. The results evaluated numerically are presented in Sec. III. Concluding remarks follow in Sec. IV.

II. MODEL AND THE f DENSITY OF STATES

We consider the Anderson lattice without orbital degeneracy and with an on-site hybridization V. The Hamiltonian is given by

$$H_0=\sum_{\mathbf{k},\sigma}\varepsilon_{\mathbf{k}}c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}+\varepsilon_f\sum_{i,\sigma}f^{\dagger}_{i\sigma}f_{i\sigma}+U\sum_i n_{i\uparrow}n_{i\downarrow}+V\sum_{\mathbf{k},\sigma}(c^{\dagger}_{\mathbf{k}\sigma}f_{\mathbf{k}\sigma}+f^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}) , \tag{2.1}$$

where ε_f is the f-level energy, U is the Coulomb repulsion in the f shell, $n_{i\sigma}=f^{\dagger}_{i\sigma}f_{i\sigma}$, $c^{\dagger}_{\mathbf{k}\sigma}$ ($f^{\dagger}_{\mathbf{k}\sigma}$) creates a conduction electron (f electron) with momentum $\mathbf{k}$ and spin σ, and $f^{\dagger}_{i\sigma}$ is the Wannier state at site $\mathbf{R}_i$. An isolated Kondo hole at site $\mathbf{R}$ can be introduced by the scattering potential

$$H_1=\Delta\varepsilon_f N^{-1}\sum_{\mathbf{k},\mathbf{k}',\sigma}\exp[-i(\mathbf{k}-\mathbf{k}')\mathbf{R}]f^{\dagger}_{\mathbf{k}\sigma}f_{\mathbf{k}'\sigma} , \tag{2.2}$$

where $\Delta\varepsilon_f$ is large and positive for the impurity to be nonmagnetic and N is the number of sites.

Since the impurity potential is factorizable, the $U=0$ scattering problem can be solved exactly.[10] It is convenient to introduce the matrix Green's function

$$\hat{G}_{\mathbf{k},\mathbf{k}'}(z)=\begin{bmatrix}\langle\langle f_{\mathbf{k}};f^{\dagger}_{\mathbf{k}'}\rangle\rangle_z & \langle\langle f_{\mathbf{k}};c^{\dagger}_{\mathbf{k}'}\rangle\rangle_z\\ \langle\langle c_{\mathbf{k}};f^{\dagger}_{\mathbf{k}'}\rangle\rangle_z & \langle\langle c_{\mathbf{k}};c^{\dagger}_{\mathbf{k}'}\rangle\rangle_z\end{bmatrix} , \tag{2.3}$$

where for simplicity we dropped the spin index (for $U=0$, up and down spins decouple). Using the equation of motion for $\hat{G}$, we obtain, after some algebra,

$$\hat{G}_{\mathbf{k},\mathbf{k}'}(z)=\hat{G}^0_{\mathbf{k}}(z)\delta_{\mathbf{k},\mathbf{k}'}+\Delta\varepsilon_f N^{-1}\hat{G}^0_{\mathbf{k}}(z)\hat{v}_{\mathbf{k}}\left[\hat{1}-\Delta\varepsilon_f N^{-1}\sum_{\mathbf{k}''}\hat{v}^{*}_{\mathbf{k}''}\hat{G}^0_{\mathbf{k}''}(z)\hat{v}_{\mathbf{k}''}\right]^{-1}\hat{v}^{*}_{\mathbf{k}'}\hat{G}^0_{\mathbf{k}'}(z) , \tag{2.4}$$

where $\hat{G}^0_{\mathbf{k}}(z)$ is the Green's function in the absence of impurity and

$$\mathbf{v}_{\mathbf{k}}=\begin{bmatrix}e^{-i\mathbf{k}\cdot\mathbf{R}} & 0\\ 0 & 0\end{bmatrix} . \tag{2.5}$$

In the limit $\Delta\varepsilon_f\rightarrow\infty$, the impurity has no f character and Eq. (2.4) reduces to

$$\hat{G}_{\mathbf{k},\mathbf{k}'}(z)=\hat{G}^0_{\mathbf{k}}(z)\delta_{\mathbf{k},\mathbf{k}'}-\hat{G}^0_{\mathbf{k}}(z)\hat{v}_{\mathbf{k}}\frac{1}{\sum_{\mathbf{k}''}G^0_{f\mathbf{k}''}(z)}\hat{v}^{*}_{\mathbf{k}'}\hat{G}^0_{\mathbf{k}'}(z) , \tag{2.6}$$

where $G^0_{f\mathbf{k}''}(z)$ is the f-electron Green's function in the absence of interactions. The imaginary part of the function (times $-1/\pi$)

$$N^{-1}\sum_{\mathbf{k}}G^0_{f\mathbf{k}}(z)=\frac{1}{z-\varepsilon_f}+\frac{V^2}{(z-\varepsilon_f)^2}\sum_{\mathbf{k}}\frac{1}{z-\varepsilon_{\mathbf{k}}-V^2/(z-\varepsilon_f)} \tag{2.7}$$

is the f DOS, which has a gap around ε_f. The real part

of this function has also a zero at one point inside this gap, giving rise to a pole in Eq. (2.6). This pole corresponds to the Kondo-hole bound state. While in our previous reports[10,11] we considered the spatial dependence of the impurity state on a simple cubic lattice, for the sake of simplicity in this paper we restrict ourselves to the continuum limit. We assume an elliptic density of states for the conduction electrons, i.e.,

$$F(z)=N^{-1}\sum_{\mathbf{k}}\frac{1}{(z-\varepsilon_{\mathbf{k}})}=\frac{2}{D^2}\left[z-(z^2-D^2)^{1/2}\right], \quad (2.8)$$

where D is the band half-width. Equations (2.6)–(2.8) then completely determine the f-electron Green's function for one Kondo hole in the absence of Coulomb repulsion.

In order to generalize this result to a finite concentration of impurities, it is convenient to rewrite the perturbed Green's function in terms of a self-energy for the f electrons. The Dyson equation reads

$$[\hat{G}^0_{\mathbf{k}}(z)^{-1}-\hat{\Sigma}_{\rm imp}(z,\varepsilon_f)]\hat{G}_{\mathbf{k}}(z)=\hat{1}\ , \quad (2.9)$$

where

$$\Sigma_{\rm imp}(z,\varepsilon_f)=\begin{pmatrix}-\dfrac{c}{N^{-1}\sum_{\mathbf{k}}G^0_{f\mathbf{k}}(z)} & 0\\ 0 & 0\end{pmatrix}, \quad (2.10)$$

with c being the impurity concentration. In this way we can interpret the Kondo-hole self-energy as a renormalization of the f-level energy. A self-consistent treatment of this self-energy immediately leads to the following implicit equation for $\tilde{\varepsilon}_f$:

$$\tilde{\varepsilon}_f(z)=\varepsilon_f+\Sigma_{\rm imp}(z,\tilde{\varepsilon}_f(z))\ , \quad (2.11)$$

which corresponds to the sum of all diagrams with noncrossing impurity lines. This equation leads to a complex f-level energy, the imaginary part broadening the δ function of the Kondo-hole bound state, giving rise to an impurity band of finite width.

The solution discussed so far corresponds to $U=0$. The main effect of the Coulomb interaction is to introduce an f-electron self-energy. For heavy electrons the momentum dependence of the self-energy is much less important than its energy dependence. We limit ourselves to a self-energy to second-order perturbation[13] in U about the Hartree-Fock solution. Schweitzer and Czycholl[12] have extensively discussed the self-energy for the periodic Anderson model to that order and developed a systematic approach to overcome the tedious $\mathbf{k}$ integrations. Their approach is based on a $1/d$ expansion,[14] where d is the dimension of the hypercubic lattice. The calculation is greatly simplified in leading order ($d\to\infty$), which corresponds to the local approximation (momentum independent). This result already contains the most relevant correlations. The $\mathbf{k}$ dependence is introduced by $1/d$ corrections,[12] which indeed turn out to be small for $d=3$. In this sense properties of the three-dimensional periodic Anderson model are quite close to those for $d=\infty$. The self-energy to second order in U and within the local approximation ($d\to\infty$) has the correct analytic properties and, qualitatively, the expected physical features.

In view of its success, we adopt the local approximation by Schweitzer and Czycholl.[12] The self-energy is then momentum independent, and correlations are straightforwardly incorporated into the $U=0$ solution for the Kondo hole if the bare f-level energy ε_f is renormalized according to

$$\varepsilon_f\to\varepsilon_f+\tfrac{1}{2}Un_f+\Sigma_U(z)\ , \quad (2.12)$$

where n_f is the f-level occupation. Note that the self-energy is not calculated self-consistently[15] with dressed Green's functions, i.e., propagators with self-energy, since a renormalized vertex would also be needed in this case in order to avoid violations of the charge-conservation Ward identity. In the same spirit we do not self-consistently incorporate the effects of the Kondo hole into the self-energy. The impurity breaks the translational invariance; this affects the f-electron propagator, giving rise to an additional $\mathbf{k}$ dependence in the self-energy, which is neglected here. In other words, the self-energy is evaluated to second order in U with the bare Green's functions for the Anderson lattice, but with the Hartree-Fock shift of the f-level energy $\varepsilon_f+\frac{1}{2}Un_f$.

A minor modification of the Schweitzer-Czycholl scheme is, however, necessary, since we consider an elliptic density of states rather than a simple cubic lattice. To second order in U and within the local approximation, we have, after carrying out the sums over the Matsubara poles,

$$\Sigma_U(z)=U^2(-i)\int d\lambda\, e^{i\lambda z}\{[A(\lambda)]^2B(-\lambda)+[B(\lambda)]^2A(-\lambda)\}\ , \quad (2.13)$$

where z is the external energy and $A(\lambda)$ and $B(\lambda)$ are defined by

$$A(\lambda)=\int_{-\infty}^{\mu}d\omega\, e^{-i\lambda\omega}\rho(\omega)\ , \quad (2.14a)$$

$$B(\lambda)=\int_{\mu}^{\infty}d\omega\, e^{-i\lambda\omega}\rho(\omega)\ , \quad (2.14b)$$

and $\rho(\omega)$ is given by

$$\rho(\omega)=\frac{2}{\pi}\frac{V^2}{D^2}\frac{1}{(\omega-\varepsilon_f)^2}\left[D^2-\left[\omega-\frac{V^2}{\omega-\varepsilon_f}\right]^2\right]^{1/2}. \quad (2.15)$$

Here μ is the chemical potential and $\rho(\omega)$ is the local DOS of the f electrons, where ε_f already contains the Hartree-Fock shift due to the Coulomb interaction.

The next step consists in incorporating the Coulomb self-energy $\Sigma_U(z)$ into the self-consistency condition (2.11), which now takes the form

$$\tilde{\varepsilon}_f(z)=\varepsilon_f+\Sigma_U(z)+\Sigma_{\rm imp}(z,\tilde{\varepsilon}_f(z))\ . \quad (2.16)$$

Note that $\Sigma_{\rm imp}(z,\tilde{\varepsilon}_f(z))$ is evaluated self-consistently with the Coulomb interaction, but in $\Sigma_U(z)$ we use only the bare Green's functions. The self-energy $\Sigma_U(z)$ has more a quantitative than qualitative effect on the Kondo-hole band.

If the concentration of Kondo holes is nonzero, the impurity band has a finite width with the Fermi level being

pinned inside the band. Fermi-liquid properties are then expected at very low temperatures. In particular, the specific heat is proportional to T and the charge and spin susceptibilities are finite as $T\rightarrow 0$. Within the local approximation the expressions for γ, $\chi_{\rm ch}$, and χ_s are then given by the standard relations[16,17]

$$\gamma=\frac{2\pi^2}{3}\rho_f(0)\left[1-\frac{\partial\Sigma_{\rm imp}(i\omega)}{\partial i\omega}-\frac{\partial\Sigma_U(i\omega)}{\partial i\omega}\right]_{\omega=0+}, \tag{2.17a}$$

$$\chi_{\rm ch}=2\rho_f(0)\left[1+\frac{\partial\Sigma_{\rm imp}(i\omega)}{\partial\varepsilon_f}+\frac{\partial\Sigma_U(i\omega)}{\partial\varepsilon_f}\right]_{\omega=0+}, \tag{2.17b}$$

$$\chi_s=\rho_f(0)\left[2+\sum_{\sigma,\sigma'}\sigma\sigma'\left[\frac{\partial\Sigma_{{\rm imp}\,\sigma}(i\omega)}{\partial B_{\sigma'}}+\frac{\partial\Sigma_{U\sigma}(i\omega)}{\partial B_{\sigma'}}\right]_{\omega=0+}\right], \tag{2.17c}$$

where $\rho_f(0)$ is the f DOS at the Fermi level and B_σ is the Zeeman shift of the energy levels. In a similar way, within the local approximation, the spin and charge relaxation rates T_{1s} and $T_{1\rm ch}$ at zero temperature are given by[18]

$$\lim_{\omega\rightarrow 0}\left[{\rm Im}\frac{\chi''(\omega)}{\omega}\right]=\frac{\pi}{2}[\chi(\omega=0)]^2 \tag{2.18a}$$

or

$$T_1=\frac{\pi}{2}\chi(\omega=0)\ . \tag{2.18b}$$

The relaxation time in (2.18b) is the low-frequency one (long-time relaxation), and we dropped the subindices s and ch for simplicity.

III. RESULTS

In this section we present the physical consequences of the equations derived in Sec. II. We first address the properties of an isolated Kondo hole and then discuss our results for an impurity band in an Kondo insulator.

For the properties of an isolated Kondo hole, we have to distinguish between a heavy-fermion metal and a Kondo insulator. In an insulator a δ-function-like bound state develops in the gap[10,11] and the Fermi level is pinned at this impurity state. On a lattice the spectral weight of this bound state in the local f DOS falls off rapidly with the distance from the impurity, so that the bound state is almost completely localized on the nearest-neighbor sites to the Kondo hole. Since there are no f electrons at the site of the Kondo hole, its local f DOS is zero. Both the size of the gap and the spectral weight of the bound state decrease with U via the self-energy as a consequence of the reduction of charge fluctuations. This bound state also appears in the d-electron DOS. Since the δ function is at the Fermi level, the Kondo hole in an insulator has magnetic properties. Its zero-field susceptibility follows a Curie law. Even a small magnetic field polarizes the bound state at $T=0$ and induces a Schottky anomaly in the specific heat, in analogy to a free spin $\frac{1}{2}$. This spin will precess in a homogeneous field if a small oscillating transversal field is applied and should in principle be observable by electron paramagnetic resonance. To be observable, however, the linewidth of the resonance has to be smaller than a fraction of one-tenth of a meV. A linewidth may originate from relaxation processes and/or from inhomogeneous broadening. Inhomogeneities caused by defects (for instance, the Kondo holes themselves) could introduce a distribution of g factors broad enough so that the line is not observable. On the other hand, inhomogeneities also introduce a distribution of bound-state energies, reducing in this way its magnetic character. Very large magnetic fields, however, would still polarize Kondo holes with a distribution of bound-state energies, but as pointed out by Millis,[19] they would also modify the bulk properties of the Kondo insulator and, in particular, reduce its gap.

In a metallic environment low-energy electron-hole excitations are allowed and the imaginary part of the self-energy is then nonzero everywhere except at the Fermi level. The hybridization gap is smeared to a pseudogap; i.e., the f DOS is nonzero over the entire range of interest. The Kondo hole now forms a pseudo-bound-state of finite width,[11] which is small if we have very heavy fermions. The energy of this bound state lies in the pseudogap, i.e., not at the Fermi level, but its spectral weight is still located in the neighboring unit cells to the impurity. The magnetic and thermal properties of this pseudo-bound-state are those of a resonant-level off-resonance with the Fermi level. As a function of T, the susceptibility is expected to have a maximum due to the thermal population of the state and be Curie-Weiss like at intermediate temperatures. The Weiss temperature is antiferromagnetic and of the order of the level width. The specific heat of the impurity is Schottky like with the position of the maximum determined by the energy of the resonance.

We now consider finite concentrations of Kondo holes in an insulator. To gain insight we first analyze the symmetric situation ($\varepsilon_f=0$) with $U=0$ analytically for small concentrations, and then we present the numerical solution for the general case. Because of the impurity self-energy $\Sigma_{\rm imp}$ in Eq. (2.11), the renormalized f-level energy acquires an imaginary part for small frequencies. In particular, for $\omega=0$, $\tilde{\varepsilon}_f$ is purely imaginary, and for small concentrations we obtain

$$\tilde{\varepsilon}_f=-2i\sqrt{c}\,\frac{V^2}{D}\ . \tag{3.1}$$

Hence the height of the impurity band is nonanalytic in the concentration of impurities. A similar analysis with $\omega\neq 0$ yields an impurity bandwidth proportional and of the order of $\tilde{\varepsilon}_f$. The impurity band is approximately semielliptic with both height and width proportional to $\sqrt{c}$ for small c; hence, as expected, the number of states in the impurity band is proportional to c. Because of the nonanalytic dependence on c, the self-consistency of Eq. (2.11) and the limit $c\rightarrow 0$ cannot be interchanged. In the Appendix we show that our result $\tilde{\varepsilon}_f\propto -i\sqrt{c}\,V^2/D$ is independent of the model density of states.

In order to obtain quantitative results, we must first

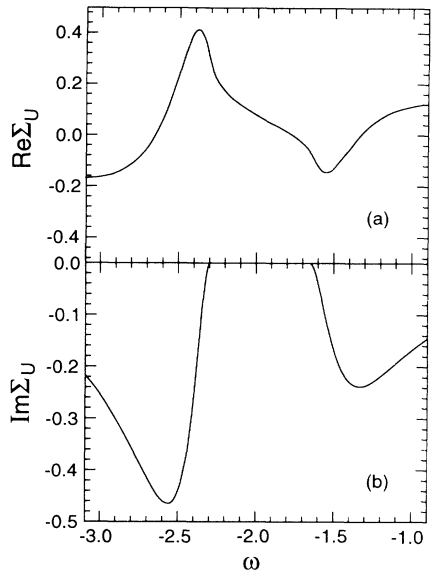

FIG. 1. (a) Real and (b) imaginary parts of the self-energy Σ_U as a function of frequency for $U=1$, $V=1$, $D=10$, and $\varepsilon_f=-2$ (Hartree-Fock corrected).

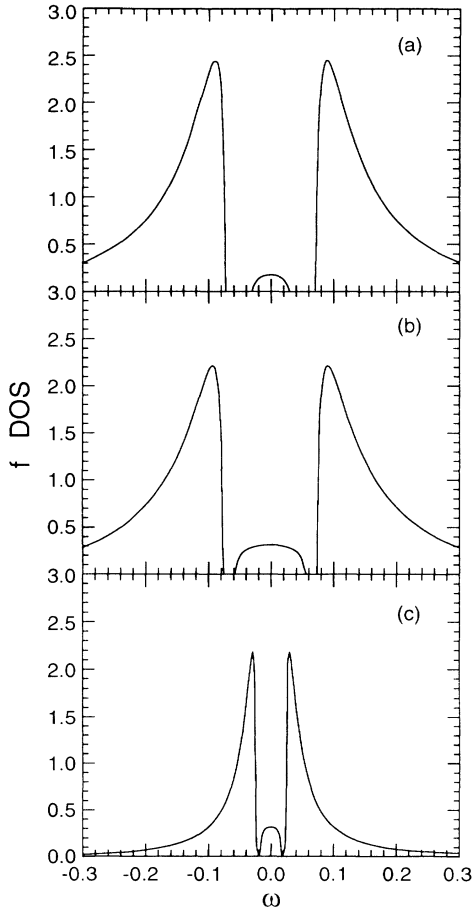

FIG. 2. f density of states for $V=1$, $D=10$, and $\varepsilon_f=0$ (Hartree-Fock corrected) and (a) $c=0.01$ and $U=1$, (b) $c=0.04$ and $U=1$, and (c) $c=0.04$ and $U=3$. The structure inside the hybridization gap is the Kondo-hole impurity band.

calculate the self-energy due to the Coulomb interaction $\Sigma_U(z)$ according to the scheme indicated by Eqs. (2.13)–(2.15). The chemical potential lies in the gap and is otherwise not relevant at this point. For a Hartree-Fock-shift f-level position $\varepsilon_f=-2$, $V=1$, $D=10$, and $U=1$, the real and imaginary parts of the self-energy are shown in Fig. 1. Since the self-energy involves a double convolution of three f Green's functions, the gap in the imaginary part is about 3 times the gap in the DOS of the bare f electrons (i.e., about $6V^2/D$). Also, the real part of $\Sigma_U(z)$ has a zero within the gap and two further zeros at larger energies, which give rise to two shoulders in the f DOS. The slope of $\Sigma_U(z)$ inside the gap is negative, so that qualitatively the effect of the correlations on the impurity band is to narrow the band. This can be seen from Eq. (2.11), where ω is to be replaced by $\gamma\omega$, with

$$\gamma=1-\frac{\partial\Sigma_U}{\partial\omega}>1\ . \tag{3.2}$$

Three examples of the f-electron DOS, as obtained by the self-consistent solution of Eq. (2.16), for $\varepsilon_f=0$, $V=1$, and $D=10$ are shown in Fig. 2. The case $U=1$ and $c=0.01$ is displayed in Fig. 2(a), Fig. 2(b) corresponds to the situation $U=1$ and $c=0.04$, and in Fig. 2(c) we show the DOS for $U=3$ and $c=0.04$. The DOS of the impurity band grows with the concentration of Kondo holes, and the main effect of the Coulomb repulsion is to narrow the hybridization gap. The critical concentration of impurities that closes the gap of the insulator decreases with the correlations. The Fermi level in this symmetric case is at zero. For sufficiently small c all states in the impurity band will be localized, but an insulator-metal transition is expected as a function of concentration. When the

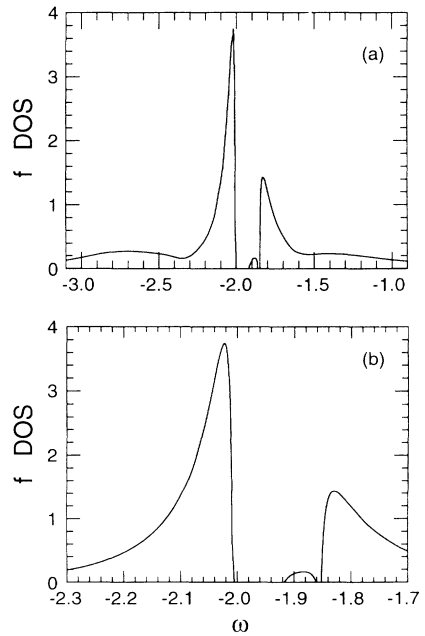

FIG. 3. (a) f density of states for $V=1$, $D=10$, $\varepsilon_f=-2$ (Hartree-Fock shifted), $c=0.01$, and $U=1$. (b) Expanded view of the hybridization gap and impurity band.

number of Kondo holes is increased, the bound states (located at the nearest-neighbor sites to the impurity) start to overlap and electrons may percolate through the crystal, giving rise to conductivity.

Figure 3(a) and 3(b) show the f DOS for the asymmetric situation $\varepsilon_f=-2$, $V=1$, $U=1$, $D=10$, and $c=0.01$. Here ε_f is the Hartree-Fock-shifted f-level energy. Figure 3(a) shows two shoulders developing as a consequence of the two additional zeros (the third one is in the gap of the insulator) of the real part of the self-energy. The peaks of the DOS are now asymmetric, the Fermi level being pinned in the impurity band. An expanded view of the hybridization gap and impurity band is shown in Fig. 3(b).

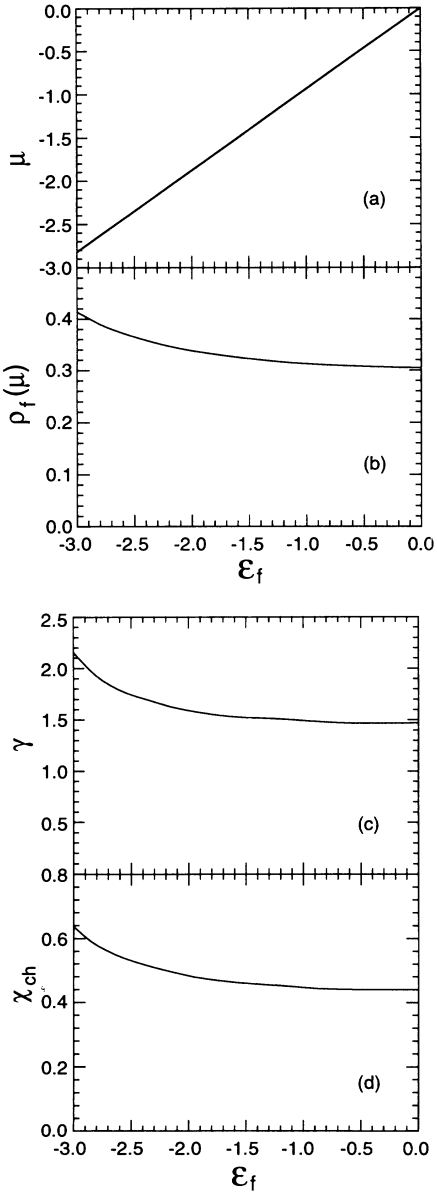

FIG. 4. (a) Chemical potential μ, (b) f density of states at the Fermi level, ρ_f, (c) linear T specific-heat coefficient γ, and (d) charge susceptibility χ_{ch} as a function of the (Hartree-Fock-corrected) f-level energy for $V=1$, $U=1$, $c=0.04$, and $D=10$.

The Fermi energy or chemical potential μ, determined as the self-consistent solution of

$$\mu=\mathrm{Re}[\tilde{\varepsilon}_f(\mu)]\ , \tag{3.3}$$

is displayed in Fig. 4(a) as a function of ε_f for $V=1$, $U=1$, $D=10$, and $c=0.04$. Note that $\mu(\varepsilon_f)$ is proportional to ε_f with a slope that is only slightly smaller than 1. The corresponding f-electron DOS at the Fermi level (i.e., the height of the impurity band at μ) is shown in Fig. 4(b). There is only a small increase of $\rho_f(\mu)$ with the asymmetry. On the other hand, $\rho_f(\mu)$ strongly depends on the Kondo-hole concentration; it grows monotonically with c, being proportional to $\sqrt{c}$ for small c. The finite f DOS at the Fermi level gives rise to a specific-heat contribution proportional to T. The range of this linear T dependence is of the order of the width of the impurity band. The γ coefficient was obtained by numerical differentiation of the self-energies at the Fermi level [see Eq. (2.17a)] and is shown as a function of ε_f for $V=1$, $U=1$, $D=10$, and $c=0.04$ in Fig. 4(c). The same slight increase with the asymmetry as in $\rho_f(\mu)$ is observed. These γ values correspond to an effective-mass enhancement of 15–20 over the mass of the conduction electrons. The charge susceptibility χ_{ch}, which was also obtained by numerical differentiation according to Eq. (2.17b), is plotted as Fig. 4(d). Again, the same slight increase with the asymmetry as for ρ_f is observed. The numerical differentiation with respect to a magnetic field to obtain the spin susceptibility is more involved, but χ_s is expected to have a similar behavior as χ_{ch} for the U values considered here.

IV. CONCLUDING REMARKS

In this paper we considered a finite concentration of Kondo holes forming an impurity band in a Kondo insulator. The formation of a Kondo insulator is perhaps the most dramatic implication of "coherent scattering." Kondo holes destroy the translational invariance and, hence, the coherence. This work extends previous reports on isolated Kondo holes in heavy-fermion compounds.[10,11] A Kondo hole in a Kondo insulator introduces a bound state in the gap, whose spectral weight is localized in the neighboring unit cells to the impurity. This bound state pins the Fermi level and consequently has magnetic properties, i.e., a Curie zero-field susceptibility and a Schottky anomaly in the specific heat if a small field is applied. If the concentration of Kondo holes is finite, an impurity band arises in the f DOS, whose height and width are proportional to $\sqrt{c}$ for small c. This impurity band is expected to have consequences on the optical properties in the infrared range of Kondo insulators.

The Coulomb interaction within the f shell is introduced via a self-energy, which has been calculated to second order in U using (a minor variant of) the $(1/d)$-expansion method by Schweitzer and Czycholl[12,14,15] to leading order in $1/d$. This method properly takes into account the momentum and energy integrations. It corresponds to the local approximation in which the $\mathbf{k}$ dependence of Σ_U is neglected, but the more important energy dependence of the heavy particles is kept. The

main effect of the Coulomb interaction is to narrow the hybridization gap as well as the impurity band. Although our calculation is restricted to small U, the effects and trends are not expected to change qualitatively for larger values of U, so that our conclusions are valid quite generally. At very low temperatures the specific heat has a component proportional to T, arising from the impurity band. The mass enhancement associated with the γ value depends on the concentration of Kondo holes and is roughly proportional to $\sqrt{c}$ for small c. The temperature range of this linear T dependence is given by the width of the impurity band. The susceptibility is Pauli like at low T. We also speculated that an insulator-metal transition should occur as a function of c.

In this paper we limited ourselves to applications of the Anderson lattice to heavy-fermion or Kondo insulators. There exists another class of materials, namely, the cuprate high-temperature superconductors, with similar properties. These systems also involve high correlations, and as a function of impurity concentration, an insulator-metal transition is induced. Since current models[20,21] for highly correlated bands of hybridized Cu $3d$ and O $2p$ orbitals are closely related to the Anderson lattice, it is expected that an analogous approach for these models will lead to conclusions similar to the ones presented here.

Note added in proof. In a recent paper Doniach and Fazekas (Philos. Mag., to be published) considered the formation of an antiferromagnetic ground state in a doped Kondo insulator. The antiferromagnetism is induced via exchange coupling between the heavy particles introduced by the Kondo holes.

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APPENDIX

We show here that the dependence of ε_f [Eq. (3.1)] on c, V, and D is independent of the model density of states. Combining Eqs. (2.7), (2.10), and (2.11) for the symmetric situation, we have

$$-[z-\tilde{\varepsilon}_f(z)]\frac{c}{\tilde{\varepsilon}_f(z)}=[z-\tilde{\varepsilon}_f(z)]\frac{1}{N}\sum_{\mathbf{k}}G^0_{f\mathbf{k}}(z)$$
$$=1+\frac{V^2}{z-\tilde{\varepsilon}_f(z)}F\left[z-\frac{V^2}{z-\tilde{\varepsilon}_f(z)}\right], \tag{A1}$$

where $F(z)$ is the Cauchy transform of an arbitrary symmetric single-band density of states. Inside the gap the argument of $F(z)$ is large, so that an expansion in $1/z$ is allowed:

$$F(z)=\frac{1}{N}\sum_{\mathbf{k}}\frac{1}{z-\varepsilon_{\mathbf{k}}}$$
$$=\frac{1}{z}+\frac{1}{z^2}\langle\varepsilon_{\mathbf{k}}\rangle+\frac{1}{z^3}\langle\varepsilon^2_{\mathbf{k}}\rangle+\cdots . \tag{A2}$$

For a symmetric band, $\langle\varepsilon_{\mathbf{k}}\rangle=0$. Inserting (A2) into (A1), we obtain for $\omega=0$, solving for $\tilde{\varepsilon}_f$,

$$\tilde{\varepsilon}_f=-i\sqrt{c}\,V^2/\langle\varepsilon^2_{\mathbf{k}}\rangle^{1/2} . \tag{A3}$$

Obviously, $\langle\varepsilon^2_{\mathbf{k}}\rangle^{1/2}\propto D$.

In the asymmetric situation, when either $\varepsilon_f\neq 0$ or $\langle\varepsilon_{\mathbf{k}}\rangle\neq 0$, the maximum of the DOS of the impurity band is not at $\omega=0$. An expansion about the shifted maximum, however, still would yield the same dependence of the impurity band on c, V, and D. Our numerical results quite convincingly show that not much changes as a function of ε_f.

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