Alloying effects of Kondo insulators

Zheng-zhong Li, Wang Xu, Chun Chen, and Ming-wen Xiao
Department of Physics, Nanjing University, Nanjing 210008, People's Republic of China
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The effects of nonmagnetic impurities (Kondo holes) in Kondo insulators (KI's) are studied based on the $U=\infty$ Anderson model in the framework of a slave-boson mean-field theory under the coherent-potential approximation (CPA). The density of states for f electrons and its variation with the concentration of Kondo holes are calculated self-consistently. The specific-heat coefficient, residual resistivity, and the $T=0$ static susceptibility in the alloying system are obtained. The results show that the insulating gap in KI's can be easily smeared out by Kondo holes, and the system changes gradually from an insulator to a heavy-fermion metal with increasing concentration, which is in qualitative agreement with experiments. Furthermore, the appearance of an impurity band in the gap comes out naturally in the dilute limit of our CPA calculations.

I. INTRODUCTION

Recently, a new class of Ce-based compound with insulating ground states in heavy-fermion systems has been discovered, namely that of Kondo insulators (KI's), which includes CeNiSn,[1,2] $Ce_3Bi_4Pt_3$,[3,4] CeRbSb,[5] etc. At low temperatures, Kondo insulators show unexpected semiconducting behavior different from the properties of heavy-fermion metals. The semiconducting behavior of KI's is thought to be caused by a small real gap at the Fermi level that separates the filled and empty renormalized bands. The gap results from the hybridization between a half-filled conduction band and local f electrons of periodically placed Kondo ions. This picture is frequently referred to as a Kondo lattice (KL) with insulating ground states.[6] Experimentally, evidence for the picture comes primarily from thermodynamic and transport properties[1,3] as well as from neutron scattering.[2,4] Theoretically, a slave-boson formalism in a mean field of a $U=\infty$ single-band Anderson lattice Hamiltonian with a degeneracy $N=2$ and two electrons per site is adopted to construct an insulating KL model. As a consequence of the coherence in the KL, a hybridization gap opens at the Fermi level between the two renormalized bands, and small-gap semiconducting properties of KI's can be naturally evolved.[7,8]

The formation of the coherence (i.e., the nature of the small gap) in KI's can also be studied by adding nonmagnetic impurities (Kondo holes) which are concerned with the alloying effect of KI's. Experimental results for $(Ce_{1-x}La_x)_3Bi_4Pt_3$ (Ref. 3) show that alloying with La decreases the resistivity and increases the specific heat toward values expected for the metallic case, and a smearing of the gap is attained by a moderate La substitution (about $x=7\%$ La). Thus adding Kondo holes to an insulating KL breaks the lattice periodicity, suppresses the gap, and leads the system to change from an insulator into a heavy-fermion metal. A theoretical study of magnetism in doped KI's was first given by Doniach and Fazekas[9] using a simplified Gutzwiller variational approximation, which can be applied only at $T=0$. The impurity bands in the gap of KI's at low doping concentrations was discussed by Schlottmann and coworkers[10,11] with a special perturbation expansion to the second order of U, which allows for a consistent description of the high- and low-temperature behavior,[12] but it is more suitable to the small-U cases. However, in actual heavy-fermion systems correlation U is believed to be very large, and also a slave-boson mean-field theory for the $U=\infty$ Anderson lattice model (ALM) has been used successfully to explain the semiconducting behavior of pure KI's.[7,8] Therefore, a theory of doped KI's which can be applied to cases of infinite U and finite temperature as well as over the whole La-concentration range $(0\le x\le 1)$ is needed.

In recent publications[13–16] we have provided a coherent-potential approximation (CPA) theory of heavy-fermion alloys in the framework of slave-boson mean-field approximation (SBMFA) upon doping of Kondo holes in metallic KL's, which is different from the previous CPA treatments of the ALM.[17–19] The purpose of this paper is to extend the above theory to the insulating case. We expect to give a unified explanation of alloying effects in KI's, including the formation of the impurity band in the dilute limit, the crossover from KI's to a heavy-fermion metal for moderate concentrations, and also the concentration dependence of thermodynamic and transport properties in doped KI's.

The rest of this paper is organized as follows: In Sec. II, we describe the disorder model and CPA formalism of Kondo insulators in the SBMFA. In Sec. III, we present the self-consistent results of the f-electron density of states (f DOS) in an alloying KI. This involves the appearance of an impurity band in the dilute limit, and the gradual smearing out of a real gap with the increasing of Kondo holes. An attempt to explain the effect of the Kondo holes on the low-T specific-heat coefficient, residual resistivity, and $T=0$ static susceptibility will be given

in Sec. IV. Finally, our results will be summarized in Sec. V.

II. DISORDER MODEL AND CPA FORMALISM OF KI's

The disorder system that we shall investigate is modeled after $(La_xCe_{1-x})NiSn$ and $(La_xCe_{1-x})_3Bi_4Pt_3$. This doped KI system contains two kinds of rare-earth atoms A and B, where A (La like) is a nonmagnetic atom without any f electrons, and B a magnetic atom with f electrons. The substitution of A for B creates the missing f centers, which are referred to as the Kondo holes. As an appropriate starting point for discussing doped KI's, we introduce compositional disorder into the nondegenerate ALM with a half-filled conduction band. The random variable in the lattice point i is defined by

$$\xi_i=\begin{cases}1 & \text{for } i\in A\\ 0 & \text{for } i\in B.\end{cases} \tag{1}$$

Note that the random average $\overline{\xi_i^2}=\overline{\xi_i}=x$, where x is the normalized concentration of A atoms (Kondo holes). The disorder Hamiltonian of the alloying KI's with Kondo holes can be written as

$$\begin{aligned}H=&\sum_{\mathbf{k}\sigma}[\epsilon_{\mathbf{k}}c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}+(-E_f)f^{\dagger}_{\mathbf{k}\sigma}f_{\mathbf{k}\sigma}]\\&+\sum_{i\sigma}\xi_i(E_L+E_f)f^{\dagger}_{i\sigma}f_{i\sigma}\\&+V\sum_{i\sigma}(1-\xi_i)(f^{\dagger}_{i\sigma}c_{i\sigma}+c^{\dagger}_{i\sigma}f_{i\sigma})\\&+\tfrac{1}{2}U\sum_{i\sigma}(1-\xi_i)f^{\dagger}_{i\sigma}f_{i\sigma}f^{\dagger}_{i-\sigma}f_{i-\sigma}\ ,\end{aligned} \tag{2}$$

where $c_{\mathbf{k}\sigma}$ ($c_{i\sigma}$) and $f_{\mathbf{k}\sigma}$ ($f_{i\sigma}$) are operators in the Bloch (Wannier) representation for the conduction (c) and localization f electrons, respectively; σ is the spin index, and $\epsilon_{\mathbf{k}}$ the band energy of c electrons from the Fermi level, which is taken to be zero. $-E_f$ is the energy of f electrons on magnetic (B) atoms, and E_L represents the f level on Kondo holes (nonmagnetic A atoms). Since the Kondo hole is a missing f center, we should take the limit in the calculation in order to ensure that there is no f-electron occupation on A sites. V is the c-f mixing parameter, and U the on-site Coulomb repulsion between two electrons with the opposite spin.

In the strong correlation limit, $U\to\infty$, double occupation is strictly forbidden on the B sites. The correlation can be accounted for by introducing Barnes'[20] and Coleman's[21] slave-boson operator b_i in the c-f mixing term instead of the Coulomb repulsion part in Eq. (2). Thus we can write Hamiltonian (2) for $U\to\infty$ in slave-boson formalism as

$$\begin{aligned}H=&\sum_{\mathbf{k}\sigma}[\epsilon_{\mathbf{k}}c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}+(-E_f)f^{\dagger}_{\mathbf{k}\sigma}f_{\mathbf{k}\sigma}]+\sum_{i\sigma}\xi_i(E_L+E_f)f^{\dagger}_{i\sigma}f_{i\sigma}+V\sum_{i\sigma}(1-\xi_i)(b_if^{\dagger}_{i\sigma}c_{i\sigma}+c^{\dagger}_{i\sigma}f_{i\sigma}b^{\dagger}_i)\\&+\sum_i(1-\xi_i)\lambda_i\left[\sum_{\sigma}f^{\dagger}_{i\sigma}f_{i\sigma}+b^{\dagger}_ib_i-1\right],\end{aligned} \tag{3}$$

where a constraint due to infinite U,

$$\sum_{\sigma}f^{\dagger}_{i\sigma}f_{i\sigma}+b^{\dagger}_ib_i=1 \quad \text{for } i\in B\ , \tag{4}$$

is added with the Lagrange multiplier λ_i. This constraint prevents the double occupancy of the f level on the B sites.

In the SBMFA, the operator b_i and constraint (4) are replaced by their mean-field values with the ansatz $r=\langle b_i\rangle=\langle b^{\dagger}_i\rangle$ and $\lambda_i=\lambda$ for all B sites. The Hamiltonian (3) can then be reduced to its SBMFA formalism:

$$\begin{aligned}H_{\mathrm{MF}}=&\sum_{\mathbf{k}\sigma}[\epsilon_{\mathbf{k}}c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}+\tilde{E}_ff^{\dagger}_{\mathbf{k}\sigma}f_{\mathbf{k}\sigma}\\&+rV(f^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}+c^{\dagger}_{\mathbf{k}\sigma}f_{\mathbf{k}\sigma})]\\&+\sum_{i\sigma}\xi_i[\varepsilon_Lf^{\dagger}_{i\sigma}f_{i\sigma}-rV(f^{\dagger}_{i\sigma}c_{i\sigma}+c^{\dagger}_{i\sigma}f_{i\sigma})]\\&+\lambda(r^2-1)\sum_i(1-\xi_i)\ ,\end{aligned} \tag{5}$$

where $\tilde{E}_f=\lambda-E_f$ and $\varepsilon_L=E_L-\tilde{E}_f$ are, respectively, the renormalized f level of the magnetic (B) atoms and the Kondo holes (A atoms). The SB parameters r and λ are determined by the following saddle-point equations:

$$r\lambda=-V\sum_{\sigma}\langle c^{\dagger}_{i\sigma}f_{i\sigma}\rangle \quad \text{for } i\in B\ , \tag{6}$$

and

$$1-r^2=\sum_{\sigma}\langle f^{\dagger}_{i\sigma}f_{i\sigma}\rangle=n_f \quad \text{for } i\in B\ , \tag{7}$$

which can also be obtained by minimizing the mean-field energy $\langle H_{\mathrm{MF}}\rangle$ with respect to r and λ. Here $\langle\ \rangle$ denotes the statistical average, and n_f is the average f electron number per B site.

Since in the SBMFA a Kondo hole is simulated by a very large f-level energy $\varepsilon_L=E_L-\tilde{E}_f$, with $\tilde{E}_f$ slightly above the Fermi level μ ($\tilde{E}_f-\mu=T_K$, T_K — Kondo temperature) and $E_L\to\infty$, a Kondo hole doping leads to a very strong scattering center, and a treatment of H_{MF} within a low-order Born approximation would not be adequate. Therefore, we attempt to use a coherent-potential approximation, which also allows us to solve the disorder SBMF Hamiltonian (5) for arbitrary concentrations of the Kondo holes.

The idea of the CPA is to replace the disorder potential

of Kondo holes by a translational invariant but frequency-dependent coherent potential of the effective medium. The coherent potential for a single-conduction-band Anderson model should be assumed to be a 2×2 matrix:[22]

$$S(\omega,x)=\begin{bmatrix} S_{cc} & S_{cf} \\ S_{fc} & S_{ff} \end{bmatrix} . \tag{8}$$

The effective-medium Hamiltonian can then be written in the following matrix form:

$$\bar{H}=\sum_{\mathbf{k}\sigma}[c^{\dagger}_{\mathbf{k}\sigma} \quad f^{\dagger}_{\mathbf{k}\sigma}] \begin{bmatrix} \epsilon_{\mathbf{k}}+S_{cc} & S_{cf} \\ S_{fc} & \tilde{E}_f+S_{ff} \end{bmatrix} \begin{bmatrix} c_{\mathbf{k}\sigma} \\ f_{\mathbf{k}\sigma} \end{bmatrix} + N_s\lambda(1-x)(r^2-1) , \tag{9}$$

where N_s is the number of unit cells in the system. In the Bloch representation, the matrix of the medium Green's function (GF) is determined by $(\omega-\bar{H})^{-1}$ in the space of basis vectors $(c_{\mathbf{k}\sigma},f_{\mathbf{k}\sigma})$, and reads

$$\bar{G}(\omega,\mathbf{k})=\frac{1}{B_{\mathbf{k}}}\begin{bmatrix} \omega-\tilde{E}_f-S_{ff} & S_{cf} \\ S_{fc} & \omega-\epsilon_{\mathbf{k}}-S_{cc} \end{bmatrix} , \tag{10}$$

with

$$B_{\mathbf{k}}=(\omega-\epsilon_{\mathbf{k}}-S_{cc})(\omega-\tilde{E}_f-S_{ff})-S_{cf}S_{fc} . \tag{11}$$

From Eq. (10), we obtain the averaged site GF of the effective medium

$$F(\omega)=\frac{1}{N_s}\sum_{\mathbf{k}}\bar{G}(\omega,\mathbf{k})=\begin{bmatrix} F_{cc}(\omega) & F_{cf}(\omega) \\ F_{fc}(\omega) & F_{ff}(\omega) \end{bmatrix} . \tag{12}$$

The only remaining thing we should do is to determine the coherent potential $S(\omega\mathbf{k})$, which is related to a self-consistent requirement of the CPA. In the single-site CPA, the potential $S(\omega,\mathbf{k})$ has to be determined in such a way, that, on the average, the scattering t matrix for the difference between potentials of the disorder system and the effective medium vanishes on each site. According to Yonezawa,[23] this requirement is equivalent to a self-consistent equation in the single-site CPA:

$$xt_A+(1-x)t_B=0 , \tag{13}$$

where t_A and t_B, respectively, are the scattering t matrices for A and B atoms.

$$t_{A(B)}=V_{A(B)}[1-F(\omega)V_{A(B)}]^{-1} , \tag{14}$$

with scattering potentials of A and B atoms in the effective medium

$$V_A=\begin{bmatrix} -S_{cc} & -S_{cf} \\ -S_{fc} & \epsilon_L-S_{ff} \end{bmatrix} , \quad V_B=\begin{bmatrix} -S_{cc} & rV-S_{cf} \\ rV-S_{fc} & -S_{ff} \end{bmatrix} , \tag{15}$$

which are deduced from $H_{\mathrm{MF}}-\bar{H}=\Sigma_i V_i$ with the use of Eqs. (5) and (9), denoting the difference of the scattering potentials between the disorder system and effective medium of A and B atoms. Only when the self-consistent equation (13) is satisfied can the effective medium be considered well chosen.

Substituting Eqs. (14) and (15) into Eq. (13), and taking $\epsilon_L\to\infty$ (because $\tilde{E}_f\ll E_L$, $E_L\to\infty$) to ensure zero f-electron occupation on Kondo holes, after some algebraic manipulations (the details of which will be given in the Appendix) we find a simple analytical solution of the coherent potential:

$$S(\omega,x)=\begin{bmatrix} 0 & rV \\ rV & S_{ff} \end{bmatrix} , \tag{16}$$

where only the matrix element S_{ff} is unknown. At the same time, the self-consistent CPA equation (13) can be simplified as

$$S_{ff}F_{ff}=-x . \tag{17}$$

The averaged site GF's are expressed as

$$F_{cc}(\omega)=\frac{1}{N_s}\sum_{\mathbf{k}}\frac{\omega-\tilde{E}_f-S_{ff}}{(\omega-\epsilon_{\mathbf{k}})(\omega-\tilde{E}_f-S_{ff})-(rV)^2} , \tag{18}$$

$$F_{cf}(\omega)=F_{fc}(\omega)=\frac{rV}{\omega-\tilde{E}_f-S_{ff}}F_{cc}(\omega) , \tag{19}$$

$$F_{ff}(\omega)=\frac{1}{\omega-\tilde{E}_f-S_{ff}}\left\{1+\frac{(rV)^2}{\omega-\tilde{E}_f-S_{ff}}F_{cc}(\omega)\right\} . \tag{20}$$

As shown in Eq. (20), $F_{ff}(\omega)$ is also related to the self-consistent determination of the slave-boson (SB) parameter r and $\tilde{E}_f(=\lambda-E_f)$. Therefore, we have to solve the CPA equation (17) in combination with SB equations (6) and (7). Noting that the SB saddle-point equations (6) and (7) only appear on the magnetic (B) sites, we can rewrite them by taking an average over the randomness and using GF spectral theorem as follows:

$$(1-x)r\lambda=\frac{2V}{\pi}\int_{-\infty}^{+\infty}d\omega\, f(\omega)\mathrm{Im}F_{fc}(\omega+i0^+) , \tag{21}$$

$$(1-x)(1-r^2)=-\frac{2}{\pi}\int_{-\infty}^{+\infty}d\omega\, f(\omega)\mathrm{Im}F_{ff}(\omega+i0^+) , \tag{22}$$

where $f(\omega)$ is the Fermi distribution function.

Equations (17)–(22) constitute a set of fundamental equations for determining the coherent potential (S_{ff}) and the SB parameters (r and λ); it smoothly and naturally interpolates two mean-field theories for the Anderson impurity and the Anderson lattice,[24] and can easily be applied to calculate the electronic DOS of the HF alloys with arbitrary Kondo-hole concentrations.

III. THE f DOS IN DOPED KI's

The f-electron density of states (f DOS) in doped Kondo insulators is defined by the imaginary part of the effective medium GF, $F_{ff}(\omega)$. The f DOS per magnetic (A) atom for each spin can be written as

$$N_f(\omega,x)=-\frac{1}{x(1-x)}\mathrm{Im}F_{ff}(\omega+i0^+) , \tag{23}$$

where $F_{ff}(\omega)$ should be calculated self-consistently from Eqs. (17), (20), (21), and (22) by numerical method. In calculations the unperturbed DOS of conduction electrons, $N_0(\omega)$, is needed. For simplicity, a constant DOS of $N_0(\omega)$ is assumed:

$$N_0(\omega)=\begin{cases}\dfrac{1}{2D} & \text{for } |\omega|\le D \\ 0 & \text{for } |\omega|>D,\end{cases} \tag{24}$$

where D is the half-width of the conduction band.

The f DOS can be solved analytically in the case of $x\to 0$ and $x\to 1$. However, in the region of $0<x<1$, we have to proceed with a numerical calculation. The numerical results are shown in Figs. 1 and 2. In the limit of $x=0$, a real hybridization gap opens near the Fermi level due to the translational invariance of the insulating KL system as shown in Fig. 1(a). Adding Kondo holes into the KI's, an impurity band emerges within the gap, and

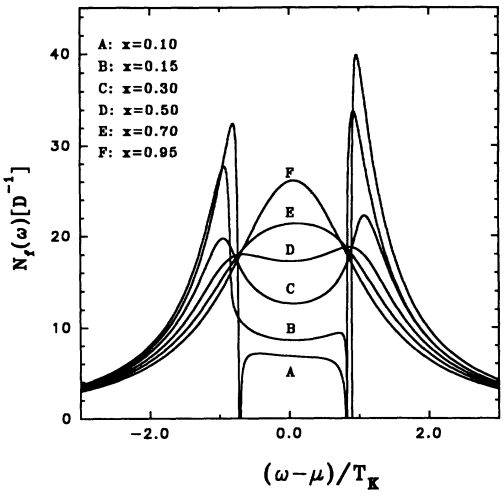

FIG. 2. The concentration dependence of f DOS for the doped KI's, where V and E_f are the same as in Fig. 1.

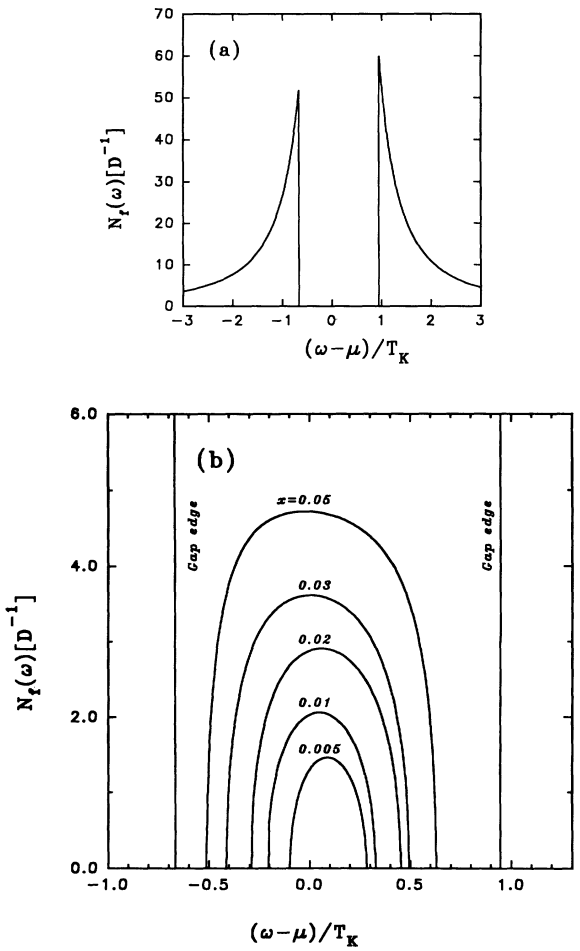

FIG. 1. (a) The f DOS of a pure Kondo insulator. (b) The f DOS of the impurity band inside the gap for dilute doping cases. Here the parameters for the numerical calculations are chosen as $V=\sqrt{0.2}D$, $E_f=1.2D$, and $T_K=1.14D\exp(-2DE_f/V^2)$.

the band is broadened with an increase in the Kondo-hole concentration x [Fig. 1(b)]. In the moderate doping concentration when $x>15\%$ La, the real gap will gradually be smeared out and, instead, there will occur a "two-peak" pseudogap structure indicating the metallic behavior of the system (see Fig. 2). Therefore, Figs. 1 and 2 can be used to explain the experimental result that upon doping the system will change from a Kondo insulator into a heavy-fermion metal.[3] We will discuss this problem in Sec. IV.

The height of the impurity band at the Fermi level can be obtained analytically in the dilute limit of our CPA formalism. Since in the dilute limit, when Kondo-hole concentration $x\to 0$, Eq. (17) gives the coherent potential $S_{ff}\to 0$. Substituting this result into $F_{cc}(\omega)$, we can easily derive an approximate expression of the $\mathrm{Im}F_{ff}(\mu+i0^+)$ from Eq. (20):

$$\mathrm{Im}F_{ff}(\mu+i0^+)=\frac{\mathrm{Im}S_{ff}(\mu+i0^+)}{(\tilde{E}_f-\mu)^2+[\mathrm{Im}S_{ff}(\mu+i0^+)]^2}\ , \tag{25}$$

where we have set

$$\mathrm{Re}[S_{ff}(\mu+i0^+)]=0 \tag{26}$$

due to the electron-hole symmetry of the system as we have pointed out in Ref. 13. Now, the CPA equation (17) at the Fermi level μ can be rewritten as

$$\mathrm{Im}S_{ff}(\mu+i0^+)\mathrm{Im}F_{ff}(\mu+i0^+)=x\ . \tag{27}$$

From Eqs. (25), (26), and (27), one can immediately obtain

$$\mathrm{Im}S_{ff}(\mu+i0^+)=-\left[\frac{x}{1-x}\right]^{1/2}(\tilde{E}_f-\mu)\ . \tag{28}$$

Thus the f DOS at the Fermi level in the limit of the small Kondo-hole concentration turns out to be

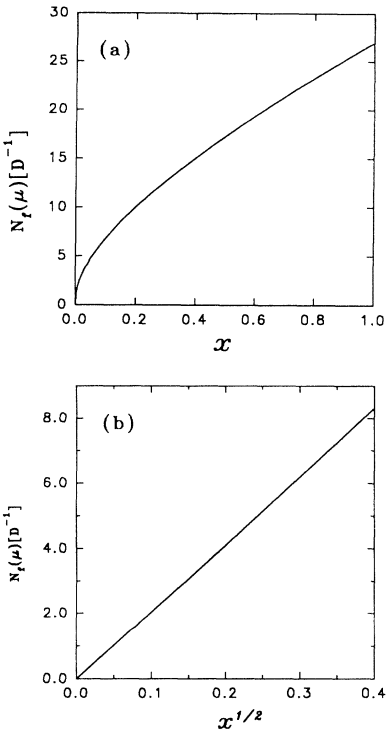

FIG. 3. (a) The f DOS at the Fermi level $N_f(\mu)$ varies with the Kondo-hole concentration x. (b) $N_f(\mu)$ vs $\sqrt{x}$ in dilute cases. Here the necessary parameters are chosen as in Fig. 1.

$$N_f(\mu,x\to 0)=\left[\frac{x}{1-x}\right]^{1/2}\frac{1}{(\tilde{E}_f-\mu)}\simeq\frac{2D}{(rV)^2}\sqrt{x}\ . \quad (29)$$

The result predicts that the height of the impurity band at the Fermi level is proportional to $\sqrt{x}$ for small x in analogy to the result of Schlottmann.[10] Furthermore, we have also calculated $N_f(\mu,x)$ in the whole concentration region $(0<x<1)$ by the numerical method, and the results are sketched in Fig. 3(a). The numerical results for small x are shown in Fig. 3(b). It is easily found that $N_f(\mu,x)\sim\sqrt{x}$ in accordance with our prediction in the dilute limit.

IV. COHERENCE IN DOPED KI's

We now turn to a discussion of coherence effects on the low-temperature properties of a doped Kondo insulator. We have calculated the low-temperature specific-heat coefficient, residual resistivity, and zero-temperature magnetic susceptibility of our alloy system. The results are as follows.

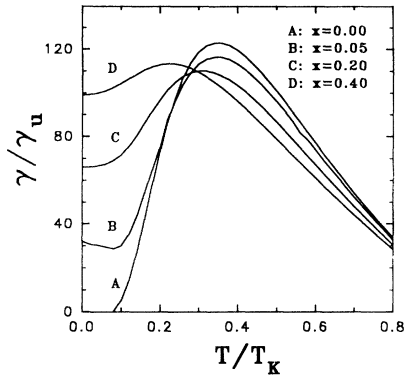

FIG. 4. Specific-heat coefficient of doped KI's where $\gamma_u=k_B^2/D$. We take V and E_f to be the same as in Fig. 1.

(a) Specific-heat coefficient of doped KI: In the low-temperature region, the main contribution of the specific heat comes from f electrons near the Fermi level, and the specific-heat coefficient of the doped KI can be written in terms of f DOS as

$$\gamma(T,x)=\tfrac{1}{2}k_B^2\beta^3\int_{-\infty}^{+\infty}d\omega\,\omega^2N_f(\omega,x)\,\mathrm{sech}^2\left[\frac{\beta(\omega-\mu)}{2}\right], \quad (30)$$

where $\beta=1/k_BT$, and $N_f(\omega,x)$ is the f DOS of alloying KI's. The numerical results of the low-temperature γ-T curves for various Kondo-hole concentrations are given in Fig. 4. From Fig. 4 we see that, in a pure Kondo insulator where $x=0$ (curve A), γ vanishes at $T=0$, due to the existence of a real gap in the excitation spectrum. However, upon doping a nonzero coefficient of specific heat at $T=0$ occurs (curve B), and for moderate doping $(x>15\%)$ the γ-T curves behave like a heavy-fermion metal with a pseudogap, as shown in curve C and D. This indicates that the substitution of La for Ce gradually smears out the gap, and leads the system to a disordered-induced metallic phase, which is in qualitatively agreement with experiments.[3]

(b) Coherence effect in residual resistivity: Once the effective medium S is found, the CPA expression of the electrical conductivity for doped KI's can be obtained easily. In the single-site CPA the conductivity of our system reads[25]

$$\sigma(T,x)=\frac{2e^2}{3\pi\hbar^2\Omega}\int_{-\infty}^{+\infty}d\omega\left[-\frac{\partial f}{\partial\omega}\right]\sum_{\mathbf{k}}v^2(\mathbf{k})[\mathrm{Im}\bar{G}_{cc}(\mathbf{k},\omega+i0^+)]^2\ , \quad (31)$$

where $v(\mathbf{k})$ is the velocity of the conduction electrons, Ω is the volume of the system, and

$$\bar{G}_{cc}(\mathbf{k},\omega)=\frac{\omega-\tilde{E}_f-S_{ff}}{(\omega-\epsilon_{\mathbf{k}})(\omega-\tilde{E}_f-S_{ff})-(rV)^2} \quad (32)$$

is the matrix element of the effective-medium GF for the conduction electrons. At zero temperature, Eq. (31) becomes

$$\sigma(T=0,x)=\frac{2e^2v_F^2}{3\pi\hbar^2\Omega}\sum_{\mathbf{k}}[\mathrm{Im}\bar{G}_{cc}(\mathbf{k},\mu+i0^+)]^2 , \tag{33}$$

where we have approximated $v(\mathbf{k})$ by the Fermi velocity v_F, which is reasonable when the system is assumed to be isotropic. After a straightforward calculation,[26] we find that

$$\sigma(T=0,x)=\frac{2e^2v_F^2}{3\pi\hbar^2\Omega_c}\frac{1}{2D}\int_{-D}^{+D}d\epsilon\frac{\left[\dfrac{(rV)^2}{\mathrm{Im}S_{ff}(\mu+i0^+)}\right]^2}{\left\{\left[\dfrac{(rV)^2-(\tilde{E}_f-\mu)(\epsilon-\mu)}{\mathrm{Im}S_{ff}(\mu+i0^+)}\right]^2+(\epsilon-\mu)^2\right\}^2} , \tag{34}$$

where Ω_c denotes the volume of the unit cell. We have calculated the residual resistivity $\rho(T=0,x)=1/\sigma(T=0,x)$ from Eq. (34). Numerical results of residual resistivity versus Kondo-hole concentration x are given in Fig. 5. As mentioned above, in the case of pure KI's where $x=0$, the system stays in an insulating state with infinite resistivity. Alloying a small amount of Kondo holes destroys the lattice periodicity, and results in an impurity band, on which the Fermi level is pinned. At this time, a finite resistivity is obtained. The residual resistivity of the doped KI's will decrease dramatically with the increasing of the Kondo-hole concentration, and the system will undergo a change from insulating to metallic ground states in accordance with experimental observations.[3,27]

Equation (34) can be solved analytically in the dilute Kondo-hole limit where $x\to 0$. Taking into account that $(\tilde{E}_f-\mu)\simeq(rV)^2/2D\ll(rV)^2$, and also that the main contribution of the integral in Eq. (34) comes from the energy region near $\epsilon=\mu$, we can neglect the term containing $(\tilde{E}_f-\mu)(\epsilon-\mu)$ in the denominator of the integrand, and Eq. (34) can be simplified as

$$\sigma(T=0,x)=\frac{2e^2v_F^2}{3\pi\hbar^2\Omega_c}\frac{1}{2D}\int_{-D}^{+D}d\epsilon\frac{\delta^2}{[\delta^2+(\epsilon-\mu)^2]^2} , \tag{35}$$

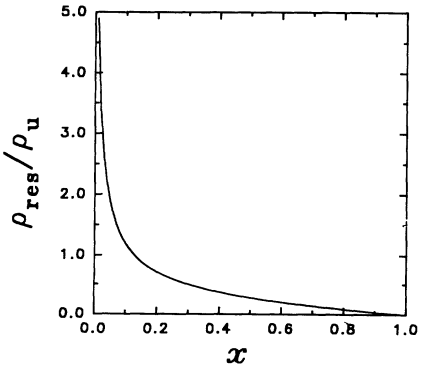

FIG. 5. Residual resistivity vs Kondo-hole concentration, where $\rho_u=3\pi\hbar^2D^2\Omega_c/2e^2v_F^2$. Here V and E_f take the same values as in Fig. 1.

where

$$\delta=\frac{(rV)^2}{\mathrm{Im}S_{ff}(\mu+i0^+)} . \tag{36}$$

In the case of $x\to 0$, where δ is very large due to the $\mathrm{Im}S_{ff}(\mu+i0^+)\to 0$, the integral in Eq. (35) then becomes $2D/\delta^2$. In this case, we obtain the residual resistivity in the form

$$\rho_{\mathrm{res}}(x\to 0)=\frac{3\pi\hbar^2\Omega_c^2}{2e^2v_F^2}\frac{(rV)^4}{[\mathrm{Im}S_{ff}(\mu+i0^+)]^2} . \tag{37}$$

Substituting Eq. (28) into Eq. (37), we find an asymptotic expression of the residual resistivity in the small Kondo-hole concentration as

$$\rho_{\mathrm{res}}(x\to 0)=\frac{6\pi\hbar^2D^2\Omega_c^2}{e^2v_F^2}x^{-1} , \tag{38}$$

which indicates that ρ_{res} approaches infinity following the power-law x^{-1} when $x\to 0$.

(c) Zero-temperature magnetic susceptibility: The static magnetic susceptibility of the pure KI can be expressed as

$$\chi=\chi_{\mathrm{V.V.}}+\chi_{\mathrm{Pauli}} , \tag{39}$$

where $\chi_{\mathrm{V.V.}}$ is an interband Van Vleck contribution to the susceptibility and is of order $g_L^2\mu_B^2/4D$ as pointed out by Riseborough,[7] where μ_B is the Bohr magneton, and g_L the Lande factor of f electrons. χ_{Pauli} represents the Pauli spin susceptibility, which has been discussed in Ref. 8 for pure KI's. At zero temperature, one can easily find that $\chi_{\mathrm{Pauli}}(T=0,x=0)=\frac{1}{4}g_L^2\mu_B^2N_f(\mu,x=0)$. Since the f DOS for pure KI's at the Fermi level vanishes, i.e., $N_f(\mu,x=0)=0$, due to the existence of a real gap near the Fermi level μ, the Pauli term makes no contribution to the susceptibility at $T=0$. However, a nonzero value of χ_{Pauli} occurs even in the dilute limit of doped KI's, where an impurity band emerges inside the gap of f DOS. We have calculated the $T=0$ Pauli susceptibility for doped KI's from the well-known formula

$$\chi_{\mathrm{Pauli}}(T=0,x)=\tfrac{1}{4}g_L^2\mu_B^2N_f(\mu,x) . \tag{40}$$

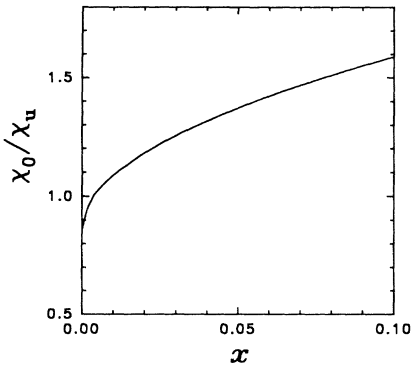

FIG. 6. Magnetic susceptibility at $T=0$ K for small Kondo-hole concentrations, where we take $V=0.6D$ and $E_f=1.2D$ for the numerical calculation, and $\chi_u=\mu_B^2/D$.

The numerical results in the limit of small Kondo-hole concentrations are shown in Fig. 6, where a constant contribution at $x=0$ is of the Van Vleck origin as mentioned above. An analytical expression for the Pauli susceptibility in the limit $x\to 0$ can be easily obtained from Eqs. (29) and (40):

$$\chi_{\text{Pauli}}(T=0,x\to 0)=\tfrac{1}{4}g_L^2\mu_B^2\left[\frac{x}{1-x}\right]^{1/2}\frac{1}{\tilde{E}_f-\mu}\sim\sqrt{x}\ , \tag{41}$$

which shows the magnetic susceptibility of doped KI's goes up with an increase in the Kondo-hole concentration x as observed experimentally.[3]

V. CONCLUSIONS

In this paper, we introduced compositional disorder into the nondegenerate Anderson lattice model with a half-filled conduction band as an appropriate starting point to discuss the substitution of La for Ce in a Kondo insulator. We have presented a single-site CPA theory for doped KI's in the framework of the slave-boson mean-field approximation. The f-electron density of states in the whole La-concentration range $0\le x\le 1$ can be calculated self-consistently in our CPA formalism. The obtained f DOS clearly shows many interesting features of the coherence in doped KI's with an increase in the Kondo-hole concentration x. For instance, in the small x an impurity band appears inside the gap and its height at the Fermi level goes up according to $x^{1/2}$; in the moderate doping concentration the real gap of the insulating ground state will gradually be smeared out and, instead, a pseudogap with a two-peak structure of the metallic ground state will occur. Using this result, alloying effects on the low-temperature specific-heat coefficient, residual resistivity, and $T=0$ magnetic susceptibility in doped KI's can be explained qualitatively. Our results reveal that upon doping the system undergoes a gradual change from a Kondo insulator into a heavy-fermion metal, which is in agreement with the experiment observations.

Finally, we would like to point out that the above discussion is valid only in the framework of SBMFA, where the fluctuations have been neglected. In order to extend our theory to study the transport properties of doped KI's at elevated temperatures, we have to go beyond the mean-field theory.[28] This problem is under investigation.

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APPENDIX

Now we give the major steps toward a simple analytical solution of the coherent potential. Setting Eq. (15) into Eq. (14), after taking $\varepsilon_L\to\infty$, we obtain the scattering t matrices of A and B atoms in the effective medium as

$$t_A=\frac{1}{B_1}\begin{bmatrix}-S_{cc}F_{ff} & S_{cc}F_{cf}\\ S_{cc}F_{cf} & -(1+S_{ff}F_{cc})\end{bmatrix}, \tag{A1}$$

$$t_B=\frac{1}{B_2}\begin{bmatrix}-S_{cc}(1+S_{ff}F_{ff})+F_{ff}\Sigma & S_{cc}S_{ff}F_{cf}-F_{cf}\Sigma\\ S_{ff}S_{cc}F_{fc}-F_{fc}\Sigma & -S_{ff}(1+S_{cc}F_{cc})+F_{cc}\Sigma\end{bmatrix}, \tag{A2}$$

where

$$B_1=F_{ff}+S_{cc}(F_{cc}F_{ff}-F_{cf}F_{fc})\ , \tag{A3}$$

$$B_2=(1+S_{ff}F_{ff})(1+S_{cc}F_{cc})-S_{cc}S_{ff}F_{cf}F_{fc}+(F_{cf}F_{fc}-F_{cc}F_{ff})\Sigma+[(S_{cf}-rV)F_{fc}+(S_{fc}-rV)F_{cf}]\ , \tag{A4}$$

$$\Sigma=(S_{cf}-rV)(S_{fc}-rV)\ . \tag{A5}$$

By combining Eqs. (A1)–(A5) with the single-site CPA equation (13), we obtain a set of four self-consistent equations of the coherent potential as follows:

$$S_{cc}\left[x\frac{F_{ff}}{B_1}+(1-x)\frac{1+F_{ff}S_{ff}}{B_2}\right]=(1-x)\frac{F_{ff}}{B_2}(S_{cf}-rV)(S_{fc}-rV)\ , \tag{A6}$$

$$S_{cc}F_{cf}\left[x\frac{1}{B_1}+(1-x)\frac{1}{B_2}\right]=(1-x)\frac{F_{cf}}{B_2}(S_{cf}-rV)(S_{fc}-rV)\ , \quad \text{(A7)}$$

$$S_{cc}F_{fc}\left[x\frac{1}{B_1}+(1-x)\frac{1}{B_2}\right]=(1-x)\frac{F_{fc}}{B_2}(S_{cf}-rV)(S_{fc}-rV)\ , \quad \text{(A8)}$$

$$(1+F_{cc}S_{cc})\left[x\frac{1}{B_1}+(1-x)\frac{S_{ff}}{B_2}\right]=(1-x)\frac{F_{cc}}{B_2}(S_{cf}-rV)(S_{fc}-rV)\ . \quad \text{(A9)}$$

Obviously, Eqs (A6)–(A8) have the following exact solution:

$$S_{cc}=0,\quad S_{cf}=S_{fc}=rV\ . \quad \text{(A10)}$$

By substituting Eq. (A10) into Eq. (A9), we finally obtain

$$S_{ff}F_{ff}=-x\ , \quad \text{(A11)}$$

which is just the simplified self-consistent equation (17).

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