Transport properties of Kondo-insulator alloys

L. Peche,[1] E. V. Anda,[1] and C. A. Büsser[2]

[1]*Departamento de Física, Pontificia Universidade Católica do Rio de Janeiro, C.P. 38071-970, Rio de Janeiro, RJ, Brazil*
[2]*National High Magnetic Field Lab and Department of Physics, Florida State University, Tallahassee, Florida 32310, USA*

We study the transport properties of disordered Kondo insulators. The compound $(Ce_{1-x}La_x)_3Bi_4Pt_3$ is taken as a paradigmatic example to study the properties of these systems. The metal-nonmetal transition is analyzed as a function of the impurity concentration x. The system is described by a periodic Anderson Hamiltonian. The many-body effects are treated by diagonalizing the site Hamiltonian and embedding this solution into the lattice, using a cumulant expansion calculated in the chain approximation. The disorder is treated through a numerical simulation. We calculate the position of the Fermi level and the mobility edges as a function of concentration, temperature, and the external applied potential. We propose a scenario where the metal-insulator transition, driven by the impurity concentration x, occurs when the Fermi level is inside the conduction band. The results are discussed under the light of several experimental results.

I. INTRODUCTION

Highly correlated electrons are present in a variety of different systems as is the case of superconductors, ferromagnets and antiferromagnets, metals, Kondo insulators, and Fermi and non-Fermi liquids. A great effort has been devoted to the understanding of the metal-nonmetal transition that occurs in these materials as a function of external pressure, composition, doping, temperature, and external magnetic field.[1] Among a large number of highly correlated systems some rare-earth and actinide compounds, the so-called Kondo insulators, have a small gap at the Fermi level, although they are expected to be metallic from their *f*-series analogs.[2,3]

Some studies emphasize the hybridization character of the small gap. This point of view has been developed using different techniques to diagonalize the Hamiltonian. Functional integral and the equation of motion methods were used to calculate the one-particle propagator[4,5] and to describe temperature-driven aspects of the metal-nonmetal transition. These theoretical approaches require, as established by band theory, an even number of valence electrons per unit cell and the same center for the *f* and *s* bands to obtain a temperature-dependent gap at the Fermi level. This seems to be a very restrictive condition to be realistic for a variety of possible situations.

Other approaches sustain that the properties of these materials are derived from the low-energy excitations produced by the Kondo effect.[6] The insulating character of these compounds is supposed to be driven by the hybridization of the *s* band with the Abrikosov-Suhl (AS) resonance,[7] which, due to its location at the vicinity of the Fermi level, generates a small insulating gap. In this case the metal-insulator transition produced by increasing the temperature of the system is a consequence of the disappearance of the AS resonance when the temperature is above the Kondo temperature T_k. Adopting this point of view, the system becomes metallic when it loses its heavy-fermion character. However, it is well known that, when the compound is doped by a small amount of a non-Kondo element (the Kondo hole), the gap disappears as a function of the doping concentration when the system is still in the Kondo regime, in which case the metallic phase is a heavy-fermion phase. This scenario is capable of explaining various experimental results.

The point of view that sustains that the metal-insulator transition is associated with the Kondo effect was developed using several formalisms such as slave-boson,[8] second-order perturbation in the Coulomb repulsion U,[9] or exactly diagonalized embedded cluster approximations.[10] For the case of $(Ce_{1-x}La_x)_3Bi_4Pt_3$, some of these studies have concluded that the incorporation of the La Kondo hole to the Kondo semiconductor induces a bound state in the gap. The spectral weight of this bound state results in being spatially localized at the immediate vicinity of the impurity. From this point of view a finite concentration of impurities creates an impurity band inside the energy gap at the Fermi level that controls the properties of the system.[9] This scenario provides a satisfactory explanation for the heavy-fermion behavior of these systems reflected by the abrupt increase of the *T*-linear contribution to the specific heat (γ) as a function of x. However, a very small concentration of impurities ($x \simeq 0.005$) is enough to produce the metal-insulator transition,[11–13] suggesting that the metal-insulator transition does not take place within the impurity band, which would require much larger concentrations to reach the quantum percolation.[14]

The experimental results are consistent with the assumption that the La impurity, in this Kondo insulator, generates a level that hybridizes significantly with the Ce states creating, even for a small concentration of impurities, a delocalized level inside the conduction band, where the Fermi level is shifted due to doping.[10]

The dynamical mean-field approach has also been applied to these systems emphasizing the non-Fermi-liquid character of some Kondo alloys.[15] It is a powerful self-consistent formalism, developed to treat infinite-dimensional systems. Although a local self-energy can be satisfactorily used to study three-dimensional (3D) systems,[16] its application in the case of an alloy is a very difficult task because the dynamical mean-field approach requires a self-consistent calculation for

each site of the lattice, as they are all different due to disorder.

This paper is dedicated to the study of the metal-nonmetal transition taking place in Kondo insulator alloys as a function of the concentration of the non-Kondo element. We study the conductivity of a disordered system, emphasizing the crucial role played by fluctuations and localization on the transport properties. We determine the mobility edges as a function of the concentration of the doping element. We treat the spin-spin correlations among the localized and conducting electrons by diagonalizing the Hamiltonian of a site in a numerical exact way, including the s and f wave functions. This procedure incorporates all the local contributions to the Kondo effect.[10,17–20] We use the chain approximation[21,22] to embed the renormalized site into the lattice. This approximation, although very simple, provides a qualitatively correct description of the many-body properties. It has the advantage of introducing very simple real-space self-energies from which we calculate the dressed propagator on the disordered lattice, without requiring a self-consistent calculation for each configuration that would require a much greater numerical effort. Due to its simplicity, it permits one to incorporate the complexity introduced by the disorder and, in particular, the localization effects that are crucial in the study of the transport properties. The system is defined on a Bethe lattice since this hierarquical lattice permits one to use a very efficient numerical algorithm to simulate disorder. Although with low connectivity, this is the simplest lattice which preserves the interference effects that give rise to localization, as was emphasized decades ago.[23] There is nothing essential in this choice, adopted because of numerical convenience.

We concentrate our attention on the transport properties, in particular on the dependence of the insulating and mobility gaps on the impurity concentration. The conductivity is obtained using the Kubo formula because as the external applied potential is supposed to be infinitesimal it is possible to use linear response theory.

Undoubtedly these are very interesting materials where to study the metal-nonmetal transition in the presence of disorder and correlation. This problem has been extensively investigated, for instance, in the case of Si doped with P.[24] However, the Kondo insulator seems to be to some extent a different situation as the Fermi energy region is, in this case, associated with an Abrikosov-Suhl resonance with no upper and lower Hubbard bands.[25]

The paper is organized as follows: Section II describes the model represented by a periodic Anderson Hamiltonian and the calculation of the one-particle Green function using the chain approximation within the context of a diagrammatic cumulant expansion. In Sec. III the problem of a doped Kondo insulator is discussed, taking as an example the compound $(Ce_{1-x}La_x)_3Bi_4Pt_3$ and treating the disorder using a numerical simulation. This section is devoted to the study of the metal-nonmetal transition and the conductivity as a function of temperature, frequency of the external applied voltage, and impurity concentration. Finally Sec. IV, includes a summary and some conclusions.

II. MODEL

Heavy-fermion systems have been largely studied adopting the periodic Anderson Hamiltonian. It is written as

$$H = \sum_i H_i + H_k, \tag{1}$$

where H_i is the Hamiltonian that corresponds to site i given by

$$H_i = \sum_\sigma \left[\epsilon_c^\alpha n_{i\sigma}^c + \epsilon_f^\alpha n_{i\sigma}^f + V_{c-f}^\alpha (c_{i\sigma}^\dagger f_{i\sigma} + \text{c.c.}) \right] + U^\alpha n_{i\uparrow}^f n_{i\downarrow}^f. \tag{2}$$

The Hamiltonian includes the e-e interaction and is represented on a Hilbert space of two localized wave functions, the s and f orbitals. The supraindex in the parameters ϵ_c^α, ϵ_f^α, V_{c-f}^α, and U^α takes into account that at each site, with certain probability, the alloy is composed of two different chemical elements. The kinetic contribution to the Hamiltonian considers the hopping among different nearest-neighbor sites,

$$H_k = t_c \sum_{\langle i,j \rangle \sigma} c_{i\sigma}^\dagger c_{j\sigma}. \tag{3}$$

The direct hybridization term among the localized f has not been included in the Hamiltonian because the width of the f band is much smaller than the conduction band. Although these matrix elements have some effect on the value of the insulating gap of the compound,[10] for the sake of simplicity, we have neglected them.

The above Hamiltonian is studied by calculating various Green functions and their derived properties. The propagators are obtained by exactly diagonalizing a cluster of atoms and embedding it into a lattice of equivalent clusters through a perturbation series. The simplest possible starting point for a perturbation theory includes the one-site cluster, which is exactly diagonalized,[19] as the unperturbed Hamiltonian and the kinetic energy as the perturbation. This procedure gives rise to a cumulant diagrammatic expansion that, for the sake of simplicity, has been restricted to the so-called chain approximation.[22] It consists of taking high-order self-energy cumulants as a sum of all possible ways in which they can be decoupled as a product of two-operator cumulants. This approximation is equivalent to the imposition of the Wick theorem to construct a diagrammatic expansion on the kinetic energy, where the zero-order Green functions are obtained from local many-body Hamiltonian.[21] This approach considers local aspects of the Kondo effect in an exact way. A similar formalism has been used with success to study the properties of Kondo systems described by the Anderson lattice Hamiltonian[10,19] and taking numerically diagonalized clusters of several atoms when studying the transport properties of mesoscopic systems described by the impurity Anderson Hamiltonian.[26] For these cases, this approximation correctly introduces a shift to the Fermi level of part of the f density of states to create the Kondo peak. For the impurity problem the Friedel sum rule and the Fermi liquid properties

of the system are automatically fulfilled.[26] For the problem we are studying, the approximation provides, correctly as well, a gap at the Fermi level, which results from the coherent interference of the Kondo peaks at each site. This describes the essential physics of the Kondo systems, their insulating properties.

To calculate the undressed atomic matrix Green function $g^{AB}(\omega) = \langle\langle A;B\rangle\rangle_\omega$, where the operators A and B are taken to be the creation and destruction operators for the s and f atomic orbitals, we use the spectral representation of the retarded propagator in a grand canonical ensemble such that

$$g^{AB}(\omega) = \frac{1}{Z} \sum_{l,m,N,N'} [\exp(-\beta E_l^N) + \exp(-\beta E_m^{N'})]$$
$$\times \frac{\langle l,N|B|m,N'\rangle\langle m,N'|A|l,N\rangle}{\omega - (E_l^N - E_m^{N'})}, \qquad (4)$$

where Z is the partition function, β is the Boltzmann factor, N is the number of particles, and the energies E_l^N are defined by

$$E_l^N = E_n - \mu N, \qquad (5)$$

where μ is the Fermi level.

The eigenvalues E_l and the wave functions $|l,N\rangle$ are obtained by diagonalizing the atomic Hamiltonian represented in a 16×16 Hilbert space. This space is spanned by the s and f orbitals, the spin, and all possible occupation states of each atomic site ($N=0,1,2,3,4$). The nearest-neighbor hopping matrix between the clusters $\hat{W}_{ij}$ is defined by

$$\hat{W}_{ij} = \begin{pmatrix} t_c & 0 \\ 0 & 0 \end{pmatrix}_{ij}. \qquad (6)$$

We propose a diagrammatic expansion taking the Hamiltonian H_k, which connects the sites among themselves, as the perturbation. The simplest infinite family of diagrams possible to be summed up gives rise to what is called the chain approximation.[21,22] The dressed propagator is given within this approximation by the Dyson equation

$$\hat{G}_{ij}(\omega) = \hat{g}(\omega)\delta_{ij} + \hat{g}(\omega)\sum_l \hat{W}_{il}\hat{G}_{lj}(\omega), \qquad (7)$$

with $\hat{g}(\omega)$ given by

$$\hat{g}(\omega) = \begin{pmatrix} g^{cc}(\omega) & g^{cf}(\omega) \\ g^{fc}(\omega) & g^{ff}(\omega) \end{pmatrix}, \qquad (8)$$

where, for simplicity, we have neglected the spin index σ. The density of states (DOS), the electronic transport, and other derived thermodynamic properties can be obtained from the dressed Green function $\hat{G}_{ij}(\omega)$.

The site parameters ϵ_c^α, ϵ_f^α, $V_{c\text{-}f}^\alpha$, and U^α of the Hamiltonian (2) are binary random variables. Their two possible values, which depend upon the atom sitting at site i, are represented by the supraindex α. The binary character of the variables neglects the local parameter variation produced by

different possible environments. This hypothesis is compatible with the nature of the doping we are studying. In our case the doping is performed directly in the f sites, while the conduction lattice has a small, although important, change since the sizes of both atoms (Ce and La) are approximately the same. This permits us to neglect possible changes of the parameter t_c, assuming it to be independent of site and environment. In this case we have to solve a problem restricted to diagonal disorder.[27] It is important to emphasize that the diagonal matrix elements of the conduction band ϵ_c^α of both atoms are taken to be different. The adoption of a diagonal element value ϵ_c^α larger for the La than for Ce ion, required to describe their different distribution of charges, is responsible for the strong hybridization of the La conduction doping impurity state with the conduction band of $Ce_3Bi_4Pt_3$. As is shown in Figs. 4 and 6, the Fermi level of the alloy enters into the conduction band as soon as the content of La increases. This point will be discussed in detail below.

The two kinds of rare-earth atoms play different roles. The La atom is nonmagnetic with the f and d levels above the Fermi energy and the Ce is a magnetic atom in the mixed-valence regime with an f level below the Fermi energy, but inside the conduction band of the compound. The substitution of Ce by La gives rise to a missing f center, which can be thought to be a Kondo hole. This is so because, as the conduction electrons at that site are not spin polarized due to the absence of the f state, they do not constitute the local singlet responsible for the Kondo effect.[28]

The disorder of a Kondo insulator alloy has been previously studied by us using a real-space renormalization procedure.[10] Although this technique is very accurate to study thermodynamic properties derived from the mean-value DOS of the system, it destroys the information derived from localization produced by disorder.[14] This is an essential property to be preserved in order to study the flowing of carriers in an alloy.

To treat the disorder we use a numerical simulation algorithm, which is extremely efficient from the numerical point of view when applied to hierarquical lattices.[29] In order to benefit from it, we assume that the Kondo insulator is defined on a Bethe lattice. Although the Bethe lattice has less connectivity than a Bravais lattice, it preserves the interference effects that give rise to localization.[23] This algorithm consists in generating randomly, N sites corresponding to isolated La or Ce and their many-body dressed Green functions, with a probability that depends upon their concentration in the alloy. These Green functions are dressed randomly, connecting these sites with other randomly generated N sites, according to the topology of a Bethe lattice of coordination number z. This process is continued M times, creating in this way a lattice of $[(z-1)^M-1]N/(z-2)$ sites, which tends very rapidly to the thermodynamic limit as M increases. The Green functions $g_{sb}^{(i)}(w)$ of the last N sites obtained after M iterations, $0 > i > N$, correspond to the propagators of N different realizations of a semi-Bethe lattice. Combining them in all possible ways to obtain N^2 realizations of the Bethe lattice we obtain the configurational average of the local Green function given by

$$\langle G_{11}(\omega_0)\rangle = \sum_{i,j=1}^{N} G_{11}^{i,j}(\omega_0), \qquad (9)$$

where the subindex 1 of $\langle G_{11}(\omega_0)\rangle$ refers to an arbitrary site of the lattice and the sum is over all spatial configurations of the alloy we have numerically created. The propagator $G_{11}^{i,j}(\omega_0)$ is given by

$$G_{11}^{i,j}(\omega_0) = g_{sb}^{i}(\omega_0)[1 - t_c^2 g_{sb}^{i}(\omega_0)g_{sb}^{j}(\omega_0)]^{-1}, \qquad (10)$$

where $g_{sb}^{i}(\omega_0)$ corresponds to the propagator of the semi-Bethe lattice at the border site i. To find the variation of the Fermi level μ with the impurity concentration it is necessary to solve the self-consistent equation

$$n = \int_{-\infty}^{\mu} \Omega(\omega)d\omega, \qquad (11)$$

where

$$\Omega(\omega) = \frac{-1}{\pi}\sum_{m} \mathrm{Im}\langle G_{00}^{mm}(\omega)\rangle \qquad (12)$$

is the average DOS of the system and we have written explicitly the supraindex m in the Green function to identify the different bands (conduction and f bands).

From the mean value of the one-particle Green function $\langle \hat{G}_{00}(\omega)\rangle$ we obtain the properties associated to the DOS, as it could be the case of the specific heat, etc.

For the case of the transport properties it is necessary to calculate other mathematical objects. According to linear response theory, the current circulating along two adjacent arbitrary sites $n, n+1$, due to the application of an external bias, can be calculated from the Kubo formula

$$I_{n,n+1} = 2et_c h^{-1}\sum_{\sigma} \int_{-\infty}^{\infty} [\langle G_{n,n+1}^{-+}(w)\rangle - \langle G_{n+1,n}^{-+}(w)\rangle]dw, \qquad (13)$$

where the two adjacent sites are connected through the matrix element t_c and $\langle G_{n,n+1}^{-+}(w)\rangle$ is the configurational average of the out-of-equilibrium Keldysh Green function that determines the probability of an electron of energy w to hop from site $n+1$ to site n. Assuming, as discussed above, that the many-body effects can be obtained by diagonalizing the Hamiltonian corresponding to a site and that the external applied potential is infinitesimal and depends upon the frequency ω_0, the configurational average of the conductance can be written as

$$\sigma^T(\omega_0) = -\sum_{i,j=1}^{N} \frac{2\pi e^2}{h\omega_0}(e^{-\omega_0/KT}-1)\int_{-\infty}^{\infty} d\epsilon I^{i,j}(\epsilon,\omega_0)f(\epsilon)$$
$$\times [1-f(\epsilon+h\omega_0)], \qquad (14)$$

$$I^{i,j}(\epsilon,\omega_0) = t_c^2[2G_{12}^{i,j}(\epsilon+h\omega_0)G_{12}^{i,j}(\epsilon) - G_{11}^{i,j}(\epsilon+h\omega_0)$$
$$\times G_{22}^{i,j}(\epsilon) - G_{22}^{i,j}(\epsilon+h\omega_0)G_{11}^{i,j}(\epsilon)], \qquad (15)$$

where 1 and 2 are two arbitrary first neighbor sites of the lattice and

$$G_{22}^{i,j}(\omega_0) = G_{11}^{j,i}(\omega_0),$$

$$G_{12}^{i,j}(\omega_0) = g_{sb}^{i}(\omega_0)t_c G_{22}^{i,j}(\omega_0), \qquad (16)$$

where $f(\epsilon)$ is the Fermi-Dirac distributions. For zero temperature and in the static limit $\omega_0 \to 0$, Eq. (14) reduces to

$$\sigma_0(E_f) = \sum_{i,j=1}^{N} 2et_c h^{-1}\rho_{sb}^{(i)}(E_f)\rho_{sb}^{(j)}(E_f)$$
$$\times |1-t_c^2 g_{sb}^{(i)}(E_f)g_{sb}^{(j)}(E_f)|^{-2}, \qquad (17)$$

where the DOS of the i realization of the semi-Bethe lattice is obtained from the expression $\rho_{sb}^{(i)}(E_f) = \mathrm{Im}[g_{sb}^{(i)}(E_f)]$. To obtain the conductance, we need to take the spatial average over all possible configurations of the alloy. The average implied in Eq. (17) permits us to find the values of the Fermi energy for which the conductance is finite and the mobility edges, where it becomes zero. In general terms, the support of the conductance obtained from Eq. (17) is included within the larger support of the DOS defining the region in ω within which, although $\Omega(\omega) \neq 0$, all states are localized. If the Fermi level happens to be in this region, the system is an Anderson insulator. However, in the case of an ordered Kondo insulator, as the gap is due to correlation, the insulator is of the Mott type.

III. RESULTS

To study the physics proposed above we take the paradigmatic example of the Kondo alloy $Ce_3Bi_4Pt_3$ when doped with La. The one-body parameters of the tight-binding Hamiltonian are obtained by comparing, at the vicinity of the Fermi level, the DOS of $U=0$ with the result that provides a simplified density functional calculation.[10] The Ce compound is modeled with the Hamiltonian parameters $t_c = W/\sqrt{4(z-1)}$ (where z is the coordination of the Bethe lattice and W is the half-width band), $\epsilon_c^{Ce}=0$, $\epsilon_f^{Ce} = -0.7 W$, $V_{c\text{-}f}^{Ce}=0.09 W$, and $U^{Ce}=1.4 W$. We take for La the same t_c as for Ce and $\epsilon_c^{La}=0.2 W$. The correlation parameter U has been estimated from the size of the f and d states of Ce and La, respectively. However, the results obtained are weakly dependent on U if the condition $U \gg \epsilon_c - \epsilon_f$ is satisfied. It is important to emphasize that the diagonal element of the s band for La is greater than for Ce, $\epsilon_c^{La} > \epsilon_c^{Ce}$. This can be understood in the following way. The Ce ion in the compound $(Ce_{1-x}La_x)_3Bi_4Pt_3$ possesses a Xe core of four positive charges and two electrons at the $4f$ and $6s$ orbitals, while the La ion has a Xe core of three positive charges and one $6s$ electron. As the $4f$ state does not screen completely the extra charge of the Xe core belonging to Ce, the s electron of Ce is more strongly bounded than its equivalent of La. The fact that the conduction electrons of La are less bounded than that of Ce is very important to determine the physical properties of the alloys. As discussed below, it is responsible for the shift of the Fermi level into the conduction band, where the metal-nonmetal transition takes place when the concentration of La is increased.

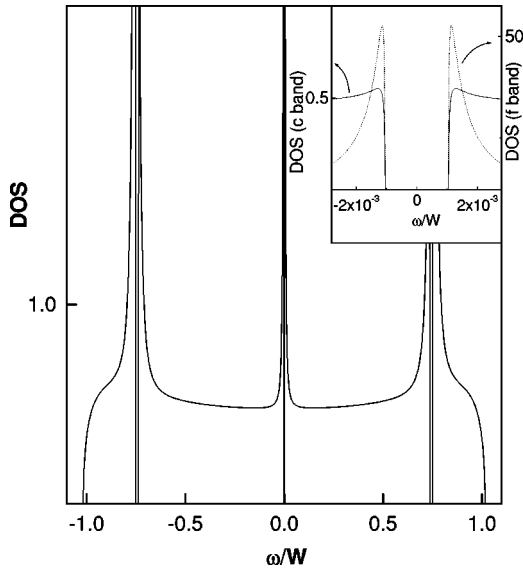The DOS of the pure material presents the known features

FIG. 1. The DOS of the compound $Ce_3Bi_4Pt_3$ for Ce. The inset shows the gap produced by the Kondo resonance [solid lines (c band) and dashed lines (f band)].

of a Kondo insulator. The coherent hybridization creates two gaps: one of no physical importance at low energies near the energy of the f state and the other at the Fermi level that results from the hybridization of the Kondo resonance with the conduction band. The DOS of this heavy-fermion material has two very important and well-known properties. It is a semiconductor with a very narrow gap of very high edges due to the Abrikosov-Suhl resonance split by hybridization at the borders of the valence and conduction bands. This is shown in Fig. 1. In the inset, we show the different contributions in the vicinity of the Fermi level. It is clear from the figure that the Kondo peak is mainly of f nature, while its existence is reflected in the conduction band by the creation of the insulating gap.

In Figs. 2–5 we show, for different values of the impurity concentration of the alloy, the DOS as a function of fre-
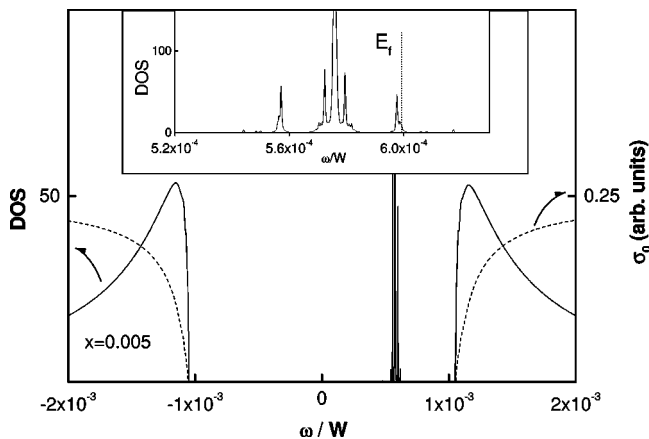

FIG. 2. DOS (solid line) as a function frequency w and the static conductivity (dashed line) as a function of the Fermi level E_f ($E_f = w$) at the gap vicinity for $x = 0.005$. The inset shows the localized states at the gap.
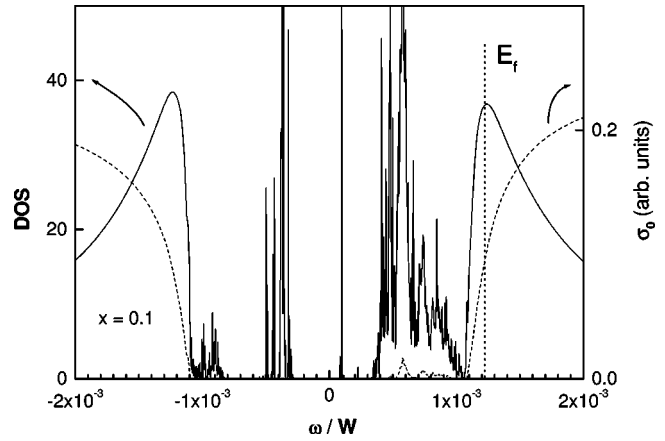

FIG. 3. The same as Fig. 2 for $x = 0.1$.

quency w and the static conductance as a function of possible values of the Fermi energy E_f taken to be $w = E_f$. The DOS for a very low concentration ($x = 0.005$) is depicted in Fig. 2. The presence of La originates an impurity band within the insulating gap, where the Fermi energy is localized, which is displaced towards the edge of the conduction band because the s electron of La is less bounded than that of the Ce. This impurity band is formed mainly by states localized at the La sites surrounded by essentially Ce atoms adopting different configurations. These states are not extended and accordingly their conductance is zero, as shown in the figure. The states localized at the neighborhood of an atom of La, with energy in the gap region, do not connect other atoms of La. They do not create a percolating path involving the whole system. As shown in the inset of Fig. 2, when the La atoms are incorporated, the Fermi level is displaced from the middle of the gap into the impurity band formed by localized states. From the figure, we can conclude that the localized states are restricted to the impurity band, as the edges of the DOS and the conductance inside the valence and conduction bands is almost coincident. Although for this concentration of impurities the system is an insulator, the liner temperature contribution to the specific heat is finite because the Fermi level is located at the localized impurity band.

As the impurity concentration is increased several processes take place. The Kondo holes destroy the translational
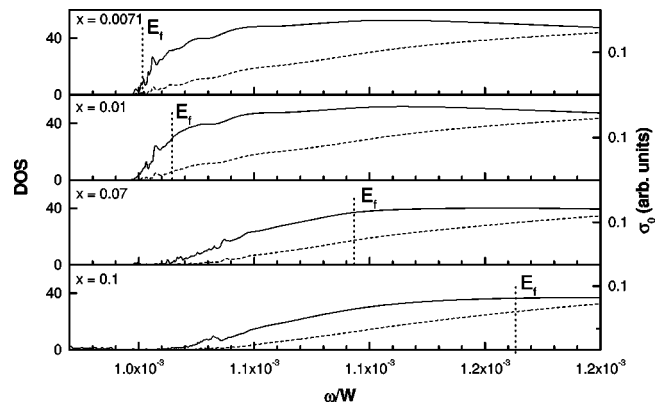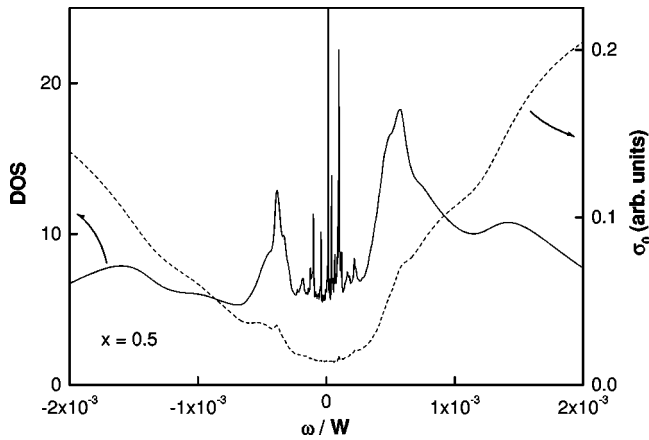

FIG. 4. The same as Fig. 3 for various values of x.

FIG. 5. The same as Fig. 3 for $x=0.5$.

FIG. 6. (a) DOS at the Fermi level vs x. (b) Fermi level vs x. The inset shows a zoom of this figure for $x<0.4$. (c) Conductivity vs x. The inset shows a zoom in the region of the metal-nonmetal transition.

invariance of the lattice and, as a consequence, the coherent hybridization responsible for the existence of the gap. The top and bottom of the valence and conduction bands, respectively, are modified as shown in Fig. 3. The impurity band increases its width and weight with x and for $x\sim0.1$ some of its states are delocalized, as reflected by the finite conductivity inside it. However, for this concentration, the Fermi level, which is displaced towards the conduction band when the impurity content increases, has already entered into it. The system is already a metal as the Fermi level has passed the mobility edge and is localized in a region where the conductance is finite. This process has a more detailed presentation in Fig. 4, where the DOS and conductivity at the neighborhood of the conduction band are depicted for various values of La concentration. For $x\sim0.0071$, the system is at the threshold of being a metal because the Fermi level, inside the conduction band, is below, although very near, the mobility edge. For greater values of x the system is conducting. According to the experimental results[11,12] a very small concentration of impurities ($x<0.01$) is enough for the system to undergo a metal-nonmetal transition. Our results confirm that the concentration of impurities capable of delocalizing the states inside the impurity band ($x\sim0.1$) is much greater than this experimental value. Moreover, we show that the Fermi level is not pinned but displaced from the middle of the gap to the interior of the conduction band due to the presence of the impurities. These two results give support to the scenario according to which the metal-nonmetal transition takes place within the conduction band and not inside the impurity band[9] as the La concentration is increased. From this point of view the metallic side of the transition is controlled by electrons that contribute to the conductivity inside the Kondo resonance; the system is a heavy-fermion and very much influenced by disorder.

We show in Fig. 5 the DOS and conductivity for large values of the concentration $x=0.5$ in a region of energy inside the gap of the pure material. Although the Fermi energy is already inside the conduction band for this value of x, as shown in Fig. 6, it is interesting to realize that for this concentration there is still a pseudogap in the conductivity. This gives rise to a rapid oscillating DOS, showing that these
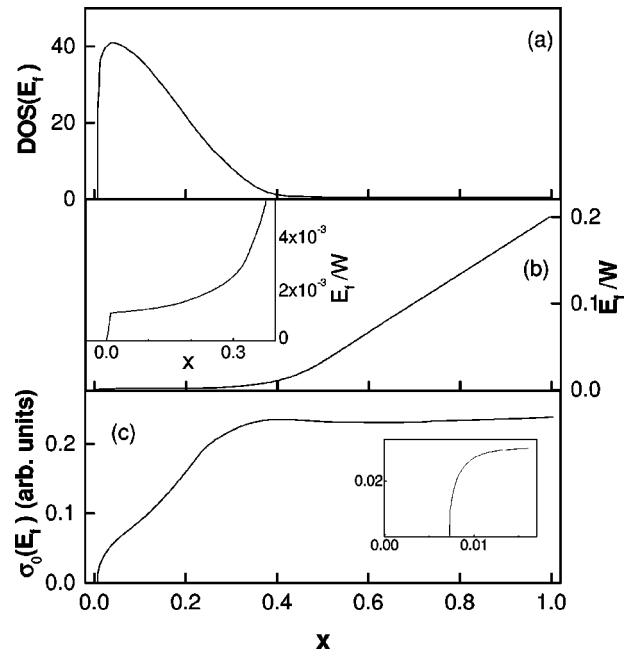
states, although above the percolation threshold, have some local character.

In Figs. 6(b) and 6(c) we represent the conductivity and Fermi level as a function of concentration. As is clear from the behavior of the conductivity, a very small concentration of Kondo holes gives rise to a metal-nonmetal transition, above which the conductivity is different from zero. Because the Ce atoms attract the conduction electron more strongly than the La ones, a small concentration of impurities is enough to displace the Fermi level into the conduction band. However, it depends slowly on x for $x<0.4$. This is a consequence of the fact that up to that concentration the system behaves as a heavy fermion with a large DOS in the neighborhood of the Fermi level. In agreement with the experimental results[1] for $x>0.4$, the DOS reduces drastically with x as shown in Fig. 6(a), the heavy-fermionic behavior disappears and the Fermi level shifts rapidly to compensate the weaker attraction of the La atom.

In Fig. 7 we present the dependence of the conductivity in a logarithm scale, as a function of temperature for various values of the concentration x. For the pure Ce compound, as the system is an insulator the resistance has, at low temperatures ($T<T_k$), an activation behavior. This permits to obtain from the curve the gap value. At higher temperatures as the gap disappears for $T\gg T_k$, the system behaves as a metal. For finite values of x, although still very small ($x>0.007$), the figure shows that the resistance has an activation behavior for small values of T, but as the temperature is reduced even further, it saturates and diminishes reaching a finite value at $T=0$. This last behavior reflects the fact that the system is already a conductor. At very low temperature, it is possible to expand the conductivity σ at the Fermi level in
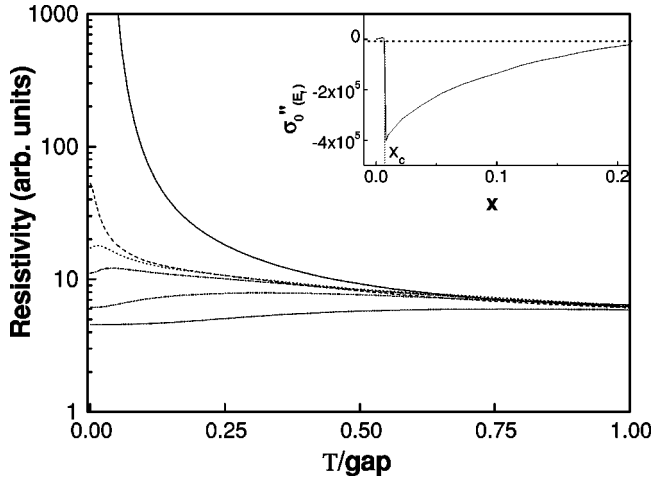
FIG. 7. Resistivity vs temperature for various values of x; from top to bottom $x=0.005, 0.01, 0.07, 0.1, 0.2, 0.3$. The inset shows the second derivative of the conductivity at the Fermi level vs x.

FIG. 8. The optical conductivity of $Ce_3Bi_4Pt_3$ as a function of w_0, for various values of temperature.

powers of the temperature, following the traditional Sommerfeld expansion of the Fermi distributions, such that

$$\sigma = \sigma_0(E_f) + \frac{\pi^2}{12}\left(\frac{d^2}{d^2E}\sigma_0(E)\right)_{E=E_f} T^2.$$

The second derivative of the conductivity controls the behavior of the resistivity at very low temperature. Its dependence upon the concentration x is shown in the inset of Fig. 7. As x is increased, the derivative, which is positive for $x < 0.007$, has an abrupt change into a large negative quantity and reduces its modulus as the concentration is increased. The value of the impurity concentration at which this quantity changes sign can be considered to be an upper limit for the metal-nonmetal transition concentration because, when the resistivity increases with temperature, it has to be finite at $T=0$. The behavior of the resistivity with temperature and impurity concentration, depicted in Fig. 7, coincides qualitatively and semiquantitatively with the experimental results,[11,31] giving further basis for the scenario we propose for the metal-nonmetal transition.

Finally, we study the optical conductivity $\sigma(\omega_0)$ given in Eq. (14), measured for the pure compound,[30] for different temperatures as a function of frequency ω_0. The results are shown in Fig. 8. They are in qualitative and semiquantitative agreement with the experiments. For high temperatures the conductivity shows a low dependence on ω_0. For lower temperatures the conductivity exhibits a strong dependence for low frequencies, a typical behavior of a system with a gap. This manifestation is clearer as the temperature is reduced. The theoretical result shows an abrupt discontinuity of the conductivity for a value of ω_0 of the order of the gap that tends to disappear by increasing the temperature. It reflects the abrupt increase of the conductivity when the incident light has enough energy to excite electron from the valence to the conduction band. We believe that this abrupt change is not reflected in the experimental result because the real system possesses impurities that create states in the gap from
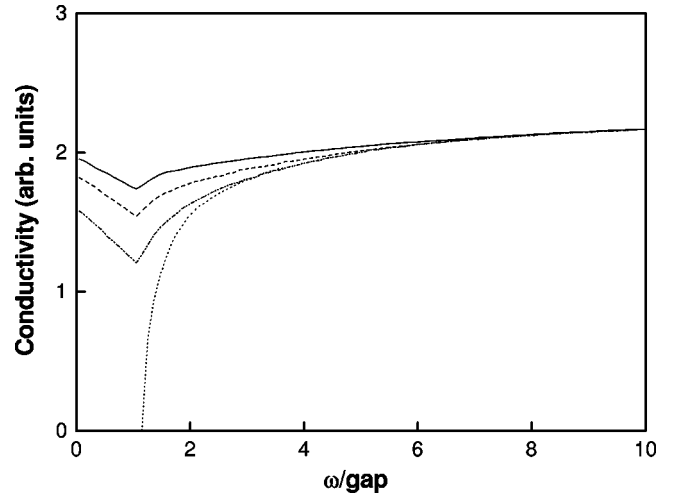
which the electrons are excited to the conduction band in a more continuous way. In fact the linear contribution to the specific heat, experimentally observed for the real material,[11,32] gives support to this interpretation.

IV. SUMMARY

We have studied the metal-insulator transition in disordered Kondo compounds, using a periodic Anderson Hamiltonian. The Green functions that describe the system were obtained diagonalizing the site Hamiltonian, which contains all the many-body interactions, and by taking as the perturbed Hamiltonian the intersite matrix elements. The perturbation expansion is calculated in the chain approximation.[21] Although the many-body problem is treated in a simple way, which could restrict the validity of the results obtained, we believe it provides the essential physics that could be expected from more sophisticated approaches. We are referring to the appearance of a gap at the Fermi level, its behavior with temperature, and the heavy-fermion properties obtained. The relative simplicity of the many-body treatment permitted to use a numerical algorithm that considers disorder in an exact way. Although not essential, with the purpose of reducing the numerical effort, we have supposed that the system is defined on a Bethe lattice.

It was studied in particular the DOS and the conductivity dependence upon the concentration of impurities for the alloy $[(Ce_{1-x}La_x)_3Bi_4Pt_3]$. The simultaneous study of these two quantities permitted us to find the mobility edges and to establish that the metal-nonmetal transition is a result of the interplay of correlation and disorder when the Fermi level is inside the conduction band. We have compared the transport properties obtained with various available experiments.

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