The metal-non-metal transition and specific heat of Kondo insulators

2000 J. Phys.: Condens. Matter 12 9885

(http://iopscience.iop.org/0953-8984/12/48/306)

J. Phys.: Condens. Matter **12** (2000) 9885–9896. Printed in the UK PII: S0953-8984(00)12443-9

The metal–non-metal transition and specific heat of Kondo insulators

C A Büsser†, E V Anda† and G Chiappe‡

† Departamento de Física, Pontificia Universidade Católica do Rio de Janeiro, CP 38071-970, Rio de Janeiro, RJ, Brazil

‡ Departamento de Física, Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires Ciudad Universitaria, 1428, Buenos Aires, Argentina

Received 8 March 2000, in final form 12 October 2000

Abstract. The metal–non-metal transition in Kondo insulators of the type $(Ce_{1-x}La_x)_3Bi_4Pt_3$ is studied as a function of the La (Kondo hole) concentration x. We explore the transition under variation of the applied magnetic field, the pressure, and the temperature. The many-body effects are treated by diagonalizing the site Hamiltonian and embedding this solution into the lattice, using the chain approximation. The alloy states at the Fermi energy are obtained using a real-space renormalization technique. The metal–insulator transition produced by the incorporation of La impurities is explained by the appearance of a delocalized level inside the conduction band rather than by the creation of an impurity band at the gap.

1. Introduction

Heavy-fermion materials are characterized by properties derived from their highly correlated electrons. These systems can be superconductors, ferromagnets and antiferromagnets, metals, Kondo insulators, and Fermi and non-Fermi liquids. They undergo a variety of phase transitions as functions of different thermodynamic variables. In particular the metal–non-metal transition has been studied as function of external pressure, composition, doping, temperature, and external magnetic field [1].

Non-Fermi-liquid behaviour in metals represents one of the most challenging problems for these highly correlated systems. A large class of f-electron non-magnetic materials present this behaviour, probably due to proximity to a quantum critical point or, in the case of alloy materials, because of correlation enhanced by disorder [2, 3].

Among the large number of rare-earth and actinide compounds, some have small gaps although they are expected to be metallic by analogy with their f-series analogues [4].

These Kondo insulators, due to their small gaps, are good candidates for displaying a metal–non-metal transition when subjected to alloying, external pressure, or a magnetic field or when their temperature is increased.

This problem has been studied theoretically by several authors in the last few years using a two-band model (a large uncorrelated conduction s band and another narrow correlated band which describes the f electrons) and different techniques for diagonalizing the Hamiltonian. Functional integral approaches [5] and approximations based on decoupling procedures [6] for the equation of motion of the one-particle propagator were able to provide a description of some aspects of the metal–non-metal transition driven by temperature and f–f hybridization, emphasizing the s–f hybridization character of the small gap. These theoretical approaches,

0953-8984/00/489885+12$30.00

however, are not suitable for describing the low-energy excitations derived from the Kondo effect. As a consequence, to obtain the gap at the Fermi level these approximations require an even number of valence electrons per unit cell and the same centre for the f and s bands, as established by band theory. The insulating properties of these compounds are more probably derived from the hybridization of the s band with the Abrikosov–Suhl (AS) resonance [7] that, due to its location in the vicinity of the Fermi level, generates a small insulating gap. From this viewpoint, it is natural that a metal–insulator transition is obtained by increasing the temperature, since the AS resonance disappears for temperatures above the Kondo temperature T_K. Adopting this scenario, the metallic regime is outside the Kondo regime. However, as is well known, under an external or chemical pressure or an external magnetic field, the gap can be closed while maintaining the system in the Kondo regime, in which case the metallic phase is a heavy-fermion phase.

Other important approaches used to study Kondo insulators have adopted slave-boson techniques [8] or second-order perturbation of the Coulomb repulsion U [9]. For the case of $(Ce_{1-x}La_x)_3Bi_4Pt_3$, it was concluded that the incorporation of the La Kondo hole into the Kondo semiconductor induces a bound state in the gap. The spectral weight of this bound state turns out to be spatially localized in the immediate vicinity of the impurity. In view of this, it is clear that a finite concentration of impurities creates an impurity band inside the energy gap that, in principle, controls the specific heat and the conductivity of the system. This scenario gives a satisfactory explanation for the abrupt increase of the T-linear contribution to the specific heat (γ), which is typical behaviour for a heavy-fermion system. It is known that when the Fermi energy is within an impurity band, the metal–non-metal transition is described by quantum percolation as there are no delocalized states of the bulk in a condition to hybridize significantly with the impurity band levels. Some experiments [10, 11] show that a very small concentration of impurities ($x \simeq 0.005$), much lower than the quantum percolation threshold for localized states of a 3D system, is sufficient for transforming the semiconductor $Ce_3Bi_4Pt_3$ into a metal (10) [12]. This suggests that the incorporation of a La impurity in this Kondo insulator is more likely to generate a level which hybridizes significantly with the Ce states, creating a delocalized level inside the band. In this scenario the Fermi level of the alloy, for moderate impurity concentrations, turns out to be inside the valence band of the semiconductor, near the top.

Very recently a dynamical mean-field approach has been applied to the study of the non-Fermi-liquid properties of other Kondo alloys [2]. It is a powerful self-consistent formalism, developed to treat infinite-dimensional systems. Although a local self-energy can be satisfactorily used to study 3D systems [13], when a self-consistent calculation is required, as is the case for the dynamical mean-field approach, its application in studying disordered systems is very difficult.

We study in this paper alloy Kondo insulators, emphasizing the fact that they are finite coordinated systems for which disordered fluctuations, in the vicinity of the Fermi level, could play an important role in determining properties. The many-body effects are treated in a simple approximation which, due to its simplicity, permits a very accurate treatment of disorder. We incorporate all the local contributions to the Kondo effect [14, 15], exactly diagonalizing the Hamiltonian of a site, including the s and f electrons [16]. We use the chain approximation [17, 18] to embed this renormalized atom into the lattice. Since the many-body spin–spin correlations are restricted to the nearest neighbours, the approximation does not provide the correct energy scales. In particular, the Kondo temperature does not scale properly with the parameters of the system. However, this calculation has the advantage of introducing very simple real-space self-energies from which we can calculate the dressed propagator on the lattice. This generates a very natural and numerically feasible procedure for incorporating

disorder. The disorder is treated using real-space renormalization techniques. Some versions of this procedure permit us to obtain very accurate results when disorder fluctuations are properly treated in calculating the Green functions [19].

We study one-particle propagator properties of Kondo insulators. We concentrate our attention on the physical properties of these systems, emphasizing two aspects. The first one is the important role played by the effective f–f hybridization in the electronic properties near the Fermi energy [6]. The second refers to the necessity of considering a more sophisticated approximation than the traditional CPA to study the alloy states at the Fermi level, whether it is in the impurity band within the gap or in the neighbourhood of the band edges. This is due to the fact that dilution and band edges are ill described by mean-field CPA-type approximations for a finite coordinated system [20].

Undoubtedly these materials provide very interesting cases for which to study the metal–non-metal transition in the presence of disorder and correlation. This problem has been extensively investigated, for instance, in the case of Si doped with P [21]. However, the Kondo insulator seems to present 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 [22]. A proper study of the transport properties of these systems would require the calculation of two-body propagators; this is not developed in this paper. However, this study does constitute an excellent test for the approximation used, having in mind its application to the study of transport properties.

The paper is organized in the following way. Section 2 describes the model represented by a periodic Anderson Hamiltonian and the calculation of the one-particle propagator from a cumulant expansion which exactly diagonalizes a minimum cluster of one site that is afterwards embedded into the lattice. Section 3 discusses the problem of a doped Kondo insulator, taking as an example the compound $(Ce_{1-x}La_x)_3Bi_4Pt_3$ and treating the disorder using a real-space renormalization technique. Section 4 is dedicated to the discussion of the density of states of this material in the vicinity of the Fermi level and the specific heat as a function of the impurity concentration. Section 5 is devoted to the study of the metal–non-metal transition driven by temperature, pressure, and external magnetic field, and finally section 6 includes a summary and some conclusions.

2. The model

The peculiarities of heavy-fermion systems have been traditionally studied by adopting the periodic Anderson Hamiltonian. To study Kondo alloys, we incorporate an effective first-neighbour f–f hybridization term induced by the mixing of the f states with the ligands. The direct one is almost negligible, for most compounds, due to the local character of the f states. Although this is normally a very small contribution, the very small gap of a Kondo insulator turns out to be very sensitive to this term [6]. The total Hamiltonian is written as

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

where H_i which is given by

$$H_i = \sum_\sigma (\epsilon_c^\alpha n_{i\sigma}^c + \epsilon_f^\alpha n_{i\sigma}^f + V_{c-f}^\alpha (c_{i\sigma}^+ f_{i\sigma} + \text{c.c.}) + U^\alpha n_{i\uparrow}^f n_{i\downarrow}^f + \mu_B g B (n_{i\uparrow}^f + n_{i\uparrow}^c - n_{i\downarrow}^f - n_{i\downarrow}^c) \tag{2}$$

is the atomic Hamiltonian that includes the e–e interaction and the electronic coupling with an external magnetic field B and is represented in a Hilbert space with two localized wave functions, the s and f orbitals. The superscript α in the parameters ϵ_c^α, ϵ_f^α, V_{c-f}^α, and

U^{α} introduces the possibility of representing a system doped by another chemical element. The kinetic contribution to the Hamiltonian considers the hopping among different nearest-neighbour sites:

$$H_k = \sum_{\sigma} \left(t_c \sum_{\langle i,j \rangle} c^{+}_{i\sigma} c_{j\sigma} + t_f \sum_{\langle i,j \rangle} f^{+}_{i\sigma} f_{j\sigma} \right). \tag{3}$$

The system described by the above Hamiltonian is studied by calculating the one-particle propagator and its derived properties.

The propagator is obtained by exactly diagonalizing a cluster of atoms and embedding it into a lattice of equivalent clusters through a perturbation series that takes the hopping between them as the perturbation Hamiltonian. The simplest possible starting point for the perturbation theory which already includes all the local aspects of the Kondo effect is to take as the unperturbed Hamiltonian the one-site clusters that are exactly diagonalized [16] 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 [18]. This consists in taking high-order self-energy cumulants as sums of all of the possible ways in which they can be decoupled as products of two-operator cumulants. This approximation is equivalent to the imposition of the Wick theorem for constructing a diagrammatic expansion on the kinetic energy, where the zero-order Green functions are obtained from the local many-body Hamiltonian [17]. This approximation has been used with success to study the properties of Kondo systems described by the Anderson lattice Hamiltonian [16, 25].

To calculate the undressed atomic matrix Green function $g^{AB} = \langle\langle A; B \rangle\rangle_0$ 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

$$g^{AB}(\omega) = \frac{1}{Z} \sum_{l,m,N,N'} (\exp(-\beta E^N_l) + \exp(-\beta E^{N'}_m)) \frac{\langle l, N|B|m, N'\rangle \langle m, N'|A|l, N\rangle}{\omega - (E^N_l - E^{N'}_m)} \tag{4}$$

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

$$E^N_l = E_n - \mu N \tag{5}$$

where μ is the Fermi level.

The eigenvalues E_l and 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 conduction and f orbitals, the spin, and all of the possible occupation states of each atomic site ($N = 0, 1, 2, 3, 4$). The nearest-neighbour hopping matrix connecting the clusters $\hat{W}_{ij}$ is defined by

$$\hat{W}_{ij} = \begin{pmatrix} t_c & 0 \\ 0 & t_f \end{pmatrix}_{ij}. \tag{6}$$

The chain approximation [17] gives rise to a Dyson equation for the dressed propagator given by

$$\hat{G}_{ij}(\omega) = \hat{g}(\omega)\delta_{ij} + \hat{g}(\omega) \sum_{l} \hat{W}_{il} \hat{G}_{lj}(\omega) \tag{7}$$

where $\hat{g}(\omega)$ is given by

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

where we have neglected the spin index σ.

The density of states, the specific heat, and other derived thermodynamic properties are obtained from the dressed Green function $\hat{G}$.

3. The disorder

The parameters ϵ_c^α, ϵ_f^α, V_{c-f}^α, and U^α of the Hamiltonian (2) that describe site i are, in the case of doped Kondo insulators, binary random variables. Their two possible values that depend upon the atom sitting at site i are represented by the superscript 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 that we are studying. In our case the doping is performed directly at the f sites, while the conduction lattice undergoes a small, although important, change since the sizes of the atoms (Ce and La) are approximately the same. This is why the hopping matrix elements t_c of the conduction band are not considered to be random variables. The t_f matrix element is important for determining the gap of the compound, but is irrelevant as a random variable not only due to its small value but also because the difference between the local diagonal energy levels in Ce and La is large. In this case, we have to solve a problem restricted to diagonal disorder [20]. It is important to emphasize that the diagonal matrix elements of the conduction band ϵ_c^α of the two atoms are taken to be different. The adoption of different diagonal elements ϵ_c^α makes possible a strong hybridization of the La conduction state with the conduction band of $Ce_3Bi_4Pt_3$ when it enters as a doping impurity. This is shown in the density of states of figure 1. This point will be discussed in detail below. The two kinds of rare-earth atom play different roles. The La atom is non-magnetic 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 La for Ce gives rise to a missing f centre, which can be thought of as 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 local singlets responsible for the Kondo effect [23].

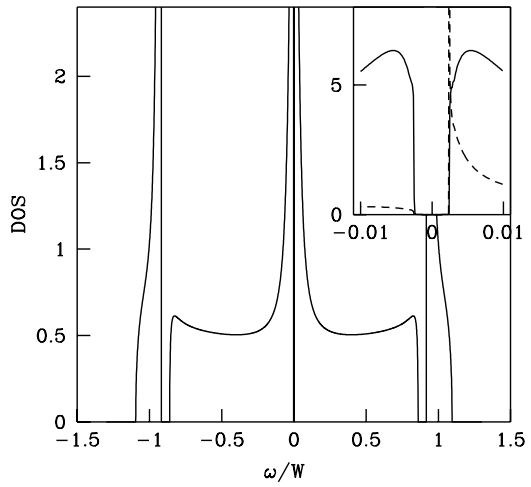

Figure 1. The DOS for the Ce compound in a Bethe lattice of coordination 4. We can see, in the inset, the hybridization gap of the Kondo resonance (solid lines) and the DOS of an isolated La Kondo hole in a matrix of Ce (dashed lines). This Kondo hole does not induce bound states in the gap.

In order to treat the disorder produced by doping, we use a real-space renormalization procedure which consists of an iterative decimation of the lattice sites which permits us to calculate the mean value of the Green function. To use this decimation technique in a simple

way, we restrict ourselves to the study of hierarchical lattices [19]. In particular we suppose that the Kondo insulator can be represented on a Bethe lattice. This lattice can be constructed as a limit of an iterative procedure in which the linear chain is the basic structure. So the real-space renormalization process reduces to a procedure of decimating sites in a linear chain, averaging the propagator in relation to the decimated degrees of freedom, and constructing at each step the Bethe lattice from the linear chain. This treatment is superior to a mean-field CPA approximation particularly in the case of a dilute lattice below or in the vicinity of the percolation threshold at the centre of the band [19] (the dilution peak), which in our case corresponds to the gap of the compound. At this particular energy, localized states are associated with isolated atoms, clusters of atoms, and some atomic configurations which appear in the connected part of the lattice. This is also true at the edges of the bands, which is precisely the region of interest.

Following along the lines developed in [19], we generalize the decimation procedure to the case of two states per site. We adopt the linear chain as the initial structure for constructing the Bethe lattice. The Dyson equation for a 1D system is given by

$$\hat{G}_{00}(\omega) = \hat{g}^{\nu}(\omega) + \hat{g}^{\nu}(\omega)\hat{W}_{01}\hat{G}_{10}(\omega) + \hat{g}^{\nu}(\omega)\hat{W}_{0-1}\hat{G}_{-10}(\omega) \tag{9}$$

where the superscript ν indicates the possibility for the atom to be La or Ce.

We can decimate the sites 1 and -1 in the equation and rewrite equation (9), coupling the central site 0 with sites 2 and -2. This procedure defines a renormalization process where the renormalized relations to be iterated are given by

$$\hat{g}^{\nu(N+1)}(\omega) = \sum_{\alpha\beta}\big(\hat{1} - \hat{g}^{\nu(N)}(\omega)\hat{W}^{\nu(N)}(\omega)(\hat{g}^{\alpha(N)}(\omega)\hat{W}^{\alpha(N)}(\omega) + \hat{g}^{\beta}(N)(\omega)\hat{W}^{\beta(N)}(\omega))\big)^{-1}\hat{g}^{\nu(N)}(\omega)c_\alpha c_\beta \tag{10}$$

$$\hat{W}^{\nu(N+1)}(\omega) = \sum_{\alpha\beta}\big(\hat{1} - \hat{g}^{\nu(N)}(\omega)\hat{W}^{\nu(N)}(\omega)(\hat{g}^{\alpha(N)}(\omega)\hat{W}^{\alpha(N)}(\omega) + \hat{g}^{\beta}(N)(\omega)\hat{W}^{\beta(N)}(\omega))\big)^{-1}\hat{W}^{\nu(N)}(\omega)\hat{g}^{\alpha(N)}(\omega)\hat{W}^{\alpha(N)}(\omega)c_\alpha c_\beta \tag{11}$$

where the iteration process is begun by adopting the initial values

$$\hat{g}^{\nu(0)}(\omega) = \hat{g}^{\nu}(\omega) \tag{12}$$

$$\hat{W}^{\nu(0)}(\omega) = \hat{W}_{01} = \hat{W}_{0-1}. \tag{13}$$

The configurational average is taken over the decimated degrees of freedom at each iteration step and c_α is the concentration of the species α in the system. In principle, when $N \to \infty$ we obtain the solution for the propagator corresponding to the linear chain as the fixed point of the renormalization process:

$$\hat{G_{00}}(\omega) = \lim_{N\to\infty}\sum_{\alpha} c_\alpha \hat{g}^{\alpha(N)}(\omega). \tag{14}$$

The DOS of the Bethe lattice can be calculated by superposing linear chains where the central atom always has to be undressed in order to conserve the finite coordination number of the lattice. This procedure gives us the dressed Green function of the system. To find the variation of the Fermi level μ with the impurity concentration, it is necessary to solve the self-consistent equation

$$n = \int_{-\infty}^{\mu} \rho(\omega)\,\mathrm{d}\omega \tag{15}$$

where

$$\rho(\omega) = \frac{-1}{\pi}\sum_{m} \operatorname{Im} G_{00}^{mm}(\omega) \tag{16}$$

and n is the number of electron per site, contained in the m bands (conduction and f bands), given by $n = \sum_\alpha c_\alpha n_\alpha$, where n_α is the number of electrons of the α-specimens.

4. Specific heat and DOS

We discuss in this section the physics associated with the compound $Ce_3Bi_4Pt_3$ when doped with La. We have calculated the density of states produced by the periodic Anderson Hamiltonian taking $U = 0$ and we have compared it with the results obtained using a simplified density functional calculation [24]. The one-body parameters used to study these compounds result from the best fit that can be obtained from these two sets of results in the vicinity of the Fermi energy. The Ce compound will be modelled with the Hamiltonian parameters $t_c = W/\sqrt{4(z-1)}$ (where z is the coordination of the Bethe lattice and W is the band halfwidth), $t_f = 0.035t_c$, $\epsilon_c^{\mathrm{Ce}} = 0$, $\epsilon_f^{\mathrm{Ce}} = -0.7W$, $V_{c-f}^{\mathrm{Ce}} = 0.2W$, and $U^{\mathrm{Ce}} = 1.4W$, and La with $t_c = W/\sqrt{4(z-1)}$, $t_f = 0.035t_c$, $\epsilon_c^{\mathrm{La}} = 0.2W$, $\epsilon_f^{\mathrm{La}} = 0.6W$, $V_{c-f}^{\mathrm{La}} = 0.01W$, and $U^{\mathrm{La}} = 2.4W$. 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 the U-values 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, $\epsilon_c^{\mathrm{La}} > \epsilon_f^{\mathrm{Ce}}$. This can be understood in the following way. In the compound $(Ce_{1-x}La_x)_3Bi_4Pt_3$ the Ce ion possesses a Xe core of four positive charges and two electrons in the 4f6s orbitals while the La ion has a Xe core of three positive charges and one 6s electron. As the 4f state does not completely screen the extra charge of the Xe core belonging to Ce, it is natural to think that the s electron of Ce is more strongly bound than its equivalent for La.

The density of states of the pure material presents the known features of a Kondo insulator. The coherent hybridization creates two gaps: one at low energies near the f state and the other at the Fermi level that results from the hybridization of the Kondo resonance with the conduction band. The density of states of this heavy-fermion material has two very important and well known properties. It turns out to be a semiconductor of very narrow gap and it has very high edges due to the Abrikosov–Suhl resonance split by hybridization to the borders of the valence and conduction bands. This is shown in figure 1.

It is important to notice that the physical properties of this gap and, in particular, its temperature behaviour are governed by the nature of the Kondo peak.

The value of the gap is extremely dependent on the f–f hybridization parameter V_f, as discussed in detail below.

We have calculated the density of states of the alloy for different concentrations of impurities. An isolated La Kondo hole in a matrix of Ce Kondo insulator does not induce a bound state in the gap of the semiconductor because the La hybridizes strongly with the conduction states of the bulk. This is clearly seen in the inset of figure 1, where the density of states projected over the isolated La impurity is shown. The extra La state appears as a resonant state within the conduction band of the compound, almost at its edge. As a consequence, the Fermi level is not pinned but displaced from the middle of the gap to the upper edge of the conduction band due to the presence of the impurity. This precludes the formation of an impurity band at the gap as the La concentration is increased [9].

On increasing the concentration of impurities, the Kondo hole destroys the translational invariance of the lattice and as a consequence the coherent hybridization responsible for the existence of the gap. The top of the valence band is greatly modified as shown in figure 2 and, through the self-consistent calculation proposed in [14], the Fermi level is found to enter into the conduction band (figure 3). In this situation the electrons that contribute to the conductivity

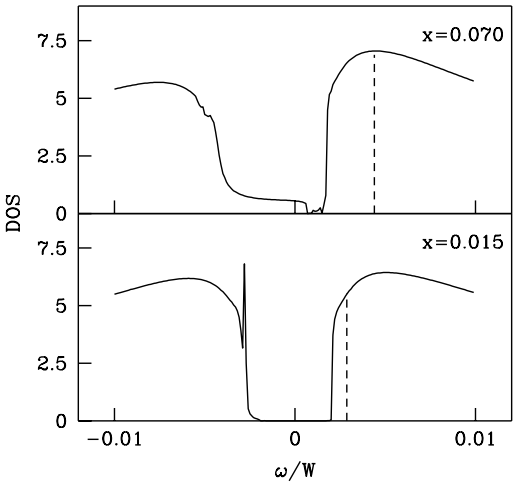

Figure 2. The DOS in the vicinity of the gap for different La concentrations (x). Dashed lines show where the Fermi level lies for each concentration. The Fermi level enters into the conduction band.

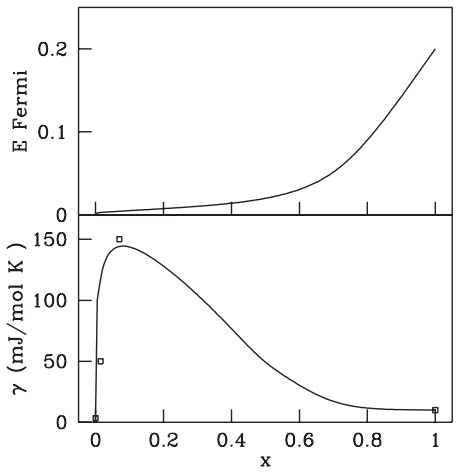

Figure 3. The T-linear contribution to the specific heat (γ) and Fermi level as a function of La concentration. Experimental data from reference [10] (squares) are shown. For small concentration, the Fermi level lies in the Kondo resonance region, increasing the γ-coefficient very rapidly.

of the system are within the Kondo resonance and very much influenced by disorder. According to the experimental results [10, 11], a very small concentration of impurities are sufficient to cause the Fermi level to go through the mobility edge to a region of delocalized states.

From the density of states we have calculated the coefficient γ corresponding to the T-linear contribution to the specific heat. Due to the fact that the Fermi level enters into the conduction band in the Kondo resonance region, the γ-coefficient increases very rapidly with the impurity concentration. We have plotted in figure 3 the coefficient γ as a function of impurity concentration and compared it with experimental measurements.

Two series of experimental results [10, 11] show that the value of γ is very sample dependent. The positions of the theoretical points are very sensitive to the values of the parameters V_{c-f} and t_f. Small changes of these parameters permit the results to be near one of the series or the other. We have chosen a set of parameters which give a γ-dependence on the La concentration x which is very close to that for one of the two series of data. The very

rapid increase of the linear coefficient of the specific heat with x is a common characteristic of all of the experimental and theoretical results. As is shown in the figure, the curve is asymmetric, reflecting the fact that while the Ce compound is a Kondo insulator, the La one is not a heavy-fermion material.

5. Metal–non-metal transitions driven by temperature, pressure, and magnetic field

We have already seen that a low concentration of La impurities take the $Ce_3Bi_4Pt_3$ to a disordered, although metallic, heavy-fermion phase. The heavy-fermion nature of this metal is reflected in the large value of the linear specific coefficient γ. Besides doping, which introduces disorder, external perturbations like pressure, external magnetic field, or temperature could promote a metal–non-metal transition in these very small-gap materials. For a system described by the periodic Anderson Hamiltonian, the value of the gap is of the order of the Kondo temperature, which turns out to be the energy spacing between the singlet and the triplet state, describing a local spin coupled antiferromagnetically or ferromagnetically with the spin of the nearby conduction electrons, respectively. The gap stems from the hybridization of the Abrikosov–Suhl resonance, at the Fermi level, and the conduction band of the material [7]. It is clear that on increasing the temperature above T_K, the Kondo peak responsible for the gap, and the gap itself, disappear [1]. From this viewpoint, the metal–non-metal transition driven by temperature is governed by the way in which the Abrikosov–Suhl resonance reduces its weight and increases its width as temperature rises. In this case the metallic phase is not a heavy-fermion phase because it only exists at $T > T_K$. The application of a magnetic field creates a similar scenario. The $S_z = 1$ state belonging to the triplet $S = 1$ is pushed down in energy by the field, and for large enough fields it becomes the ground state of the system. The Kondo correlation among the spins is destroyed and a metal–non-metal transition produced by the external applied magnetic field takes place.

As in the case of the temperature-driven transition, the system is a metallic but not a heavy-fermion one.

It is the non-heavy-fermion nature of the metallic phase implied in this standard description that emphasizes the importance of the non-diagonal matrix element connecting adjacent f orbitals, t_f. An f–f hybridization of the order of T_K is sufficient to close the gap of the system, although it does not change the Kondo temperature in any significant way. This is the mechanism which probably plays an important role in the constitution of the metallic heavy-fermion ground state of some compounds that become insulators under the effect of an external or chemical pressure. As in this case V_{c-f} increases due to a reduction of the unit cell, it can overcome the f–f hybridization that was big enough to eliminate the gap of this system without pressure, opening the insulating gap. This behaviour is shown in figure 4 where the densities of states are represented for four different values of the relation t_f/t_c in the vicinity of the Fermi level.

For the Kondo insulator, the f–f hybridization could also be very important as it reduces the gap to a value that is always less than the Kondo temperature. This creates the possibility of having a metal–non-metal transition driven by temperature and magnetic field, within the Kondo regime.

In figure 5 we show the behaviour of a typical Kondo insulator under the influence of a magnetic field. The densities of states for up and down spins are displaced in opposite directions when the field is increased. For applied magnetic fields less than the semiconductor gap, the numbers of up- and down-spin electrons do not change and the system remains an insulator. However, as shown in the figure, as $t_f \neq 0$, for a large enough magnetic field the gap disappears; the system becomes metallic although without destroying the Kondo ground

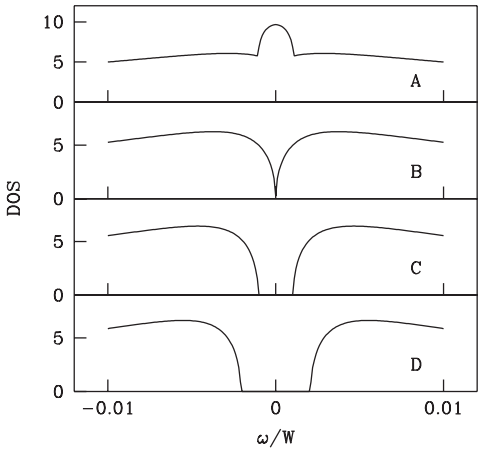

Figure 4. The DOS for Ce compounds for several values of the hybridization parameter t_f: (A) $t_f = 0.0425t_c$; (B) $t_f = 0.040t_c$; (C) $t_f = 0.0375t_c$; (D) $t_f = 0.0350t_c$.

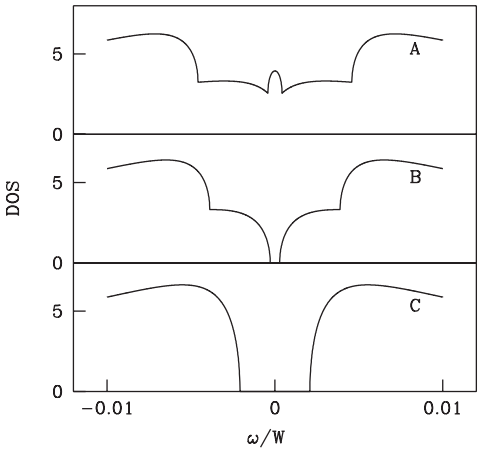

Figure 5. The DOS for several magnetic fields: (A) $B = 0.15$ kiloteslas; (B) $B = 0.108$ kiloteslas; (C) $B = 0$.

state of the system. This is reflected in the clear Kondo peak appearing in the total density of states at the Fermi level in the metallic phase. In figure 5(B) we can see a double band gap, which results from the superposition of the magnetic displaced spin-up and spin-down bands. A similar result based on a mean-field approach is found in reference [28]. This double band gap is consistent with the double activation energy found by Sugiyama *et al* [27] for YbB_{12}.

In order to encourage an experimental investigation of this process, we calculate the specific heat parameter γ as a function of the magnetic field for a set of parameters corresponding to $Ce_3Bi_4Pt_3$. It is clear from figure 6 that for small magnetic field the system behaves as a heavy-fermion material while for values of the magnetic field greater than the Kondo temperature the specific heat turns out to be almost independent of the applied field, as expected. A similar transition can be obtained just by increasing the temperature of the system. In figure 7 we show the behaviour of the gap as a function of temperature. There is a critical temperature T_c above which the insulator becomes a metal. The Kondo peak at the Fermi level reflects the heavy-fermion nature of the phase. In all cases where the metal–non-metal transition is due to pressure, magnetic field, or temperature, as shown in the figures 4, 5, and 7, the gap of the insulating phase in the vicinity of the transition has a linear dependence on the driving variable. This behaviour corresponds to the universality class of the so-called density-driven metal–insulator transitions [5], a situation that was already indicated by a completely different approach to the problem where the Kondo effect plays no role in the process.

6. Summary

We have discussed the metal–non-metal transition in Kondo insulators using a periodic Anderson Hamiltonian where a correlated f level is hybridized with a conduction band. The density of states is obtained from the Green function of the system. The dressed propagators were obtained from an exact atom diagonalization followed by the insertion of the atom into the lattice using the chain approximation. We have studied in particular the alloy compound $((Ce_{1-x}La_x)_3Bi_4Pt_3$ for which disorder was treated using a real-space renormalization technique. We found that the introduction of the La Kondo holes into the

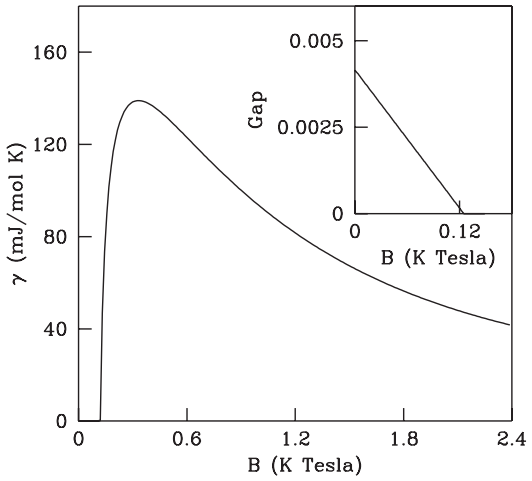

Figure 6. The T-linear contribution to the specific heat (γ) as a function of the magnetic field. The critical field ($B_c \sim 0.121$ kiloteslas) is close the hybridization gap (inset), giving a metal–insulator transition. For $B \geqslant B_c$ the Kondo peak lies at the Fermi level, giving a strong contribution to γ.

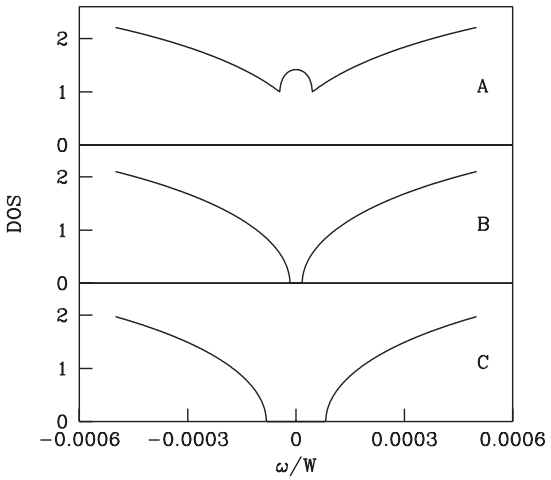

Figure 7. The DOS for Ce compound parameters for $B = 0.12$ kiloteslas and several temperatures: (A) $kT = 200\times10^{-4}W$; (B) $kT = 180\times10^{-4}W$; (C) $kT = 10^{-4}W$.

system shifts the Fermi level to the upper edge of the conduction band producing a metal–non-metal transition of the Anderson type inside the band. This precludes the formation of an impurity band at the gap, which is compatible with the fact that the metal–non-metal transition occurs at very low concentrations. At moderate concentrations of La, the Fermi level lies in the Kondo peak region, giving a strong contribution to the electronic specific heat. This fact is in agreement with the experimental results [10, 11]. For large concentrations of La the system is not a heavy-fermion one.

When a magnetic field is applied, the insulating gap decreases linearly with the field, driving the system into a metal–insulator transition. A similar gap dependence is present as a function temperature and pressure. Due to the f–f hybridization this transition could occur without destroying the Kondo state, giving rise to the heavy-fermion behaviour in the metallic phase.

References

[1] Hewson A C 1993 *The Kondo Problem to Heavy Fermions* (Cambridge: Cambridge University Press)
[2] Miranda E, Dobrosavljevic V and Kotliar G 1997 *J. Phys.: Condens. Matter* **9** 9871
Miranda E, Dobrosavljevic V and Kotliar G 1993 *Phys. Rev. Lett.* **70** 290
Bernal O, MacLaughlin D E, Lukefahr H G and Andraka B 1995 *Phys. Rev. Lett.* **75** 2023
[3] von Löhneysen H *et al* 1994 *Phys. Rev. Lett.* **72** 3262
Continentino M A 1993 *Phys. Rev.* B **47** 1158
Millis A J 1993 *Phys. Rev.* B **48** 7183
Grosche F M *et al* 1996 *Physica* B **223+224** 50
[4] Aeppli G 1992 *Comment. Condens. Matter Phys.* **16** 155
[5] Tovar M V Costa, Toper A, de Oliveira N A, Japiassú G M and Continentino M A 1998 *Phys. Rev.* B **57** 6943
[6] Continentino M A, Japiassú G M and Troper A 1994 *Phys. Rev.* B **49** 4432
Continentino M A, Japiassú G M and Troper A 1995 *J. Phys.: Condens. Matter* **7** L701
[7] Newns D M and Read N 1987 *Adv. Phys.* **36** 799
[8] Chen C, Li Z Z and Xu W 1993 *J. Phys. C: Solid State Phys.* **5** 95
Li Z Z, Xu W, Chen C and Xiao M W 1994 *Phys. Rev.* B **50** 11 332
Xu X H, Li Z Z and Xiao M W 1996 *Phys. Rev.* B **45** 12 993
[9] Schlottmann P 1992 *Phys. Rev.* B **46** 998
[10] Hundley M F, Canfield P C, Thompson J D, Fisk Z and Lawrence J M 1990 *Phys. Rev.* B **42** 6842
[11] Hundley M F, Canfield P C, Thompson J D and Fisk Z 1994 *Phys. Rev.* B **50** 18 142
[12] Latge A and Anda E V 1990 *Solid State Commun.* **76** 1387
[13] Louis E, Verges J A, Flores F and Anda E V 1985 *Solid State Commun.* **54** 961
Verges J A, Louis E, Flores F and Anda E V 1987 *Phys. Rev.* B **35** 7146
[14] Fulde P 1991 *Electronic Correlations in Molecules and Solids* (Berlin: Springer)
[15] Nozières P 1974 *J. Low Temp. Phys.* **17** 31
[16] da Rosa Simoes A S, Iglesias J R, Rojo A and Alascio B R 1941 *J. Phys. C: Solid State Phys.* **21** 1987
[17] Anda E V 1981 *J. Phys. C: Solid State Phys.* **14** L1037
[18] Metzner W 1991 *Phys. Rev.* B **43** 8549
[19] Anda E V and Latge A 1988 *J. Phys. C: Solid State Phys.* **21** 4251
[20] Elliott R J, Krumhansl J A and Leath P L 1974 *Rev. Mod. Phys.* **46** 465
[21] Aoki H and Kamimura H 1976 *J. Phys. Soc. Japan* **40** 6
[22] Makler S and Anda E V 1983 *J. Phys. C: Solid State Phys.* **16** 45
[23] Schlottmann P 1989 *Phys. Rep.* **181** 1
[24] Llois A M and Weissman M 1999 Private communication
[25] Sanchez-Castro C S, Bedell K S and Copper B R 1993 *Phys. Rev.* B **47** 6879
[26] Foglio M and Figueira da Silva M S 1998 *Int. J. Mod. Phys.* B **12** 837
[27] Sugiyama K, Iga F, Kasaya M, Kasuya T and Date M 1988 *J. Phys. Soc. Japan* **57** 3946
[28] Rappoport T G, Figueira M S and Continentino M A 2000 *Phys. Lett.* A **264** 497
(Rappoport T G, Figueira M S and Continentino M A 1999 *Preprint* cond-mat/9904221)