A simple model for the two-site Anderson Hamiltonian

A simple model for the two-site Anderson Hamiltonian

J Arispe†§, B Coqblin†, Acirete S da Rosa Simões‡ and J R Iglesias‡

† Laboratoire de Physique des Solides associé au CNRS, Bâtiment 510, Université Paris-Sud, 91405 Orsay, France
‡ Instituto de Física, Universidade Federal do Rio Grande do Sul, CP 15051, 91501 Porto Alegre, Brazil

Abstract. We consider a two-site Anderson Hamiltonian which includes hybridization both inside the same and between different sites, as well as Coulomb and exchange interactions between them. An exact diagonalization of this Hamiltonian is performed and the competition between the Kondo and RKKY interactions is studied as a function of the exchange, J, and the hybridization parameters. The local, uniform and staggered magnetic susceptibilities are calculated. From the correlation functions it is possible to see that the existence of the Kondo effect depends strongly on the ratio between the on-site and inter-site hybridizations. No divergence of the susceptibility was found at the critical J value for finite temperatures.

1. Introduction

The properties of Kondo alloys and compounds containing cerium or other anomalous rare earths have been studied extensively over the last few years [1]. It is well known that the susceptibility of a single Kondo impurity has a Curie–Weiss behaviour at high temperatures, i.e. above the characteristic temperature T_K (the Kondo temperature), and becomes non-magnetic below T_K. In Ce compounds or concentrated alloys, there is substantial competition between the Ruderman–Kittel–Kasuya–Yosida (RKKY) interaction and the Kondo effect itself, which yields either a non-magnetic ground state, as in the single-Kondo-impurity problem, or a magnetically ordered state at low temperatures. Many cerium compounds have been found experimentally to order magnetically at low temperatures (for example $CeAl_2$, CeB_6) or to have a non-magnetic behaviour (as in $CeAl_3$, $CeCu_2Si_2$, $CePd_3B$, etc) or even to present superconductivity as in $CeCu_2Si_2$ and some uranium systems. However, neutron diffraction experiments have recently shown evidence of the existence of short-range magnetic correlations in non-magnetic cerium compounds which do not present any long-range order [2, 3]. Non-magnetic cerium compounds are characterized at low temperatures by a Fermi liquid (so called 'heavy fermion') behaviour with very large values of the linear coefficient of the electronic specific heat, γ, magnetic susceptibility and, in some cases, the coefficient of the T^2 term of the resistivity [4].

Thus, the competition between the RKKY interaction and the Kondo effect has been extensively studied for a lattice, called the 'Kondo lattice' or the 'Anderson lattice' according to the different models studied. However, the problem of the lattice is not really solved. The two-impurity Kondo or Anderson model has recently been studied again in detail, as

---

§ Permanent address: Universidad Central de Venezuela, Departamento de Física, Apartado 47586, Caracas, Venezuela.

it is a step towards solving the lattice problem and also allows the study of short-range magnetic correlations.

The two-impurity Kondo problem has firstly been studied by the numerical renormalization group method in order to investigate the ground state and the properties at $T = 0$ [5, 6]. In addition to the two s–f exchange interaction Hamiltonians (on two sites) that define the Kondo temperature, T_K, for the isolated impurity, a direct interaction $-J S_1^f \cdot S_2^f$ is introduced between the spins of the localized f electrons with the resulting behaviour depending on the ratio J/T_K, with a critical value $J_c/T_K = -2.2$. For $J > J_c$ the ground state, which corresponds to a triplet wave function for the localized electrons, is that of a correlated Kondo effect, while for $J < J_c$, the ground state is an uncompensated singlet with strong spin interactions and no Kondo effect occurs. Both regimes represent a Fermi liquid ground state. The $J = J_c$ value corresponds to an unstable fixed point and renormalization group calculations predict a divergence of γ and of the staggered susceptibility $\chi^{(s)}$ at J_c. The two-impurity Kondo model has also been extensively studied by several theoretical methods; numerical Monte Carlo simulations for both the Kondo [7] and the Anderson [8] Hamiltonians, a critical theory using conformal field-theory methods [9], renormalization group [10] and variational methods for the Anderson Hamiltonian [11, 12]. It is also found that the Kondo effect occurs for large J values and disappears for small J values and that these two regimes are separated by a multicritical point. The behaviour of the staggered susceptibility $\chi^{(s)}$ around the critical point generates some controversy, since it is either weakly divergent or not diverging according to simulation calculations [7] or variational method calculations for the classical s–f exchange Hamiltonian [12], while some variational theory calculations predict a divergence of $\chi^{(s)}$ at the critical value of J in the Coqblin–Schrieffer limit [12].

The competition between the Kondo effect and the RKKY interaction has also been studied within the so called 'molecular model' which starts from the Anderson Hamiltonian in two atoms, with only one level at each atom for the conduction electron, and only a simple hopping term for the interaction between the two impurities [13]. Results depend on the ratio between the hopping temperature t and Kondo temperature, T_K; for $t \ll T_K$ two independent Kondo singlets are formed, while for $t \gg T_K$ the impurity spins have strong antiferromagnetic correlations. The periodic Anderson Hamiltonian in one-dimensional chains of from three to six sites has also been studied by exact diagonalization [13]. In the weak coupling limit, the results for the short-range magnetic correlations suggest a smooth transition from a ferromagnetic state at low electron concentration to an antiferromagnetic state at half-filling [13].

The purpose of the present paper is to study the two-site problem within the 'molecular' model of two atoms with two localized (f like) and conduction (d or s like) electron states, described by the Anderson Hamiltonian but including hopping, exchange and inter-site hybridization interactions between the two sites. The direct f–f hopping term is neglected as usual [5, 7, 11], because the 4f electrons are strongly localized and the 4f bandwidth is zero or negligible, so that the exchange interaction between f electrons in rare-earth materials arises from the indirect RKKY-type mechanism via the conduction electrons. In this paper, we have introduced both the on-site (V_1) and inter-site (V_2) hybridization terms and we give an exact analytical solution for the case $V_1 = V_2$. We will study the influence of the new term V_2 on the Kondo effect and then we present the results for the magnetic susceptibility and correlation function as a function of the different parameters.

2. The two-site problem

The Hamiltonian of the two-site problem is the sum of two on-site terms and an inter-site term

$$H = H_0 + H_{12} \tag{1}$$

with the on-site Hamiltonian defined by the Anderson Hamiltonian

$$H_0 = \sum_{i=1}^{2} \sum_{\sigma} \left[E_0 n_{i\sigma}^f + E_B n_{i\sigma}^d + \frac{U_{ff}}{2} n_{i\sigma}^f n_{i\bar{\sigma}}^f + V_1 (d_{i\sigma}^\dagger f_{i\sigma} + f_{i\sigma}^\dagger d_{i\sigma}) \right] \tag{2}$$

and the inter-site Hamiltonian written as

$$H_{12} = t \sum_{\sigma} (d_{1\sigma}^\dagger d_{2\sigma} + d_{2\sigma}^\dagger d_{1\sigma}) + V_2 \sum_{\sigma} (d_{1\sigma}^\dagger f_{2\sigma} + d_{2\sigma}^\dagger f_{1\sigma} + \text{HC})$$
$$+ (U - \tfrac{1}{2}J) n_1^f n_2^f - 2J S_1^f \cdot S_2^f \tag{3}$$

where E_0 is the energy of the f electrons, E_B that of the d electrons, U_{ff} is the Coulomb repulsion between f electrons at the same site, V_1 is the on-site hybridization, V_2 is the inter-site hybridization, t is the d–d hopping, U and J are the Coulomb and exchange integrals, respectively, between the f electrons at different sites and

$$n_i = n_{i\uparrow} + n_{i\downarrow}$$
$$S^{f+} = f_{i\uparrow}^\dagger f_{i\downarrow}$$
$$S^{f-} = f_{i\downarrow}^\dagger f_{i\uparrow} \tag{4}$$
$$S_{iz}^f = \tfrac{1}{2}(n_{i\uparrow} - n_{i\downarrow})$$
$$S_1^f \cdot S_2^f = \tfrac{1}{2}(S_1^{f+} S_2^{f-} + S_1^{f-} S_2^{f+}) + S_{1z}^f S_{2z}^f.$$

In the inter-site Hamiltonian given by equation (3), we have considered the d–d hopping, corresponding to the d band in the case of a real compound and the inter-site hybridization between the localized 4f and the band-like d electrons. However, we have completely neglected the f–f hopping term, because the 4f electrons are well localized. The Hamiltonian (1) can be exactly solved analytically in the case $V_1 = V_2 = V$ and $U_{ff} \to \infty$, while it is exactly solvable numerically in the general case with different V_1 and V_2 values. In the particular case $V_1 = V_2$, we have derived an analytical solution of both the eigenvalues and eigenfunctions of H for an infinite value of the f–f Coulomb repulsion ($U_{ff} \to \infty$). If one writes

$$S_i = S_i^f + S_i^d \tag{5}$$

and

$$S = S_1 + S_2 \tag{6}$$

the Hamiltonian (1) commutes with S_z and S^2

$$[H, S^2] = [H, S_z] = [S^2, S_z] = 0 \tag{7}$$

so the eigenstates of H are also eigenstates of S^2 and S_z.

We have studied the problem with two electrons per atom, i.e. $N = 4$ electrons, and we have built up the different eigenstates, starting from the eight states $f_{i\sigma}^\dagger |0\rangle$ and $d_{i\sigma}^\dagger |0\rangle$ (with $i = 1, 2$ and $\sigma = \uparrow, \downarrow$). For $V_1 = V_2$ there are 70 different eigenstates in the case of a finite

U_{ff} value and 41 in the limit $U_{ff} \to \infty$. In this case we can derive an analytical solution for the eigenstates; there are 13 different eigenvalues given in table 1. The energies are measured with respect to the energy of the d electrons; $E_B = 0$. In table 1, we give also the degeneracy of each eigenenergy and the values of S and S_z for the different eigenfunctions.

The eigenstates are found here by an analytical diagonalization and we will see in the next section that the ground state depends on the different parameters and in particular on J. Then we calculate the three on-site χ, uniform $\chi^{(u)}$ and staggered $\chi^{(s)}$ susceptibilities, that we define respectively by

$$\chi = \int_0^\beta d\tau \langle S_{1z}^f(\tau) S_{1z}^f \rangle \tag{8}$$

$$\chi^{(u)} = \frac{1}{2} \int_0^\beta d\tau \langle [S_{1z}^f(\tau) + S_{2z}^f(\tau)][S_{1z}^f + S_{2z}^f] \rangle \tag{9}$$

$$\chi^{(s)} = \frac{1}{2} \int_0^\beta d\tau \langle [S_{1z}^f(\tau) - S_{2z}^f(\tau)][S_{1z}^f - S_{2z}^f] \rangle \tag{10}$$

with $\beta = (k_B T)^{-1}$ and $S^f(\tau) = e^{\tau H} S^f e^{-\tau H}$. Here, we take $k_B = \hbar = 1$. A straightforward calculation yields the values of the susceptibilities as a function of the 13 eigenenergies E_m

$$\chi = \sum_{m,m'} F(E_m, E_{m'}) |\langle m|S_{1z}^f|m' \rangle|^2 \tag{11}$$

$$\chi^{(u)} = \frac{1}{2} \sum_{m,m'} F(E_m, E_{m'}) |\langle m|(S_{1z}^f + S_{2z}^f)|m' \rangle|^2 \tag{12}$$

$$\chi^{(s)} = \frac{1}{2} \sum_{m,m'} F(E_m, E_{m'}) |\langle m|(S_{1z}^f - S_{2z}^f)|m' \rangle|^2 \tag{13}$$

with

$$F(E_m, E_{m'}) = \frac{1}{\mathrm{Tr}(e^{-\beta H})} \frac{e^{-\beta E_{m'}} - e^{-\beta E_m}}{E_m - E_{m'}}. \tag{14}$$

Thus, the three susceptibilities as well as the correlation functions $\langle S_1^f \cdot S_2^f \rangle$ between the two impurity spins and $\langle S_i^f \cdot S_i^d \rangle$, between f and d electrons at the same site, are computed analytically for $V_1 = V_2$. The results are presented in the next section.

3. Discussion of the theoretical results for $V_1 = V_2 = V$

First of all, we compute the eigenvalues and we see that the ground state is the energy E_{12}, corresponding to $S = 0$ for J values smaller than the critical value J_c and then the energy E_8 corresponding to $S = 1$ for J values larger than J_c. The critical value J_c, which is very close to zero, does not vary very much with U and negative E_0 values and increases with increasing V.

The 41 eigenfunctions corresponding to the 13 eigenenergies have been computed analytically for $V_1 = V_2 = V$, but we do not present them here; however, see appendix A for the eigenfunctions corresponding to the energy E_{12} with total spin $S = 0$ and the three eigenfunctions corresponding to the energy E_8 with a total spin $S = 1$. Thus, one goes from a state, for J smaller than J_c, with an antiferromagnetic coupling between the f electrons on the two sites, to a state, for J larger than J_c, with a ferromagnetic coupling between the f electrons on the two sites.

Table 1.

Energy	Degeneracy	Values of S and S_z
$E_1 = 2E_0 + U - J$	8	$S = 2, S_z = \pm 2, \pm 1, 0$ $S = 1, S_z = \pm 1, 0$
$E_2 = 2(E_0 + t) + U - J$	3	$S = 1, S_z = \pm 1, 0$
$E_3 = \dfrac{3E_0 + t + U + J}{2} + \sqrt{\left(\dfrac{E_0 - t + U + J}{2}\right)^2 + 2V^2}$	4	$S = 1, S_z = \pm 1, 0$ $S = 0, S_z = 0$
$E_4 = \dfrac{3E_0 + t + U + J}{2} - \sqrt{\left(\dfrac{E_0 - t + U + J}{2}\right)^2 + 2V^2}$	4	$S = 1, S_z = \pm 1, 0$ $S = 0, S_z = 0$
$E_5 = \dfrac{3E_0 + t + U - J}{2} + \sqrt{\left(\dfrac{E_0 - t + U - J}{2}\right)^2 + 6V^2}$	4	$S = 1, S_z = \pm 1, 0$ $S = 0, S_z = 0$
$E_6 = \dfrac{3E_0 + t + U - J}{2} - \sqrt{\left(\dfrac{E_0 - t + U - J}{2}\right)^2 + 6V^2}$	4	$S = 1, S_z = \pm 1, 0$ $S = 0, S_z = 0$
$E_7 = \dfrac{3(E_0 - t) + U - J}{2} + \sqrt{\left(\dfrac{E_0 - t + U - J}{2}\right)^2 + 4V^2}$	3	$S = 1, S_z = \pm 1, 0$
$E_8 = \dfrac{3(E_0 - t) + U - J}{2} - \sqrt{\left(\dfrac{E_0 - t + U - J}{2}\right)^2 + 4V^2}$	3	$S = 1, S_z = \pm 1, 0$
$E_9 = E_0 - t$	4	$S = 1, S_z = \pm 1, 0$ $S = 0, S_z = 0$
$E_{10} = 2(E_0 + t) + U + J$	1	$S = 0, S_z = 0$
$E_{11} = 2\sqrt{q} \cos \dfrac{\alpha}{3} - \dfrac{c_2}{3}$	1	$S = 0, S_z = 0$
$E_{12} = -\sqrt{q} \cos \dfrac{\alpha}{3} - \dfrac{c_2}{3} - \sqrt{3q} \sin\left(\dfrac{\alpha}{3}\right)$	1	$S = 0, S_z = 0$
$E_{13} = -\sqrt{q} \cos \dfrac{\alpha}{3} - \dfrac{c_2}{3} + \sqrt{3q} \sin\left(\dfrac{\alpha}{3}\right)$	1	$S = 0, S_z = 0$

Where

$$q = \frac{1}{9}c_2^2 - \frac{1}{3}c_1 \tag{15}$$

$$\alpha = \arctan\left(\frac{\sqrt{q^3 - r^2}}{r}\right) \tag{16}$$

$$r = \frac{1}{6}(c_1 c_2 - 3c_0) - \frac{1}{27}c_2^3 \tag{17}$$

$$c_0 = 8V^2 (2E_0 + U + J - 2t) \tag{18}$$

$$c_1 = (E_0 - t)(2E_0 + U + J - 2t) - 12V^2 \tag{19}$$

$$c_2 = 3(t - E_0) - U - J \tag{20}$$

We present now the calculations performed for the susceptibilities and the correlation functions as a function of temperature, for a reasonable set of parameters: $E_B = 0$, $E_0 = -1$, $t = 3$, $U = 1$ and $V = 0.3$, in units of $\Delta = E_B - E_0$, equal to 1. In the experimental case of cerium compounds, we can take this arbitrary unit approximately equal to 1 eV. Thus, all the quantities, which are listed in the following, have to be multiplied by Δ, if one would like to have the parameters expressed in real energy units.
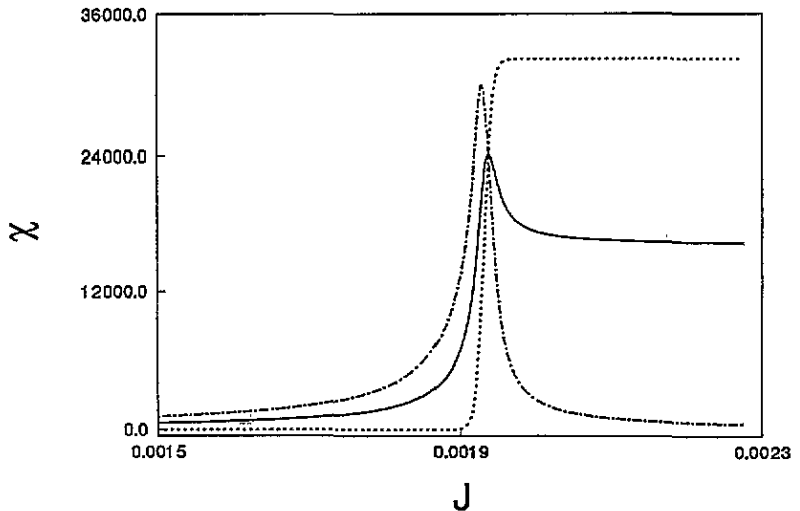

Figure 1. Plot of the local (full line), uniform (dashed) and staggered (dot-dashed) susceptibilities as a function of J for $t = 3$, $U = 1$, $V = 0.3$ and $T = 10^{-5}$. The critical value of J is near 0.0019

Figure 1 exhibits the three uniform, local and staggered susceptibilities as a function of J for a very low temperature, $T = 10^{-5}$; as an example, if we take $\Delta = 1$ eV, T is almost equal to 1 K. We see that the staggered susceptibility is passing through a maximum at a J value approximately equal to the critical value J_c separating the two domains $S = 0$ and $S = 1$. This maximum happens for all finite temperatures, the staggered susceptibility diverging only at strictly zero temperature and $J = J_c$. In the present case, one obtains $J_c = 0.00194$ or $J_c = 225$ K for $\Delta = 1$ eV.

Let us examine the behaviour of the three susceptibilities in the zero-temperature limit. First, the expression $F(E_m - E_{m'})$ diverges when the energies E_m and $E_{m'}$ are equal to each other and equal to the ground state energy. Then in addition, the susceptibilities diverge only if the matrix elements in front of $F(E_m, E_{m'})$ are non-zero when the temperature tends to zero. For $J < J_c$, the ground state is E_{12} and $S = 0$; according to the formula (25) of appendix A, all the matrix elements are equal to zero and the three susceptibilities remain finite for $T \rightarrow 0$ and $J < J_c$. In contrast, for $J > J_c$, the ground state is E_8 and $S = 1$; the matrix elements in equations (11) and (12) are non-zero and χ and $\chi^{(u)}$ diverges, while $\chi^{(s)}$ remains finite for $T \rightarrow 0$. Finally, at $J = J_c$, $E_{12} = E_8$ and the three susceptibilities are diverging. Thus, the staggered susceptibility diverges at $J = J_c$ for $T \rightarrow 0$, while the two other susceptibilities χ and $\chi^{(u)}$ diverge for $J \geqslant J_c$.

The next question to answer is that of the occurrence of the Kondo effect in the two domains with $S = 0$ and $S = 1$. In this oversimplified model with a zero-width conduction band, the relevant quantity for studying the 'Kondo effect' on each site, i.e. the compensation of the f magnetic moment by the d magnetic moment, is the d–f correlation
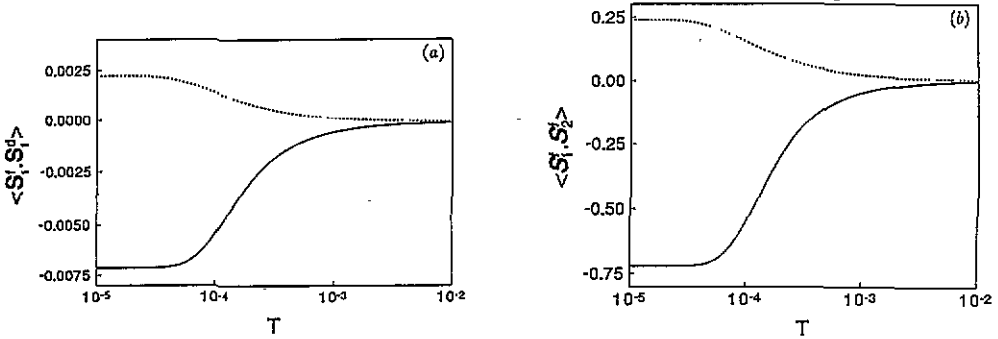
Figure 2. Plot of the local d–f correlation function $\langle S_1^f \cdot S_1^d \rangle$ (a) and of the two-site f correlation function $\langle S_1^f \cdot S_2^f \rangle$ (b) for $J < J_c$ (dashed lines) and $J > J_c$ (full) as a function of temperature, for $V = 0.3$, $t = 3$, and $U = 1$.

function on the same site, $\langle S_i^d \cdot S_i^f \rangle$. Figure 2(a) gives the temperature dependence of the d–f correlation function on the same site $S_i^f \cdot S_i^d \rangle$, for two values of the parameter J below and above J_c. We can see that the on-site correlation function remains very small and that there is almost no spin compensation due to the Kondo effect: at very low temperatures the correlation function corresponds to roughly $1/100$ of the $S = 1$ value for $J > J_c$ and of the $S = 0$ value for $J < J_c$. Thus, there is a very weak Kondo effect for $J < J_c$. On the other hand, figure 2(b) shows the f–f correlation function $\langle S_1^f \cdot S_2^f \rangle$. At low temperatures the correlation function is characteristic of an antiferromagnetic coupling ($S = 0$) for $J < J_c$ and a ferromagnetic one ($S = 1$) for $J > J_c$.

Figure 3 gives the temperature dependence of the three susceptibilities in the same system with $\Delta = 1$ for a value of J smaller than J_c and the curves are similar to the ones previously derived for the case $J = 0$ and with only an on-site hybridization term [11]. The local and staggered susceptibilities show a plateau below a temperature T_K of order 10^{-4} (or 10 K for $\Delta = 1$ eV), indicating a weak Kondo effect with a Kondo temperature T_K. The uniform susceptibility goes through a maximum with decreasing temperature tending to zero.
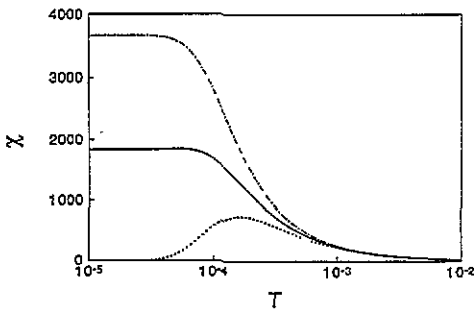

Figure 3. Plot of the local (full line), uniform (dashed) and staggered (dot-dashed) susceptibilities as a function of temperature for the same parameters as in figure 1 and $J = 0$.
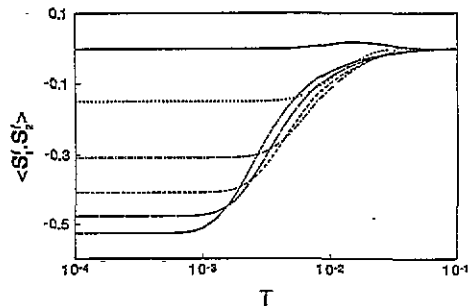
Figure 4. Plot of the two-site f correlation function $\langle S_1^f \cdot S_2^f \rangle$ as a function of temperature for six different values of t: $t = 0$ (upper curve), 0.02, 0.04, 0.06, 0.08 and 0.1 (lower curve) and $U = 1$, $V_1 = 0.06$, $V_2 = 0.02$ and $J = -10^{-4}$.

Thus the transition occurring at J_c corresponds to an antiferromagnetic–ferromagnetic transition for the f electrons, without appreciable Kondo effect on the two sides. So, the case $V_1 = V_2$ gives a very weak Kondo effect, in contrast to the classical Anderson Hamiltonian with only an hybridization term between d and f electrons on the same site.

4. Discussion of the theoretical results with different values of V_1 and V_2

In this section, we study the general case with different values of V_1 and V_2 and $U_{ff} \to \infty$. The Hamiltonian (1) with $V_1 \neq V_2$ cannot be solved analytically and the determination of both the eigenvalues and eigenfunctions needs numerical calculations. Thus, we will present here the main results obtained for V_2 different from V_1. The general behaviour of the susceptibilities versus increasing J values is similar here to that shown on figure 1 for $V_1 = V_2$; in particular, the staggered susceptibility exhibits a maximum at a critical J value for finite very low temperatures. In the zero-temperature limit, the staggered susceptibility diverges only at $J = J_c$, while χ and $\chi^{(u)}$ diverge for $J \geqslant J_c$ and remain finite for $J < J_c$.

In order to study the occurrence of the Kondo effect as a function of V_2 and V_1 we have plotted in figures 4 and 5 the two correlation functions $\langle S_1^f \cdot S_2^f \rangle$ and $\langle S_1^f \cdot S_1^d \rangle$ as a function of temperature for different values of V_1 and V_2 ($V_1 = 0.06$ and a much smaller V_2 value, $V_2 = 0.02$). The different curves are plotted as a function of t, from $t = 0$ to $t = 0.1$ (in the usual unit system with $\Delta = 1$). It is interesting to discuss here this choice of parameters; in fact, if one takes the previously chosen value $t/\Delta = 3$ of section 3, one obtains no Kondo effect, exactly as is shown in figure 2(b). The Kondo effect exists only for very small values of t and consequently we have chosen small t values in order to study clearly the influence of V_2 on the Kondo effect.
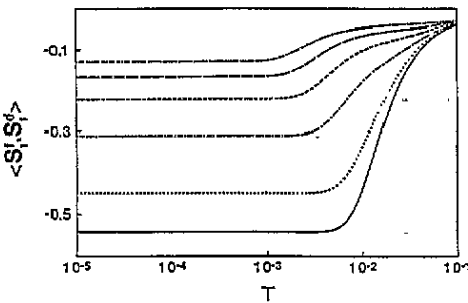

Figure 5. Plot of the local d–f correlation function $\langle S_1^f \cdot S_1^d \rangle$ as a function of temperature for six different values of t: $t = 0$ (lower curve), 0.02, 0.04, 0.06, 0.08 and 0.1 (upper curve) and $U = 1$, $V_1 = 0.06$, $V_2 = 0.02$ and $J = -10^{-4}$.
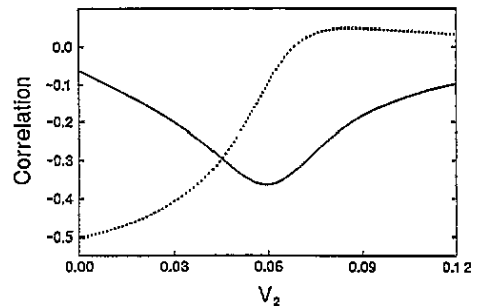
Figure 6. Plot of the local d–f correlation function $\langle S_1^f \cdot S_1^d \rangle$ (dashed) and the two-site f correlation function $\langle S_1^f \cdot S_2^f \rangle$ (full) as a function of V_2 for $t = 0.02$, $V_1 = 0.06$, $U = 1$ and $J = -10^{-4}$.

One can see that the d–f correlation function is of order -0.5 at very low temperatures, for very small values of t, while it increases rapidly with increasing t. Conversely, the two-site f–f correlation function is almost equal to zero for $t = 0$, as expected, and decreases rapidly when increasing t. Thus, at very low temperatures one goes from a Kondo-like behaviour with ferromagnetic-like coupling between the two sites for $t = 0$ to a magnetic behaviour on each site with an antiferromagnetic-like coupling between the two sites for a larger t value, of the order of 0.1.

In fact, in our approach, since there is only one d level and one f level on each site, the Kondo effect is understood as giving a negative value close to $-3/4$ for the d–f on-site correlation function $\langle S_1^f \cdot S_1^d \rangle$ indicating a 'compensation' of the f magnetic moment by the d magnetic moment. In fact, even for a very small t value, as shown on figure 5, the Kondo effect is incomplete since the negative value of the d–f correlation function remains still larger than $-3/4$.

The three susceptibilities χ, $\chi^{(u)}$ and $\chi^{(s)}$ exhibit the same behaviour for the set of parameters used in figure 4 and 5 as that previously shown in figure 3, i.e. a Curie–Weiss behaviour at high temperatures and a plateau at low temperatures below a given temperature T_K. Also, the staggered susceptibility is larger than the uniform one. The differences between the different cases lie in the value of the so-called Kondo temperature T_K and consequently in the very low-temperature values of the local susceptibility. T_K is of order 10^{-5} (in $\Delta = E_B - E_0$ units) in figure 3, with $t = 3$; and of order 10^{-3} for the previous set of parameters with $t = 0.08$ and 10^{-2} with $t = 0.01$. As a consequence, the very low temperature value of χ decreases with increasing T_K (or decreasing t) and varies usually as $1/T_K$, as expected within the Kondo theory. Thus, we see that T_K is obviously larger when the d–f correlation function is more negative at low temperatures.

Finally, figure 6 gives the very low-temperature values of both the d–f correlation function $\langle S_1^f \cdot S_1^d \rangle$ and the two-site f correlation function $\langle S_1^f \cdot S_2^f \rangle$ as a function of the parameter V_2 for a given value of V_1, from $V_2 = 0$ to a large value $V_2 = 2V_1$. The d–f correlation function increases from a value close to $-3/4$ to a value very close to 0 for V_2 equal or larger than V_1. Conversely, the two-site f correlation function decreases with increasing V_2, passes through a minimum for $V_2 = V_1$ and increases again for V_2 larger than V_1. Thus, the inter-site hybridization V_2 tends to suppress the Kondo effect which exists only when both t and V_2 are small compared to the intra-site parameters $E_B - E_0$, U and V_1.

5. Concluding remarks

Thus, our simple 'molecular' model gives a typical Kondo behaviour for the magnetic susceptibility, in agreement with previous results [12]. The staggered susceptibility passes through a maximum for non-zero temperature at the critical J value separating the two magnetic regimes. However, we have shown here that the addition of the inter-site hybridization term V_2 tends to suppress the 'Kondo effect', i.e. the compensation between f and d magnetic moments, and to restore the antiferromagnetic coupling. In particular, we have treated, analytically, the case $V_1 = V_2$ and we have shown that there remains only a very weak Kondo effect on the two atoms when there is an antiferromagnetic-like coupling between the f magnetic moments of the two atoms. Finally, in our study with different V_1 and V_2 values, we have also shown that the Kondo effect exists only for small V_2 and t values. In spite of its crudeness, our model provides interesting information on the role of the two-site hybridization term V_2 and confirms the effect of the intersite exchange coupling J and of the d–d hopping term t on the magnetic properties of the system.

Acknowledgments

Appendix A.

The three eigenfunctions corresponding to the eigenenergy E_8 are given by $|S, S_z, E_8\rangle$

$$|1, 1, E_8\rangle = \left[\frac{\sin \beta}{2} f_{1\uparrow}^\dagger f_{2\uparrow}^\dagger \left(d_{1\uparrow}^\dagger d_{2\downarrow}^\dagger + d_{2\uparrow}^\dagger d_{1\downarrow}^\dagger - d_{1\uparrow}^\dagger d_{1\downarrow}^\dagger - d_{2\uparrow}^\dagger x_{2\downarrow}^\dagger \right) \right.$$
$$\left. - \frac{\cos \beta}{2} d_{1\uparrow}^\dagger d_{2\uparrow}^\dagger \left(f_{1\uparrow}^\dagger d_{1\downarrow}^\dagger - f_{1\uparrow}^\dagger d_{2\downarrow}^\dagger - f_{2\uparrow}^\dagger d_{1\downarrow}^\dagger + f_{2\uparrow}^\dagger d_{2\downarrow}^\dagger \right) \right] |0\rangle \tag{A1}$$

$$|1, 0, E_8\rangle = \frac{1}{2\sqrt{2}} \left\{ \sin \beta \left(f_{1\uparrow}^\dagger f_{2\downarrow}^\dagger - f_{2\uparrow}^\dagger f_{1\downarrow}^\dagger \right) \left(d_{1\uparrow}^\dagger d_{2\downarrow}^\dagger + d_{2\uparrow}^\dagger d_{1\downarrow}^\dagger - d_{1\uparrow}^\dagger d_{1\downarrow}^\dagger - d_{2\uparrow}^\dagger d_{2\downarrow}^\dagger \right) \right.$$
$$+ \cos \beta \left[d_{1\uparrow}^\dagger d_{1\downarrow}^\dagger \left(f_{1\uparrow}^\dagger d_{2\downarrow}^\dagger - d_{2\uparrow}^\dagger f_{1\downarrow}^\dagger - f_{2\uparrow}^\dagger d_{2\downarrow}^\dagger + d_{2\uparrow}^\dagger f_{2\downarrow}^\dagger \right) \right.$$
$$\left. \left. + d_{2\uparrow}^\dagger d_{2\downarrow}^\dagger \left(f_{1\uparrow}^\dagger d_{1\downarrow}^\dagger - d_{1\uparrow}^\dagger f_{1\downarrow}^\dagger - f_{2\uparrow}^\dagger d_{1\downarrow}^\dagger + d_{1\uparrow}^\dagger f_{2\downarrow}^\dagger \right) \right] \right\} |0\rangle \tag{A2}$$

$$|1, -1, E_8\rangle = \left[\frac{-\sin \beta}{2} f_{1\downarrow}^\dagger f_{2\downarrow}^\dagger \left(d_{1\uparrow}^\dagger d_{2\downarrow}^\dagger + d_{2\uparrow}^\dagger d_{1\downarrow}^\dagger - d_{1\uparrow}^\dagger d_{1\downarrow}^\dagger - d_{2\uparrow}^\dagger d_{2\downarrow}^\dagger \right) \right.$$
$$\left. + \frac{\cos \beta}{2} d_{1\downarrow}^\dagger d_{2\downarrow}^\dagger \left(d_{1\uparrow}^\dagger f_{1\downarrow}^\dagger - d_{2\uparrow}^\dagger f_{1\downarrow}^\dagger - d_{1\uparrow}^\dagger f_{2\downarrow}^\dagger + d_{2\uparrow}^\dagger f_{2\downarrow}^\dagger \right) \right] |0\rangle \tag{A3}$$

with

$$\cos \beta = \left[\frac{1}{2} + \frac{E_0 - t + U - J}{4\sqrt{(E_0 - t + U - J/2)^2 + 4V^2}} \right]^{1/2} \tag{A4}$$

and the eigenfunction corresponding to the eigenenergy E_{12} is given by

$$|0, 0, E_{12}\rangle = \left\{ a_1 \left(f_{1\uparrow}^\dagger f_{2\downarrow}^\dagger + f_{2\uparrow}^\dagger f_{1\downarrow}^\dagger \right) \left(d_{1\uparrow}^\dagger d_{2\downarrow}^\dagger + d_{2\uparrow}^\dagger d_{1\downarrow}^\dagger - d_{1\uparrow}^\dagger d_{1\downarrow}^\dagger - d_{2\uparrow}^\dagger d_{2\downarrow}^\dagger \right) \right.$$
$$+ a_2 \left[d_{1\uparrow}^\dagger d_{1\downarrow}^\dagger \left(f_{1\uparrow}^\dagger d_{2\downarrow}^\dagger + d_{2\uparrow}^\dagger f_{1\downarrow}^\dagger + f_{2\uparrow}^\dagger d_{2\downarrow}^\dagger + d_{2\uparrow}^\dagger f_{2\downarrow}^\dagger \right) \right.$$
$$\left. \left. + d_{2\uparrow}^\dagger d_{2\downarrow}^\dagger \left(f_{1\uparrow}^\dagger d_{1\downarrow}^\dagger + d_{1\uparrow}^\dagger f_{1\downarrow}^\dagger + f_{2\uparrow}^\dagger d_{1\downarrow}^\dagger + d_{1\uparrow}^\dagger f_{2\downarrow}^\dagger \right) \right] + a_3 d_{1\uparrow}^\dagger d_{1\downarrow}^\dagger d_{2\uparrow}^\dagger d_{2\downarrow}^\dagger \right\} |0\rangle \tag{A5}$$

where we use both the notation of table 1 and the following

$$a_1 = Qa_2 \tag{A6}$$

$$a_3 = Pa_2 \tag{A7}$$

$$a_2 = \frac{1}{[8(Q^2 + 1) + P^2]^{\frac{1}{2}}} \tag{A8}$$

$$P = \frac{8V}{E_{12}} \tag{A9}$$

$$Q = \frac{2V}{2(E_0 - t) + U + J - E_{12}} \tag{A10}$$

References

[1] Fulde P, Keller J and Zwicknagl G 1988 *Solid State Physics* **41**, ed H Ehrenreich and D Turnbull (London: Academic) 1; Schlottmann P 1989 *Phys. Rep.* **181** 1

[2] Rossat-Mignod J, Regnault L P, Jacard J L, Vettier C, Lejoy P, Flouquet J, Walker E, Jaccard D and Amato A 1988 *J. Magn. Magn. Mater.* **76–77** 376 and references therein

[3] Mignot J M, Jacard J L, Regnault L P, Rossat-Mignod J, Haen P, Lejay P, Boutzouille Ph, Hennion B and Petitgrand D 1990 *Physica* B **163** 611 and references therein

[4] Evans S M M, Bhattacharjee A K and Coqblin B 1991 *Physica* B **171** 293

[5] Jones B A and Varma C M 1987 *Phys. Rev. Lett.* **58** 843; 1989 *Phys. Rev.* B **40** 324

[6] Jones B A 1991 *Physica* B **171** 53

[7] Fye R M and Hirsch J E 1989 *Phys. Rev.* B **40** 4780

[8] Fye R M, Hirsch J E and Scalapino D J 1987 *Phys. Rev.* B **35** 4901

[9] Affleck I and Ludwig A W W 1992 *Phys. Rev. Lett.* **68** 1046

[10] Rasul J W and Schlottmann P 1993 *Physica* B **186–188** 334
Kaneko N, Kato J, Katai O and Shimizu Y 1993 *Physica* B **186–188** 888

[11] Andreani L C, Frazzioli S and Beck H 1991 *Solid State Commun.* **77** 635
Andreani L C and Beck H 1993 *Phys. Rev.* B **48** 7322

[12] Saso T and Kato H 1992 *Prog. Theor. Phys.* **87** 331

[13] Andreani L C and Beck H 1991 *Solid State Commun.* **79** 17
Santini P, Andreani L C and Beck H 1993 *Phys. Rev.* B **47** 1130