Two-impurity Anderson model in an antiferromagnetic metal: zero-bandwidth limit

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Abstract
We study the zero-bandwidth limit of the two-impurity Anderson model in an antiferromagnetic (AF) metal. We calculate, for different values of the model parameters, the lowest excitation energy, the magnetic correlation \( \langle S_1 S_2 \rangle \) between the impurities and the magnetic moment at each impurity site as a function of the distance between the impurities and the temperature. At zero temperature, in the region of parameters corresponding to the Kondo regime of the impurities, we observe an interesting competition between the AF gap and the Kondo physics of the two impurities. When the impurities are close enough, the AF splitting governs the physics of the system and the local moments of the impurities are frozen, in a state with a very strong ferromagnetic correlation between the impurities and roughly independent of the distance. In contrast, when the impurities are sufficiently far apart and the AF gap is not too large, the scenario of the Kondo physics takes place: non-magnetic ground state and the possibility of spin-flip excitation emerges and the ferromagnetic \( \langle S_1 S_2 \rangle \) decreases as the distance increases, but the complete decoupling of the impurities never occurs. In addition, the presence of the AF gap gives a non-zero magnetic moment at each impurity site, showing a non-complete Kondo screening of the impurities in the system. We observe that the residual magnetic moment decreases when the distance between the impurities is increased.

1. Introduction

The behavior of spin correlations in heavy fermion systems is still not completely understood [1]. At high temperatures, heavy fermion materials behave like a collection of individual local moments. When the temperature goes down, correlations take place and the Kondo effect [2] can occur in this system. This screening can quench the magnetic interaction between local moments and the question is: how can spin polarizations propagate to other local moments? A first approach towards an understanding of this very interesting problem, the competition between the Kondo effect and the Ruderman–Kittel–Kasuya–Yosida interaction (RKKY) [3] has been studied in the simplified framework of the two-impurity Anderson [4] or Kondo [5] models. Recently, in the Kondo limit, a systematic study of the ground states of two Anderson impurities has been realized [6]. Both models take into account the conduction electrons in a non-magnetic band. Nevertheless, many experiments in heavy fermion systems show antiferromagnetic correlations or orderings at low temperatures. For example, inelastic neutron scattering from the antiferromagnetic heavy fermion system \( \text{U}_2\text{Zn}_{17} \) [7] shows spin fluctuations in this material. Also, \( \text{UPt}_3 \) [8] and \( \text{URu}_2\text{Si}_2 \) [9] are both heavy fermion compounds where spin fluctuations and antiferromagnetic correlations are present. This suggests that, to understand the anomalous properties of these materials, it is necessary to study also the Kondo effect in the presence of different kinds of magnetic order of itinerant electrons. Zhang and Yu [10] considered a half-filled anisotropic Kondo lattice model within a mean field theory and found a coexistence of antiferromagnetic long-range order and the Kondo singlet state. Similar results are obtained by Capponi and Assaad [11] using a Quantum Monte Carlo algorithm. Recently, the single Kondo effect in an antiferromagnetic metal was studied [12]. This work shows that, for a general location of the impurity, the Kondo singularities still occur, but the ground state has a partially unscreened moment. From the theoretical point of view, a natural extension of this problem is to consider the case of two magnetic impurities in an antiferromagnetic metal. The study of a pair of spin-1/2 impurities is a starting point for our understanding of a lattice behavior in this kind of material.
The aim of this work is to present a very simple approach to study how the competition between partial quenching of the individual moments and their indirect interaction via the antiferromagnetic conduction electrons take place. To this end, as a first approach to the solution of this problem, we extend the zero-bandwidth (ZBW) limit approximation of the two-impurity Anderson model in a paramagnetic metal [13] to include the AF conduction band [12]. Despite our simple approximation, the ZBW limit has been successfully applied to explain quantitatively most of the experimental results in valence fluctuating problems [14]. This limit also gives a good description of the magnetic reentrance phenomena in superconductors with Kondo impurities [15]. Also this method was applied to explain transport experiments on semiconductor quantum dots [16]. An attractive feature of the ZBW limit is, that all calculations can be realized exactly with a minimum of numerical effort and the results are very satisfying, since they reproduce results for properties found much more laboriously by other techniques. For example, the most important results of our previous paper [13] were obtained in [6] by means of variational wavefunctions. Nevertheless, it is important to recognize that the ZBW limit is oversimplified, specifically in not containing any band structures, and consequently we must expect to obtain a cartoon of the real picture. In summary, motivated by the experimental results in the magnetic heavy fermion systems as mentioned above and by the previous successful theoretical work and following this train of thought, we employ the ZBW limit to study this very interesting problem. In the absence of more elaborate theoretical solutions, this approach often gives results in good qualitative agreement with experimental data.

We introduce the two-impurity Anderson Hamiltonian and set up the zero-bandwidth approximation to this problem in section 2. Section 3 is devoted to presenting the numerical results and discussing their physical implications. Section 4 is devoted to conclusions.

2. Model

We start from the two-impurity Anderson Hamiltonian [17] in the absence of direct hopping between impurities extended to include the antiferromagnetism of the itinerant electrons:

\[
H = \sum_{k,\sigma} \epsilon_{k}\text{c}_{k\sigma}^\dagger \text{c}_{k\sigma} + \sum_{k} \left[ \Gamma \left( \text{c}_{k\uparrow}^\dagger \text{c}_{k+\mathbf{Q}\uparrow} + \text{c}_{k\downarrow}^\dagger \text{c}_{k+\mathbf{Q}\downarrow} \right) + \text{H.c.} \right] + \epsilon_{d} \sum_{\sigma,j=1,2} d_{j\sigma}^\dagger d_{j\sigma} + U \sum_{j=1,2} d_{j\uparrow}^\dagger d_{j\uparrow} d_{j\downarrow}^\dagger d_{j\downarrow} + \sum_{k,\sigma,j=1,2} V_{kj} \left( \text{c}_{k\sigma}^\dagger d_{j\sigma} + \text{H.c.} \right),
\]

where \( \text{c}_{k\sigma}^\dagger \) (\( \text{c}_{k\sigma} \)) creates (destroys) an electron with momentum \( \mathbf{k} \) and spin \( \sigma \) in the conduction band with energy \( \epsilon_{k} \), and \( d_{j\sigma}^\dagger \) (\( d_{j\sigma} \)) creates (destroys) a localized electron with spin \( \sigma \) on the site \( \mathbf{R}_{j} \) with energy \( \epsilon_{d,j} \). Besides, \( \Gamma \) is the AF gap, \( \mathbf{Q} \) is the ordering wavevector, \( U \) is the localized-orbital Coulomb interaction and \( V_{kj} = V e^{i \mathbf{k} \cdot \mathbf{R}_{j}} \), where \( V \) is the hybridization strength. For \( \Gamma = 0 \), \( H \) reduces to the well-known two-impurity Anderson model [17]. From the practical point of view, the ZBW approximation replaces the structureless conduction bands by a few states, located just at the Fermi energy (\( \epsilon_{F} \)); conceptually, this recognizes the fact that in most experiments essentially only levels close to the Fermi energy are relevant. As in the previous paper [13], we take here two different vectors \( \mathbf{k} (\mathbf{k}_{1} \text{ and } \mathbf{k}_{2} \text{ with } \mathbf{k}_{1} \neq \mathbf{k}_{2} \text{ and } |\mathbf{k}_{1}| = |\mathbf{k}_{2}| = |\mathbf{k}_{0}| \text{ with } \mathbf{k}_{0} \text{ the Fermi momentum) as a minimal model to compensate for the two localized spins at the impurity sites.}

The model should lead to two independent Anderson problems when the impurities are sufficiently far apart and \( \Gamma = 0 \). Accordingly, the original Hamiltonian of equation (1) reduces to

\[
H_{ZBW} = \epsilon_{F} \sum_{\sigma} \left( c_{1\sigma}^\dagger c_{1\sigma} + c_{2\sigma}^\dagger c_{2\sigma} \right) + \Gamma \left[ c_{1\uparrow}^\dagger c_{1\uparrow} - c_{1\downarrow}^\dagger c_{1\downarrow} \right] + \text{H.c.} + \epsilon_{d} \sum_{\sigma,j=1,2} d_{j\sigma}^\dagger d_{j\sigma} + U \sum_{j=1,2} d_{j\uparrow}^\dagger d_{j\uparrow} d_{j\downarrow}^\dagger d_{j\downarrow} + V \sum_{\sigma} \left( \phi_{1\sigma}^\dagger c_{1\sigma} d_{1\sigma} + \phi_{2\sigma}^\dagger c_{2\sigma} d_{1\sigma} \right) + \text{H.c.}
\]

\[
+ \epsilon_{d} \sum_{\sigma,j=1,2} d_{j\sigma}^\dagger d_{j\sigma} + U \sum_{j=1,2} d_{j\uparrow}^\dagger d_{j\uparrow} d_{j\downarrow}^\dagger d_{j\downarrow} + \sum_{k,\sigma,j=1,2} V_{kj} \left( c_{k\sigma}^\dagger d_{j\sigma} + \text{H.c.} \right),
\]
and
\[ H_1 = \sum_{\sigma} (\varepsilon_F - S_\sigma \Gamma) \alpha_{2\sigma}^\dagger \alpha_{2\sigma}, \]
(6)
where we define \( S_\sigma = +(-) \) for the spin \( \sigma = \uparrow(\downarrow) \), \( \alpha_{1\sigma}^\dagger = (c_{1\uparrow}^\dagger + c_{1\downarrow}^\dagger)/\sqrt{2} \) and \( \alpha_{2\sigma}^\dagger = (c_{2\uparrow}^\dagger + c_{2\downarrow}^\dagger)/\sqrt{2} \). This is the limit for the case in which the impurities are close together and we see that the hybridization with the conduction band electrons reduces to only one orbital (\( \alpha_{1\sigma} \)) and favors the ferromagnetic coupling between the impurities. So the \( H_{\text{ZBW}} \) reduces to an effective simplified zero-bandwidth Hamiltonian \( H_0 \) plus a diagonal term \( (H_1) \) disconnected from it. As a consequence, the mathematical problem reduces to solving \( H_0 \). For \( \phi \neq 0 \) and \( \phi^\prime = \pm \pi, \pm 3\pi, \ldots, \pm (2n + 1)\pi \) the hybridization term reduces to the case in which two orthogonal band states are coupled each to a different impurity (i.e., \( V \sum_{\sigma} \lbrack e^{i\phi} \alpha_{1\sigma}^\dagger + c_{2\sigma}^\dagger \rbrack \alpha_{1\sigma} \alpha_{2\sigma} \). \( H_{\text{ZBW}} \) reduces to \( H_{\text{model}} \) and the parameter \( \phi \) as a measure of the distance between the impurities. We start by presenting in figure 1 the energy difference of the two lowest energy levels \( E_K = (\lambda_{S,+1} - \lambda_{S,0}) /\gamma \) for a function of \( \phi, \) for \( \varepsilon_d \). \( V \). The five different values of \( V / \gamma = 0, 0.2, 0.5, 1 \) and 2, and three different values of \( U / V = 30, 10 \) and 5 (figures 1(a)–(c)), respectively, ranging from the Kondo limit (\( U \gg |\varepsilon_d - \varepsilon_F| \)) to the intermediate valence (IV) regime (\( U \sim |\varepsilon_d - \varepsilon_F| \)). We can see that \( E_K \) always decreases when \( \phi \) decreases and also \( E_K \) decreases when \( \gamma \) increases. In the Kondo limit (figures 1(a) and (b)), for any value \( V / \gamma \neq 0 \), \( E_K < 0 \) for \( \phi = 0 \) and \( E_K > 0 \) for \( \phi = \pi / 2 \). Therefore, for \( \phi = 0 \), there is a particular value \( \phi = \phi_0 \), with \( 0 < \phi < \pi / 2 \), where \( E_K = 0 \). For \( \phi < \phi_0 \), the ground state properties take place in the IV regime (figure 1(c)), for a given value of \( U / |\varepsilon_d - \varepsilon_F| \), the existence or not of \( \phi_0 \) depends on the value of \( V / \gamma \). When \( U / V \) reduces, large values of \( V / \gamma \) are needed to obtain the \( \lambda_{S,0} \) ground state at \( \phi = 0 \). To analyze these results, we consider first the limit of \( \phi = \pi / 2 \), where we have the Hamiltonian \( H_{\text{ZBW}} = H_{A1} + H_{A2} + \Gamma \lbrack (\gamma_{1\uparrow} \gamma_{2\uparrow} - \gamma_{1\downarrow} \gamma_{2\downarrow}) + \Gamma \downarrow \rbrack \) + \( H_{\text{ZBW}} \) in terms of two independent Anderson Hamiltonians plus a coupling term: \( H_{\text{ZBW}} = H_{A1} + H_{A2} + \Gamma \lbrack (\gamma_{1\uparrow} \gamma_{2\uparrow} - \gamma_{1\downarrow} \gamma_{2\downarrow}) + \Gamma \downarrow \rbrack \) + \( H_{\text{ZBW}} \) in terms of two independent Anderson Hamiltonians plus a coupling term.

For \( \phi = 0 \) equation (7) gives \( H_{\text{ZBW}} = H_0 + H_1 \). For \( \phi = \pi / 2 \) we have \( \gamma_{1\uparrow} = (i c_{2\uparrow} + c_{2\downarrow}) /\sqrt{2} \) and \( \gamma_{2\downarrow} = (c_{2\uparrow} + i c_{2\downarrow}) /\sqrt{2} \). For \( \phi = 0 \) equation (7) gives \( H_{\text{ZBW}} = H_0 + H_1 \). For \( \phi = \pi / 2 \) we have \( \gamma_{1\uparrow} = (i c_{2\uparrow} + c_{2\downarrow}) /\sqrt{2} \) and \( \gamma_{2\downarrow} = (c_{2\uparrow} + i c_{2\downarrow}) /\sqrt{2} \). For \( \phi = 0 \) equation (7) gives \( H_{\text{ZBW}} = H_0 + H_1 \). For \( \phi = \pi / 2 \) we have \( \gamma_{1\uparrow} = (i c_{2\uparrow} + c_{2\downarrow}) /\sqrt{2} \) and \( \gamma_{2\downarrow} = (c_{2\uparrow} + i c_{2\downarrow}) /\sqrt{2} \).

\[ H_{A1} = \sum_{\sigma} \gamma_{1\sigma} \gamma_{1\sigma} + \varepsilon_d \sum_{j=1}^{d_{1\sigma}} d_{1\sigma}^\dagger d_{1\sigma} + U \sum_{j=1}^{d_{1\sigma}} d_{1\sigma}^\dagger d_{1\sigma}^\dagger d_{1\sigma} + H.c. \]
(7)
\[ H_{A2} = \sum_{\sigma} \gamma_{2\sigma} \gamma_{2\sigma} + \varepsilon_d \sum_{j=1}^{d_{2\sigma}} d_{2\sigma}^\dagger d_{2\sigma} + U \sum_{j=1}^{d_{2\sigma}} d_{2\sigma}^\dagger d_{2\sigma}^\dagger d_{2\sigma} + H.c. \]
(8)

3. Results and discussion
The magnetic correlations between the impurities given by the model Hamiltonian (equation (7)) can be obtained from the four-particle states (this is the most relevant Hilbert space in relation to the two Anderson problems discussed here) or from the grand canonical ensemble adjusting the chemical potential in such a way that the mean total number of particles is always four. There is little numerical difference between these alternative calculations [14]. So that, in all the numerical results presented below, we use the four-particle states \( (N = 4) \). For this case, the full Hamiltonian matrix is \( 70 \times 70 \). Nevertheless, the solution of the problem reduces to the diagonalization of two \( 16 \times 16 \) matrices (for \( S_\sigma = \pm 1 \)) and a \( 36 \times 36 \) matrix (for \( S_\sigma = 0 \)) as the full Hilbert space is block diagonalized, with each block corresponding to a given \( S_\sigma \) component. For \( S_\sigma = \pm 2 \), the model gives two degenerate eigenvalues \( (\lambda_2 = 2(\varepsilon_F + \varepsilon_d)) \). To obtain the numerical results we take the Fermi energy \( \varepsilon_F = 0 \) and \( V \) as the unit of energy. Therefore, the model is completely characterized by \( \varepsilon_d, U, \Gamma \) and the parameter \( \phi \) as a measure of the distance between the impurities.
Therefore, for $\Gamma > 0$ and $\phi = \pi/2$ we obtain, approximately, $E_K \simeq \frac{2\epsilon_d}{\gamma} \frac{J}{\gamma}$ for $|J| \gg |\Gamma|$ and $E_K \simeq -J - \frac{10}{3} \frac{\epsilon_d}{\gamma}$ for $|J| \gg |\Gamma|$.

For $\Gamma = 0$ (solid lines in figures 1(a) and (b)), the problem reduces to solve the one impurity problem ($H_{A\phi}$) and we have obtained [13] $E_K = \Delta + R_0$, with $R_0 = \sqrt{\Delta^2 + 4V^2}$.

In the opposite limit, for $\phi = 0$, the model gives $H_{ZBW} = H_0 + H_1$ and we find that two different ground states are possible:

(A) For large Coulomb repulsion ($|\epsilon_d - \epsilon_F| \ll U$), the three-particle states and $S_z = +1/2$ (for $\Gamma > 0$) gives the ground state energy of $H_0$ and the corresponding eigenvector ($b_1, b_2, b_3$ and $b_4$) can be obtained easily from the lowest eigenvalue $\lambda_{3,1/2}$ of the $5 \times 5$ matrix given by

$$
\begin{pmatrix}
2\epsilon_d + J & \sqrt{2}\Gamma & 0 \\
\sqrt{2}\Gamma & 2\epsilon_d + J/2 & \sqrt{2}\Gamma \\
0 & \sqrt{2}\Gamma & 2\epsilon_d
\end{pmatrix}.
$$

The lowest eigenvalue gives $\lambda_{3,1} = 2\epsilon_d + \frac{J}{\Gamma} - \sqrt{(\frac{J}{\Gamma})^2 + 4\Gamma^2}$. Therefore, for $\Gamma > 0$ and $\phi = \pi/2$ we obtain, approximately, $E_K \simeq \frac{2\epsilon_d}{\gamma} \frac{J}{\gamma}$ for $|J| \gg |\Gamma|$ and $E_K \simeq -J - \frac{10}{3} \frac{\epsilon_d}{\gamma}$ for $|J| \gg |\Gamma|$.
and 5 (c). In (a) and (b) we take $\frac{|/Gamma_1|}{|/Gamma_1|}$ state of $Sz$

The first excited state corresponding to obtained from the previous matrix, changing $|\rangle$ as:

$$
|\alpha, \epsilon| = \frac{1}{\sqrt{2}}(|d^{\uparrow}_1 d^{\uparrow}_2 - d^{\downarrow}_1 d^{\downarrow}_2|0) \text{ and } |h5\rangle = \frac{1}{\sqrt{2}}(|d^{\uparrow}_1 d^{\downarrow}_1 - d^{\downarrow}_1 d^{\uparrow}_1|0).
$$

In a similar manner, we obtain the first excited state as $|3, -1/2\rangle = \sum b^i|hi\rangle$, where we define $|h1\rangle = a^{\dagger}_{1\uparrow}(\Theta)$, $|h2\rangle = a^{\dagger}_{1\downarrow}(\Theta)$, $|h3\rangle = \frac{1}{\sqrt{2}}a^{\dagger}_{1\uparrow}a^{\dagger}_{1\downarrow}(d^{\uparrow}_1 - d^{\downarrow}_1|0)$, $|h4\rangle = \frac{1}{\sqrt{2}}a^{\dagger}_{1\uparrow}a^{\dagger}_{1\downarrow}(d^{\downarrow}_1 - d^{\uparrow}_1|0)$, and $|h5\rangle = \frac{1}{\sqrt{2}}(d^{\uparrow}_1 d^{\downarrow}_1 - d^{\downarrow}_1 d^{\uparrow}_1|0)$, with the corresponding eigenvalue $\lambda_{3,-1/2}$, obtained from the previous matrix, changing $\Gamma$ by $-\Gamma$. From these two states, we obtain the four-particle states for $H_{ZBW}$ by adding one electron in the decoupled $\alpha_{2\uparrow}$ state (the ground state of $H_1$) and we have $a^{\dagger}_{2\uparrow}|3, -1/2\rangle_0$ with $S_z = +1$ and the corresponding ground state energy $\lambda_{S,z+1} = \epsilon_F - \Gamma + \lambda_{3,-1/2}$. The first excited state corresponding to $S_z = 0$ is given by $a^{\dagger}_{2\uparrow}|3, -1/2\rangle_0$ with $\lambda_{S,z=0} = \epsilon_F - \Gamma + \lambda_{3,-1/2}$. Therefore, the lowest energy difference gives $E_K = \lambda_{S,z+1} - \lambda_{S,z=0} = \lambda_{3,1/2} - \lambda_{3,-1/2} < 0$, and we cannot identify this energy with a Kondo excitation because in the process there is no spin-flip excitation ($d^{\downarrow}_1$ is absent in both states). For $\Gamma = 0$, the model Hamiltonian gives $\lambda_{3,1/2} = \lambda_{3,-1/2} = \lambda_3$. For very large Coulomb repulsion ($U/|\Delta| \to \infty$), equation (11) reduces to a $3 \times 3$ matrix and we can solve it to obtain $\lambda_3 = 3(\epsilon_F + \epsilon_d)/2 - R$, with $R = \sqrt{\Delta^2 + 6\epsilon^2}$ and the corresponding eigenvector ($b_1$, $b_2$ and $b_3$) gives: $b_1 = -\frac{1}{\sqrt{2}}\sqrt{\Gamma + \Delta/R}$, $b_2 = \sqrt{\Gamma + \Delta/R}$ and $b_3 = \frac{1}{\sqrt{2}}\sqrt{\Delta/R}$.

For small values of $\Gamma$ ($\Gamma \ll V$ and $\epsilon_F = 0$), we can write from equation (11), $\lambda_{3,1/2} \simeq 3\Delta - R - \Gamma V^2/(R^2 + R\Delta)$ and $\lambda_{3,-1/2} \simeq 3\Delta - R + \Gamma V^2/(R^2 + R\Delta)$. So that $E_K = -2\Gamma V^2/(R^2 + R\Delta)$. For $V \ll \Gamma$ and $\Gamma \ll |\epsilon_d|$, we can write $\lambda_{3,1/2} \simeq 2\epsilon_d - \Gamma - 4\epsilon^2/(\Gamma - \epsilon_d)$, $\lambda_{3,-1/2} \simeq 2\epsilon_d - \Gamma - 2\epsilon^2/(\Gamma - \epsilon_d)$, and therefore $E_K = -2\epsilon^2/(\Gamma - \epsilon_d)$. From the above considerations, for $\Gamma \neq 0$ and large values of $U$, we can see that $E_k < 0$ for $\phi = 0$ and $E_k > 0$ for $\phi = \pi/2$. Therefore, there is always a particular value $\phi = \phi_c$, with $0 < \phi_c < \pi/2$, where $E_k = 0.
(B) For small Coulomb repulsion, in the IV regime \((U \lesssim |\varepsilon_d - \varepsilon_F|)\) and small values of \(\Gamma/V\) (see figure 1(c)), we can see that the ground state corresponds to \(S_z = 0\) \((E_0 > 0)\). We can obtain this state solving \(H_0\) in the four-particle subspace with \(S_z = 0\). So we obtain the ground state energy of \(H_{ZW}\) and the corresponding eigenvector \((c_1, c_2, c_3, c_4, c_5)\) from the lowest eigenvalue \(\lambda_{\phi,0}'\) of the 5 \(\times\) 5 matrix given by

\[
\begin{pmatrix}
\varepsilon_1' - 2V & 2V & 0 & 0 \\
-2V & \varepsilon_2' - \Gamma & 0 & -\sqrt{2V} \\
2V & 0 & \varepsilon_3' + \Gamma & \sqrt{2V} \\
0 & -\sqrt{2V} & \varepsilon_4' & -\sqrt{2V} \\
0 & \sqrt{2V} & 0 & \varepsilon_4' \\
\end{pmatrix},
\]

with \(\varepsilon_1' = 2(2\varepsilon_d + U), \varepsilon_2' = 3\varepsilon_d + U + \varepsilon_F, \varepsilon_3' = 2\varepsilon_d + U + 2\varepsilon_F\) and \(\varepsilon_4' = 2\varepsilon_d + 2\varepsilon_F\). The ground state is: \([4, 0, 0] = \sum_{c|f} \langle f | 1 \rangle = d_{t1}^\dagger d_{t2}^\dagger d_{t3}^\dagger d_{t4}^\dagger |0\rangle, \langle f | 2 \rangle = \frac{1}{2}\alpha_{1}^\dagger (d_{t1}^\dagger d_{t2}^\dagger + d_{t3}^\dagger d_{t4}^\dagger) |0\rangle, \langle f | 3 \rangle = \frac{1}{2}\alpha_{1}^\dagger (d_{t1}^\dagger d_{t3}^\dagger + d_{t2}^\dagger d_{t4}^\dagger) |0\rangle, \langle f | 4 \rangle = \frac{1}{2}\alpha_{1}^\dagger (d_{t1}^\dagger d_{t4}^\dagger + d_{t2}^\dagger d_{t3}^\dagger) |0\rangle, \text{and} \langle f | 5 \rangle = \frac{1}{2}\alpha_{1}^\dagger (d_{t1}^\dagger d_{t2}^\dagger - d_{t3}^\dagger d_{t4}^\dagger) |0\rangle\). The last term shows the antiferromagnetic state \(|\Omega\rangle\) for the impurities in this ground state. When this limit take place, we can see (figure 1(c)) that \(E_0 > 0\) and the fundamental state always has \(S_z = 0\) for any value of \(\phi\).

In figure 2 we show the zero-temperature magnetic correlations \(|S_i S_j\rangle\) between the impurities \((S_i 1, S_j 2)\) as a function of \(\phi\), for the same parameters of figure 1.

For \(\phi \rightarrow 0\) and large Coulomb repulsion \((|\varepsilon_d - \varepsilon_F| < U)\) we always observe ferromagnetic correlations between the impurities (figures 2(a) and (b)). For \(\phi = 0\), we have the ground state \(\alpha_{1}^\dagger |3, +1/2\rangle\) and we can write \(|S_1 S_2\rangle = 0.25(b_1^+ b_2^+)\). When \(\Gamma\) is increased, we can see that \(|b_1\rangle\) increases (see equations (11)) and we can write \(|S_1 S_2\rangle = \alpha_{1}^\dagger |+\rangle\) for the impurities in the ground state. As a consequence, we can see that the ferromagnetic correlation increases with \(\Gamma\) for \(\phi = 0\) at zero temperature. For \(U/|\Delta| \rightarrow \infty\) and \(\Gamma = 0\), this ferromagnetic correlation reduces to \((1 - \Delta/R)/8\). When \(\phi\) increases up to \(\phi_1\), we can observe a ‘jump’ or discontinuity in \(S_1 S_2\) showing the transition from the \(S_z = +1\) ground state to \(S_z = 0\). For \(\phi = \pi/2\), the magnetic correlation take the minimum value. This value, in the Kondo limit of each impurity \((U/|\Delta| \rightarrow \infty, V/|\Delta| \ll 1)\), gives \(|S_1 S_2\rangle = \langle \hat{S}_z \rangle = \langle \hat{S}_\uparrow \rangle = 1/2\). For \(\Gamma = 0, a_2 = a_3 = 0\) and \(\langle S_1 S_2 \rangle = 0\). In figure 2(c) we show the IV regime \((U \leq |\varepsilon_d - \varepsilon_F|)\). For large values of \(\Gamma/V\), we have \(S_z = +1\) ground state at \(\phi = 0\) and we can see that \(|S_1 S_2\rangle\) has the same behavior observed in figures 2(a) and (b). For small values of \(\Gamma/V\), the \(S_z = 0\) ground state takes place and using \([4, 0|0\rangle\) we can write \(|S_1 S_2\rangle = \frac{1}{2}\alpha_{1}^\dagger \alpha_{1}^\dagger\). So we have always antiferromagnetic correlation between the impurities. Finally, for intermediate values of \(\Gamma/V(0.6)\), we observe the transition from ferromagnetic to antiferromagnetic correlation at \(\phi = \phi_1\). In figure 1(c), for \(\Gamma/V = 0.6\) and \(\phi = 0\), we can see that a very small value of \(|E_0|\) occurs. Due to this fact, the transition can take place only at small values of \(\phi_1\).

For \(\Gamma = 0\) (solid lines in figures 1 and 2), the antiferromagnetic coupling between itinerant electrons disappears and the model Hamiltonian is spin conserving. Therefore, the first triplet excited state has the lower eigenvalue \(\lambda_{s=1}\) (three times degenerate \(S_z = \pm 1, 0\)) and we can see that \(E_K\) gives the low energy spin excitation in this model (Kondo energy). This energy decreases continuously from the maximum value at \(\phi = \pi/2\), where two independent \((H_{K})\) Anderson models take place, to zero for \(\phi = 0\), with the impurities in the limit of the very strong interaction regime, where the states \(|3, \pm 1/2\rangle\) play the role of an effective localized spin 1/2 coupled to the band states \(\alpha_{2}^\dagger\) to produce the physics that governs the ground state of the Kondo model. Therefore, when the distance between the impurities decreases, the interaction between the impurities via the conduction electrons increases and reduces the \(E_K\) energy. Furthermore, in accordance to the Kondo physics, the magnetic moment at each impurity site \(j, \phi\) given by: \(m_j = \sum_{\sigma,\sigma'} \langle d_{j}^\dagger \sigma S_{\sigma,\sigma'} d_{j}^\sigma \rangle\), where \(S_{\sigma,\sigma'}\) are the standard Pauli matrices, always gives zero for any value of \(\phi\). In contrast, for \(\Gamma \neq 0\), the model Hamiltonian is spin non-conserving and we obtain \(m_j \neq 0\). We show in figure 3, for \(|\varepsilon_d - \varepsilon_F| < U\), the magnetic moment of the magnetic moment \(|m_j|\) as a function of \(\phi\).

The figure shows the region for \(\phi < \phi_c\), where we observe a very weak dependence on \(\phi\) for the corresponding magnetic moment at \(\phi = 0\), where we can write \(|m_j| = 0.25 \times (2b_1^+ + 2b_2^+)\). For \(\phi_c\), we observe the discontinuity showing the transition from \(S_z = +1\) ground state to \(S_z = 0\) and, finally, for \(\phi < \phi_c\) we can see that \(|m_j|\) decreases and reduces to zero at \(\phi = \pi/2\) (see figure 4(c)). For \(U/V = 6\), far from the strong Kondo limit, we can observe an important reduction of the magnetic moment.

In figure 4, we show the magnetic correlations \(|S_1 S_2\rangle\) as a function of \(\phi\), for \(\varepsilon_d + V = -5\), \(\Gamma/V = 0.5\) and different values of temperature \((T)\). For \(U/V = 10\), in the Kondo region, figure 4(a) shows different behavior depending on the value of \(\phi\) related to \(\phi_c\). For small values \((\phi < \phi_c \approx 0.61)\) and very low temperatures, results show very strong ferromagnetic...
Figure 4. Zero-temperature magnetic correlation $\langle S_1 S_2 \rangle$ as a function of $\phi$, for $\varepsilon_d/V = -5$, $\Gamma/V = 0.5$ and different values of temperature. In (a) we show the case of $U/V = 10$ and (b) shows $U/V = 5$.

Figure 5. The magnetic correlations $\langle S_1 S_2 \rangle$ as a function of temperature, for $\varepsilon_d/V = -5$, $U/V = 10$, $\Gamma/V = 0.5$ and different values of $\phi$ around $\phi_c = 0.61$.

correlation due to the ground state $\alpha^\dagger_2 \left| 3, +\frac{1}{2} \right>_0$. Therefore, as the temperature increases, the contribution of the low energy levels reduces the magnetic correlation. In contrast, for $\phi > \phi_c$, it is interesting to note that, at low temperatures, thermodynamical excitations to the low excited states give additional contributions to the ferromagnetic correlation. This is an expected result in a Kondo energy level scheme (singlet–triplet structure). Therefore, we consider that $\phi_c$ as the lowest limit of $\phi$ below which the breakdown of Kondo theory occurs. Finally, for $\phi \to \pi/2$, the splitting of the low energy levels decreases, so that correlation decreases with increasing temperature.

For $U/V = 5$, in the IV regime, figure 4(b) shows the antiferromagnetic correlation between the impurities. We can see that $\langle S_1 S_2 \rangle$ increases when $T$ increases. In figure 5, we show the temperature dependence of $\langle S_1 S_2 \rangle$ for $U/V = 10$, $\varepsilon_d/V = -5$, $\Gamma/V = 0.5$ and different values of $\phi$, around $\phi_c = 0.61$.

At low temperatures, for $\phi \geq \phi_c$, the curves show a maximum. This maximum is due to excitation from the $S_z = 0$ ground state to the low excited states $S_z = +1, 0, -1$. When $\phi$ is increased from $\phi_c$, the maximum becomes more significant and, according to the above discussion in figure 4, we consider that the temperature at the maximum gives a rough measure of the Kondo temperature in this model. The curves also show how the maximum moves to low temperatures (the Kondo temperature goes down) when $\phi$ (the distance between impurities) is decreased. For $\phi < \phi_c$, the maximum disappears and the Kondo regime is impossible.

4. Conclusions

We have extended the zero-bandwidth limit of the two-impurity Anderson model to include the effect of an antiferromagnetic gap in the conduction band states. We have studied, as a function of $\phi = k_F \cdot r$, the lowest excitation energy, the magnetic moment at each impurity site and the magnetic correlation between the impurities in this model. In the region of the parameters where the impurities are in the Kondo regime, as a function of $\phi$, we have shown that a very interesting competition between the AF gap and the Kondo physics of the two impurities takes place. At zero temperature, when the impurities are close enough ($\phi < \phi_c$), the AF splitting governs the physics of the system and the local moments of the impurities are frozen in a state with very strong ferromagnetic correlation between the impurities, roughly independent of the distance. In contrast, when the impurities are sufficiently far apart ($\phi > \phi_c$) and the AF gap is not too large, the scenario of Kondo physics takes place: a non-magnetic ground state with the possibility of spin-flip excitation can occur. Here, the ferromagnetic $\langle S_1 S_2 \rangle$ decreases
when $\phi$ is increased from $\phi_c$, but the complete decoupling of the impurities never occurs. In addition, the presence of the AF gap gives a non-zero magnetic moment $m_j$ at each impurity site, showing a non-complete Kondo screening of the impurities. Also, we can see that the residual magnetic moment decreases when $\phi$ is increased. Finally, the zero-bandwidth limit approach used here gives a new contribution to understand the very relevant and difficult problem of two-magnetic impurities in an antiferromagnetic metal. We expect that new experimental results in nanodevices will confirm some of the theoretical predictions obtained here.

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References

[1] Lee P A, Rice T M, Serene J W, Sham L J and Wilkins J W 1986 Comments Condens. Matter Phys. 12 99 and references therein
[2] Kondo J 1969 Solid State Phys. 23 183
[3] Ruderman M A and Kittel C 1954 Phys. Rev. 96 99
[4] Fye R M, Hirsch J E and Scalapino D J 1987 Phys. Rev. B 35 4901
[5] Jones B A and Varma C M 1987 Phys. Rev. Lett. 58 843
[6] Simonin J 2006 Phys. Rev. B 73 155102
[7] Broholm C, Kjems J K, Aeppli G, Fisk Z, Smith J L, Shapiro S M, Shirane G and Ott H R 1987 Phys. Rev. Lett. 58 917
[8] Aeppli G, Goldman A, Shirane G, Bucher E and Ch Lux-Steiner M 1987 Phys. Rev. Lett. 58 808
Aeppli G, Bucher E, Broholm C, Kjems J K, Baumann J and Hufnagl J 1988 Phys. Rev. Lett. 60 615
[9] Broholm C, Kjems J K, Buyers W J L, Matthews P, Palstra T T M, Menovsky A A and Mydosh J A 1987 Phys. Rev. Lett. 58 1467
Broholm C, Lin H, Matthews P T, Mason T E, Buyers W J L, Collins M F, Menovsky A A, Mydosh J A and Kjems J K 1991 Phys. Rev. B 43 12809
[10] Zhang G-M and Yu L 2000 Phys. Rev. B 62 76
[11] Capponi S and Assaad F F 2001 Phys. Rev. B 63 155114
[12] Aji V, Varma C and Vekhter I 2007 arXiv:0708.1950
Aji V, Varma C and Vekhter I 2008 Phys. Rev. B 77 224426
[13] Allub R 2003 Phys. Rev. B 67 144416
[14] Alascio B, Allub R and Aligia A A 1980 J. Phys. C: Solid State Phys. 13 2869
[15] Allub R, Wiecko C and Alascio B 1981 Phys. Rev. B 23 1122
[16] Allub R and Proetto C R 2009 Phys. Rev. B 62 10923
[17] See, for example Kim D and Nagaoka Y 1963 Prog. Theor. Phys. 30 743
Alexander S and Anderson P W 1964 Phys. Rev. 133 A1594
Gottlieb P and Suhl H 1964 Phys. Rev. 134 A1586
Caroli B 1967 J. Phys. Chem. Solids 28 1427