Two Anderson Impurities in the Kondo Limit
Doublet States

J. Simonin
Centro Atómico Bariloche and Instituto Balseiro,
8400 S.C. de Bariloche, Río Negro, Argentina
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We analyze two pairs of doublet states for the two Anderson impurity problem. We found that for short interimpurity distances they have a lower energy than the ferro triplet and the antiferro singlet. For medium to long distances between the impurities, the doublets also have a lower energy than the two decoupled Kondo-singlet state for most of the range of interest. The mechanism behind their energy gain is a coherence enhanced Kondo-like interaction.

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The two Anderson impurity problem, i.e., how two magnetic impurities interact when they are embedded in a metallic host, has been the subject of many theoretical studies, ranging from perturbation theory and narrow band approximation to renormalization group analysis. Besides its natural presence in alloys, today this system can be tailor made by means of quantum dots and promises to be a relevant circuit component in quantum electronics. Here we present a variational wave function analysis that, as in the single impurity case, gives a clear description of the system. When needed, we specialize in the one dimensional (1D) case because of its technological applications.

The Anderson Hamiltonian for magnetic impurities diluted in a metallic host is:

\[ H = \sum_{k\sigma} c_{k\sigma}^\dagger c_{k\sigma} + \frac{V}{N_c} \sum_{j\sigma}(\epsilon_{k\sigma} r_j d_{j\sigma}^\dagger c_{k\sigma} + h.c.) - E_d \sum_{j} d_{j\sigma}^\dagger d_{j\sigma} + U \sum_{j} d_{j\uparrow}^\dagger d_{j\downarrow}^\dagger d_{j\downarrow} d_{j\uparrow}, \] (1)

where the fermion operators \( c_{k\sigma} \) act on the conduction band states and \( d_{j\sigma} \) on the orbital of the magnetic impurity situated at \( r_j \). Single state energies \( \epsilon_k, -E_d \) are referred to the Fermi energy \( (E_F = k_F^2/2m) \), i.e., there is an implicit \( -\mu \) \( N \) term in the Hamiltonian that regulates the population of the system \( (\mu = E_F \) is the chemical potential and \( N \) the total number operator), \( V \) is the \( d - c \) hybridization and \( N_c \) is the number of cells in the metal. In the Kondo limit the impurity levels are well below the Fermi energy \((E_d \gg 0)\), and they can not be double occupied due to the Coulomb repulsion in them \((U \gg 2E_d)\). In order to simplify calculations we renormalize the vacuum (denoted by \( |F\rangle \)) to be the conduction band filled up to the Fermi energy and we make an electron-hole transformation for band states below the Fermi level: \( b_{k\sigma}^\dagger = c_{-k,-\sigma} \) for \( |k| \leq k_F \). In this way the energy of a hole excitation (i.e., to remove an electron from below the Fermi level) is explicitly positive.

We consider here the two impurities case, one impurity at \(-r/2\) (the Left impurity) and the other at \(r/2\) (the Right impurity). Although calculations were made with the second quantization operators, we use in the text a “ket” notation for the impurity states: the first symbol indicates the population status of the Left impurity and the second the status of the Right impurity, e.g. \(|\downarrow, \uparrow\rangle \equiv |\downarrow \rangle \otimes |\uparrow \rangle \), \(|\downarrow \rangle \otimes |\uparrow \rangle \), \(|\downarrow \rangle \otimes |\downarrow \rangle \), \(|\downarrow \rangle \otimes |\uparrow \rangle \rangle\) and the antiferro singlet \(|\uparrow \downarrow, \downarrow \uparrow \rangle \rangle\), with energies \(-2E_d\). These states are not eigenstates of the system; the hybridization mixes these states with configurations having excitations in the band. Perturbation theory allows for the calculation of the corresponding corrections. These energy corrections are the same for both the ferro (FF) and antiferro (AF) states (and twice the single impurity corrections) up to the well known RKKY-like four order term, which has opposite contributions on them:

\[ E_{FF} = -2E_d - \Sigma_R, \quad E_{AF} = -2E_d + \Sigma_R, \] (2)

\[ \Sigma_R = 2v^4 \sum_{k,q} \cos((q + k) \cdot r) \cos(|q| \cdot r), \] (3)

where the \( q \) \((k)\) sum is over hole (electron) excitations \(|\eta\rangle \leq k_F \), \(|\eta| \geq k_F \) and \( v = V/\sqrt{N_c} \).

A related state is the Kondo singlet, the ground state when just one impurity is considered. If only the Left impurity is present, this singlet is described by the variational wave function:

\[ |S_L\rangle = |\uparrow \rangle - \sum_{q} \alpha^K_q e^{iq \cdot r/2}(b_{q\uparrow}^\dagger |\downarrow L\rangle + b_{q\downarrow}^\dagger |\uparrow L\rangle), \] (4)

where the variational parameter results to be \( \alpha^K_q = \sqrt{|E_S + E_d - \epsilon_q|} \) and a self-consistent equation is obtained for the singlet energy \( E_S \):

\[ E_S = 2v^2 \sum_{q} \frac{1}{E_S + E_d - \epsilon_q}, \] (5)

after the pole in the sum, \( E_S = -E_d - \delta_K \) is proposed \((E_d \gg \delta_K)\), and Eq. 16 becomes an equation for the Kondo energy \( \delta_K \):

\[ E_d = 2v^2 \sum_{q} \frac{1}{\delta_K + \epsilon_q}, \] (6)
from which
\[ \delta_K = D \ e^{-1/(2Jn)} \] (7)
is obtained. \( Jn \) \((V^2/E_d) \) \( n_o, \ n_o \) being the density of states at the Fermi level) is the relevant parameter for these theories, and \( D \), the half band-width, becomes the energy scale \((\delta_K, \Sigma_R \) are proportional to it). \( Jn = 0.07238 \) gives \( \delta_K \) one thousandth of \( D \), a reasonable value.

We study two doublet states, the even doublet, \( |D_e\rangle = (|\uparrow, 0\rangle + |0, \uparrow\rangle) + \sum_q \{ \)
\[ -i \alpha^F_q \sin \frac{q \cdot r}{2} \left[ 2 b^\dagger_{q\uparrow} |\uparrow, \uparrow\rangle + b^\dagger_{q\downarrow} (|\uparrow, \downarrow\rangle + |\downarrow, \uparrow\rangle) \right] \]
\[ + \alpha^A_q \cos \frac{q \cdot r}{2} b^\dagger_{q\uparrow} (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) \} \] (8)
and the odd doublet,
\[ |D_o\rangle = (|\uparrow, 0\rangle - |0, \uparrow\rangle) + \sum_q \{ \)
\[ + \alpha^F_q \cos \frac{q \cdot r}{2} \left[ 2 b^\dagger_{q\uparrow} |\uparrow, \uparrow\rangle + b^\dagger_{q\downarrow} (|\uparrow, \downarrow\rangle + |\downarrow, \uparrow\rangle) \right] \]
\[ -i \alpha^A_q \sin \frac{q \cdot r}{2} b^\dagger_{q\uparrow} (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) \} \] (9)

After a standard minimization procedure, the variational parameters are obtained
\[ \alpha_q^{F(A)} = \frac{\nu}{E_X + 2E_d + \Sigma_R - e_q} \] (10)
where \( E_X \) stands for the energy of the doublet (\( E_E \) or \( E_O \)) and the plus sign in front of \( \Sigma_R \) holds for the ferro \( \alpha \) factor \((\alpha^F)\) and the minus for the antiferro. For the energies, self-consistent equations result
\[ E_E = -E_d + \nu^2 \sum_q \frac{3 \sin^2 \frac{q \cdot r}{2}}{E_E + 2E_d + \Sigma_R - e_q} \]
\[ + \nu^2 \sum_q \frac{\cos^2 \frac{q \cdot r}{2}}{E_E + 2E_d - \Sigma_R - e_q} \] (11)
For \( E_O \) a similar equation holds, with the sin and cos interchanged. This behavior, as well as the sign of \( \Sigma_R \), is due to the spatial symmetry of the ferro and antiferro states. As is the case of the Kondo singlet, the dominant pole in the sums of Eq.(11) determines the value of \( E_E \).

First, let us analyze the situation when \( \Sigma_R \) vanishes. This situation corresponds to the zeros of the RKKY interaction and the \( k_{FR} \geq \pi \) limit.

For \( \Sigma_R = 0 \), after expanding the \( \sin^2, \cos^2 \) functions, Eq.(11) reads
\[ E_E = -E_d + \nu^2 \sum_q \frac{2 - \cos q \cdot r}{E_E + 2E_d - e_q} \] (12)
Proposing \( E_E = -2E_d - \delta_E \) we obtain
\[ E_d = \nu^2 \sum_q \frac{2 - \cos q \cdot r}{\delta_E + e_q} \] (13)
Therefore for very large \( r \), such that the contribution from the cos term vanishes, the energy gain of the doublet \((\delta_E)\) tends to that of one Kondo singlet. This is not surprising, given that the doublets, when \( \Sigma_R = 0 \), can be written as
\[ |D_X\rangle = |\uparrow_L\rangle \otimes |S_R\rangle \pm |S_L\rangle \otimes |\uparrow_R\rangle, \] (14)
i.e., the combination of a Kondo singlet in one impurity and the other single occupied plus (minus) their mirror image.

This energy, \( \delta_E \), must be compared with twice the Kondo energy, because, for very large \( r \), the latter is the energy gain for a state that has simultaneously both impurities forming a Kondo singlet \((|S_L\rangle \otimes |S_R\rangle)\).

Now, we examine the effect of the coherence term in Eq.(13); here we present the 1D analysis. The sums in Eq.(13) can be done exactly. The first one is the Kondo coherence integral,
\[ \frac{1}{N_e} \sum_{q} \frac{1}{\delta + e_q} = n_o \ I_K(\delta) = n_o \ln \left(1 + \frac{D}{\delta} \right), \] (15)
\[ \frac{1}{N_e} \sum_{q} \frac{\cos q \cdot r}{\delta + e_q} = n_o \ I_X(\delta, x), \] (16)
where \( x = k_{FR} \). The Coherence integral has a logarithmic dependence on \( \delta \) that goes like \( I_K \), so it is useful to define \( C_D(\delta, x) = I_X(\delta, x)/I_K(\delta) \), which is a decaying oscillatory function that depends lightly on \( \delta \). We will see that \( C_D \) plays the role of a coherence driven extra connectivity between the components of the doublet wave function. In Fig.1 we plot \( C_D \) as a function of \( k_{FR} \) for various values of \( \delta \) and the \( r \) dependence of the 1D-RKKY is also plotted. It can be seen that the RKKY reaches its asymptotic form \(( -\cos(2\pi x)/\pi x) \) very quickly, at \( k_{FR} \geq \pi \), whereas \( I_X \) approaches a similar form \(( \sin(\pi x) / x \delta) \) but at \( k_{FR} \delta / \pi \geq 1 \), a distance about one thousand times greater, the Kondo length.

As a function of \( I_K \) and \( C_D \) Eq.(13) becomes
\[ 1/Jn = |2 - C_D(\delta_E, k_{FR})| I_K(\delta_E), \] (17)
from which \( \delta_E \) can be obtained numerically. It is interesting to write it the Kondo way (Eq.16),
\[ \delta_E = D \exp \left[ \frac{-1}{|2 - C_D(\delta_E, k_{FR})| Jn} \right], \] (18)
which can be taken as an approximate solution by evaluating \( C_D \) at \( \delta_K \), or used iteratively to find the exact result with fast convergency. Note that \( C_D \) couples to the "connectivity" factor (the 2 in the exponent of Eq.(16)), and small changes in this factor produce huge changes in \( \delta_E \). For \( \delta_O \) the sign in front of \( C_D \) is positive. These energies are plotted in Fig.2 as a function of \( k_{FR} \) for \( \delta_K = 0.001 \ D \). They alternatively surpass \( 2 \, \delta_K \) up to \( k_{FR} \approx 50 \pi \).

This effect, \( \delta_E, \delta_O \geq \delta_K \), is present for values of \( Jn \) lower than \( Jn_{ic} = 0.240 \) (which gives \( \delta_K = D/8 \)); the
proposing $E_E = -2E_d - \Sigma_R - \delta_E$, Eq. (11) is transformed to
\begin{equation}
E_d + \Sigma_R + \delta_E = \frac{3}{2} v^2 \sum \frac{1 - \cos qr}{q^2 + \delta_E + e_q} + \frac{1}{2} v^2 \sum_q \frac{1 + \cos qr}{2\Sigma_R + \delta_E + e_q},
\end{equation}
and then, using the definitions for $I_K$ and $I_X$, we have,
\begin{equation}
\frac{E_d + \Sigma_R + \delta_E}{n_o V^2} = \frac{3}{2} [I_K(\delta_E) - I_X(\delta_E)]
+ \frac{1}{2} [I_K(2\Sigma_R + \delta_E) + I_X(2\Sigma_R + \delta_E)],
\end{equation}
a self-consistent equation for $\delta_E$ (in Eq. (20) $I_X$ is also a function of $k_F r$, but only the “energy” dependence is quoted). If $E_d \gg \Sigma_R, \delta_E$ the left side of Eq. (20) is just $1/Jn$; if not, a new parameter must be introduced: the $E_d/D$ ratio. In the present work we keep it simple (just $Jn$). For $\delta_O$ and $\Sigma_R > 0$ the sign of the $I_X$ terms are inverted. Therefore when $\delta_O$ decreases $\delta_E$ increases and vice versa, following the oscillations of $C_D$ as a function of $k_F r$, just as in the $\Sigma_R = 0$ case. For $\Sigma_R < 0$ the dominant pole is that of the antiferro component of the doublets and $\delta_E, \delta_O$ swap equations, with $|\Sigma_R|$ instead of $\Sigma_R$ and one important difference: the bare connectivity of the antiferro component is $1/2$, instead of the $3/2$ of the ferro one, and hence these energy gains are lower than in the $\Sigma_R > 0$ case.
thus this is the only surviving configuration of the ones that compose the doublet, and a FF (AF) state with just one hole at the Fermi level is simply a FF (AF) state. The kinks of $\Delta_E$ in these regions are because $\Delta_E = |\Sigma_R|$. In the relevant regions ($\delta_E > \delta_O$) usually $\delta_E > |\Sigma_R|$, thus the dominant pole configurations (FF (AF) based) have just a little more weight in the doublet than the “dominated” one (AF (FF) based), and the $\Sigma_R = 0$ regime is soon reached.

Finally, in Fig. 4, we plot both $\Delta_E$ and $\Delta_O$ as function of $r$, $\Sigma_R$ is also shown ($\delta_K = 0.001D$). For this value of $Jn$, in the measure that $r$ increases the system alternates between the odd and even doublets, just as in the $\Sigma_R = 0$ case, except for a small region above $k_F r = \pi/2$. At this point $\Sigma_R$ is near an AF maximum and $C_D$ is at its first zero. Hence there is not connectivity enhancement, neither for the odd, nor for the even doublet, and they collapse into the AF state.

\[ \Sigma_R \simeq 2 \frac{\sqrt{d}}{E_d} \sum_{k q} \frac{\cos(q r) \cos(k r)}{(e_k + e_q)} = \left( \frac{\pi}{2} Jn \right)^2 D J_R(2k_F r), \quad (A.21) \]

where the $r$ dependence is given by $d = \delta/D$. 

\[ J_R(2k_F r) = \frac{2}{\pi} \left[ \frac{\pi}{2} - \text{Si}(2k_F r) \right] . \quad (A.22) \]

The 1D Doublet Coherence integral is given by

\[ I_X(\delta, x) = \cos(x + xd)[\text{Ci}(x + xd) - \text{Ci}(x)] + \sin(x + xd)[\text{Si}(x + xd) - \text{Si}(x)] , \quad (A.23) \]

where $d = \delta/D$. $\text{Ci}$ (Si) is the CosIntegral (SinIntegral) function, as defined in Mathematica®.

The upper critical value of $Jn$, given that $|C_D| \leq 1$, is defined by the equation

\[ e^{-1/(3Jn_c)} = 2 e^{-1/(2Jn_c)} , \quad (A.24) \]

which gives $Jn_c = 1/6 \ln 2$. 

\begin{figure}
\centering
\includegraphics[width=0.5\textwidth]{fig4.png}
\caption{$\Delta_E$ and $\Delta_O$ as a function of $r$, for $\delta_K = 0.001D$.}
\end{figure}

In conclusion, we give a clear description of the behavior of these doublet states of the Two Anderson Impurity System and their interplay with the RKKY interaction. A remarkable point of the model is the long distances at which the impurities remain in a correlated state. A full understanding of this property, which our model provides in detail, allows these systems to be used in the design of quantum devices.

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Appendix: In 1D, $\Sigma_R$, Eq. (2), half the RKKY interaction, is

\[ \Sigma_R \simeq 2 \frac{\sqrt{d}}{E_d} \sum_{k q} \frac{\cos(q r) \cos(k r)}{(e_k + e_q)} = \left( \frac{\pi}{2} Jn \right)^2 D J_R(2k_F r), \quad (A.21) \]

where the $r$ dependence is given by $d = \delta/D$. 

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