Two Anderson Impurities in the Kondo Limit.
Systematic Study

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We analyze the two Anderson impurity problem, in the strong Coulomb repulsion limit, by means of variational wave functions whose equations we solve analytically. We found two pairs of Doublet states, one odd and one even with respect to the midplane between the impurities. These Doublets make a significatively strong use of the hybridization terms of the Hamiltonian, and have a much larger Kondo-like correlation energy than a single impurity (the Kondo energy). Furthermore, these Doublets combine to form a Super-Singlet. This Super-Singlet makes use of the remaining hybridization probability to improve its energy with respect to the Doublets energy, but for low-Dimensional systems and at the inter-impurity distances where the Doublets are full developed, its energy gain is exponentially small. The interaction behind the Doublets is a first-order (in the effective Kondo coupling) one, it also generates a parallel alignment of the impurity-spins. This ferromagnetic impurity-impurity response is thus generated without resort to the RKKY interaction. The effective range of this first-order Doublet interaction is also much larger than the one of the RKKY interaction.

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I. INTRODUCTION

The two-impurity Anderson (TIA) model is a classic problem in condensed matter physics, where it represents the interaction of two magnetic impurities embedded in a metallic host. The Anderson Hamiltonian is a generic Hamiltonian that describes how localized orbitals with a strong internal Coulomb repulsion behave when they are connected to/through a metallic bath. The current advance in nanotechnology allows for several man-made realizations of such systems. Quantum Dots in the Coulomb blockade regimen connected via a low-dimensional electron gas, magnetic atoms individually deposited on metallic surfaces, nanoclusters or magnetic impurities connected to/through metallic carbon-nanotubes, etc. This kind of circuits, characterized by the low-dimension of the metallic host, promises to be a relevant circuit component in quantum electronics.

The TIA Hamiltonian has been the subject of many theoretical studies, ranging from perturbation theory, and narrow band approximations to renormalization group analysis, conformal field theory and Quantum Monte Carlo simulations. With some approximations/simplifications, as detailed in Ref., some analytical results has been obtained. An other theoretical approach to Anderson Impurity systems has been the use of variational wave functions (VWF) and conformal field theory and Quantum Monte Carlo simulations. In Ref. a set of VWF equations that describes the lower energy state of the TIA system has been numerically analyzed. In this paper we present a systematic VWF analysis of the TIA in the strong-Coulomb-repulsion Kondo Limit. By means of VWF we obtain several set of equations that describe the lower energy states of different subspaces of the system. We analytically solve those equations, identifying two Kondo-like energy scales that depend strongly in the inter-impurity distance. The higher one corresponds to the formation of Kondo-like Doublets states and the lower one corresponds to the formation of a “composite” Kondo Singlet, based upon the screening of the Doublets states. Our equations depend on the details of the metallic host through a simple Coherence factor that, when needed, we evaluate in the one Dimensional (1D) case because of its importance for technological applications. The 2D and 3D scenarios are also analyzed.

We found that the Doublets states generates a ferromagnetic impurity spin-spin correlation without resort to the RKKY interaction. The effect of the RKKY terms in the Doublets structure and energy is also analyzed.

Whereas our analytical results confirm the general picture of the system behavior that is already known from numerical simulations, they also point out that the main interaction between the impurities, contrary to the general belief, is not given by the RKKY process but by the simplest electronic process behind the formation of the Kondo-Doublet states.

This paper is organized as follows: In Section III we write down the TIA Hamiltonian and we make a basis change to the mirror symmetric basis. In Section III we make a preliminary study of the system, analyzing the main features of the Hamiltonian at some special distances between the impurities. In Section IV we make a systematic analysis of the different subspaces of the Hamiltonian. The effects of the intrinsic RKKY interaction in our states are analyzed in Section IV. The high-Dimension scenarios are analyzed in Section V. The Impurity spin-spin correlation is evaluated in Section VI. In Section VII we discuss the conclusions and perspectives open by the method, its possible extension to similar situations and its relation to previous work.
II. THE HAMILTONIAN

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

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

(1)

where \(c_{k\sigma}\) and \(d_{j\sigma}\) are fermion operators which act respectively on the conduction band states and on the orbital states of the magnetic impurity placed at \(r_j\). Single state energies \(e_k\), \(-E_d\) 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 that we analyze here the impurity levels are well below the Fermi energy \((-E_d \ll 0)\), and can not be doubly occupied due to the Coulomb repulsion in them \((U \to \infty)\). 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: \(b_{k\sigma}^{\dagger} \equiv c_{k\sigma}\) for \(|k| \leq k_F\). In this way the energy of a hole excitation is explicitly positive.

We consider here two impurities placed one at \(-r/2\) (the Left impurity) and the other at \(r/2\) (the Right impurity).

In this situation \((-E_d < 0, U \to \infty)\) the lower energy configurations of the system are the ferromagnetic (ferro, FM) triplet \((d_{L\uparrow}^{\dagger} d_{R\uparrow}^{\dagger},|F\rangle, \ldots\) ) and the antiferromagnetic (antiferro, AF) singlet \((d_{L\uparrow}^{\dagger} d_{R\uparrow}^{\dagger} - d_{L\downarrow}^{\dagger} d_{R\downarrow}^{\dagger},|F\rangle\), with energies \(-2E_d\). These states are not eigenstates of the system because the hybridization terms \((H_V)\) mixes these states with configurations having excitations in the band.

An important state for magnetic impurities in a metal is the Kondo singlet, the ground state when a single impurity is considered. If this impurity is at the origin, this singlet is described by the VWF state:

\[
|S\rangle = |F\rangle - \sum_{q} Z(q) (b_{q\uparrow}^{\dagger} b_{q\downarrow}^{\dagger} |F\rangle + b_{q\downarrow}^{\dagger} b_{q\uparrow}^{\dagger} |F\rangle),
\]

(2)

where the function \(Z(q)\) is to be determined variationally. It turns out that \(Z(q) = \sqrt{V/(E_K + E_d - e_q)}\). A self-consistent equation is obtained for the singlet energy \(E_K\)

\[
E_K = 2 \sqrt{V} \sum_{q} \frac{1}{E_K + E_d - e_q},
\]

(3)

where the \(q\) sum is over hole excitations \(|q| \leq k_F\), and \(\sqrt{V} = \sqrt{N_c}\). After the form

\[
E_K = -E_d - \delta_K
\]

(4)

is assumed Eq.(3) becomes an equation for the Kondo energy gain \(\delta_K\)

\[
E_d + \delta_K = 2 \sqrt{V} \sum_{q} \frac{1}{\delta_K + e_q}.
\]

(5)

From here, in the \(E_d, D \gg \delta_K\) regime, it is obtained

\[
\delta_K = D \exp \left( - \frac{1}{2J_n} \right).
\]

(6)

In this equation \(J_n \equiv n_o V^2/E_d\), \(n_o\) being the density of states at the Fermi level and \(D\) the half band-width. \(J_n\), the effective Kondo coupling, is the relevant parameter for these systems, and \(D\) gives the energy scale. If we demands that \(\delta_K\) be one thousandth of \(D\), a reasonable value, it follows \(J_n = 0.07238\).

Note that although all the \(b_{q\sigma}^{\dagger} d_{p\sigma}^{\dagger} |F\rangle\) configurations enter in the definition of the Kondo singlet only the holes with \(e_q \lesssim \delta_K\) make a significant contribution given that the \(Z(q)\) variational amplitude results proportional to \(1/(\delta_K + e_q)\). The Fermi state \(|F\rangle\) plays the role of a nearly virtual state in the Kondo singlet.

The Hamiltonian Eq.(1) conserves the total number of electrons \(N_T\), the total spin \(S_T\), its projection \(S_z\), and has also a mirror symmetry plane at the middle point between the impurities. For example, the FM state has \(N_T = 2\) (plus a half filled conduction band), \(S_T, S_z = 1, 1\) and is odd under the mirror reflection \((d_{L\uparrow}^{\dagger} d_{R\uparrow}^{\dagger} |F\rangle = -d_{R\uparrow}^{\dagger} d_{L\uparrow}^{\dagger} |F\rangle\) ), the AF state has \(N_T = 2\), \(S_T = 0\) and is even under reflection. Assuming a canonical ensemble in the thermodynamic limit, this allows the Hamiltonian to be analyzed by subspaces corresponding to different quantum numbers.

It is useful to rewrite the Hamiltonian Eq.(1) in terms of one-electron operators of well defined mirror symmetry. This is easily done by changing to the symmetric and antisymmetric combinations

\[
c_{Xk\sigma} = \frac{1}{\sqrt{2}} (c_{k\sigma} + c_{-k\sigma}), \quad c_{Xk\sigma} = \frac{1}{\sqrt{2}} (c_{k\sigma} - c_{-k\sigma}),
\]

\[
d_{X\sigma} = \frac{1}{\sqrt{2}} (d_{R\sigma} + d_{L\sigma}), \quad d_{A\sigma} = \frac{1}{\sqrt{2}} (d_{R\sigma} - d_{L\sigma}),
\]

(7)

where \(X\) stands for \((-k_x, k_y, k_z)\). The impurities are on the \(x\)-axis, at \(x = \pm r/2\) and the mirror plane is the \(x = 0\) plane. The transformed Hamiltonian is

\[
H = \sum_{Xk\sigma} c_{Xk\sigma}^{\dagger} c_{Xk\sigma} - E_d \sum_{X\sigma} d_{X\sigma}^{\dagger} d_{X\sigma} + 2\sqrt{V} \sum_{k\sigma} \frac{k_{x\sigma}}{2} d_{X\sigma}^{\dagger} c_{Xk\sigma} + i \frac{k_{x\sigma}}{2} d_{A\sigma}^{\dagger} c_{Xk\sigma} + h.c.
\]

(8)

plus eight four-\(d\)-operator \(U\) Coulomb terms, which can be evaluated when needed. In the Hamiltonian above \(X = \{A, S\}\) and the \(k\)-sum runs only in the right \(k\)-halfspace \((k_x > 0)\). The electron-hole transformation for the conduction band states in this basis is just \(b_{Xk\sigma}^{\dagger} \equiv c_{Xk\sigma}\) for \(|k| \leq k_F\).
The effect of the $U$ terms in the $U \to \infty$ limit is to inhibit two of the six two-electrons in the two-impurity states. The forbidden configurations are

$$(d^\dagger_{A\uparrow} d^\dagger_{A\uparrow} + d^\dagger_{S\uparrow} d^\dagger_{S\uparrow}) , \quad (d^\dagger_{A\uparrow} d^\dagger_{S\uparrow} - d^\dagger_{A\uparrow} d^\dagger_{S\uparrow}) ,$$

(9)
i.e. the symmetric and antisymmetric combinations of the forbidden configurations in the direct basis, $d^\dagger_{L\uparrow} d^\dagger_{L\uparrow}$ and $d^\dagger_{R\uparrow} d^\dagger_{R\uparrow}$. The four allowed configurations are

$$|AF⟩ = (d^\dagger_{A\uparrow} d^\dagger_{A\uparrow} - d^\dagger_{S\uparrow} d^\dagger_{S\uparrow}), \quad |FM\uparrow⟩ = d^\dagger_{A\uparrow} d^\dagger_{S\uparrow} ,$$

$$|FM0⟩ = (d^\dagger_{A\uparrow} d^\dagger_{S\uparrow} + d^\dagger_{A\uparrow} d^\dagger_{S\uparrow}), \quad |FM\downarrow⟩ = d^\dagger_{A\uparrow} d^\dagger_{S\uparrow} ,$$

(10)

the first one is the AF two-impurity configuration, an even state, the last three are the $S_z = 1, 0$ and $-1$ components of the FM triplet. Higher impurity population states are forbidden.

III. THE MODEL

We base our theory on a careful analysis of the Hamiltonian in the symmetrized basis, Eq. (5). First we notice that in this basis the hybridization terms are decoupled, i.e. symmetric $d_S$ impurity orbitals only mix with symmetric $c_S$ conduction band states and the same is true for the antisymmetric ones. Thus it is appropriate to think in terms of two nearly independent magnetic impurities, the symmetric impurity (SI) and the antisymmetric impurity (AI), keeping in mind that these are linear combinations of the two original impurities. The symmetrized impurities are correlated through the action of the Coulomb interaction because the forbidden impurity occupations are not the double occupied SI (or AI) configurations ($d^\dagger_{S\uparrow} d^\dagger_{S\uparrow}$ and $d^\dagger_{A\uparrow} d^\dagger_{A\uparrow}$) but the combinations thereof given in Eq. (9).

Secondly, we notice the factor of 2 in the hybridization term of Eq. (5), which originates in the change in the matrix elements of the Hamiltonian due to the change of basis states. This has important consequences because the correlation energy for a magnetic impurity Eqs. (9,6) depends on the effective hybridization raised to the power two.

A. A singlet

As a consequence of the above, when the two impurities are at a distance such that $|\cos(k_{FR}/2)| \approx 1$ and given that only the conduction holes near the Fermi level are relevant for the formation of a Kondo singlet, the effective coupling for the SI impurity is nearly twice the bare coupling $V$ whereas the effective coupling for the AI impurity is near zero. Therefore, the maximum Kondo-like correlation energy $\delta_4$ that can be obtained by forming a SI Kondo singlet is given by

$$\delta_4 = D \exp \left(-\frac{1}{4J_n}\right) .$$

(11)

Notice the factor 4 in the exponential, while the single impurity Kondo energy $\delta_K$ has only a factor of 2. The effective hybridization coupling provides a $2^2$ factor but half the $q$-states in the sum of Eq. (5) have already been summed in doing the basis change, and this is the reason for the change from 2 to 4 in going from $\delta_K$ to $\delta_4$. This result is exact for $r = 0$ and a good approximation for the next few maxima of the effective SI hybridization coupling ($r \approx n\lambda_F$, $\lambda_F$ the Fermi wave length). This is a very large correlation energy gain for the two impurity case compared with the single impurity Kondo energy. For the above given value of $J_n = 0.07238$, and assuming $D = E_F = 10,000K$, one obtains $\delta_K = 10K$ and $\delta_4 = 316K$, an remarkable effect. In fact the $\delta_4/D$ ratio is given by the square root of the $\delta_K/D$ ratio, thus this magnification effect is higher the lower $\delta_K/D$.

Let us examine this situation in more detail. Consider first the values of $r$ for which the effective symmetric hybridization coupling is enhanced and the antisymmetric one is depressed, $|\cos(k_{FR}/2)| \approx 1$, $|\sin(k_{FR}/2)| \approx 0$, i.e. $r \approx n\lambda_F$. To analyze these regions we can write down the two-impurity SI singlet $|S⟩$, changing $b_q^\dagger d^\dagger_{L-\sigma}$ by $b_q^\dagger d^\dagger_{S-\sigma}$ in the Kondo singlet Eq. (2). The maximum correlation energy gain for such an state is $\delta_4$, thus the energy of the SI singlet is $E_{SI} \geq -E_d - \delta_4$, i.e. a very high correlation energy gain but a not too low total energy because the average total population of the impurities is 1 for such an state. In the appendix A we show that $E_{SI}$ is always greater than the ground state energy expected when the two impurities are far apart,

$$E_{2K} = 2E_K = -2E_d - 2\delta_K ,$$

(12)

the ground state energy for the two magnetic impurity problem in the $r \to \infty$ uncorrelated limit.

B. A doublet

We can try to take advantage of the correlation energy gain $\delta_4$ of the $|S⟩$ singlet by making the SI singlet the core of an odd doublet formed by adding an electron in the inactive AI impurity, i.e. forming the doublet $|D⟩ = d^\dagger_{A\uparrow} |S⟩$. This state has an average total population of 2 electrons in the impurities but it contains the $d^\dagger_{A\uparrow} d^\dagger_{S\uparrow}$ impurity configuration, which is not within the configurations allowed by the $U$ terms of the Hamiltonian, Eqs. (9,10). This can be corrected by noting that

$$2 d^\dagger_{A\uparrow} d^\dagger_{S\uparrow} = (d^\dagger_{A\uparrow} d^\dagger_{S\uparrow} + d^\dagger_{A\uparrow} d^\dagger_{S\uparrow}) + (d^\dagger_{A\uparrow} d^\dagger_{S\uparrow} - d^\dagger_{A\uparrow} d^\dagger_{S\uparrow}) .$$

(13)

The first combination is the $|FM0⟩$ allowed state and the second a forbidden one, thus we project it out of the wave function. In doing this we are loosing 1/4 of the active states of the $|S⟩$ singlet, we will see that this lose reduce the factor 4 of Eq. (11) to a maximum of 3 for the
correlation energy of the doublet. Thus, the odd doublet is given by

$$|D_{ot}\rangle = d_A^\dagger |F\rangle + \sum_k S_k \{ 2 \, Z_1(k) \, b_{S_k}^\dagger |FM\rangle + Z_2(k) \, b_{S_k}^\dagger |FM0\rangle \}$$  \hspace{1cm} (14)$$

where $S_k = cos \frac{k_F r}{2}$. We use the notation of Eq.10 for the doubly occupied impurity states. We apply the standard analytical Euler/Lagrange minimization procedure to the expectation value of the energy, $E_X = \langle X | H | X \rangle / \langle X | X \rangle$, of this state. For the variational functions in the amplitudes of the wave function components we obtain

$$Z_1(k) = Z_2(k) = \frac{v}{E_{D_o} + 2E_d - e_k}.$$  \hspace{1cm} (15)$$

We see that they depend on the energy of the doublet $E_{D_o}$, which is determined by the selfconsistent relation

$$E_{D_o} = -E_d + 3v^2 \sum_q \frac{1 + cos q_F r}{E_{D_o} + 2E_d - e_q},$$ \hspace{1cm} (16)$$

where the sum index runs over the symmetric hole states, i.e. $|q| \leq k_F$ and $q_F r \geq 0$. As we are looking for the lowest energy solution of this equation, we assume $E_{D_o} = -2E_d - \delta_o$. Eq.(16) becomes a selfconsistent equation for $\delta_o$,

$$E_d + \delta_o = 3v^2 \sum_q \frac{1 + cos q_F r}{\delta_o + e_q}.$$  \hspace{1cm} (17)$$

Two limits can be immediately obtained by just comparing this equation with the selfconsistent equation for $\delta_K$, Eq.14. At $r = 0$ one has $cos q_F r = 1$ for all $q$’s, thus

$$\delta_3 = \delta_o(r = 0) = D \ exp - \frac{1}{3J_n}.$$  \hspace{1cm} (18)$$

This is still a great enhancement. For the values used in the previous analysis we obtain $\delta_3 = 100K$ (whereas $\delta_K = 10K$). This is an exact result because the AI impurity is strictly inactive for $r = 0$, this result has been previously found in Ref [15]. For $r \gg 0$ the contribution from the $cos q_F r$ term in the sum vanishes by decoherence effects, therefore $\delta_o(r \gg 0) = D \ exp(-1/(3J_n)) \ll \delta_K$. This is a physically wrong result, one expects $\delta_o = \delta_K$ in this limit, but by the same decoherence effects the AI impurity is active in this limit even if $r = M\lambda_F$, $M$ being a very big integer, and its contribution to the odd doublet can no longer be ignored. We correct this point in Section IV-A.

For the values of $r$ other than the analyzed limits, we must evaluate the sums in Eq.(17). The first one is the Kondo integral

$$I_K(\delta) = \frac{2}{n_oN_c} \sum_q \frac{1}{\delta + e_q} = \ln \left( \frac{D + \delta}{\delta} \right),$$ \hspace{1cm} (19)$$

and the second one can also be summed analytically. We call it the Quantum Coherence Integral, and in 1D we obtain

$$I_Q(\delta, r) = \frac{2}{n_oN_c} \sum_q \frac{cos q_F r}{\delta + e_q} = \ln \left( \frac{D + \delta}{\delta} \right),$$  \hspace{1cm} (20)$$

where $\rho = k_F r$, $\chi = \frac{\rho}{\delta}$ and $C_i (Si)$ is the CosIntegral (SinIntegral) function, as defined in Mathematica®. The Quantum Coherence Integral has a logarithmic dependence on $\delta$ that goes like $I_K$. Notice that $I_Q(\delta, 0) = I_K(\delta)$, so it is useful to define the two-impurity Coherence factor $C_Q(\delta, r) = I_Q(\delta, r)/I_K(\delta)$, which is a decaying oscillatory function that depends weakly on $\delta$. In Fig.1 we plot $C_Q$ as a function of $r$ for various values of $\delta$, the $r$-dependence of the 1D-RKKY interaction, $J_K(r)$, is also plotted for comparison. It can be seen that $J_K(r)$ decays rather rapidly, with range $r \gg \lambda_F$, whereas $C_Q$ has the much larger range $\xi_F$ ( $\equiv \lambda_F E_F/\delta_K$), the Kondo length. In 1D the dominant decoherence effect is that of the energy width ( $\delta$) of the packet of holes that forms the Kondo cloud. In higher Dimensions they appear also angular effects that contributes to the decoherence with typical length of the order of $\lambda_F$.

![FIG. 1: The two-impurity 1D Coherence factor, $C_Q(\delta, r)$ and the $r$-dependence $J_K(r)$ of the RKKY interaction as function of $r$. See that $C_Q$ depends weakly on $\delta$. The period of $J_K(r)$ is half the one of $C_Q$ and its amplitude decays rather rapidly. These characteristics are due to the fact that the RKKY depends on two excitations, whereas the Coherence factor involves just one.](image)

Using the results of the sums Eqs.19, 20, Eq.17 reads

$$E_d + \delta_o = \frac{3}{2} \left( 1 + C_Q(\delta_o, r) \right) \left[ \frac{D + \delta_o}{\delta_o} \right],$$  \hspace{1cm} (21)$$

which can be recast as

$$\delta_o(r) = D \ exp - \frac{1}{2} \left[ 1 + C_Q(\delta_o, r) \right] J_n.$$  \hspace{1cm} (22)$$
still a selfconsistent equation but given the weak dependence of $C_Q$ on $\delta$, it converges very rapidly when used iteratively. It can be easily checked that it gives the two limits already discussed, corresponding to $C_Q = 1$ ($r \to 0$) and $C_Q = 0$ ($r \to \infty$). We will show later, by evaluating the energy of the full odd doublet, that this approximation is in fact good enough at $r \simeq n \lambda_F$, more precisely, around the maxima of $C_Q$. At $r \simeq (n + 1/2) \lambda_F$ the more active impurity is the AI one. Therefore for these points we could repeat all the arguments of this section but for an even doublet based on the AI singlet, however it is enough to observe that the square of the effective hybridization coupling of the AI impurity goes however it is enough to observe that the square of the odd doublet is in fact this effective hybridization coupling of the AI impurity goes amplified. See also that when $\delta_o$ is at one maximum $\delta_e$ is very small and viceversa, for the first maxima their ratio is exponentially small.

\[ |SS\rangle = |F\rangle - i \sum_k Z(k) A_k (b_{Ak}^\dagger b_{Ak}^\dagger + b_{Ak}^\dagger b_{Ak}^\dagger) |F\rangle \]

\[ - i \sum_{k,q} Y(k,q) A_k S_q \{ (b_{Ak}^\dagger b_{S_q}^\dagger + b_{Ak}^\dagger b_{S_q}^\dagger)|FM0\rangle + 2 b_{Ak}^\dagger b_{S_q}^\dagger |FM\rangle \} , \quad (23) \]

where $A_k = \sin \frac{k r}{\lambda_F}$.

\[ Y(k,q) = v Z(k)/(E_S + 2E_d - e_k - e_q) , \quad (24) \]

\[ Z(k) = 2 v/D_S(k) , \quad (25) \]

\[ E_S = 2 v \sum_k (1 - \cos (k r)) Z(k) , \quad (26) \]

where the denominator of $Z(k)$ is

\[ D_z(k) = E_S + E_d - e_k - 3v^2 \sum_q \frac{1 + \cos q r}{E_S + 2E_d - e_k - e_q} . \]

To find $E_S$ we must transform this denominator. It closely resembles Eq. (14) for $E_{D_o}$, with the change $E_{D_o} \to E_S - e_k$. In fact $D_z(k)$ comes from the contribution of the odd doublet to the $|SS\rangle$ energy. Therefore we assume

\[ E_S = E_{D_o} - \gamma = -E_d - \delta_o - \gamma . \quad (27) \]

Thus, using \{ $I_K$, $I_Q$, $C_Q$ \} for the sums in $D_z$, and then Eq. (21) for $E_d + \delta_o$, $-D_z(k)$ becomes

\[ -D_z(k) = (\gamma + e_k) + \frac{3}{2} v^2 n_o (1 + C_Q(\delta_o)) \ln \frac{\delta_o + \gamma + e_k}{\delta_o} , \quad (28) \]

now, note that if $\gamma > 0$, i.e. $E_S < E_{D_o}$, $-D_z(k)$ is always positive. Furthermore, we expect this reduced version of the supersinglet to be good just in the regions in which the odd doublet is. In those regions the contribution to be expected from the AI hybridization channel is very small, i.e. $\delta_o \gg \gamma$, and thus the holes that will contribute the most to the sum in the $E_S$ equation Eq. (20) are the ones at an energy distance of the order of $\gamma$ from de Fermi level. In these conditions the argument of the logarithm
in Eq. (28) is very close to one, and thus is safe to take $-D_0(k) = (\gamma + e_k)$ when used in the sum of Eq. (29). The next order correction $(\ln(1 + x) \simeq x)$ can be included at no mathematical cost, but it requires introducing a new parameter, the $E_d/D$ ratio. We keep it simple just disregarding this correction. Therefore, Eq. (28) becomes

$$2E_d + \delta_o + \gamma = 4\sqrt{2} \sum_k \frac{(1 - \cos(kx))}{\gamma + e_k} \ln D + \gamma$$

from which

$$\gamma(\gamma) = D \exp -\frac{1}{[1 - C_Q(\gamma, r)]J_n}.$$ (30)

This is a very small number when $\delta_o(r)$ is strong ($C_Q$ near 1). Notice that the $C_Q$ factor in Eq. (30) depends on $\gamma$, not on $\delta_o$, thus it is closer to 1 than $C_Q(\delta_o)$.

Near the second maximum of $\delta_o$, at $r = 1.11\lambda_F$, and for $J_n = 0.07238$ Eq. (29) converges in five iterations to $\delta_o = 0.00324$ (and $C_Q = 0.607$) starting with $\delta_o = \delta_k$ as iteration seed. Eq. (30) converges in seven iterations to $\gamma = 1.39410^{-29}$ ($C_Q = 0.792$). Near the first maximum, at $r = 0.1\lambda_F$ we obtain $\delta_o = 0.00922$, $\gamma = 5.7010^{-24}$.

These are very small numbers indeed, but $\gamma$ is positive and small enough to justify the approximations made to reduce Eq. (29), and thus the supersinglet is a better option as a possible ground state of the system than the odd doublet. At $r = 0$, $C_Q \equiv 1$ and $\gamma \equiv 0$, thus $E_S \equiv E_{D_o}$ and the supersinglet collapses into the odd doublet, i.e. it is an uncorrelated combination of the $b_{A(k\gamma)}^{\dagger} |D_{o\gamma}\rangle$ and the $b_{A(k\gamma)}^{\dagger} |D_{o\gamma}\rangle$ states. At $r \rightarrow \infty$ ($C_Q = 0$), or at the $C_Q(r) = 0$ points, this version of the supersinglet fails to give some expected results, mainly that it must be $E_S \simeq -2E_d - 2\delta_K$ for $r \rightarrow \infty$. This is not surprising since we already expect this “partial” supersinglet not to give good results outside the $r \approx n\lambda_F$ regions.

The previous analysis gives us a clear indication of what to look for in the different subspaces of the Hamiltonian, the chemical potential tell us no to go too far from $N_T = 0$ (plus the half filled conduction band) then, given the limits that $U$ impose in the population of the impurities, $N_T = 2$ seems to be a reasonable upper value. In the next section we proceed to a systematic analysis of those subspaces, looking for the lowest energy state of each one of them. We start with the $N_T = 1$ one and finish with the one corresponding to $N_T = 2$. This order is not arbitrary because the $N_T = 1$ subspace is the less explored of them and $N_T = 2$ the most explored one.

IV. SYSTEMATIC ANALYSIS

A. Doublets subspace, $N_T = 1$

The $N_T = 1$, odd subspace is the odd doublet subspace. As follows from the previous analysis the odd doublet lacks the action of the $\uparrow$ hybridization channel on its vertex state, i.e the $b_{A(k\gamma)}^{\dagger} |D_{o\gamma}\rangle$ and $b_{A(k\gamma)}^{\dagger} |D_{c\gamma}\rangle$ configuration groups. The last group is forbidden by Pauli exclusion principle and must thus be ignored. For the first group we must use the same procedure as in Eq. (12). Thus we analyze the following variational wave function in this subspace

$$|D_{o\gamma}\rangle = d_{A(k\gamma)}^{\dagger}|F\rangle + i \sum_k Z_A(k) A_k b_{A(k\gamma)}^{\dagger}|AF\rangle$$

$$+ \sum_k Z_S(k) S_k \{ 2b_{S(k)}^{\dagger} |FM\rangle - b_{S(k)}^{\dagger} |FM\rangle \},$$ (31)

the now full odd doublet. The selfconsistent equations for the variational amplitudes and energy are

$$Z_A(k) = Z_S(k) = \frac{v}{E_{D_o} + 2E_d - e_k},$$ (32)

$$E_{D_o} = -E_d + 2\sqrt{2} \sum q \frac{(3S_q^2 + A_q^2)}{E_{D_o} + 2E_d - e_q}.$$ (33)

After expanding the $S_q^2$, $A_q^2$ factors in Eq. (32), and assuming $E_{D_o} = -2E_d - \delta_o$, Eq. (33) transforms into

$$E_d + \delta_o = 2\sqrt{2} \sum q \frac{2 + \cos q_x r}{\delta_o + e_q},$$ (34)

now, using $\{ I_K(\delta), C_Q(\delta, r), E_{D_o}, E_{D_o} \}$, Eq. (34) becomes

$$\delta_o(\gamma) = D \exp -\frac{1}{[2 + C_Q(\delta_o, \gamma)]J_n}.$$ (35)

in the $D, E_d \gg \delta$ limit. This formula for $\delta_o(\gamma)$ replaces the previous partial result Eq. (22). It can be taken as an approximate solution by evaluating $C_Q$ at $\delta_o$, or used iteratively to find the exact result with fast convergency. At its first maxima, i.e. at $\{ C_Q \simeq 1, r \sim n\lambda_F \}, \delta_o \leq \delta_3$ as previously analyzed. At the $C_Q(\delta, r) = 0$ points, including the $r \rightarrow \infty$ limit, Eq. (35) gives $\delta_o(\gamma) / C_Q(\gamma) = 0 = \delta_K(\gamma \equiv 0) = \delta_K(\gamma \equiv 0)$, the physically expected result.

In the $N_T = 1$, even subspace, the relevant state is the even doublet, its construction process is the same as for the odd doublet but taking $d_{c\gamma}^{\dagger} |F\rangle$ as the vertex state. The definition of the even doublet is similar to that of the odd doublet, Eq. (24), but with the change $A \leftrightarrow S$ in the creation operators and in the hybridization amplitude factors $A_k, S_k$. A global minus sign appears for the $Z_S(k)$, given that for the AF, FM states we use the $d^\dagger$ operators ordering shown in Eq. (11), the one of the allowed impurity configurations. The energy $E_{D_o}$ of the even doublet states is given by

$$E_{D_o}(\gamma) = -2E_d - \delta_e(\gamma),$$

$$\delta_e(\gamma) = D \exp -\frac{1}{[2 + C_Q(\delta_e, \gamma)]J_n}.$$ (36)

If we compare Eq. (36) for $\delta_e(\gamma)$ with Eq. (35) for $\delta_o(\gamma)$, we see that the sign in front of $C_Q$ changes, this is because
of the $A_k \leftrightarrow S_k$ change, i.e. the SI and AI impurities interchange roles. The analysis of $\delta_c$ as a function of $r$ is also very similar to that of $\delta_o(r)$. The odd doublet correlation energy gain $\delta_o(r)$ is higher than the even doublet gain $\delta_e$ when $C_Q(\delta_K, r) > 0$, and the opposite is true for $C_Q(\delta_K, r) < 0$. They are equal, and equal to $\delta_{K} = \delta_{2}$, at the $r_K$ distances for which $C_Q(\delta_K, r_K) = 0$.

These correlation energy gains of the odd and even doublets, $\delta_o$ and $\delta_e$, are plotted in Fig.3 as a function of $r$ for $\delta_K = 0.001 D$. For very large $r$, such that $C_Q(\delta_K, r)$ vanishes, the energy gain of the doublets tends to that of one Kondo singlet. This is not surprising since the doublets, in this limit, can be written as

$$|D_X\rangle = |L\rangle \otimes |S_R\rangle \pm |S_L\rangle \otimes |R\rangle,$$

i.e., the combination of a Kondo singlet in one of the original impurities and the other single occupied plus (minus) the mirror image of that state. The total energy of this state is $-2E_d - \delta_K$, as for the doublets in the uncorrelated limit $(r \to \infty)$.

![1D Correlation energy gains of the odd $\delta_o$ and even $\delta_e$ doublets as a function of the distance between the impurities, for $J_o = 0.07238$ ($\delta_K = 0.001 D$). The inset is $\delta_e$ up to very long distances, it periodically beats $2\delta_K$ up to $r \simeq 2\xi_K$.](image)

These energies gains 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, and in an uncorrelated way, both impurities forming a Kondo singlet $(|S_L\rangle \otimes |S_R\rangle)$. The doublet gains $\delta_D$ alternatively surpass $2\delta_K$ up to $r \simeq 2\xi_K$.

This effect, $\delta_o = \max(\delta_o, \delta_e) \geq 2\delta_K$, is present for values of $J_o$ lower than $J_{nc} = 0.240$ (defined by $\delta_o = 2\delta_e$); the lower $J_o$, the greater this effect. The periodicity with which $|D_o\rangle$, $|D_e\rangle$ alternate as ground states of the $N_T = 1$ subspace is twice the RKKY period (they are ruled by $C_Q(\delta_K)$), and they stand in this situation up to very long distances. These properties are due to the fact that the doublet coherence integral involves just one hole excitation. At the intersection points one has $\delta_c, \delta_o = \delta_K$ and $C_Q = 0$.

The electronic process behind these correlated Doublets is second order in the hybridization coupling $V$. The jump of a band electron from below the Fermi level to the impurities and then back to its initial place is the only process allowed by the Doublet VWF Eq.\(\text{[31]}\).

## B. SuperSinglet, $N_T = 0$

In the $N_T = 0$ subspace there is the supersinglet, its full expression, taking into account both the even and odd doubles components, is

$$|SS\rangle = |F\rangle - \sum_k\{(i Z_O(k) A_k \left( b_{Ak}^\dagger d_{A1}^\dagger + b_{Ak} d_{A1} \right) + Z_E(k) S_k \left( b_{Sk}^\dagger d_{S1}^\dagger + b_{Sk} d_{S1} \right) |F\} - \sum_{k,q}\{(Y_O(k, q)A_k A_q b_{Ak} b_{Aq}^\dagger + Y_E(k, q)S_k S_q b_{Sk} b_{Sq}^\dagger) |AF\) + i Y(k, q) S_k A_q \left[ (b_{Ak} b_{Sk}^\dagger + b_{Aq} b_{Sq}^\dagger) |FM0\right) + 2 b_{Aq} b_{Sk}^\dagger |FM1\rangle \}.$$

The $Q_O(E)(k)$ configurations are the odd (even) doublet component of the supersinglet. The “origin” of each one of its components can also be traced down looking at the $A_k$, $S_k$ factors and/or the results obtained for their variational amplitude functions. After the functional minimization procedure, these functions turn out to be

$$Y_O(k, q) = \nu (Z_O(k) + Z_O(q)) / D_Y(k, q),$$
$$Y_E(k, q) = \nu (Z_E(k) + Z_E(q)) / D_Y(k, q),$$
$$Y(k, q) = \nu (Z_O(k) + Z_E(q)) / D_Y(k, q),$$

where $D_Y(k, q) = (E_S + 2E_d - e_k - e_q)$ and

$$Z_O(k) = -[2\nu + \nu^2 \sum_q(1-cqr) Z_O(q)/D_Y(k, q) + 3\nu^2 \sum_q(1+cqr) Z_E(q)/D_Y(k, q)]/D_{Z_O}(k),$$

$$D_{Z_O}(k) = -E_S - E_d + e_k + 2\nu^2 \sum_q 2 + cqr / D_Y(k, q).$$

where $cqr = \cos q_d x$. For $Z_E(k)$ a symmetric expression holds, with the changes, in Eqs.\(\text{[40]}\), $E \leftrightarrow O, A \leftrightarrow S, cqr \leftrightarrow -cqr$. For the supersinglet energy $E_S$, the following expression is obtained

$$E_S = 2\nu \sum_k \left[ (1-c qr) Z_O(k) + (1+c qr) Z_E(k) \right].$$

To solve these equations, which are self consistent and recursive, one must proceed in a similar way as in the case of the partial supersinglet analyzed in Section III C.

We work them out in the same approximation as before disregarding higher order terms that depend on the $E_d/D$ ratio.
First, we analyze the points at which coherence effects are suppressed, i.e. \( r \to \infty \) and the \( r_K \) points such that \( C_Q(\delta_K, r_K) = 0 \). For these points \( \delta_o = \delta_e = \delta_K \) and thus, assuming \( E_S = -2E_d - \delta_K - \gamma \), we obtain

\[
Z_X = -2v/DZ_X , \quad (43)
\]
\[
DZ_X = (\gamma + \epsilon_k) , \quad (44)
\]
\[
2E_d + \delta_K + \gamma = 8v^2 \sum_k \frac{1}{\gamma + \epsilon_k} , \quad (45)
\]

from which \( \gamma = \delta_K \) follows. Therefore, the energy of the supersinglet at these points is

\[
E_S = -2E_d - 2\delta_K . \quad (46)
\]

The value \( C_Q(\delta_K, r_K) = 0 \) marks the boundary between two regions. For \( C_Q(\delta_K, r) > 0 \) the odd doublet is the lower energy doublet and it is the main component of the supersinglet, conversely, for \( C_Q(\delta_K, r) < 0 \) the behavior of the supersinglet is determined by the even doublet. We work out now the energy of the supersinglet in the odd doublet region. In these regions \( \delta_o > \delta_e \) and thus we take \( E_S = -2E_d - \delta_o - \gamma \). With this replacement Eqs. 10, 12 become

\[
DZ_o = (\gamma + \epsilon_k) , \quad DZ_e = (\gamma + \Delta_d + \epsilon_k) , \quad (47)
\]
\[
E_S = -4v^2 \sum_k \left[ \frac{1 - ckr}{DZ_o(k)} + \frac{1 + ckr}{DZ_e(k)} \right] . \quad (48)
\]

Using the definitions of \( \{I_K, I_Q, C_Q\} \) and the proposed form of \( E_S \), Eq. 47 transforms into

\[
\frac{1}{J_n} = I_K(\gamma)(1 - C_Q(\gamma, r)) + I_K(\gamma + \Delta_d)(1 + C_Q(\gamma + \Delta_d, r)) , \quad (49)
\]

from which one obtains

\[
\gamma(r) = D e^{\frac{-r_{\text{lat}} - 4C_Q(\gamma)}{\gamma}} \left( \frac{D}{\Delta_d + \gamma} \right)^{1 + C_Q(\gamma + \Delta_d)} \left( \frac{1}{1 - C_Q(\gamma)} \right) , \quad (50)
\]

where \( \Delta_d = \delta_o - \delta_e \); only the energy dependence of \( C_Q \) is shown. This is the full expression for \( \gamma \) when the odd doublet is the dominant one. For \( C_Q(\delta_K) = 0 \) one has \( \delta_o = \delta_e = \delta_K \), and Eq. 40 reduce to \( \gamma^2 = D^2 \exp(-1/J_n) \), i.e. \( \gamma = \delta_K \), see Eq. 10.

At the maxima of \( C_Q \) \( (r \simeq n\lambda_F) \) one has \( \delta_o \gg \delta_e, \gamma \), thus \( \Delta_d \approx \delta_o \), and using Eq. 45 one obtains

\[
\gamma = D \exp \left\{ -\frac{1}{J_n[1 - C_Q(\gamma)]} \left[ 1 + \frac{1 + C_Q(\delta_o)}{2 + C_Q(\delta_o)} \right] \right\} , \quad (51)
\]

i.e. nearly Eq. 30, the previous “partial” result for \( \gamma \) at those regions. For these maxima, \( \gamma \) is exponentially small if \( C_Q(\gamma, r) \) is still strong, as discussed in Section III C.

To analyze the \( r \)-regions in which \( C_Q(\delta_K, r) < 0 \) one must propose \( E_S = -2E_d - \delta_e - \gamma \) given that for these regions \( \delta_o < \delta_e \). The result for \( \gamma \) is just Eq. 19 with the changes \( \delta_o \leftrightarrow \delta_e \) and \( C_Q \rightarrow -C_Q \). In Fig. 4 we plot the correlation energy gains of the Doublets and the Super-Singlet.

At the first maxima of the doubles energy gains, i.e. the minima of their total energy, the additional energy gain of the Super-Singlet \( \gamma \) is very small and therefore small thermal activation will destroy the correlation that generates it. This is not the case for the energy gain of the Doubles at those points, \( \delta_o \) or \( \delta_e \), which is very strong, as discussed in Section III E.

C. The \( N_T = 2 \) subspace

In this subspace there are the lower energy configurations of the system, the AF singlet and the FM triplet, whose configurational energy is \(-2E_d\). Given that these configurations are already the lower energy configurations of the subspace the effects of the hybridization on them can be directly evaluated by standard perturbation methods. For the sake of completeness we recalculated the result of reference 8 in the same variational wave functions framework as the previously analyzed subspaces. We use the “perturbation” property of the AF, FM states to solve their selfconsistent energy equation by series expansion. For these AF and FM states two hybridization (\( H_V \)) steps are needed to bring out the RKKY energy term. For the \( S_z = 1 \) component of the FM triplet, the
expanded VWF is

\[
|\text{FM}^\uparrow\rangle = |\text{FM}^\uparrow\rangle - \sum_k Z(k)(S_k c_k^\dagger d_A^k + iA_k c_k^\dagger d_s^k) + \sum_{k,q} Y(k,q)
\]

\[
(2A_k A_q b_A^k c_{q7}^\dagger + 2S_k S_q b_{sk}^k c_{sq7}^\dagger) |\text{FM}^\uparrow\rangle + (A_{k} b_{sk1}^k c_{q7}^\dagger + S_k S_q b_{sk1}^k c_{sq7}^\dagger) |\text{FM}^0\rangle
\]

\[
i(S_k A_q b_{sk1}^k c_{q7}^\dagger - A_k S_q b_{sk1}^k c_{sq7}^\dagger) |\text{AF}\rangle.
\]

(52)

After minimization, it turns out that

\[
Y(k,q) = \frac{v Z(q)}{D_Y(k,q)},
\]

(53)

\[
Z(k) = \frac{2v}{D_Z(k)},
\]

(54)

\[
D_Z(k) = E_{FM} + E_d - e_k - 2v^2 \sum_q \left\{ \frac{2 + c q r c k r}{D_Y(k,q)} \right\},
\]

(55)

\[
E_{FM} = -2E_d + 2v \sum_k Z(k),
\]

(56)

where \( D_Y(k,q) = E_{FM} + 2E_d - e_k - e_q \). As in the previous cases, the energy is to be determined selfconsistently. We can make a Taylor series expansion on \( v^2 \) on the right of Eq.(50), taking into account that \( E_{FM} \) is also a function of \( v^2 \). If this expansion is carefully analyzed, it turns out that the expansion parameter is \( J_n \). The final result for \( E_{FM} \), to order \( v^4 \), is the well known perturbation theory expression

\[
E_{FM} = -2E_d - v^2 \sum_k \left\{ \frac{4}{E_d + e_k} + v^4 \sum_{k,q} \left\{ \frac{16}{(E_d + e_k)^2(E_d + e_q)} - \frac{16 + 8 \cos q_x r \cos k_x r}{(E_d + e_k)^2(e_k + e_q)} \right\} \right\},
\]

(57)

the first \( v^4 \) term in the right is the second order contribution of the \( v^2 \) correction, this a well known property of variational wave functions like the Kondo Varma-Yafet singlet. In the second \( v^4 \) term there is a contribution that depends on the interimpurity distance \( r \),

\[
\Sigma_R(r) \approx 8 \frac{v^4}{E_d} \sum_{k,q} \frac{\cos(q_x r) \cos(k_x r)}{(e_k + e_q)}
\]

\[
= 4 \ln 2 \frac{D J_n^2}{J_R(r)},
\]

(58)

this is half the RKKY energy. The prefactor 8 appears because the sum in Eq.(55) is over \( k_x > 0, q_x > 0 \) electron (hole) excitations. The \( r \) dependent part \( J_R(r) \) of the 1D-RKKY is given by

\[
J_R(r) = \frac{2}{\pi} \left( \frac{r}{2} - \text{Si}(2k_F r) \right),
\]

(59)

which is plotted in Fig.1. It decays very fast, its first extreme values are 1.0 at \( r = 0.0 \lambda_F \), and -0.179 at \( \lambda_F / 4 \).

At \( r = 2.0 \lambda_F \) its value, 0.025, is already very small. The \( r = 0 \) value of \( \Sigma_R \) is determined by integration of Eq.(55) in the half filled flat band approximation for the conduction band of the metallic host. The Kondo energy, Eqs.(56, 57), is also evaluated in that approximation. For the AF state, expanded to the same order as the FM state, there appear the same terms as in Eq.(57) but with a minus sign in front of \( \Sigma_R \), thus the RKKY interaction, i.e., the energy difference between the FM and AF states, is twice \( \Sigma_R \).

D. The RKKY and the Doublets

The Doublets states are the results of a first-order interaction present in the TIA Hamiltonian. Only the configurations that are reached with one \( H_V \) step from the corresponding vertex state are included in the VWF we use to study them. See also that it depends on \( J_n \) (although in a non-perturbative way) and that just one hole excitation is involved in the calculus of \( C_Q \). The RKKY is a second-order interaction, two \( H_V \) steps are needed in their VWF, it depends on \( J_n^2 \) and both a hole and an electron excitation are involved in its evaluation. In fact, the correlation energy of the dominant Doublet is higher than the corresponding to the RKKY in most of the \( (J_n, r) \) parameters space of the Hamiltonian. At \( r = 0 \) the equation \( \Sigma_R(0) = \delta_3 \) determines that for \( J_n > 0.085 \) the Doublets correlation energy is greater than the RKKY energy. Note that the one-impurity Kondo energy \( \delta_k \) is never greater than \( \Sigma_R(0) \). As a function of \( r \) the RKKY interaction decays at shorter distances than the Doublet one. In Fig.4 we show the “Doublets-RKKY” “Parameters Space Phase Diagram” for the 1D two-impurity system, determined by max \( (\delta_0, \delta_e) = |\Sigma_R| \). This is not a true Quantum phase diagram given that not the Doublets nor the FM (AF) states are the ground state of the system. But it indicates in what \( (J_n, r) \) regions is relevant to include the second-order RKKY effects in the analysis of the Doublets structure. Over the near vertical dashed lines that mark the limits between the odd and even Doublets, determined by \( C_Q(\delta_K) = 0 \), there is little enhancement of the Doublets energies. These zones coincide with the AF maxima of the RKKY interaction and thus over these lines there are the highest indents of the RKKY regions.

How \( \Sigma_R(r) \) modifies the internal structure of the Doublets has been analyzed in Ref., where the Doublets where first introduced. To include the RKKY effects in the VWF of the odd Doublet, two more \( H_V \) generations of configurations must be added to it. In the odd Doublet VWF, Eq.(51), see that the configurations with the \( Z_A(k) \) amplitude factor correspond to a AF state of the impurities, whereas the ones with the \( Z_S(k) \) factor are configurations with their impurity part in a FM state. As in Section IV A we cut our VWF at that order both amplitude factors result to be equal, \( Z_A = Z_S = v/(E_d - (-2E_d + e_k)) = -v/(\delta_0 + e_k) \).
We show in Appendix B that the main effect of the configurations needed to include the RKKY interaction in our Doublet VWF is to modify those amplitude factors. Their denominators will reflect now the different energies of the FM and AF impurity configurations. The self-consistent equation for the odd Doublet energy when these higher order process are included is given by

\[
E_D = -E_d + \sum_k \frac{3v^2(1 + \cos(k_x r))}{E_D + 2E_d + 2\Sigma_0 + \frac{1}{4}J_X + \Sigma_R - \epsilon_k}
+ \sum_k \frac{v^2(1 - \cos(k_x r))}{E_D + 2E_d + 2\Sigma_0 - \frac{1}{4}J_X - \Sigma_R - \epsilon_k}. 
\]

where the first sum in the right comes from the contribution of the ferro configurations in the Doublet and the second one from the antiferro configurations, \(\Sigma_0\) is the one impurity corrections (up to second order in \(J_n\)) and the terms proportional to \(J_X\) appears, just with the VWF used in Section IV A if an external RKKY-like term \((-J_X S_L . S_R)\) is added to the TIA Hamiltonian. The effect of \(\Sigma_0\) is to shift the “zero” of energy and the effect of \(J_X\) is similar to the one of the intrinsic RKKY term \(\Sigma_R\), thus in what follows we discuss just the effects of this last term in the Doubles structure and energy. With the considerations above, the variational amplitude factor of the FM configurations in the Doublet is given by \(Z_S(k) = -v/(-\Delta_0 - \Sigma_R + \epsilon_k)\) when RKKY effects are taken into account. And for the AF configurations \(Z_A(k) = -v/(-\Delta_0 + \Sigma_R + \epsilon_k)\) holds. \(\Delta_0 = |\Sigma_R(r)| + \delta^o_0(r)\) is the total correlation energy gain of the Doublet, composed by the RKKY and Kondo-Doublt contributions.

For \(\Sigma_R > 0\) (which corresponds also to the maxima of \(|C_Q|\)), the dominant components of the dominant doublet are the FM configurations, thus we assume \(E_D = -2E_d - \Sigma_R - \delta^o_0\); and using the definitions of \(J_k\) and \(C_Q\), we obtain

\[
\frac{1}{J_n} = \frac{3(1 + C_Q(\delta^o_0))}{2} \ln \frac{D}{\delta^o_0} + \frac{(1 - C_Q(\delta^o_0 + 2\Sigma_R))}{2} \ln \frac{D}{\delta^o_0 + 2\Sigma_R} + \frac{D}{\delta^o_0 + 2\Sigma_R},
\]

a self-consistent equation that easily gives the value of the odd-doublet correlation energy \(\delta^o_0\) in a RKKY-FM region. In the extreme case \(\Sigma_R \gg \delta^o_0\) one can neglect the AF-configurations contributions to Eq.(61) (this is equivalent to use for the Doubles a VWF with \(Z_A(k) \equiv 0\) and thus

\[
\delta^o_0 = D \exp \frac{-1}{(3/2)(1 + C_Q)J_n},
\]

which gives \(\delta^o_0 > \delta_K\) for values of \(|C_Q|\) down to 1/3. Note also that for high values of \(C_Q\) there is little reduction of \(\delta^o_0\) compared with its bare (\(\Sigma_R = 0\)) value \(\delta_0\), because the AF-configurations contribution \((1 - C_Q)/2\) is already very small in this case.

Similarly, in the RKKY-AF regions (\(\Sigma_R < 0\), and \(C_Q \simeq 0\)), we assume \(E_D = -2E_d - |\Sigma_R| - \delta^o_0\) and, with the notation \(\Sigma_A = |\Sigma_R| - \Sigma_R\), the general equation Eq.(61) can be expressed as

\[
\frac{1}{J_n} = \frac{3(1 + C_Q(\delta^o_0 + 2\Sigma_A))}{2} \ln \frac{D}{\delta^o_0 + 2\Sigma_A} + \frac{(1 - C_Q(\delta^o_0))}{2} \ln \frac{D}{\delta^o_0},
\]

that in the extreme case \(\Sigma_A \gg \delta_K\) can be reduced to

\[
\delta^o_0 = D \exp \frac{-1}{(1/2)(1 - C_Q)J_n},
\]

which gives very small values for the correlation energy of the Doublet in this situation: for \(J_n = 0.07238\), which corresponds to \(\delta_k = 0.001D\) and \(\delta^o_0 = \delta_k(r = 0) = 0.01D\), one obtains \(\delta^o_0 = 0.0000000001D\). Therefore the formation of the Doubles in an extreme RKKY-AF region will be very difficult to detect in a numerical simulation of the system. Experimentally, nearly any thermal activity will destroy the doublets in this regime.

The previous equations (Eqs.(63) to (66)) are for the odd Doublet, which dominates for \(C_Q > 0\). As the equations corresponding to the even Doublet (which dominates for \(C_Q < 0\)) are the same but with a minus in front of \(C_Q\), the final result is that Eqs.(63 and 64) also apply to the even Doublet with the change \(C_Q \rightarrow -C_Q\). In Fig.6 we show a “generic” analysis of Eq.(64): for \(J_n = 0.07238\) and fixed values of \(C_Q\) we plot \(\delta^o_0\) as a function of \(\Sigma_R\) (\(-\Sigma_R\) on the right (left) panel, energies are in units of \(\Delta_k\). Actually, both \(C_Q\) and \(\Sigma_R\) are precise functions of \((J_m, r)\) and not any value of \(\Sigma_R\) can be obtained for a given \(J_m\). Anyway, we use this figure to show the general trend of the solutions of Eq.(64). It can be seen that a positive \(\Sigma_R\) has little effect in the dominant Doublet.
structure and it nearly has just an additive effect in the total energy of the Doublet. This response is due to the fact that the dominant Doublet is primary formed upon FM-like configurations. By the same reason a negative $\Sigma_R$, which energetically penalize the FM-like configurations, has a catastrophic effect on the energy gained by forming the Doublet. The corresponding extreme limits are well described by Eqs. 62 and 64.

In Fig. 7 we plot the total correlation energy of the Doublets ($\Delta_x = \delta_x^2 + |\Sigma_R|$, $x = \{o, e\}$) as a function of the distance between the impurities and for $J_n = 0.07238$. As discussed previously the main contribution to the energy of the dominant Doublet comes from the Kondo-Doublet interaction, the RKKY contribution becomes negligible very rapidly when the distance between the impurities is increased beyond $\lambda_F/2$. For the dominated Doublet, instead, nearly all the energy gain comes from the RKKY contribution. Only at $k_Fr = \pi/2$, a crossing point for the Doublets ($C_Q = 0$), the RKKY-AF interaction provides “all” the energy gain of the dominant Doublet. This point is an extreme RKKY-AF case, as described in Eq. 64.

These extreme RKKY-AF regions, which for the actual TIA Hamiltonian are only present for low values of $J_n$, are the subject of contradictory results in the literature. Numerical Renormalization Group (NRG) calculations seem to support a crossover from a Kondo-Singlet to an AF-Singlet for these regions. Instead, Quantum Monte Carlo and numerical VWF calculations do not give support for such a quantum phase transition to occur in the $U \rightarrow \infty$ limit of the TIA Hamiltonian. Our analytical VWF analysis is in line with these latter results for these extreme RKKY-AF cases: although with a very low correlation energy the Kondo-Doubet is formed on top of the AF configurations. Note that this result only applies in the analyzed limit of the TIA Hamiltonian and assuming that the RKKY-AF effects can be analyzed in a perturbative way. We have use this last property to obtain the standard RKKY result in Section IV C and also in Appendix C to obtain Eq. 60. Note also that in this limit one has $|Z_\delta(k)| \gg |Z_\delta(k)|$ and $|Z_{\delta}(k)|$ and thus the properties of the Doublet are determined mainly by its AF group of configurations.

We have restricted our previous analysis to the scenarios that are actually present in the analyzed limit of the TIA Hamiltonian: ferromagnetic RKKY regions coincide with the maxima of $|Z_Q(r)|$ and antiferromagnetic RKKY regions are in correspondence with $C_Q(r) \approx 0$. If one takes $C_Q$ and $\Sigma_R$ as free parameters, as is often done in NRG simulations using the Kondo Hamiltonian, one can achieve the following situation: a strong AF RKKY and $C_Q = 1$. In this case the self-consistent solution of Eq. 41 gives $\delta_o^2 \equiv 0$ and the doublet is not formed. This is a possible explanation for the contradictory numerical results present in the literature.

V. $C_Q$ IN THE 2D AND 3D SCENARIOS

In the previous Sections, when needed for graphical purposes, and because of its technological applications, we have evaluated our equations in the 1D case. In 1D the only decoherence factor, both for $C_Q$ and the RKKY, is the energy width of the packet of excitations involved in the interaction. In higher dimensions the angular decoherence effect dominates the behavior of $C_Q$ at values of $r$ lower than $\xi_K$. In “sintetic” TIA systems (magnetic impurities deposited over a carbon-nanotube, Quantum Dots connected to a Quantum wire or to a confined 2D electron gas in a semiconductor heterostructure, etc.) the effective Dimension is generally within 1D and 2D. The “classical” Two-Impurity Anderson problem corresponds to two magnetic impurities in a 3D metallic host. Here we analyze the behavior of $\delta$ and $\gamma$ in the 2D and
higher the lower ones. We have shown in Section III that the RKKY interaction generates a ferromagnetic alignment of the impurity spins without resort to the RKKY mechanism. We have also shown that the correlation energy of the Doublets is greater than the RKKY correlation energy for most of the Hamiltonian parameter-space. Here we show that the Kondo-Doublents interaction generates a ferromagnetic alignment of the impurity spins without resort to the RKKY mechanism.

Using for the Doublets VWF the simplest form given in Eq. (34), i.e. without the inclusion of the higher order RKKY effects discussed in Section V, the Doublet impurity spin-spin correlation \( \langle S_L S_R \rangle \) is given by

\[
\frac{\langle D | S_L S_R | D \rangle}{\langle D | D \rangle} = \frac{3}{4} \frac{D_Q(\delta, r)}{(2 \pm D_Q(\delta, r))},
\]

where \( D_Q = (\partial \delta I_Q)/(\partial \delta I_K) \) and the upper (lower) signs hold for the odd (even) Doublet.

In Fig. 10 it can be seen that the dominant Double favor a parallel (ferromagnetic) alignment of the impurity
spins. Note that this mainly ferromagnetic response is obtained without include the effects of the RKKY interaction in the Doublets structure.

This magnetic response can be clearly understood by a closer look to the first-order interaction behind the Doublets. Correlations between the impurities are the consequence of closed electron-paths that involve both impurities, paths driven by \( H_V \) in configurational space. For example, the second-order RKKY-FM path starts when one electron (say the one in the left impurity) hops to a band state \( k(>k_F) \) and then a second electron hops into the impurity, letting a hole \( q(<k_F) \) in the band. The path is closed by reversing these steps but at the other impurity. The matrix element for this loop, taking into account the mirror path, is

\[
\langle \uparrow\uparrow | H_V^4 | \uparrow\uparrow \rangle_{\text{RKKY}} = \mp \nu^4 \cos(k + q) \cdot r,
\]

where the plus sign holds for the FM state. This connectivity path produces the energy correction \( \mp \Sigma_R(r) \) for the FM (AF) state, which splits the FM and AF states. We use in this Section the direct orbital representation used for the FM (AF) state, which splits the FM and AF states. We use in this Section the direct orbital representation used in the unsymmetrized Hamiltonian, Eq. (11). Therefore, in the equation above, \( \langle \uparrow\uparrow \rangle \equiv \langle \text{FM} \uparrow \rangle \equiv d_{L,A}^\dagger d_{R,\uparrow}^\dagger |F\rangle \).

In this representation the vertex state of the odd Doublet, \( d_{A\uparrow}^\dagger |F\rangle \), is given by

\[
|A_\sigma \rangle \equiv \frac{1}{\sqrt{2}} (d_{R,\sigma}^\dagger \pm d_{L,\sigma}^\dagger) |F\rangle = \frac{1}{\sqrt{2}} (|0\sigma \rangle \mp |\sigma 0\rangle),
\]

where the plus sign is for the vertex of the even Doublet. As the starting state of the loop has a higher energy than the bunches of “visited” ones the energy associated with this interaction can not be obtained by perturbative methods.17,20 This situation, a single state connected to bunches of lower energy states, is the hallmark of a Kondo structure, in this case the Kondo Doublets that we have analyzed in the previous Sections.

With the analysis above at hand, the “ferromagnetic” behavior of the impurities induced by the Doublets is easy to understand. The correlated channel is the \( \sigma \sigma \) one, which corresponds to a ferromagnetic arrangement of the impurities (Eqs. (70a), (71b)). The configurations connected via the non-correlated \( \sigma \bar{\sigma} \) channel are also mainly ferromagnetic configurations at the maxima of \( \delta_D \). See also Eqs. (63), (64), for the dominant Doublet the connectivity factor of the ferro configurations is \( \sim 3(1 + |C_Q|)/2 \), whereas that of the antiferro ones is \( \sim (1 - |C_Q|)/2 \). Clearly, the screening action of the hole is more effective when the impurity-spins are aligned and the distance between them is near the resonant condition for the lowest energy holes \( (r \approx n\lambda_F^2/|\cos k_F r|) \sim 1 \), see Eq. (71b).

At the transition points from one Doublet to the other it is shown in Fig. 11 a little negative value for \( \langle S_L S_R \rangle \) and then a jump to positive values. Actually, at those transition points the Super-Singlet has a maximum in its correlation energy \( (\gamma \approx \delta_K) \) and it is formed with similar weights in both Doublets, thus an average of the response of the odd and even Doublets is to be expected at those regions, given a smooth transition with a \( \langle S_L S_R \rangle \) value near zero from one Doublet region to the next one. In Fig. 11 it is shown also the RKKY prediction, based upon \( \Sigma_R(r) \geq 0 \). Taking into account both interactions, the stronger of them determines the \( \langle S_L S_R \rangle \) response of the system, for \( \max(\delta_a,\delta_b) \gg |\Sigma_R| \) the response is determined by the Doublets curve (Eq. (67), Fig. III) whereas in the opposite situation the impurity-spin correlation tends to that of the RKKY.
Now we include the RKKY effects in the Doublets wave functions, and thus in their \( \langle S_L S_R \rangle \) correlation. Following the analysis of Section IV.D and Appendix C we take the variational amplitudes in the Doublets to be
\[
Z_S \sim \frac{1}{(\Delta_D - \Sigma_R + e_k)} \quad \text{for the ferro configurations and}
\]
\[
Z_A \sim \frac{1}{(\Delta_D + \Sigma_R + e_k)} \quad \text{for the antiferro ones, where}
\]
\[
\Delta_D = |\Sigma_R| + \gamma \delta_D(k) \]
as evaluated in the RKKY-Doublets section. Thus, including RKKY effects, the impurity-spin correlation of the odd Doublet is given by
\[
\langle S_L S_R \rangle = \frac{1}{A} \sum_k \frac{1}{(\Delta_D + \Sigma_R + e_k)^2},
\]
where \( D_Q^{S(A)} = D_Q(\Delta_D + \Sigma_R, r) \) and
\[
J^S(A) = \frac{1}{n_0 N_c} \sum_k \frac{1}{(\Delta_D + \Sigma_R + e_k)^2},
\]
and for the even Doublet the change \( D_Q \rightarrow -D_Q \) must be done. The \textit{supra} \( S(A) \) terms come from the contribution of the ferro (antiferro) configurations of the Doublet. Eq.\( (2) \) reduces to the previous Eq.\( (2) \) for \( \delta_D(r) \gg |\Sigma_R(r)| \). Eq.\( (2) \) reflects the changes in the energies of the FM and AF impurity configurations produced by the RKKY interaction. Thus in a RKKY-FM region the relative variational amplitude of the ferro configurations is greater than the one of the antiferro ones
\[
1/(\Delta_D + e_k) > 1/(2\Sigma_R + \Delta_D + e_k),
\]
given a ferro-like \( \langle S_L S_R \rangle \) correlation. The opposite is true in a RKKY-AF region. Note instead that the ferromagnetic response induced by the Kondo-Doublet interaction depends on the interference enhanced matrix elements, the \( (1 \pm D_Q) \) factors in Eq.\( (2) \), not in the difference of energy between the FM and AF impurity configurations.

In Fig.\( 12 \) we plot the \( \langle S_L S_R \rangle \) response of the Doublets, RKKY effects included, for the same 1D case plotted in Fig.\( 10 \). There is an abrupt change in the response of the dominated Doublet (thin lines): as \( \delta_\perp \) is exponentially small (see Fig.\( 8 \) the RKKY effects determine the response of the dominated Doublet. Thus the thin lines closely follow the RKKY response, jumping from 1/4 to \(-3/4 \) (and back) at the \( \Sigma_R(r) = 0 \) points. Instead, the dominant Doublet response (thick sections) is little modified by the RKKY interaction excepts at the extreme RKKY-AF point at \( k_F r \approx 2 \), where \( |\Sigma_R(r)| \gg \delta_\perp(r) \) and thus the RKKY-AF behavior dominates. As discussed in Fig.\( 4 \) this point corresponds to a maximum of the antiferromagnetic RKKY and to a minimum of the Kondo-Doublet interaction \( (C_Q \approx 0) \). Note also that the ferromagnetic response induced by the Kondo-Doublet interaction persists well into the RKKY-AF region.

For the Super-Singlet, Eq.\( (55) \), the \( \langle S_L S_R \rangle \) correlation is approximately given by a weighted average of the dominant and dominated Doublets response. The weighting factors are proportional to the average of the square of the corresponding amplitudes in the Super-Singlet VWF,
\[
Z_O(k) \sim 1/(\gamma + e_k) \quad \text{and} \quad Z_E(k) \sim 1/(\gamma + \Delta_\delta + e_k) \quad \text{respectively (in the \( \delta_\perp > \delta_\parallel \) case, that turn out to be proportional to \( 1/\gamma \) and \( 1/(\gamma + \Delta_\delta) \)).}
\]

VII. CONCLUSIONS

We have presented a simple and complete analysis of the two Anderson Impurity system. The variational wave
functions we use to analyze the problem are generated in each subspace of the Hamiltonian starting with the simplest configuration, and applying to it the hybridization terms, i.e., the non diagonal part of the Hamiltonian. The configurations so generated are grouped together with a variational amplitude function according with their internal symmetry. This step is repeated as many times as needed to bring out the physics of the state. One step is necessary for the Doublet states, two for the Super-Singlet, one to connect the Doublets through the Fermi Sea state and one to retain the internal structure of the Doublets, two more are included in Appendix C to show how the Doublets are affected by the RKKY interaction. In this aspect, the technical method we use is in fact an analytical Lanczos method, to some point similar to the one used in Ref.\textsuperscript{[23]}, but with variational functions as amplitude coefficients. Such variational functions are found by the classical method, i.e. Euler-Lagrange minimization of the energy functional, which is also evaluated analytically.

This method can be also applied to the case of $M$ impurities, specially if the symmetry group of the impurity arrangement is contained in the symmetry group of the metallic host. In such a case $M$ steps will be needed in the variational $M$-supersinglet to arrive to the states with $M$ electrons in the impurities, starting from the $|F\rangle$ vacuum state. But our conjecture is that, for a given set of system parameters the physical relevant state is the $M$-multiplet constructed by forming a Kondo singlet in the higher effective hybridization channel and filling the other effective impurities with one electron, as we do in Section III B to form our first approximation to the odd doublet. Starting from this $M$-multiplet, and going down, step after step, towards the $|F\rangle$ state, each successive step will introduce a exponentially small correction to the $M$-multiplet energy, as $\gamma$ correct $\delta_D$ in the case we analyzed, Section III C. Other impurity configurations, like three in a row, are also of interest. The equations of the three-in-a-row case can be easily obtained from the present study, by adding an impurity at the origin. In Appendix B we outline this case and show that for certain values of $r$ the effective hybridization is very large in the active channel. A full analysis will be presented elsewhere.

The TIA Kondo Doublet states generates a ferromagnetic Impurity-spin correlation, without resort to the RKKY interaction. The correlation energy gain of these Doublets, which is driven by a first-order direct coherence effect of the hybridization, exceeds that of the second-order RKKY interaction for most of the Hamiltonian parameter space $(J_n, r)$. These properties put the states we found well in the experimentally accessible range for Quantum Dots systems built on semiconductors devices\textsuperscript{[24]}, were most of the relevant parameters can be controlled by gate voltages.

A milestone of the Two Magnetic Impurities problem is the renormalization group analysis of Ref.\textsuperscript{[25,26]}, this work was carried out in the symmetrized basis too, but the $r$ dependence of the effective hybridization was treated in a crude fashion, just taking its value at $k = k_F$, the relevance of the increased value of the effective hybridization was missed. Nevertheless, the two energy scales found in that work can be traced to be the $\gamma$ and $\delta_D$ correlation energy gains of the supersinglet and the doublets. Their coupling parameters $J_n, J_e$ are related to the square of our effective hybridization terms, i.e., $\sim (1 \pm C_Q(\delta, r))$, and their “Kondo temperatures” $T_K(J_n), T_K(J_e)$ to our $\delta_D$ and $\gamma$, which are not the Kondo energies corresponding to $J_e$ and $J_n$, but Eq.\textsuperscript{[55]} and Eq.\textsuperscript{[56]}. We show that their relative relevance depends on the value of $C_Q(\delta_K, r)$, for $C_Q(\delta_K) \simeq 0$ both are equally relevant and both tend to $\delta_K$. Our results are also in perfect accord with the VWF numerical analysis of L. C. Andreani and H. Beck\textsuperscript{[20]}

Summarizing, our results confirm the general picture of the system behavior already known from numerical simulations but, thanks to our explicit VWF that we analytically solve in the different subspaces of the TIA, they also point out important differences with the usual interpretation of that numerical data. The main interaction between the impurities, contrary to the general belief, is not generated by the RKKY process but by the interference enhanced hybridization that generates the Kondo-Doubt states. The strength of this Kondo-Doublt interaction depends on the one-hole quantum interference factor $C_Q(r)$.

For inter-impurity distances $r$ around the maxima of $C_Q(r)$ a two-stage Kondo screening takes place. It is a correlated quenching of the total spin of the system, not the successive “one-impurity” Kondo screening of the odd and even hybridization channels\textsuperscript{[15]}\textsuperscript{[19]}. It also generates a strong ferromagnetic correlation between the impurity spins because the interference effects increase the weight of the ferro-like impurity configurations in the dominant Doublet. The ferromagnetic $r$-regions of the RKKY interaction are comprised in these zones. For low values of both the coupling constant $J_n$ and $r$ the RKKY interaction is strongest than the Kondo-Doublt interaction $(\Sigma_R > \delta_\gamma \gg \delta_K)$. However this has little effect in the structure of the TIA Kondo states because the ferro-like impurity configurations are already their main component. In a “temperature scheme”\textsuperscript{[15]} this situation $(\Sigma_R > \delta_\gamma)$ generates the intermediate triplet spin 1 phase between the high temperature uncorrelated impurity spins phase and the Doublet spin 1/2 region.

For $r$ near the zeros of $C_Q(r)$ there is not enhancement of the Kondo-Doublt energies $(\delta_\delta, \delta_\delta \simeq \delta_K)$ and the system behavior tends to that of two uncorrelated Kondo impurities. The maxima of the antiferromagnetic RKKY coincide with these points. If $-\Sigma_R > \delta_K$ the antiferro-like impurity configurations dominate the structure and response of the TIA Kondo states but, between the limits of our calculation, there is not a true quantum phase transition from the Kondo super-singlet to a AF-singlet\textsuperscript{14}.

We provide detailed formulas for the evaluation, in all
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APPENDIX A: M-CHANNEL SINGLET

Given that for an arrangement of $M$ magnetic impurities is always possible to construct an $M$-channel singlet, the first step of the $M$-supersinglet, is worthwhile to show that, although $\delta_{2M} \gg \delta_K$, its total energy, $E_M = -E_d - \delta_{2M}$ is always greater than the energy of $M$ decoupled Kondo singlets, $E_{dc} = M(-E_d - \delta_K)$. Therefore, Eq. (3), we must show that

$$-E_d - \delta_{2M} = -2M \nu^2 \sum_q \frac{1}{\delta_{2M} + e_q} , \quad (A1)$$

is always greater than

$$-M(E_d + \delta_K) = -M 2 \nu^2 \sum_q \frac{1}{\delta_K + e_q} . \quad (A2)$$

Comparing the sums term to term, we see that in each of them $\frac{1}{\delta_{2M} + e_q} > \frac{1}{\delta_{2M} + e_q}$ for $\delta_{2M} > \delta_K$. Thus $E_M > E_{dc}$ independently of the $D$, $E_d \gg \delta$ usual approximation and for any distribution of the conduction band hole states ($q$). In particular, this applies for $M= 2$, Section III A.

APPENDIX B: THREE-IN-A-ROW

For the three-in-a-row impurity case, two as analyzed in this paper plus one at the origin, one can take as normal modes of the impurities the following symmetrized combinations of the impurity orbitals

$$A = (-1/\sqrt{2}, \quad 0 \quad , \quad 1/\sqrt{2}) , \quad (B1)$$

$$S_1 = (1/\sqrt{3}, \quad 1/\sqrt{3}, \quad 1/\sqrt{3}) \quad , \quad (B2)$$

$$S_2 = (1/\sqrt{6}, \quad -2/\sqrt{6}, \quad 1/\sqrt{6}) \quad , \quad (B3)$$

In each of these combinations the first coefficient is the amplitude of the normal mode at the Left impurity, the second coefficient is the amplitude at the impurity at the origin and the third coefficient is the one corresponding to the Right impurity. The hybridization matrix elements, with the symmetric ($\sqrt{2} \cos k_x x$) and antisymmetric ($i\sqrt{2} \sin k_x x$) conduction band orbitals are

$$V_A = \langle d_A | H_{hyb} | c_{Ak} \rangle = 2 i \nu \sin k_x r/2 , \quad (B4)$$

for the combination $A$, as before, see Eq. (5), and

$$V_S_1 = \langle d_{S1} | H_{hyb} | c_{Sk} \rangle = \sqrt{\frac{2}{3}} \nu (1 + 2 \cos k_x r/2) , \quad (B5)$$

$$V_S_2 = \langle d_{S2} | H_{hyb} | c_{Sk} \rangle = \sqrt{\frac{2}{6}} \nu (-2 + 2 \cos k_x r/2) \quad (B6)$$

for the symmetric combinations $S$. Therefore for $r = 2\lambda_F$, one has $\{V_A \simeq 0, \; V_S_1 \simeq \sqrt{6} \nu, \; V_S_2 \simeq 0\}$ and a strong 3-multiplet can be proposed, formed upon a Kondo singlet in the $S_1$ impurity plus one electron in each one of the other impurity normal modes.

APPENDIX C: THE ODD DOUBLET IN AN EXTREME RKKY-AF REGION

In order to show the validity of Eq. (3) to analyze the RKKY effects in our doublets, we present here a partial deduction of it. Assuming we are in an extreme RKKY-AF region, we can drop the contribution of the FM-like impurity configurations to the odd doublet. Therefore we start with

$$|D_{or}\rangle = d_{Ak}^\dagger |F\rangle + i \sum_k Z_A(k) A_k b_{Ak}^\dagger |AF\rangle , \quad (C1)$$

applying $H_V$ to the $Z_A$ configurations one electron is removed from the impurities and transferred to the band states. Given the structure of $|AF\rangle$ there are four possibilities, two corresponding to the transfer of a symmetric electron (with a probability amplitude proportional to $S_q$) and the other two corresponding to the transfer of an antisymmetric electron ($\sim iA_q$), therefore the following states are added to the VWF

$$+ \sum_{k,q} A_k b_{Ak}^\dagger \{ i S_q [ Y_1(k,q) c_{Sq}^\dagger d_{S1}^\dagger |F\rangle - Y_2(k,q) c_{Sq}^\dagger d_{S1} |F\rangle ] - A_q [ Y_3(k,q) c_{AQ}^\dagger d_{Ak}^\dagger |F\rangle - Y_4(k,q) c_{AQ}^\dagger d_{Ak} |F\rangle ] \} \quad (C2)$$

applying again $H_V$, a big set of new configurations is generated. The ones with one electron in each impurity are the ones of lower energy, and of these, in order to maintain this presentation as simple as possible, we include here only the ones that contribute to the RKKY
interaction

\[ E_D = \langle D_{\sigma \uparrow}|H|D_{\sigma \uparrow}\rangle / \langle D_{\sigma \uparrow}|D_{\sigma \uparrow}\rangle . \]  \hspace{1cm} (C4)

The variational equations are solved in a progressive way, starting with the higher order amplitude factors

\[ X_1(k, q, p) = -2 \, v \, Y_1(k, q)/D_X(k, q, p), \]
\[ X_2(k, q, p) = -v \, (Y_2(k, q) - Y_2(p, q))/D_X(k, q, p), \]
\[ X_3(k, q, p) = -2 \, v \, Y_3(k, q)/D_X(k, q, p), \]
\[ X_4(k, q, p) = -2 \, v \, Y_4(k, q)/D_X(k, q, p), \]  \hspace{1cm} (C6)

where

\[ D_X(k, q, p) = -E_D - 2E_d + e_k + e_q + e_p. \]  \hspace{1cm} (C7)

Using the above results, the \( Y_i \) factors are found

\[ Y_1(k, q) = -2 \, v \, Z_A(k)/D_Y S(k, q) , \]
\[ Y_2(k, q) = -2 \, v \, Z_A(k)/D_Y S(k, q) + 4v^2 \sum_p (A^2_p Y_2(p, q)/D_X(k, q, p)) D_Y S(k, q) , \]
\[ Y_3(k, q) = -2 \, v \, Z_A(k)/D_Y C(k, q) , \]
\[ Y_4(k, q) = -2 \, v \, Z_A(k)/D_Y C(k, q) , \]  \hspace{1cm} (C8)

where

\[ D_Y S(k, q) = -E_D - E_d + e_k + e_q \]
\[ -4v^2 \sum_p A^2_p /D_X(k, q, p) , \]
\[ D_Y C(k, q) = -E_D - E_d + e_k + e_q \]
\[ -4v^2 \sum_p S^2_p /D_X(k, q, p) . \]  \hspace{1cm} (C9)

The \( Y_i \) factors carry the RKKY effects into the variational equation obtained for \( Z_A \), which is

\[ (E_D + 2E_d - e_k)Z_A(k) = v + \sum_q \{ \cos^2 \left( \frac{q \cdot r}{2} \right)(Y_1(k, q) + Y_2(k, q)) \]
\[ + \sin^2 \left( \frac{q \cdot r}{2} \right)(Y_3(k, q) + Y_4(k, q)) \} . \]  \hspace{1cm} (C10)

This is a self-consistent equation, the \( Y_i \) factors depend themselves on \( Z_A \). In order to solve it, and to obtain the standard expression for the RKKY contribution, the \( Y_i \) factors must be expanded in powers of \( v \), as already done in Section IV C

\[ Y_1(k, q) = Z_A(k)[v y_0(k, q) + v^2 y_{2S}(k, q)] , \]
\[ Y_2(k, q) = Y_1(k, q) + v^3 y_{2X}(k, q) , \]
\[ Y_3(k, q) = Z_A(k)[v y_0(k, q) + v^2 y_{2C}(k, q)] , \]
\[ Y_4(k, q) = Y_3(k, q) , \]  \hspace{1cm} (C11)

where, with \( D_Y (k, q) = -E_D - E_d + e_k + e_q, \)
\[ y_0(k, q) = -2/D_Y (k, q) , \]
\[ y_{2S}(k, q) = -8/D_Y^2(k, q) \sum_p \sin^2 \left( \frac{p \cdot r}{2} \right)/D_X(k, q, p), \]
\[ y_{2C}(k, q) = -8/D_Y (k, q) \sum_p \cos^2 \left( \frac{p \cdot r}{2} \right)/D_X(k, q, p), \]
\[ y_{2X}(k, q) = -8/D_Y (k, q) \sum_p \frac{Z_A(p) \sin^2 \left( \frac{p \cdot r}{2} \right)}{D_Y (k, q) D_X(k, q, p)}. \]  \hspace{1cm} (C12)

Using the above equations in the variational equation for \( Z_A(k) \), it is obtained

\[ Z_A(k) = \frac{-v(1 - v^3 \Gamma_Z)}{-E_D - 2E_d + e_k - \Sigma_Z} , \]  \hspace{1cm} (C13)

where

\[ \Gamma_Z = 8 \sum_{q, p} \frac{Z_A(p) \sin^2 \left( \frac{p \cdot r}{2} \right) \cos^2 \left( \frac{q \cdot r}{2} \right)}{D_Y (k, q) D_Y (q, p) D_X(k, q, p)} . \]
\[ \Sigma_Z = 4v^2 \sum_q \frac{1}{D_Y (k, q)} \]
\[ + 8v^4 \sum_{q, p} \frac{1 - \cos(q \cdot r) \cos(p \cdot r)}{D_Y^2 (k, q) D_X(k, q, p)} \]
\[ \approx 2\Sigma_{01} + \Sigma_{02} - \Sigma_R (r) . \]  \hspace{1cm} (C14)

Both \( \Gamma_Z \) and \( \Sigma_Z \) are very weakly dependent on \( e_k \), in fact it is a common practice to substitute factors of the kind \( 1/(E_d + e_k) \) by \( 1/E_d \) in the available calculus of the RKKY interaction, a notable exception is ref.\[27\] . In any case, such approximation overestimates the RKKY effects. \( \Sigma_{0i} \) is the order \( J_{ni} \) “one impurity” correction. \( \Gamma_Z \) can be evaluated by substituting \( Z_A(p) \) by its first-order approximation \( v/(E_D + 2E_d - e_p) \). \( \Gamma_Z \) gives a \( J_{ni} \) correction to the “connectivity” factor of the AF configurations.
involved in the odd doublet. In the equations above the sums over $k, p$ ($q$) are over “symmetrized” hole (electron) excitations. From Eqs. (C5, C13, and C14) the last term in the right side of Eq. (60) immediately follows.

We have analyzed the general situation, i.e. including the $Z_S$ FM-like configurations in the doublet (and the corresponding secondary configurations), in order to fully certify Eq. (60). Our “second quantization” Mathematica® package does the calculations needed for Eq. (C4) on the fly, a primitive version of this package was used in Refs. 28, 29. To bring those equations to ink, instead, will take a considerable amount of pages and time. The general procedure is similar to the one we outlined here for the extreme RKKY-AF case.

1. B. Coqblin and J. R. Schieffer, Phys. Rev. 185, 847 (1969).
2. N. J. Craig, J. M. Taylor, E. A. Lester, C. M. Marcus, M. P. Hanson, and A. C. Gossard, Science 304, 565 (2004).
3. P. Simon, Phys. Rev. B 71, 155319 (2005).
4. D. Goldhaber-Gordon, H. Shtrikman, D. Mahalu, D. Abusch-Magder, U. Meirav, and M. A. Kastner, Nature (London) 391, 156 (1998).
5. C. R. Proetto and A. López, Phys. Rev. B 25, 7037 (1982).
6. S. Galkin, C. A. Balseiro, and M. Avignon, Euro. Phys. J. B 38, 519 (2004).
7. R. Allub, Phys. Rev. B 67, 144416 (2003).
8. C. Jayaprakash, H. R. Krishna-murthy, and J. W. Wilkins, J. Appl. Phys. 53, 2142 (1982).
9. B. A. Jones and C. M. Varma, Phys. Rev. Lett. 58, 843 (1987).
10. C. Jayaprakash, H. R. Krishna-murthy, and J. W. Wilkins, Phys. Rev. Lett. 47, 737 (1981).
11. B. A. Jones, C. M. Varma, and J. W. Wilkins, Phys. Rev. Lett. 61, 125 (1988).
12. K. Ingersent, B. A. Jones, and J. W. Wilkins, Phys. Rev. Lett. 69, 2594 (1992).
13. J. B. Silva, W. L. C. Lima, W. C. Oliveira, J. N. L. Mello, L. N. Oliveira, and J. W. Wilkins, Phys. Rev. Lett. 76, 275 (1996).
14. B. A. Jones, Ph.D. thesis, Cornell University (1987).
15. R. M. Fye and J. E. Hirsch, Phys. Rev. B 40, 4780 (1989).
16. P. Schlottmann, Phys. Rev. Lett. 80, 4975 (1998).
17. C. M. Varma and Y. Yafet, Phys. Rev. B 13, 2950 (1976).
18. T. Saso, Phys. Rev. B 44, 450 (1991).
19. T. Saso and H. Kato, Progress of Theoretical Physics 87, 331 (1992).
20. L. C. Andreani and H. Beck, Phys. Rev. B 48, 7322 (1993).
21. P. Simon, R. López, and Y. Oreg, Phys. Rev. Lett. 94, 086602 (2005).
22. G. V. Vavilov and L. I. Glazman, Phys. Rev. Lett. 94, 086805 (2005).
23. V. I. Litvinov and V. K. Dugaev, Phys. Rev. B 58, 3584 (1998).
24. J. Simonin, cond-mat 0503163 (2005).
25. J. D. Mancini and D. C. Mattis, Phys. Rev. B 28, 6061 (1983).
26. H. Tamura, K. Shiraishi, and H. Takayanagi, J. J. Applied Phys. 43, L691 (2004).
27. C. R. Proetto, Ph.D. thesis, Instituto Balseiro (1985).
28. M. E. Simon and A. A. Aligia, Phys. Rev. B 49, 13061 (1994).
29. J. Simonin and R. Allub, Phys. Rev. Lett. 74, 466 (1995).