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Magnetic correlations between two Kondo impurities with two magnetic configurations: Narrow-band limit

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ABSTRACT

The lowest excitation energy and the magnetic correlations $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle$ between two magnetic impurities are analyzed within the two-magnetic-impurity model Hamiltonian. The model includes two magnetic ions that can exist in two valence states and a band of conduction electrons. The two localized states represent the ground states of the ionic configurations $(5f)^n$ and $(5f)^{n+1}$, assumed to be a doublet and a triplet, respectively. In the zero band-width limit, three parameters characterize this model: the energy difference between the magnetic configurations (Δ), the localized-extended-state hybridization energy (V), and the relationship between the Fermi wavelength and the distance $\vec{\mathbf{r}}$ between the magnetic ions ($\phi = \vec{\mathbf{k}}_F \cdot \vec{\mathbf{r}}$). For $\phi \to 0$, the strong coupling regime takes place and the physics that governs the ground state depends on Δ/V. For $V \ll -\Delta$, the highest spin configuration is favored, and the model shows a triplet ground state and the coexistence of strong ferromagnetic (F) correlations between the impurities with the Kondo physics of two magnetic impurities. For $V < -\Delta$, with major charge fluctuations between the magnetic configurations, a singlet ground state occurs and antiferromagnetic (AF) correlations between the impurities appear. When ϕ increases, the decoupling of the impurities proceeds and $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle$ decreases, finally for $\phi = \pi/2$ the decoupled limit takes place and the model is reduced to two independent ions ($\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle = 0$). For a narrow region of Δ/V, when ϕ increases, the model shows the crossover from singlet (AF) ground state to triplet (F) ground state.

1. Introduction

The behavior of 4*f* or 5*f* states in heavy fermion (HF) materials is one of the most interesting open problems in solid-state physics. Experimentally, these systems show very peculiar properties including Kondo effect, magnetic order, superconductivity, etc. [1]. From the theoretical point of view, the essential physical ingredients to describe HF compounds are (i) a lattice of localized magnetic orbitals; (ii) a structureless non-interacting conduction band; and (iii) a hybridization matrix element which mixes the localized and conduction band states [2]. Therefore, at high temperatures, HF systems behave like a collection of individual local moments. On the contrary, at low temperatures, correlations take place and the Kondo effect can occur. This screening can quench the magnetic interaction between local moments. The interplay between both mechanisms is a long-standing problem and remains unclear.

In order to solve this very interesting problem and taking into account that systems with more than one impurity are considerably more complicated, much of the work has focused on the two-impurity Anderson (TIA) model [3–19], and its integer valence limit, the two-impurity Kondo (TIK) model [20–37]. The TIA is the simplest model that can be studied to analyze the interplay between the Ruderman–Kittel–Kasuya–Yosida (RKKY) interaction which favors magnetic ordering of the impurities and the Kondo effect which works against order since it tends to quench individual impurity spins. This interplay is thought to be the most relevant mechanism for understanding the magnetic properties in many heavy fermions compounds [38]. However, it is interesting to point out that the Anderson model describes transitions between one magnetic and one nonmagnetic configuration, as in Ce or Yb compounds. Nevertheless, the problem is different in some actinide systems [39], such as Uranium and Neptunium compounds, where the involved 5*f* electrons can fluctuate between two magnetic configurations and the degree of localization or mixed-valence depends on the compound. For US compounds, the experimental data suggest a mixed-valence scenario [40]. On the contrary, for UTe [40], $UCo_{0.5}Sb_2$ [41], among other compounds, the coexistence of Kondo effect and ferromagnetic order has been detected experimentally showing an important localized character of 5*f* electrons. Similar results are also obtained in Np compounds such as $NpNiSi_2$ [42] or Np_2PdGa_3 [43].

Motivated by this scenario we consider in this paper the problem of two magnetic impurities fluctuating between two magnetic configurations. To this end we resort to the theory

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of valence fluctuation phenomena. In order to calculate spin and charge dynamical susceptibilities in Tm compounds, Mazzaferro et al. [44] presented a theory of intermediate valence between two magnetic configurations. Their results can explain the most important features of the neutron-scattering spectrum of TmSe, with TmSe fluctuating between two magnetic configurations: Tm^{3+} ($J=6$) and Tm^{2+} ($J=7/2$). They show that one of the most important features of the model is the existence of two magnetic configurations, which makes the difference with the Anderson model. The effective magnetic moment does not disappear at intermediate valence if the fluctuations take place between two magnetic configurations. This model was also studied by Allub et al. [45] using Wilson's renormalization group . The aim of this work is to present the narrow-band approximation [46–51] to solve a straightforward extension of this model: the problem of two magnetic impurities fluctuating between two magnetic configurations. We consider that this is the simplest approach to describe the competition between local hybridization and magnetic order.

In the following section we introduce the model Hamiltonian and set up the zero-bandwidth approximation to this problem. Section 3 presents the numerical results and discusses their physical implications. Section 4 consists of the conclusions.

2. Model

Beginning with the model for one magnetic impurity fluctuating between two magnetic configurations [45], we extend it to include two magnetic impurities and the following model Hamiltonian may be written:

$$H = H_b + H_f + H_{hyb}. \tag{1}$$

The first term represents the band Hamiltonian

$$H_b = \sum_{\vec{k},\sigma} \epsilon_{\vec{k}} c^{\dagger}_{\vec{k}\,\sigma} c_{\vec{k}\,\sigma}, \tag{2}$$

where $c^{\dagger}_{\vec{k}\,\sigma}$ ($c_{\vec{k}\,\sigma}$) creates (destroys) an electron with momentum $\vec{\mathbf{k}}$ and spin σ in the conduction band, and $\epsilon_{\vec{k}}$ is the energy of conduction electrons.

The second term stands for the localized f states in the magnetic ions

$$H_f = E_{1/2} \sum_{j=1,2} (|\uparrow_j\rangle\langle\uparrow_j| + |\downarrow_j\rangle\langle\downarrow_j|) + E_1 \sum_{j=1,2} (|+_j\rangle\langle+_j| + |0_j\rangle\langle 0_j| + |-_j\rangle\langle-_j|), \tag{3}$$

where, in bracket notation, the lowest spin configuration of each ion at site $\vec{\mathbf{R}}_j$ is represented by the spin-1/2 states ($|\uparrow_j\rangle$ for $S_z=+1/2$ and $|\downarrow_j\rangle$ for $S_z=-1/2$), and the highest spin configuration is represented by the spin-1 states ($|+_j\rangle$ for $S_z=+1$, $|0_j\rangle$ for $S_z=0$, and $|-_j\rangle$ for $S_z=-1$). $E_{1/2}$ and E_1 are the energies of the two accessible valence states. Furthermore, in this paper we consider 1 localized electron in the lowest spin configuration and 2 electrons in the highest spin configuration [45].

The third term is the hybridization Hamiltonian, whereby the ionic configuration changes by emission or absorption of a conduction electron and is given by

$$H_{hyb} = \sum_{\vec{k}\,j} \left[V_{\vec{k}\,j} (c^{\dagger}_{\vec{k}\,\uparrow} |\uparrow_j\rangle\langle+_j| + c^{\dagger}_{\vec{k}\,\downarrow} |\downarrow_j\rangle\langle-_j|) + H.c. \right] + \frac{1}{\sqrt{2}} \sum_{\vec{k}\,j} \left[V_{\vec{k}\,j} (c^{\dagger}_{\vec{k}\,\downarrow} |\uparrow_j\rangle\langle 0_j| + c^{\dagger}_{\vec{k}\,\uparrow} |\downarrow_j\rangle\langle 0_j|) + H.c. \right], \tag{4}$$

where the matrix elements in H_{hyb} are taken as to preserve rotational symmetry and we define $V_{\vec{k}\,j} = V e^{i\vec{\mathbf{k}}\cdot\vec{\mathbf{R}}_j}$, with V the hybridization strength. The first term $c^{\dagger}_{\vec{k}\,\uparrow} |\uparrow_j\rangle\langle+_j|$ destroys at site j the ionic state with $S_z=+1$ in the highest spin configuration and creates a conduction electron in a $\vec{k}$ state with spin $\uparrow$ and a localized electron in the lowest spin configuration with spin $\uparrow$. The following terms in Eq. (4) act in similar manner with the different spin z component. Note that H_{hyb} is the term which allows, through the conduction electrons, the charge transfer from one impurity site to the other. For only one impurity (i.e., $j=1$), Eq. (1) reduces exactly to the model considered in Ref. [45].

Exact treatment of the many-body Hamiltonian (1) is an unsolvable problem. This is why, as a first approach to solve this problem and taking into account the fact that essentially, in most experiments, only levels close to the Fermi energy are relevant, here we study the zero-bandwidth (ZBW) limit of this model. For this purpose, following our previous work [16], we simplify the conduction band by a few extended states, located precisely at the Fermi energy (ϵ_F). Therefore, we represent the conduction band by two $\vec{\mathbf{k}}$ states: $\vec{\mathbf{k}}_1 = \vec{\mathbf{k}}_F$ and $\vec{\mathbf{k}}_2 = -\vec{\mathbf{k}}_F$, with $\vec{\mathbf{k}}_F$ the Fermi momentum. Accordingly, the band Hamiltonian reduces to

$$H_b = \sum_{\vec{k}_m,\sigma} \epsilon_{\vec{k}_m} c^{\dagger}_{\vec{k}_m\sigma} c_{\vec{k}_m\sigma} = \epsilon_F \sum_{\sigma} \left(c^{\dagger}_{\vec{k}_1\sigma} c_{\vec{k}_1\sigma} + c^{\dagger}_{\vec{k}_2\sigma} c_{\vec{k}_2\sigma} \right), \tag{5}$$

and H_{hyb} gives

$$H_{hyb} = V \sum_{\vec{k}_m j} \left[e^{i\vec{\mathbf{k}}_m\cdot\vec{\mathbf{R}}_j} \left(c^{\dagger}_{\vec{k}_m\uparrow} |\uparrow_j\rangle\langle+_j| + c^{\dagger}_{\vec{k}_m\downarrow} |\downarrow_j\rangle\langle-_j| \right) + H.c. \right] + \frac{V}{\sqrt{2}} \sum_{\vec{k}_m j} \left[e^{i\vec{\mathbf{k}}_m\cdot\vec{\mathbf{R}}_j} \left(c^{\dagger}_{\vec{k}_m\downarrow} |\uparrow_j\rangle\langle 0_j| + c^{\dagger}_{\vec{k}_m\uparrow} |\downarrow_j\rangle\langle 0_j| \right) + H.c. \right]. \tag{6}$$

Defining $c^{\dagger}_{1\sigma} = e^{i\vec{\mathbf{k}}_1\cdot\vec{\mathbf{R}}_2} c^{\dagger}_{\vec{k}_1\sigma}$, $c^{\dagger}_{2\sigma} = e^{i\vec{\mathbf{k}}_2\cdot\vec{\mathbf{R}}_1} c^{\dagger}_{\vec{k}_2\sigma}$, and $\phi = \vec{\mathbf{k}}_1\cdot(\vec{\mathbf{R}}_1 - \vec{\mathbf{R}}_2) = \vec{\mathbf{k}}_F\cdot(\vec{\mathbf{R}}_1 - \vec{\mathbf{R}}_2)$, we can write the ZBW limit of H as

$$\begin{aligned} H_{ZBW} = {} & \epsilon_F \sum_{\sigma} (c^{\dagger}_{1\sigma} c_{1\sigma} + c^{\dagger}_{2\sigma} c_{2\sigma}) + E_{1/2} \sum_{j=1,2} (|\uparrow_j\rangle\langle\uparrow_j| + |\downarrow_j\rangle\langle\downarrow_j|) \\ & + E_1 \sum_{j=1,2} (|+_j\rangle\langle+_j| + |0_j\rangle\langle 0_j| + |-_j\rangle\langle-_j|) \\ & + V \Big\{ \left[(e^{i\phi} c^{\dagger}_{1\uparrow} + c^{\dagger}_{2\uparrow}) |\uparrow_1\rangle\langle+_1| + (e^{i\phi} c^{\dagger}_{1\downarrow} + c^{\dagger}_{2\downarrow}) |\downarrow_1\rangle\langle-_1| + H.c. \right] \\ & + \left[(c^{\dagger}_{1\uparrow} + e^{i\phi} c^{\dagger}_{2\uparrow}) |\uparrow_2\rangle\langle+_2| + (c^{\dagger}_{1\downarrow} + e^{i\phi} c^{\dagger}_{2\downarrow}) |\downarrow_2\rangle\langle-_2| + H.c. \right] \\ & + \frac{1}{\sqrt{2}} \left[(e^{i\phi} c^{\dagger}_{1\uparrow} + c^{\dagger}_{2\uparrow}) |\downarrow_1\rangle\langle 0_1| + (e^{i\phi} c^{\dagger}_{1\downarrow} + c^{\dagger}_{2\downarrow}) |\uparrow_1\rangle\langle 0_1| + H.c. \right] \\ & + \frac{1}{\sqrt{2}} \left[(c^{\dagger}_{1\uparrow} + e^{i\phi} c^{\dagger}_{2\uparrow}) |\downarrow_2\rangle\langle 0_2| + (c^{\dagger}_{1\downarrow} + e^{i\phi} c^{\dagger}_{2\downarrow}) |\uparrow_2\rangle\langle 0_2| + H.c. \right] \Big\}. \end{aligned} \tag{7}$$

Measuring energies from the Fermi level ($\epsilon_F = 0$), the model is completely characterized by three parameters: $\Delta = (E_1 - E_{1/2})/2$ (the energy difference between the two configurations), V, and ϕ. The Hilbert space of the localized electrons in the model under consideration reduces to 25 states which we define as: 4 two-particle $|\sigma_1\sigma_2\rangle$ states, 12 three-particle $|Sz_i\sigma_j\rangle$ states, and 9 four-particle $|Sz_1Sz_2\rangle$ states, with $Sz_j = +_j, -_j$, 0_j and $\sigma_j = \uparrow_j, \downarrow_j$. The magnetic properties of H_{ZBW} can be obtained from the six-particle states ($N=6$) or from the grand canonical ensemble adjusting the chemical potential fixing the average number of particles in the system. Both methods give the same physical

results and here we consider the solution in the subspace of $N=6$. For this case, the full Hamiltonian matrix is 106×106: 4 states with 4 conduction electrons and 2 localized electrons ($c^\dagger_{1\uparrow}c^\dagger_{1\downarrow}c^\dagger_{2\uparrow}c^\dagger_{2\downarrow}|\sigma_1\sigma_2\rangle$), 48 states with 3 conduction electrons and 3 localized ($c^\dagger_{l\uparrow}c^\dagger_{l\downarrow}c^\dagger_{l'\sigma}|Sz_i\sigma_j\rangle$), and 54 states with 2 conduction electrons and 4 localized($c^\dagger_{l\sigma}c^\dagger_{l'\sigma'}|Sz_1Sz_2\rangle$).

For $\phi=\pi/2$ (or $\pm(2n+1)\pi/2$), H_{ZBW} corresponds to two independent magnetic impurities and we can write $H_{ZBW}(\phi=\pi/2)=H_{I1}+H_{I2}$, with

$$\begin{aligned}H_{Ij}=&\epsilon_F\sum_\sigma\gamma^\dagger_{j\sigma}\gamma_{j\sigma}+E_{1/2}(|\uparrow_j\rangle\langle\uparrow_j|+|\downarrow_j\rangle\langle\downarrow_j|)\\&+E_1(|+_j\rangle\langle+_j|+|0_j\rangle\langle0_j|+|-_j\rangle\langle-_j|)\\&+\sqrt{2}V\Big\{\Big[\gamma^\dagger_{j\uparrow}|\uparrow_j\rangle\langle+_j|+\gamma^\dagger_{j\downarrow}|\downarrow_j\rangle\langle-_j|+H.c.\Big]\\&+\frac{1}{\sqrt{2}}\Big[\gamma^\dagger_{j\uparrow}|\downarrow_j\rangle\langle0_j|+\gamma^\dagger_{j\downarrow}|\uparrow_j\rangle\langle0_j|+H.c.\Big]\Big\},\end{aligned}\tag{8}$$

where we define $\gamma^\dagger_{1\sigma}=(ic^\dagger_{1\sigma}+c^\dagger_{2\sigma})/\sqrt{2}$, and $\gamma^\dagger_{2\sigma}=(c^\dagger_{1\sigma}+ic^\dagger_{2\sigma})/\sqrt{2}$. In this particular case, each impurity can be solved independently in a given Hilbert space and we obtain the decoupled (DC) limit of this model. It is interesting to note that the ground state in this limit corresponds to the fixed point Hamiltonian obtained, in the strong coupling regime, by the renormalization-group approach for one impurity problem [45]. In principle, the Hilbert space corresponding to H_{Ij} comprises just 20 states: four possible occupations of the extended (γ) orbital (0, ↑, ↓, and ↑↓), and five possible localized states ($|\uparrow_j\rangle,|\downarrow_j\rangle,|+_j\rangle,|0_j\rangle$, and $|-_j\rangle$). Nevertheless, two-particle and three-particle states are only relevant for mixing in H_{Ij} and it is easy to see that the lowest energy level corresponds to three-particle states with spin $S=1/2$. Therefore, taking six-particle states in H_{ZBW}, the DC limit corresponds to two identical impurities, each one in the subspace of three-particle states. Therefore, the ground state energy is four-times degenerated: one state with $S=0$ and three states with $S=1$.

For $\phi=0$ (or $\pm n\pi$), H_{ZBW} reduces to the strong coupling (SC) limit of this model, where both impurities are coupled through only one band state and the model Hamiltonian can be written as $H_{ZBW}(\phi=0)=H'+H''$, where we define

$$\begin{aligned}H'=&\epsilon_F\sum_\sigma\alpha^\dagger_{1\sigma}\alpha_{1\sigma}+E_{1/2}\sum_{j=1,2}(|\uparrow_j\rangle\langle\uparrow_j|+|\downarrow_j\rangle\langle\downarrow_j|)\\&+E_1\sum_{j=1,2}(|+_j\rangle\langle+_j|+|0_j\rangle\langle0_j|+|-_j\rangle\langle-_j|)\\&+\sqrt{2}V\sum_{j=1,2}\Big\{\Big[\alpha^\dagger_{1\uparrow}|\uparrow_j\rangle\langle+_j|+\alpha^\dagger_{1\downarrow}|\downarrow_j\rangle\langle-_j|+H.c.\Big]\\&+\frac{1}{\sqrt{2}}\Big[\alpha^\dagger_{1\uparrow}|\downarrow_j\rangle\langle0_j|+\alpha^\dagger_{1\downarrow}|\uparrow_j\rangle\langle0_j|+H.c.\Big]\Big\}\end{aligned}\tag{9}$$

and

$$H''=\epsilon_F\sum_\sigma\alpha^\dagger_{2\sigma}\alpha_{2\sigma},\tag{10}$$

with $\alpha^\dagger_{1\sigma}=(c^\dagger_{1\sigma}+c^\dagger_{2\sigma})/\sqrt{2}$ and $\alpha^\dagger_{2\sigma}=(c^\dagger_{1\sigma}-c^\dagger_{2\sigma})/\sqrt{2}$. Therefore, the SC limit can be solved by a diagonalization of H'. The corresponding subspace includes 100 states: for each four possible occupations of the extended (α) orbital (0, ↑, ↓, and ↑↓), there are twenty-five localized states ($|\sigma_1\sigma_2\rangle$, $|Sz_i\sigma_j\rangle$, and $|Sz_1Sz_2\rangle$).

The ground state properties of H' depend on the parameter Δ/V. There is a critical value $\Delta_{C0}/V\simeq-1.49$ such that for $\Delta<\Delta_{C0}$, the ground state energy corresponds to a five-particle states with $S=3/2$. On the contrary, for $\Delta>\Delta_{C0}$, the ground state energy corresponds to a four-particle state with $S=0$. Therefore, to study the six-particle subspace of H_{ZBW}, we must take only direct products of the H' states by the H'' states: four-particle states in H' with two-particle states in H'', five-particle states in H' with one-particle states in H'', and finally six-particle states in H'.

3. Results and discussion

For the one impurity case, the coupling of the local spin to the conduction electrons is ferromagnetic if the lowest spin configuration is energetically favored ($\Delta=(E_1-E_{1/2})/2>0$) and antiferromagnetic (Kondo) if the highest spin configuration is energetically favored ($\Delta<0$) [45]. Therefore, to study the magnetic correlations between two Kondo impurities we consider in this paper $\Delta<0$. In what follow we discuss the two limiting cases ($\phi=\vec{\mathbf{k}}_F\cdot(\vec{\mathbf{R}}_1-\vec{\mathbf{R}}_2)=\pi/2$ or 0) and the general case.

3.1. The decoupled limit: $\phi=\pi/2$

Let us first consider the decoupled limit. Following our previous discussion, we solve Eq. (8) for three-particle states. Let $|N,S,S_Z\rangle_{Ij}$ denotes the eigenstate of H_{Ij} with N particles, spin S, and z component of spin S_Z. It is easy to obtain

(i) 4 states with $S=3/2$ and energy $\lambda^{(4)}_{Ij,3,3/2}=E_1$:
$|3,3/2,+3/2\rangle_{Ij}=\gamma^\dagger_{j\uparrow}|+_j\rangle$,
$|3,3/2,+1/2\rangle_{Ij}=(\gamma^\dagger_{j\downarrow}|+_j\rangle+\sqrt{2}\gamma^\dagger_{j\uparrow}|0_j\rangle)/\sqrt{3}$,
$|3,3/2,-1/2\rangle_{Ij}=(\gamma^\dagger_{j\uparrow}|-_j\rangle+\sqrt{2}\gamma^\dagger_{j\downarrow}|0_j\rangle)/\sqrt{3}$, and
$|3,3/2,-3/2\rangle_{Ij}=\gamma^\dagger_{j\downarrow}|-_j\rangle$.

(ii) 4 states with $S=1/2$ and energies $\lambda^{(2)}_{Ij,3,1/2,\pm}=0.5(E_{1/2}+E_1)\pm R$:
$|3,1/2,+1/2,\pm\rangle_{Ij}=a_{I\pm}\gamma^\dagger_{j\uparrow}\gamma^\dagger_{j\downarrow}|\uparrow_j\rangle+b_{I\pm}(\sqrt{2}\gamma^\dagger_{j\downarrow}|+_j\rangle-\gamma^\dagger_{j\uparrow}|0_j\rangle)/\sqrt{3}$,
$|3,1/2,-1/2,\pm\rangle_{Ij}=a_{I\pm}\gamma^\dagger_{j\uparrow}\gamma^\dagger_{j\downarrow}|\downarrow_j\rangle+b_{I\pm}(-\sqrt{2}\gamma^\dagger_{j\uparrow}|-_j\rangle+\gamma^\dagger_{j\downarrow}|0_j\rangle)/\sqrt{3}$,

with $a_{I\pm}=\sqrt{(1\mp\Delta/R)/2}$, $b_{I\pm}=\sqrt{(1\pm\Delta/R)/2}$, and $R=\sqrt{\Delta^2+3V^2}$.

This is the physical scenario, in the ZBW approximation, of an intermediate-valence impurity fluctuating between two magnetic configurations: the degenerate $S=1/2$ ground state, $|3,1/2,\pm1/2,-\rangle_{Ij}$, is a mixing of both magnetic configurations.

For $\Delta<0$ and $|\Delta|\gg V$, the model is reduced to the Kondo problem in this system and the ground state energy (two-times degenerate) is $\lambda^{(2)}_{IjK}\simeq E_1-1.5(V^2/|\Delta|)$ corresponding to $(\sqrt{2}\gamma^\dagger_{j\downarrow}|+_j\rangle-\gamma^\dagger_{j\uparrow}|0_j\rangle)/\sqrt{3}$ and $(-\sqrt{2}\gamma^\dagger_{j\uparrow}|-_j\rangle+\gamma^\dagger_{j\downarrow}|0_j\rangle)/\sqrt{3}$. The first excited states (spin excitations) are given in (i), and it is straightforward to see that the physics that governs the low excitation energies is given by an s–d Hamiltonian with antiferromagnetic (Kondo) coupling between conduction electrons and spin-1 local moment [45]. Here, the Kondo energy is $E_{IK}=1.5(V^2/|\Delta|)$.

As in the case of ZBW Anderson model [46,47], many physical results of the one impurity problem can be qualitatively understood in this simple theoretical picture [48].

3.2. The strong coupling limit: $\phi=0$

For $\phi=\vec{\mathbf{k}}_F\cdot(\vec{\mathbf{R}}_1-\vec{\mathbf{R}}_2)=0$, the SC limit occurs and the ground state of H' depends on Δ/V:

(a) For $\Delta<\Delta_{C0}$, H' gives four five-particle states with $S=3/2$ and energy $\lambda'^{(4)}_{5,3/2}=0.5(3E_1+E_{1/2})-R'$, with $R'=\sqrt{\Delta^2+5V^2}$. The five-particle state with $S=3/2$ and $S_z=+3/2$ reads $|5,3/2,+3/2\rangle=a_0\big[2\alpha^\dagger_{1\downarrow}|+_1+_2\rangle-\alpha^\dagger_{1\uparrow}(|+_1 0_2\rangle+|\ 0_1+_2\rangle)/\sqrt{2}\big]/\sqrt{5}+b_0\alpha^\dagger_{1\uparrow}\alpha^\dagger_{1\downarrow}(|+_1\uparrow_2\rangle+|\uparrow_1+_2\rangle)/\sqrt{2}$, where $a_0=\sqrt{(1-\Delta/R')/2}$ and $b_0=\sqrt{(1+\Delta/R')/2}$.

It is straightforward to write the other z component states: $|5,3/2,+1/2\rangle$, $|5,3/2,-1/2\rangle$, and $|5,3/2,-3/2\rangle$.

(b) For $\Delta>\Delta_{C0}$, the lowest eigenvalue ($\lambda'_{4,0}$) of H' results from the diagonalization of a 3×3 matrix (four-particle states with

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$S=0$) given by

$$\begin{vmatrix} 2E_1 & -2V & 0 \\ -2V & (E_1+E_{1/2}) & \sqrt{6}V \\ 0 & \sqrt{6}V & 2E_{1/2} \end{vmatrix}, \quad (11)$$

and the corresponding eigenvector (a'_0, b'_0, and c'_0) allows us to write the ground state as

$$|4,0,0\rangle = a'_0[|+_1-_2\rangle - |0_1 0_2\rangle + |-_1+_2\rangle]/\sqrt{3} + b'_0\left[\alpha^\dagger_{1\uparrow}(|0_1\downarrow_2\rangle + |\downarrow_1 0_2\rangle - \sqrt{2}|-_1\uparrow_2\rangle - \sqrt{2}|\uparrow_1-_2\rangle)/\sqrt{6}\right]/\sqrt{2} + b'_0\left[\alpha^\dagger_{1\downarrow}(|0_1\uparrow_2\rangle + |\uparrow_1 0_2\rangle - \sqrt{2}|+_1\downarrow_2\rangle - \sqrt{2}|\downarrow_1+_2\rangle)/\sqrt{6}\right]/\sqrt{2} + c'_0\alpha^\dagger_{1\uparrow}\alpha^\dagger_{1\downarrow}(|\uparrow_1\downarrow_2\rangle - |\downarrow_1\uparrow_2\rangle)/\sqrt{2}.$$

In Fig. 1, solid line shows the energy difference ($\lambda'_{4,0}-\lambda'_{5,3/2}$) as a function of Δ and we can see the critical value $\Delta_{C0}/V\simeq -1.494$, defined by ($\lambda'_{4,0}-\lambda'_{5,3/2}$)$=0$. The dashed line corresponds to ($\lambda'_{4,1}-\lambda'_{5,3/2}$) with $\lambda'_{4,1}$, the lowest eigenvalue (three-times degenerate $\lambda'^{(3)}_{4,1}$) of four-particle states with $S=1$, obtained from the 4×4 matrix

$$\begin{vmatrix} 2E_1 & -\frac{2\sqrt{2}}{\sqrt{3}}V & -\frac{2}{\sqrt{3}}V & 0 \\ -\frac{2\sqrt{2}}{\sqrt{3}}V & (E_1+E_{1/2}) & 0 & \frac{\sqrt{2}}{\sqrt{3}}V \\ -\frac{2}{\sqrt{3}}V & 0 & (E_1+E_{1/2}) & \frac{4}{\sqrt{3}}V \\ 0 & \frac{\sqrt{2}}{\sqrt{3}}V & \frac{4}{\sqrt{3}}V & 2E_{1/2} \end{vmatrix}. \quad (12)$$

($\lambda'_{4,1}-\lambda'_{5,3/2}$)$=0$, defines the critical value $\Delta'_{C0}/V\simeq -1.156$.

Thus, in Fig. 1 we distinguish two different ground states: a quadruplet (singlet) ground state for $\Delta<\Delta_{C0}$ ($\Delta>\Delta_{C0}$) and three different first excited states, depending on the value of Δ/V. For $\Delta<\Delta_{C0}$, the first excited state is $|4,0,0\rangle$ (solid line); for $\Delta_{C0}<\Delta<\Delta'_{C0}$, the first excited states are $|5,3/2,S_Z\rangle$ (dotted line), and finally, for $\Delta>\Delta'_{C0}$, the first excited states are $|4,1,S_Z\rangle$ (dashed line). From these results, it is easy to write (by adding one or two electrons in the decoupled α_2 orbital) the six-particle states ($|6,S,S_Z\rangle$) of $H_{ZBW}(\phi=0)$. For spin-2 states we can write

$$|6,2,+2\rangle = \alpha^\dagger_{2\uparrow}|5,3/2,+3/2\rangle,$$
$$|6,2,+1\rangle = \left[\alpha^\dagger_{2\downarrow}|5,3/2,+3/2\rangle + \sqrt{3}\alpha^\dagger_{2\uparrow}|5,3/2,+1/2\rangle\right]/2,$$

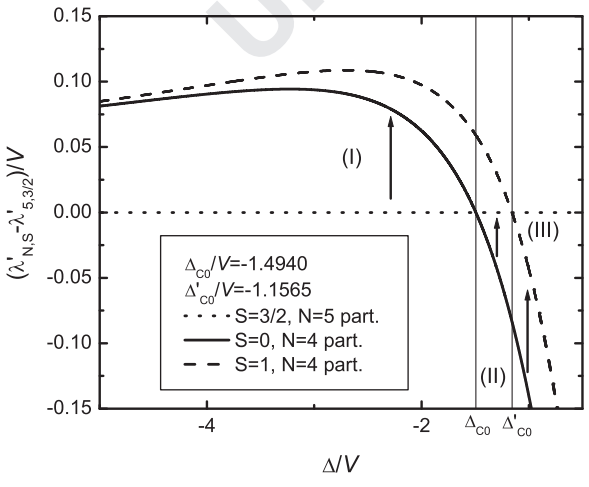

Fig. 1. Lowest energy levels of H' (measured from $\lambda'_{5,3/2}$) as a function of Δ/V. Depending on the value of Δ/V, three different regions are observed: (I) for $\Delta<\Delta_{C0}$, the ground state energy corresponds to $\lambda'_{5,3/2}$ and the first excited energy is $\lambda'_{4,0}$, (II) or $\Delta_{C0}<\Delta<\Delta'_{C0}$, the ground state energy is $\lambda'_{4,0}$ and the first excited energy is $\lambda'_{5,3/2}$, and (III) for $\Delta>\Delta'_{C0}$, where the ground state energy is $\lambda'_{4,0}$ and the first excited energy is $\lambda'_{4,1}$. Arrows show the first excited energy in (I), (II) and (III).

$$|6,2,0\rangle = \left[\alpha^\dagger_{2\downarrow}|5,3/2,+1/2\rangle + \alpha^\dagger_{2\uparrow}|5,3/2,-1/2\rangle\right]/\sqrt{2}, \text{ etc. For spin-1 states we take:}$$
$$|6,1,+1\rangle = \left[\sqrt{3}\alpha^\dagger_{2\downarrow}|5,3/2,+3/2\rangle - \alpha^\dagger_{2\uparrow}|5,3/2,+1/2\rangle\right]/2,$$
$$|6,1,0\rangle = \left[\alpha^\dagger_{2\downarrow}|5,3/2,+1/2\rangle - \alpha^\dagger_{2\uparrow}|5,3/2,-1/2\rangle\right]/\sqrt{2}, \text{ etc. For } \Delta<\Delta_{C0}, \text{ all these states correspond to the eight-times degenerate ground state energy } \lambda'_{5,3/2}. \text{ For } \Delta>\Delta_{C0}, \text{ the singlet six-particle state } |6,0,0\rangle = \alpha^\dagger_{2\uparrow}\alpha^\dagger_{2\downarrow}|4,0,0\rangle \text{ with energy } \lambda'_{4,0}, \text{ occurs. Defining the localized spin operators } S^Z_{1/2j} = (|\uparrow_j\rangle\langle\uparrow_j| - |\downarrow_j\rangle\langle\downarrow_j|)/2,\ S^+_{1/2j} = |\uparrow_j\rangle\langle\downarrow_j|, \text{ and } S^-_{1/2j} = |\downarrow_j\rangle\langle\uparrow_j| \text{ for spin-1/2 at site } j, \text{ and } S^Z_{1j} = (|+_j\rangle\langle+_j| - |-_j\rangle\langle-_j|),\ S^+_{1j} = \sqrt{2}(|+_j\rangle\langle 0_j| + |0_j\rangle\langle-_j|), \text{ and } S^-_{1j} = \sqrt{2}(|-_j\rangle\langle 0_j| + |0_j\rangle\langle+_j|) \text{ for spin-1, it is easy to obtain the magnetic correlations } \langle\mathbf{S}_1\cdot\mathbf{S}_2\rangle \text{ between the impurities. At zero temperature } (T=0), \text{ for } \Delta<\Delta_{C0} \text{ ferromagnetic correlations are obtained from } \langle 5,3/2,S_Z|\langle\mathbf{S}_1\cdot\mathbf{S}_2\rangle|5,3/2,S_Z\rangle = a_0^2 + 0.5b_0^2 = 0.25(3-\Delta/\sqrt{\Delta^2+5V^2}). \text{ Conversely, for } \Delta>\Delta_{C0}, \text{ the ground state gives antiferromagnetic correlations}$$
$$\langle 4,0,0|\langle\mathbf{S}_1\cdot\mathbf{S}_2\rangle|4,0,0\rangle = -2a_0'^2 - b_0'^2 - 0.75c_0'^2.$$

3.3. *The general case:* $0<\vec{\mathbf{k}}_F\cdot(\vec{\mathbf{R}}_1-\vec{\mathbf{R}}_2)<\pi/2$

For $0<\phi<\pi/2$, in the absence of hybridization ($V=0$), there may be 106 different six-particle states, corresponding to three possible occupations ($n=2$, 3, and 4 electrons) of the localized orbitals with the three occupations (6-n) of the extended states: (4×1) states for $n=2$, (12×4) states for $n=3$, and (9×6) states for $n=4$. Hybridization couples states with the same total spin z component and number of electrons, such that the 106×106 matrix factorizes into seven (1×1) blocks with $S=3$, five (9×9) blocks with $S=2$, three (15×15) blocks with $S=1$, and one (9×9) block with $S=0$. By diagonalizing these matrices, we obtain the eigenvalues and eigenstates of H_{ZBW}. Depending on the values of the model parameters Δ/V and $\phi=\vec{\mathbf{k}}_F\cdot(\vec{\mathbf{R}}_1-\vec{\mathbf{R}}_2)$, there are two possible ground states: a singlet, with energy $\lambda_{6,0}$ or a triplet, with energy $\lambda_{6,1}$, and three possible excited states corresponding to a singlet, a triplet, or a quintuplet, with energy $\lambda_{6,2}$. For $S=2$, it is easy to obtain the analytical expression $\lambda_{6,2}=0.5(3E_1+E_{1/2})-\sqrt{\Delta^2+0.5V^2(5+\sqrt{1+24\cos^2(\phi)})}$. For $\Delta/V=-4.5$ and $E_{1/2}/V=-1$, the lowest three energy levels ($\lambda_{6,0}$, $\lambda_{6,1}$, and $\lambda_{6,2}$) as a function of ϕ are shown in Fig. 2. For these parameters, there is always a triplet ground state, while the first excited state depends on the value of ϕ and it can be a singlet or a quintuplet. Due to the

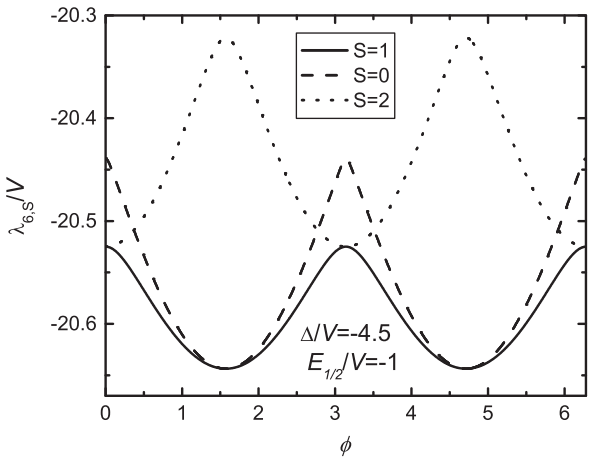

Fig. 2. Lowest energy levels of H_{ZBW} as a function of $\phi=\vec{\mathbf{k}}_F\cdot(\vec{\mathbf{R}}_1-\vec{\mathbf{R}}_2)$, for $\Delta/V=-4.5$ and $E_{1/2}/V=-1$. The solid line indicates the ground state energy $\lambda_{6,1}$, the dashed line shows $\lambda_{6,0}$, and the dotted line represents $\lambda_{6,2}$.

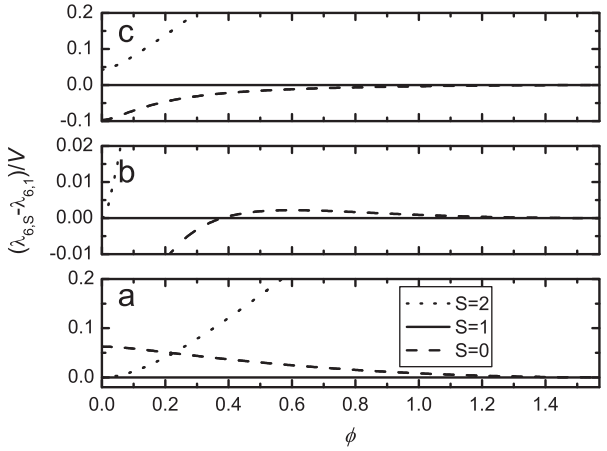

Fig. 3. Lowest six-particle energy levels of H_{ZBW} (measured from $\lambda_{6,1}$) as a function of $\phi = \vec{\mathbf{k}}_F \cdot (\vec{\mathbf{R}}_1 - \vec{\mathbf{R}}_2)$ (ranging from 0 to $\pi/2$). (a) For $\Delta/V = -2$, the ground state energy corresponds to $S=1$ (solid line) and the first excited energy level shows a crossover from total spin $S=2$ (dotted line) to $S=0$ (dashed line) at $\phi \approx 0.22$. (b) For $\Delta/V = -1.25$, the ground state energy shows a crossover from $S=0$ (dashed line) to $S=1$ (solid line) at $\phi \approx 0.38$. (c) For $\Delta/V = -1$ and any value of ϕ, the singlet ground state energy occurs (dashed line) and the first excited energy is given by the $S=1$ states (solid line).

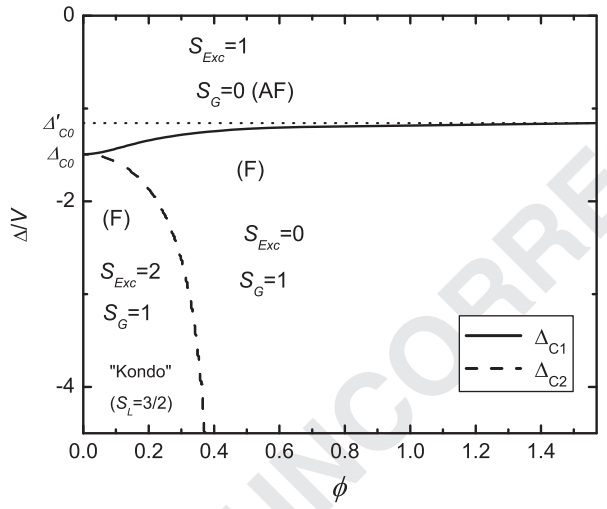

Fig. 4. ϕ dependence of the critical values Δ_{C1}, where the singlet and triplet ground states are equal in energy, and Δ_{C2}, where the first excited energy changes from $S=2$ to $S=0$ state. We can observe three different regions, in each one we represent the ground state spin by S_G and the first excited state spin with S_{Exc}. (F) and (AF) refer to ferromagnetic and antiferromagnetic character of the magnetic correlations between the impurities at zero-temperature. The dotted line is a guide to the eye.

periodical dependence on ϕ, hereafter we take this parameter ranging from 0 to $\pi/2$ [16].

In Fig. 3, for total spin $S = 0, 1, 2$ we show the lowest energy levels (measured from $\lambda_{6,1}$) as a function of ϕ. In Fig. 3(a), for $\Delta/V = -2$ ($\Delta < \Delta_{C0}$), the ground state is always a triplet but the first excited state, depending on the value of ϕ, is $S=0$ or $S=2$. For $\phi < 0.22$, the quintuplet occurs, whereas for $\phi > 0.22$, the singlet takes place. Similar results are obtained when Δ/V decreases. In Fig. 3(b), for $\Delta/V = -1.25$, depending on the value of ϕ, two different ground states occur: for $0 < \phi < 0.38$, the ground state is a singlet; conversely, for $0.38 < \phi < \pi/2$, the triplet ground state emerges. For ϕ ranging from 0 to $\pi/2$, the existence of two ground states is restricted to a narrow range of Δ between Δ_{C0} and Δ'_{C0}. In Fig. 3(c), for $\Delta/V = -1$ and ϕ ranging from 0 to $\pi/2$, we can see that the ground state energy corresponds to $S=0$ (dashed line) and the first excited state is $S=1$ (solid line). When Δ/V increases, the same results are obtained.

In Fig. 4, we put together these results showing the ϕ dependence of the critical values Δ_{C1}, where the singlet and triplet ground states are equal in energy, and Δ_{C2}, defined by $(\lambda_{6,2} - \lambda_{6,0}) = 0$. Two possible ground states can be observed: for $\Delta < \Delta_{C1}$ the triplet ground state occurs showing ferromagnetic (F) correlations between the impurities; conversely, for $\Delta > \Delta_{C1}$ the system shows a singlet ground state with antiferromagnetic (AF) correlations between the impurities. Furthermore, for $\phi < 0.41$, three different excited states can be distinguished: starting from $\Delta < \Delta_{C2}$ the system shows a quintuplet first excited state, when Δ increases we can observe first a crossover ($\Delta = \Delta_{C2}$) from $S=2$ to $S=0$ excited state and at high Δ the crossover ($\Delta = \Delta_{C1}$) from singlet to triplet excited state. For $\phi > 0.41$, only the last crossover from singlet to triplet can be observed. It is straightforward to determine the value $\phi = 0.41$ that corresponds to $\Delta < 0$ and $|\Delta| \gg V$. Since we can approximate $\lambda_{6,2} \approx 2E_1 - 0.25V^2(5 + \sqrt{1 + 24\cos^2(\phi)})/|\Delta|$ and $\lambda_{6,0} \approx 2E_1 - V^2(2 + \sin(\phi))/|\Delta|$, yields the equation of ϕ as: $5\sin^2(\phi) + 3\sin(\phi) - 2 = 0$. Furthermore, it is interesting to note that in the region of parameters where the ground state corresponds to $S=1$ and the first excited state is $S=2$ ($S_G = 1$ and $S_{Exc} = 2$ in the figure), the low excitation energies can be adjusted by an antiferromagnetic Heisenberg Hamiltonian (Kondo) where a localized spin $S = 3/2$ is coupled to $s = 1/2$ extended state. For $\Delta < 0$ and $|\Delta| \gg V$, we can approximate $\lambda_{6,1} \approx 2E_1 - 0.25V^2(9 + \sqrt{1 + 8\sin^2(\phi)})/|\Delta|$, and we can write the Kondo energy near the strong coupling regime as $(\lambda_{6,2} - \lambda_{6,1}) \approx 0.25V^2(4 + \sqrt{1 + 8\sin^2(\phi)} - \sqrt{1 + 24\cos^2(\phi)})/|\Delta|$. Therefore, in the ZBW approach at very low temperatures, for $\Delta < 0$ and $|\Delta| \gg V$, the Kondo physics occurs as in the single impurity problem, where $S=1$ localized spin is coupled to $s = 1/2$ band state [45]. According to our previous discussion ($\phi = 0$), the $S = 3/2$ localized state results from the impurities in a ferromagnetic $S=2$ state antiferromagnetically coupled to $s = 1/2$ band state. Thus, near the strong coupling regime, the Kondo physics favors the ferromagnetic coupling between the impurities.

In Fig. 5, we show the zero-temperature magnetic correlations $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle$ between the impurities as a function of ϕ for different values of Δ/V. For $\Delta/V = -4.5$ (solid line), due to the fact that the ground state of the system is a triplet, we can see only ferromagnetic correlations in the full range of ϕ, starting from $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle = a_0^2 + 0.5b_0^2 \approx 0.97$ for $\phi = 0$ to $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle = (9 + 6b_{I-}^2 + b_{I-}^4)/36 \approx 4/9$ for

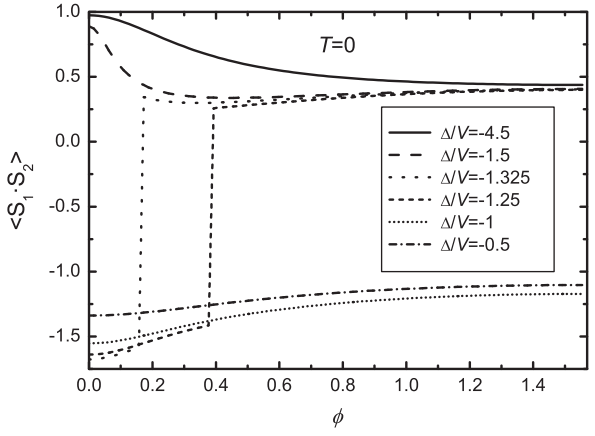

Fig. 5. Zero-temperature magnetic correlations $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle$ between the impurities as a function of $\phi = \vec{\mathbf{k}}_F \cdot (\vec{\mathbf{R}}_1 - \vec{\mathbf{R}}_2)$, for different values of Δ/V. Three different behaviors can be distinguished: the ferromagnetic local moments regime, for $\Delta < \Delta_{C0}$ ($\Delta/V = -4.5$ or -1.5), the antiferromagnetic local moments regime, for $\Delta > \Delta'_{C0}$ ($\Delta/V = -1$ or -0.5), and the crossover regime for $\Delta_{C0} < \Delta < \Delta'_{C0}$ ($\Delta/V = -1325$ or -1.25).

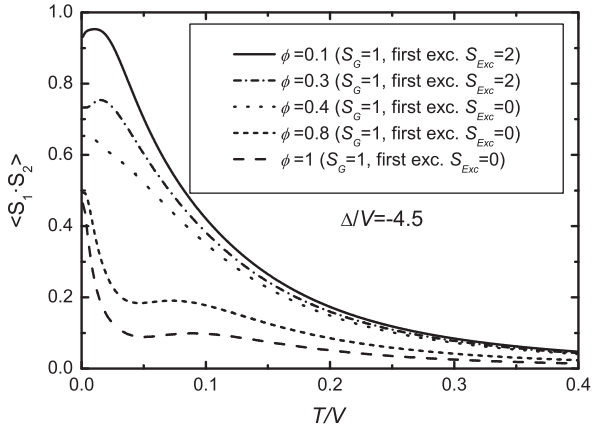

Fig. 6. Magnetic correlations $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle$ between the impurities as a function of temperature, for $\Delta/V = -4.5$ and different values of $\phi = \vec{\mathbf{k}}_F \cdot (\vec{\mathbf{R}}_1 - \vec{\mathbf{R}}_2)$. At low temperatures, we can see different behaviors depending on ϕ. For $\phi = 0.1$ we can observe, at very low temperatures, the Kondo peak due to excitation from triplet ground state to first excited quintuplet state. When ϕ increases, the peak diminishes and it moves to high temperatures due to the increases in the Kondo energy (see $\phi = 0.3$). The temperature at the peak is a measure of the Kondo energy. For $\phi = 0.4$, the curve shows the interplay of excitations to singlet (AF) and quintupled (F) exited states. For $\phi = 0.8$, the curve shows the effect of excitation from triplet ground state to first excited singlet state. For $\phi = 1$, the same behavior is observed.

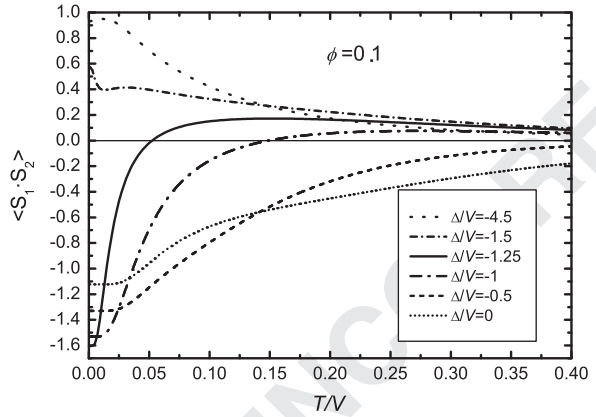

Fig. 7. Magnetic correlations $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle$ between the impurities as a function of temperature for $\phi = \vec{\mathbf{k}}_F \cdot (\vec{\mathbf{R}}_1 - \vec{\mathbf{R}}_2) = 0.1$ and different values of Δ/V. For $\Delta/V = -4.5$, we observe the peak showing the signature of the Kondo physics of two magnetic impurities. For $\Delta/V = -1.5$, the curve, at very low temperatures, diminishes rapidly due to thermal excitations from triplet ground state (F) to singlet excited state (AF). For $\Delta/V = -1.25$ or -1, as temperature increases, the curves show the changes from AF correlations to F correlations produced by thermal excitations. For $\Delta/V = -0.5$ or 0, we only observe AF correlations between the impurities with a monotonous decrease as T increases. At very low temperatures, for $\Delta > \Delta_{C0}$ ($\Delta_{C0}/V \simeq -1.49$), it is interesting to note that as the $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle$ becomes less temperature dependent due to the strong mixes of both configurations. Consequently, the figure shows the intersection of different curves.

$\phi \to \pi/2$. It is straightforward to determine this value from the decoupled limit. The same results, with lower values of $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle$ are obtained for $\Delta/V = -1.5$ (dashed line). For $\Delta/V = -1.325$ (dotted line), the figure shows antiferromagnetic correlations for $\phi < 0.17$ and ferromagnetic correlations for $\phi > 0.17$. For $\phi = 0.17$, we can see the abrupt jump of $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle$ due to the fact that the ground state changes from a singlet with AF correlations between the impurities to a triplet with FM correlations. Similarly, for $\Delta/V = -1.325$ (short dashed line), where we can observe AF correlations for $\phi < 0.39$ and F correlations for $\phi > 0.39$. For $\phi = 0$, the AF analytic solution gives $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle = -2a_0'^2 - b_0'^2 - 0.75c_0'^2$. Finally, for $\Delta/V = -1$ and $\Delta/V = -0.5$, the ground state is a singlet and only AF correlations occurs in the full range of ϕ. For $\phi \to \pi/2$, it is easy to show that $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle = -(9 + 6b_{I-}^2 + b_{I-}^4)/12$, since $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle = 0$ for $\phi = \pi/2$ (the decoupled limit).

In Fig. 6, we show $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle$ as a function of temperature, for $\Delta/V = -4.5$ and several values of ϕ. For small values of ϕ, at low temperatures, we can see a peak due to the thermodynamic excitations from triplet ground state to the quintuplet excited state given an additional FM contribution to $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle$. When ϕ increases, the peak decreases and the maximum moves to high temperatures (see $\phi = 0.1$ and 0.3). For $\phi = 0.4$, the peak disappears and $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle$ decreases monotonous as T increases. When ϕ increases, the splitting between the $S=1$ ground state and the first excited singlet state decreases, which can be observed for $\phi = 0.8$ or 1: at low temperatures, when T increases, the curves show a rapid decrease in $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle$. In Fig. 7, we show $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle$ as a function of temperature, for $\phi = 0.1$ (strong coupling region) and different values of Δ/V. At zero temperature, for $\Delta < \Delta_{C0}$ ($\Delta_{C0}/V \simeq -1.49$), we observe ferromagnetic correlations ($S_G = 1$ ground state). On the contrary, for $\Delta > \Delta_{C0}$, only antiferromagnetic correlations ($S_G = 0$ ground state) are obtained. In both cases, the magnetic correlations decrease with decreasing $|\Delta|/V$; in other words, increasing the mixes of both configurations decreases the magnetic correlations between ions. For $\Delta/V = -4.5$, we can see the low temperature peak outlined in Fig. 6. For $\Delta/V = -1.5$, the figure shows the decreasing F correlations, due to the low temperature excitation from $S_G = 1$ ground state to the $S_{Exc} = 0$ first excited state. For $\Delta/V = -1.25$, the singlet ground state occurs with strong AF correlations which are destroyed by increasing temperature, favoring F correlations due to the $S_{Exc} = 1$ first excited state. Similar behavior is observed for $\Delta/V = -1$. For $\Delta/V = -0.5$ or 0, we only observe AF correlations between the impurities. Finally, it should be noted that as the mixes of both configurations increase, the magnetic correlations decrease and the curves become less temperature dependent. This implies the intersection of curves for different Δ/V.

4. Conclusions

We have applied the narrow-band approximation to solve the problem of two magnetic impurities fluctuating between two magnetic configurations. The solution presented here enables the understanding, in simplified terms, of the behavior of two magnetic ions by the competing effects of three types of energies: (I) the energy difference between the magnetic configurations (Δ); (II) the hybridization effects which, at a given degree of strength (V), mix the f- and conduction-band states energy; and (III) the relation of the Fermi wavelength with the distance between the magnetic ions ($\phi = \vec{\mathbf{k}}_F \cdot (\vec{\mathbf{R}}_1 - \vec{\mathbf{R}}_2)$). At zero-temperature, we have obtained a Δ/V vs. ϕ "phase diagram".

For $\Delta < \Delta_{C1}$ ($-1.5 < \Delta_{C1}/V < -1.1$), the ground state is a triplet and the magnetic correlations between the impurities are ferromagnetic. On the contrary, for $\Delta > \Delta_{C1}$, the singlet ground state occurs with antiferromagnetic correlations between the impurities. For small values of ϕ (strong coupling region), $\Delta < 0$ and $|\Delta| \gg V$, the highest spin configuration, in each ion, is favored and the Kondo physics of two magnetic impurities emerges, in this case the model gives a triplet ground state with very strong ferromagnetic correlation between the impurities. The first excited state corresponds to $S=2$ and the model allows these results to be understood in terms of a Kondo Hamiltonian of an effective localized $S = 3/2$ spin state and a extended (band) $s = 1/2$ spin. For $\phi = \pi/2$, the model gives two independent ions and $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle = 0$. For $\phi \to \pi/2$ (low coupling regime), depending on Δ/V, the ground state is a triplet or a singlet with low

ferromagnetic or antiferromagnetic correlations, respectively. The effective magnetic moment in each ion, in contrast to the case of two-impurity Anderson model [16], does not disappear at intermediate-valence if the fluctuations take place between two magnetic configurations, giving rise to the possibility of magnetic order between them at any value of the coupling different from the DC limit. Finally, it would be desirable to obtain experimental results in nanodevices to confirm some of the results obtained here.

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