Two-impurity Anderson model: A variational study

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A comprehensive variational study of the two-impurity Anderson model is presented. First a lowest-order basis is introduced, which does not contain electronic excitations above the Fermi level: in this basis, the indirect f-f interaction of the form $-J\mathbf{S}_1 \cdot \mathbf{S}_2$ is not generated but is added by hand. The effect of electron-hole (EH) excitations is also studied. A suitable discretization of the continuous band spectrum allows us to obtain all eigenvalues and eigenvectors and to calculate finite-temperature magnetic properties. For a distance $R > R_c$, where $R_c \sim 2.5(k_F)^{-1}$ (k_F is the Fermi wave vector), the interference between screening clouds around the two impurities is weak and the physics depends smoothly on the ratio between the coupling J and the Kondo temperature T_K. In this regime, the effect of EH excitations is to renormalize the f-level energy and to add the magnetic interaction. At finite temperature, the results of scaling theory and of quantum Monte Carlo simulations are recovered, with growth of magnetic correlations down to temperatures $T \sim T_K$ and a two-stage Kondo effect for $J \gg T_K$. For $R \to 0$, the impurity spins lock in a triplet and the binding energy is exponentially increased, indicating that a collective Kondo effect takes place. At zero distance, only a half of the total impurity moment is compensated at low temperature. The magnetic interaction now competes with the enhanced binding energy. It is argued that the short-distance behavior of the two-impurity model is not representative of the properties of the periodic Anderson model close to half-filling.

I. INTRODUCTION

Heavy-fermion behavior in concentrated Kondo systems (Ce and U compounds) is always accompanied by anomalies in the magnetic properties, which place such systems at the borderline between magnetic and nonmagnetic behavior. Even in the absence of long-range order, short-range antiferromagnetic correlations[1] as well as metamagnetic transitions[2] are observed. A small increase of the lattice constant can drive the system to an ordered state, with a magnetic moment which depends in a sensitive way on the Kondo temperature.[3] Some heavy-fermion compounds have long-range antiferromagnetic order with moments of the order of a hundredth of a Bohr magneton.[4] These phenomena are attributed to a competition between the Kondo effect and the indirect f-f interaction, and are believed to be described by the periodic version of the Anderson impurity model.[5] A question of particular interest is to determine the regime of parameters in which either the magnetic or the nonmagnetic (Kondo) state is stable, and to describe the transition between these two states.

The two-impurity model is a highly simplified version of the periodic Anderson model, which still contains the two competing effects, namely Kondo compensation of the localized moments and the magnetic interaction between them.[6] Therefore there is some hope that a study of the two-impurity model will shed light on the properties of the Anderson lattice, and on the validity of the methods used for its investigation. However it must be emphasized that the two-impurity model is not a representation of a physical system; this is at variance with the one-impurity model, which describes a metal with diluted Kondo impurities.

The two-impurity Anderson or Kondo models have been the subject of various investigations,[7–29] yet a complete understanding of their properties has not been reached. Older works employed either the Hartree-Fock method[7] or perturbation theory.[8] The two-impurity Kondo Hamiltonian was studied in Ref. 9 by the technique of perturbative scaling: the resulting picture was found to depend on the ratio between the magnetic coupling J and Kondo temperature T_K, in particular a two-stage Kondo effect was predicted to occur for strong ferromagnetic couplings $J \gg T_K$. The numerical renormalization group applied to the two-impurity Kondo Hamiltonian[17,20] predicted a complex low-temperature behavior and a new critical point with diverging staggered susceptibility for an antiferromagnetic coupling $J \simeq -2.2T_K$. This result was confirmed by a theorem,[23,28] which shows that the critical point must exist for the particle-hole symmetric Kondo Hamiltonian. Instead, calculations on the Anderson Hamiltonian by quantum Monte Carlo,[18] slave boson,[21] and renormalization group[24] techniques did not find a divergence of the staggered susceptibility. The different phys-

ical behavior of the two models is now understood to be due to potential scattering, which is contained in the Anderson but not in the Kondo Hamiltonian.[23–25,28] Exact diagonalization on small clusters[26] and the variational method[26,27,29] have also been applied to the two-impurity Anderson model.

Each technique has its own merits and drawbacks. The numerical renormalization group is in principle an exact method, which had great success in the solution of the one-impurity model.[30,31] However it is a heavy numerical technique, and it cannot be easily extended to the lattice. The quantum Monte Carlo method is also exact, but it cannot reach very low temperatures or treat extreme limits of the parameters. Speaking of approximate methods, slave-boson–mean-field techniques are simple to implement and can be readily extended to the lattice, but the results can be modified by the inclusion of fluctuations. The variational method, pioneered by Varma and Yafet[32] and Gunnarson and Schönhammer,[33] provides a ground-state wave function and a simple picture of the physics involved: however the results may depend on the choice of the basis. Also, Fermi-liquid properties cannot be studied by this method, a fact which is often not emphasized. At present, a complete understanding of these strongly correlated systems seems to require results from different techniques.

In this work we present the results of a comprehensive study of the two-impurity Anderson model by the variational method. We calculate the following quantities: energy spectrum, spin correlation functions, and magnetic susceptibilities. Emphasis is given on the dependence of the physical properties on the interimpurity distance and on the magnetic coupling. We intepret the results in terms of the interference between the screening clouds around the two impurities, which can drive magnetic correlations even in the absence of the indirect f-f interaction. Attention to a proper choice of the variational basis is given, and the dependence on the basis is studied. In addition, we try to establish which properties of the two-impurity model remain true for the Anderson lattice.

In Sec. II we introduce the model Hamiltonian and describe the variational method used for its solution. In Sec. III we present the results for zero-temperature properties in the lowest-order variational basis which does not include electron-hole excitations: this is the "reference" calculation. In Sec. IV we study the effect of an added magnetic coupling in the lowest-order basis. In Sec. V an extension of the variational method is proposed, which allows one to study low-temperature magnetic properties. In Sec. VI we discuss the dependence of the results on the variational basis, in particular the renormalization effects associated with electron-hole excitations. Section VII gives an outlook on the results and their relation with the properties of the periodic Anderson model. Some technical details are given in the three appendices. Part of the results of the present work were already published in short form.[34] In the present paper we give details on the method and present new results on spin correlations, on finite-temperature properties, and on the effect of electron-hole excitations.

II. MODEL AND METHOD

Our model Hamiltonian is given by

$$H=\sum_{\mathbf{k}\sigma}\epsilon_k c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}+E_f\sum_{i\sigma}f^\dagger_{i\sigma}f_{i\sigma}+U\sum_{i,\sigma\neq\sigma'}f^\dagger_{i\sigma}f_{i\sigma}f^\dagger_{i\sigma'}f_{i\sigma'}+\sum_{\mathbf{k}i\sigma}(e^{i\mathbf{k}\cdot\mathbf{R}_i}V_{\mathbf{k}}f^\dagger_{i\sigma}c_{\mathbf{k}\sigma}+\text{H.c.})-J\mathbf{S}_1\cdot\mathbf{S}_2, \tag{1}$$

where $f^\dagger$ ($c^\dagger$) is the creation operator of a localized (conduction) level, $i=1,2$ labels the two impurities at positions $\mathbf{R}_i$, and σ is a spin index. The quantization axis is taken along the line connecting the two impurities. Throughout this work, we assume a Coulomb correlation $U=\infty$, so that double occupancy of a localized level is strictly forbidden. The band is taken to be free-electron-like with a lowest energy $-B$ and an upper cutoff B', both measured from the Fermi level. The f-level position $E_f<0$. The hybridization width is given by

$$\Gamma(\epsilon)=\pi\sum_{\mathbf{k}}|V_{\mathbf{k}}|^2\delta(\epsilon-\epsilon_k)\equiv\pi|V(\epsilon)|^2\rho(\epsilon), \tag{2}$$

where $\rho(\epsilon)$ is the density of states. For simplicity, $\Gamma(\epsilon)$ is assumed to be independent of energy: given the free-electron density of states, this implies that the hybridization $V_{\mathbf{k}}\propto k^{-1/2}$. The Hamiltonian (1) refers to the case of spin degeneracy only ($N_f=2$). We are mainly concerned with the weak-coupling (Kondo) regime $\Gamma\ll|E_f|$, in which the f occupation $n_f\simeq 1$.

For generality, a magnetic interaction term $-J\mathbf{S}_1\cdot\mathbf{S}_2$ between the localized spins is included in the Hamiltonian. Such a term is also generated to fourth order in the hybridization. Including this term will be useful in order to compare the lowest-order results, which do not include electron-hole excitations, with the higher-order ones (Sec. VI).

The total number of particles is a conserved quantum number: we choose to work in the subspace with an even number of electrons. We represent the many-body wave function in a variational basis.[32,33] Basis states are classified according to the total spin S and its component S_z. For the states with $S=0$, the variational basis is

$$\psi_0=\text{filled Fermi sea}, \tag{3}$$

$$\psi^{(a)}_{i\mathbf{k}}=\frac{1}{\sqrt{2}}e^{i\mathbf{k}\cdot\mathbf{R}_i}(f^\dagger_{i\uparrow}c_{\mathbf{k}\uparrow}+f^\dagger_{i\downarrow}c_{\mathbf{k}\downarrow})\psi_0, \tag{4}$$

$$\psi^{(b)}_{\mathbf{k}\mathbf{k}'} = \frac{1}{\sqrt{3}}[f^\dagger_{1\uparrow}f^\dagger_{2\uparrow}c_{\mathbf{k}\uparrow}c_{\mathbf{k}'\uparrow} + f^\dagger_{1\downarrow}f^\dagger_{2\downarrow}c_{\mathbf{k}\downarrow}c_{\mathbf{k}'\downarrow} + \tfrac{1}{2}(f^\dagger_{1\uparrow}f^\dagger_{2\downarrow} + f^\dagger_{1\downarrow}f^\dagger_{2\uparrow})(c_{\mathbf{k}\uparrow}c_{\mathbf{k}'\downarrow} + c_{\mathbf{k}\downarrow}c_{\mathbf{k}'\uparrow})]\psi_0, \tag{5}$$

$$\phi^{(b)}_{\mathbf{k}\mathbf{k}'} = \frac{1}{2}(f^\dagger_{1\uparrow}f^\dagger_{2\downarrow} - f^\dagger_{1\downarrow}f^\dagger_{2\uparrow})(c_{\mathbf{k}\uparrow}c_{\mathbf{k}'\downarrow} - c_{\mathbf{k}\downarrow}c_{\mathbf{k}'\uparrow})\psi_0, \tag{6}$$

$$\psi^{(c)}_{\mathbf{k}\mathbf{q}} = \frac{1}{\sqrt{2}}(c^\dagger_{\mathbf{q}\uparrow}c_{\mathbf{k}\uparrow} + c^\dagger_{\mathbf{q}\downarrow}c_{\mathbf{k}\downarrow})\psi_0, \tag{7}$$

$$\psi^{(d)}_{i\mathbf{k}\mathbf{k}',\mathbf{q}} = \frac{1}{\sqrt{3}}[f^\dagger_{i\uparrow}c^\dagger_{\mathbf{q}\uparrow}c_{\mathbf{k}\uparrow}c_{\mathbf{k}'\uparrow} + f^\dagger_{i\downarrow}c^\dagger_{\mathbf{q}\downarrow}c_{\mathbf{k}\downarrow}c_{\mathbf{k}'\downarrow} + \tfrac{1}{2}(f^\dagger_{i\uparrow}c^\dagger_{\mathbf{q}\downarrow} + f^\dagger_{i\downarrow}c^\dagger_{\mathbf{q}\uparrow})(c_{\mathbf{k}\uparrow}c_{\mathbf{k}'\downarrow} + c_{\mathbf{k}\downarrow}c_{\mathbf{k}'\uparrow})]\psi_0, \tag{8}$$

$$\phi^{(d)}_{i\mathbf{k}\mathbf{k}',\mathbf{q}} = \frac{1}{2}(f^\dagger_{i\uparrow}c^\dagger_{\mathbf{q}\downarrow} - f^\dagger_{i\downarrow}c^\dagger_{\mathbf{q}\uparrow})(c_{\mathbf{k}\uparrow}c_{\mathbf{k}'\downarrow} - c_{\mathbf{k}\downarrow}c_{\mathbf{k}'\uparrow})\psi_0, \tag{9}$$

$$\psi^{(f)}_{\mathbf{k}\mathbf{k}',\mathbf{q}\mathbf{q}'} = \frac{1}{\sqrt{3}}[c^\dagger_{\mathbf{q}\uparrow}c^\dagger_{\mathbf{q}'\uparrow}c_{\mathbf{k}\uparrow}c_{\mathbf{k}'\uparrow} + c^\dagger_{\mathbf{q}\downarrow}c^\dagger_{\mathbf{q}'\downarrow}c_{\mathbf{k}\downarrow}c_{\mathbf{k}'\downarrow} + \tfrac{1}{2}(c^\dagger_{\mathbf{q}\uparrow}c^\dagger_{\mathbf{q}'\downarrow} + c^\dagger_{\mathbf{q}\downarrow}c^\dagger_{\mathbf{q}'\uparrow})(c_{\mathbf{k}\uparrow}c_{\mathbf{k}'\downarrow} + c_{\mathbf{k}\downarrow}c_{\mathbf{k}'\uparrow})]\psi_0, \tag{10}$$

$$\phi^{(f)}_{\mathbf{k}\mathbf{k}',\mathbf{q}\mathbf{q}'} = \frac{1}{2}(c^\dagger_{\mathbf{q}\uparrow}c^\dagger_{\mathbf{q}'\downarrow} - c^\dagger_{\mathbf{q}\downarrow}c^\dagger_{\mathbf{q}'\uparrow})(c_{\mathbf{k}\uparrow}c_{\mathbf{k}'\downarrow} - c_{\mathbf{k}\downarrow}c_{\mathbf{k}'\uparrow})\psi_0. \tag{11}$$

A similar basis is introduced for the states with $S = 1$ and $S = 2$ (working with an even number of electrons, the values $S = 0, 1, 2$ of the total spin are the only possible ones which can be formed within our variational basis). States (5), (6), and (8)–(11) must be restricted to half of the values $(\mathbf{k}, \mathbf{k}')$ or $(\mathbf{q}, \mathbf{q}')$ (for example, $k_z < k'_z$, $q_z < q'_z$) to avoid overcompleteness of the basis. States (5) and (6) have a total impurity spin $S_{\rm imp} = 1$, $S_{\rm imp} = 0$, respectively: however, $S_{\rm imp}$ is not a good quantum number of the Hamiltonian.

The restriction to the variational basis (3)–(11) (and the analogous ones for the higher spin values $S = 1$ and 2) defines the approximation adopted in the present work. The Hamiltonian matrix restricted to the variational subspace generates linear equations for the expansion coefficients: a technique for discretizing the continuous band spectrum is needed in order to solve these equations. We formulate the Schrödinger equation in terms of a generalized eigenvalue problem, by introducing suitable nonorthogonal basis functions: this has the advantage of yielding all eigenvalues and eigenvectors, while keeping matrices of small dimension. The numerical technique is described in Appendix A. For the low-temperature results of Sec. V, we take all eigenvalues and eigenvectors resulting from the generalized eigenvalue equation and calculate finite-temperature thermodynamic properties from the partition function.

From the eigenvectors we calculate the correlation functions and impurity susceptibilities. The latter are generally defined by

$$\chi = \int_0^\beta d\tau\, \langle S_{1z}(\tau) S_{1z}\rangle, \tag{12}$$

$$\chi_u = \frac{1}{2}\int_0^\beta d\tau\, \langle (S_{1z}(\tau) + S_{2z}(\tau))(S_{1z} + S_{2z})\rangle, \tag{13}$$

$$\chi_s = \frac{1}{2}\int_0^\beta d\tau\, \langle (S_{1z}(\tau) - S_{2z}(\tau))(S_{1z} - S_{2z})\rangle, \tag{14}$$

with $\beta = (k_B T)^{-1}$, and where χ, χ_u, χ_s represent the on-site, uniform, and staggered susceptibilities, respectively; the definition $O(\tau) = e^{\tau H} O e^{-\tau H}$ is used. Expressions (12)–(14) are conveniently evaluated using the Van Vleck formula.

A schematic illustration of the basis is shown in Fig. 1, where one more state is considered [state (e)]. The crucial state for the Kondo effect is (b) [Eqs. (5) and (6)], which allows for a simultaneous screening of the two impurities and therefore is able to describe both the independent-impurity limit and a correlated Kondo effect on the two sites for finite distance. The structure of the two-impurity basis for $U = \infty$ is analogous to that of the one-impurity basis for finite U.[35] The representation of Fig. 1 corresponds to the idea of an $1/N_f$ expansion:[33] states on the same line are coupled by terms of order unity, while states on different lines are coupled by terms of order $1/\sqrt{N_f}$. Thus in the limit $N_f \to \infty$ only basis

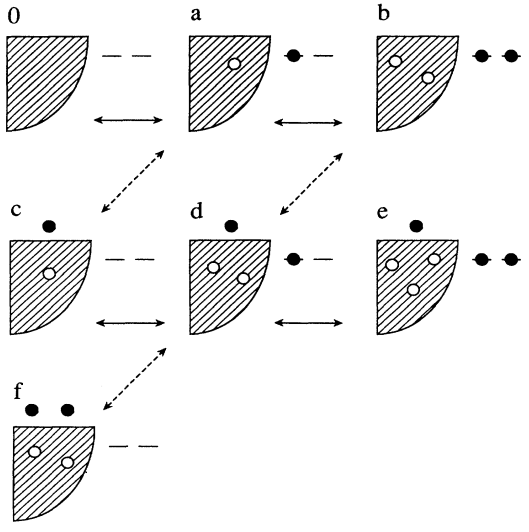

FIG. 1. Variational basis for the two-impurity problem in the limit $U \to \infty$. Solid circles represent electrons, open circles represent holes. The f levels representing the two impurities are on the right of the Fermi sea. In states (a) and (d), both impurities can be occupied. Solid arrows indicate couplings of order $(1/\sqrt{N_f})^0$, while dotted arrows indicate couplings of order $(1/\sqrt{N_f})$.

states ($0ab$) need to be considered. However we do not aim at a systematic $1/N_f$ expansion: rather, we choose to emphasize the physical effects introduced by electron-hole excitations [states ($cdef$)], which are of course important for $N_f = 2$. Our strategy is the following: in Secs. III–V we present the results in the lowest-order basis ($0ab$), which excludes electron-hole excitations (see also Appendix B). Since the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction is not generated in this basis, we must include the term $-J\mathbf{S}_1 \cdot \mathbf{S}_2$ in the Hamiltonian. In Sec. VI we present the results obtained in the basis which includes electron-hole excitations. It will be shown that electron-hole excitations have two main effects: (i) generating a magnetic interaction term, and (ii) renormalizing the parameter E_f used in the lowest-order calculation. To compare with published variational treatments of the two-impurity problem, the wave function of Ref. 26 corresponds to our lowest-order basis ($0ab$), whereas the "Kondo-singlet" wave function studied in Ref. 27 corresponds to the basis (abd) of Fig. 1.

The choice of the appropriate variational basis is not obvious. The basis of Fig. 1 is not the only possibility: another possible basis is shown in Fig. 2(a), and will be referred to as a "magnetic" basis. The bases of Figs. 1 and 2(a) have the same quantum numbers, hence they must be equivalent if the variational expansion is performed to all orders: however, if the expansion is truncated to a finite order, the two bases might give different results. The choice is then dictated by physical considerations. The important state for the correlated Kondo effect is the one with two holes in the band, i.e., state (b) in the nonmagnetic basis of Fig. 1 and state (h) in the magnetic basis of Fig. 2(a). Thus the correlated Kondo effect is already obtained to order ($0ab$) in the nonmagnetic basis, while it is only recovered to order ($bdefgh$) in the magnetic basis. On the other hand, the magnetic interaction is described by the diagrams (bde), (bdf) in both bases (see also Sec. VI), which means that the basis of Fig. 2(a) is more appropriate to study the magnetic interaction. Since it is the Kondo effect which is nonperturbative and at the heart of the problem, it is reasonable to use the nonmagnetic basis of Fig. 1, where the effect of the higher-order states ($cdef$) can to a large extent be understood by Brillouin-Wigner perturbation theory (as shown in Sec. VI).

It would also be possible to work in the subspace with an odd number of electrons, i.e., using a variational basis with half-integer values of the total spin. For the case without electron-hole excitations, such a basis is shown in Fig. 2(b). Having one more electron cannot matter in the thermodynamic limit, provided however the variational expansion is performed to all orders. A calculation in the basis of Fig. 2(b) is carried out in Appendix C, and shows that when electron-hole excitations are neglected, the basis with an odd number of electrons gives an equivalent description of the ground state for $R = 0$, but yields incorrect results for $R \to \infty$.

A similar situation occurs in the one-impurity problem, where "nonmagnetic" and "magnetic" bases can also be defined [Figs. 3(a) and 3(b)]. Here the two bases have different quantum numbers: the nonmagnetic (magnetic) basis has an even (odd) number of electrons. Here again, having one more electron is irrelevant in the thermodynamic limit: thus the two expansions of Fig. 3 must still give the same results when evaluated to all orders.[36] When truncated to a finite order, the Kondo effect is already described to order ($0a$) in the nonmagnetic basis, while one must go to order (acd) in the magnetic basis for the Kondo effect to be present.

A related problem is how to define the Kondo temperature T_K in the one-impurity case. In the Kondo problem, T_K can be defined either from perturbation theory at high temperature, or from the inverse of the zero-temperature susceptibility, the two definitions be-

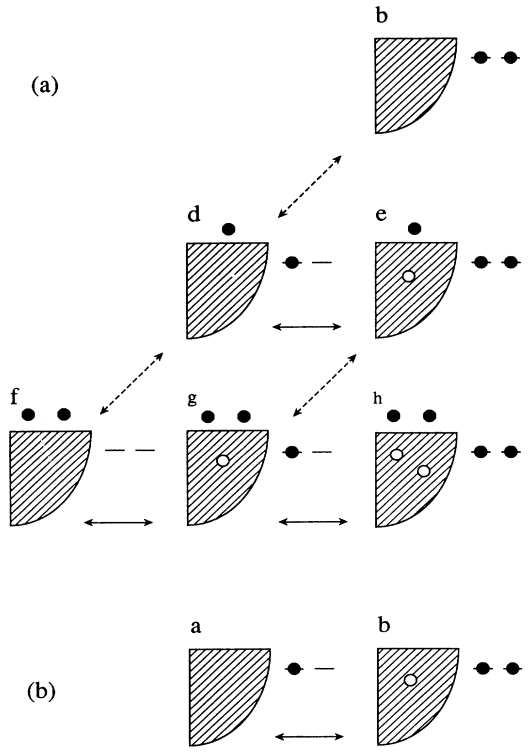

FIG. 2. (a) "Magnetic" basis for the two-impurity problem. (b) Spin-1/2 basis for the two-impurity problem. Meaning of the symbols as in Fig. 1.

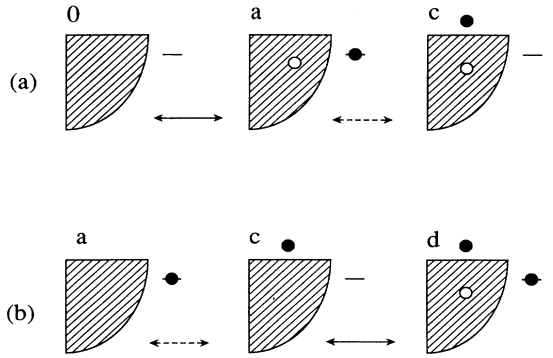

FIG. 3. (a) Nonmagnetic and (b) magnetic basis for the one-impurity problem. Meaning of the symbols as in Fig. 1.

ing related by a universal Wilson number.[30] In the variational expansion, for $n_f \to 1$, we take the definition $T_K = 1/[4\chi(T=0)]$, where χ is the impurity susceptibility.[33] Within the variational bases $(0a)$ or $(0ac)$ of Fig. 3(a), the above expression for T_K is calculated to be close to the triplet-singlet splitting $E(S=1) - E(S=0)$. Both quantities of course depend on the order of the calculation. However we note that since the one-impurity problem is known to have no gap in the excitation spectrum, performing the variational expansion to all orders the triplet-singlet splitting must eventually vanish, while the zero-temperature susceptibility remains finite.

Since the variational expansion leads to a finite gap above the ground state, Fermi-liquid properties like the specific heat cannot be studied by this method. In this sense the variational technique is closest to finite-cluster calculations,[26,37] which are also characterized by a finite gap. A finite susceptibility at zero temperature, which is one of the signatures of a Fermi-liquid ground state in the one-impurity problem, appears as Van Vleck-like magnetism in variational or finite-cluster calculations.

III. LOWEST-ORDER CALCULATION

In this section we present the results obtained in the lowest-order basis $(0ab)$ and without the magnetic interaction term. Figure 4 shows the energies of the two lowest states and the spin correlation function $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle$. There exists a critical distance $R_c \simeq 2.5/k_F$, which separates two distinct regimes. For $R > R_c$, the ground-state energy is close to $-2T_K$, where $T_K \simeq B\exp[\pi E_f/(2\Gamma)]$ is the single-impurity Kondo temperature, and interimpurity spin correlations are small. In this regime, the physics is that of two weakly coupled Kondo impurities. For $R < R_c$, the binding energy is enhanced, and tends to $\delta_- \simeq B\exp[\pi E_f/(3\Gamma)]$ as $R \to 0$ (see Appendix B). Thus the ground-state energy still depends exponentially on the hybridization width, but with a smaller exponent (in absolute value) than for the single-impurity case. Spin correlations become ferromagnetic for $R < R_c$, and for $R \to 0$ the impurity spins are locked in a triplet ($\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle$ remains slightly below 1/4 due to charge fluctuations). We take the exponential increase of the binding energy, as well as the formation of an impurity spin triplet, as an indication that a collective Kondo effect takes place for $R \to 0$. The limiting behavior for $R = 0$ can be understood analytically, as shown in Appendix B.

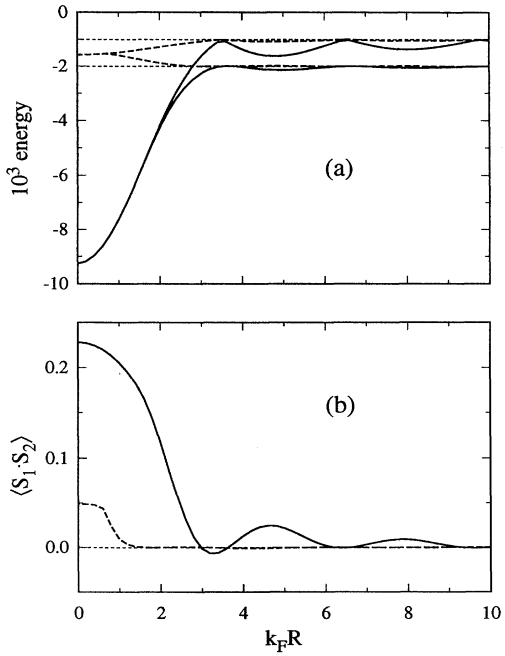

FIG. 4. (a) Energies of the two lowest states, (b) ground-state correlation function as a function of distance. Solid lines: $N_f = 2$. Dashed lines: $N_f = 14$. Other parameters: $B = 1$, $J = 0$, $N_f\Gamma = 0.2$, $T_K = 0.001$.

The ground state is always a nondegenerate singlet. The first excited level is found to be fourfold degenerate: one state with $S = 0$ and three states with $S = 1$. Starting from this first excited level, the spectrum is continuous. For $R \to 0$, the gap tends to zero and the whole spectrum is continuous.

In Fig. 4 we also show the results in the case of a high degeneracy $N_f = 14$ of the f level. Orbital degeneracy is treated by introducing an orbital index m for the f level, $f_{im\sigma}$, and assuming that the hybridization $V_{\mathbf{k}m}$ satisfies $V_{\mathbf{k}m} = V_{\mathbf{k}} e^{im\phi}$, where ϕ is the angle of $\mathbf{k}$ in the x-y plane. It can be seen that correlations between the localized spins are much weaker for large N_f. In fact, in the limit $N_f \to \infty$ the two impurities are decoupled, as is well known,[38] unless a magnetic interaction term is introduced.[21] Also, for large N_f the energy at $R = 0$ becomes higher than for $R \to \infty$. In fact, the energy in the weak-coupling limit is $-2T_K = -2B\exp[\pi E_f/[(N_f\Gamma)]$ for $R \to \infty$, and $-B\exp\{\pi E_f/[(N_f+1)\Gamma]\}$ for $R \to 0$, as one can show by a calculation similar to that of Appendix B. For small N_f, the change in exponent makes the energy for $R = 0$ lower than for $R \to \infty$, but for $N_f \to \infty$ the exponents become identical and the factor of 2 makes the energy lower for $R \to \infty$. Even for $N_f = 2$, the energy can become higher for $R = 0$ than for $R \to \infty$ if the hybridization is so large that the above formulas (valid only in the weak-coupling limit) do not hold.

We emphasize that the correlations in Fig. 4 are obtained in the absence of electron-hole excitations, and for this reason they cannot be associated to a RKKY mechanism. In fact, these correlations are closely related to the presence of a nonanalytical term in the ground-state energy, i.e., to the Kondo effect. Still, since the interimpurity correlations of Fig. 4 are mediated by the conduction electrons, their spatial dependence reflects Fermi-surface effects. The length scale π/k_F of the oscillations has nothing to do with the Kondo screening length, which is discussed below in terms of the correlations between impurity and conduction spins.

In the one-impurity problem, correlations between f and conduction spins have been shown[39] to extend over distances of the order of $\zeta = v_F/T_K$ (or $k_F\zeta = 2\epsilon_F/T_K$): the extension of the screening cloud is orders of magnitudes larger than the lattice constant, as has been verified experimentally.[40] In the two-impurity problem, the

naive expectation is that the two impurities would interact at distances $R < \zeta$. This expectation is incorrect, as can be seen from the following argument. The screening cloud around each isolated impurity consists of electrons in partial s-wave states. An s-wave at site 1 is seen from site 2 as consisting of partial waves with angular momenta up to $l_{\max} \sim k_F R$. Quantitatively, the scalar product of two normalized s waves around two sites at distance R is calculated to be $\sin(kR)/(kR)$. Thus for $k_F R \gg 1$ the two screening orbitals are almost orthogonal, the screening electrons do not "feel" each other, and the two impurities interact weakly. For $k_F R \ll 1$, on the other hand, the conduction electron wavelength is too long to "resolve" the two impurities, the screening orbital becomes the same for both impurities, and a collective effect arises with ferromagnetic correlations between the impurity spins. Considering the case of orbital degeneracy, the interference between screening clouds is an effect of order $1/N_f$, and vanishes for $N_f \to \infty$. In the rest of this paper we shall consider only the case $N_f = 2$.

In Fig. 5 we plot the correlation function $\langle \mathbf{S}_1 \cdot \mathbf{s}_c \rangle$ between one impurity spin and the total conduction spin $\mathbf{s}_c = \int \mathbf{s}(\mathbf{r}) d\mathbf{r}$; the conduction spin density is defined as

$$\mathbf{s}(\mathbf{r}) = \frac{1}{V} \sum_{\mathbf{k}\mathbf{k}'} e^{-i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}} \sum_{\alpha\beta} c^{\dagger}_{\mathbf{k}\alpha} \frac{\sigma_{\alpha\beta}}{2} c_{\mathbf{k}'\beta}. \tag{15}$$

For the one-impurity problem, since the ground state is a singlet, it can be shown that the sum rule $\langle \mathbf{S}_1 \cdot \mathbf{s}_c \rangle = -(3/4) n_f$ holds. In fact in Fig. 5 $\langle \mathbf{S}_1 \cdot \mathbf{s}_c \rangle$ is close to $-3/4$ for $R \to \infty$, the small difference coming from charge fluctuations. The correlation $\langle \mathbf{S}_1 \cdot \mathbf{s}_c \rangle$ shows weak oscillations for $R > R_c$, and tends to $-n_f$ for $R \to 0$. The value of -1 is characteristic of two spins one, antiferromagnetically coupled to each other. Thus Fig. 5 confirms that the impurity spins form a triplet for $R \to 0$, which is compensated by the conduction electrons. However it is shown in Appendix B that for $R = 0$ the spectrum is continuous, and one of the two screening holes is in a plane-wave state: its characteristic length is infinitely large. This can be understood from the following argument: since the screening orbital becomes the same for both impurities as $R \to 0$, the Pauli principle forbids its occupation by more than one hole, and the second hole occupies a plane-wave state close to the Fermi energy. A similar calculation can be performed working with an odd number of electrons (see Appendix C). The hole in a plane-wave state, appearing for $R = 0$, is not present in this basis. The basis with an odd number of electrons gives an equivalent physical description of the ground state for $R \to 0$, but now the correlation $\langle \mathbf{S}_1 \cdot \mathbf{s}_c \rangle = -n_f/2$.

To study in more detail the spatial correlations between f and c spins, we show in Fig. 6 the correlation function $G(z) = 4\pi z^2 \langle \mathbf{S}_1 \cdot \mathbf{s}(\rho = 0, z) \rangle$, where (ρ, z) are the cylindrical coordinates along the axis connecting the two impurities. The general form of $G(z)$ consists of oscillations with a period π/k_F, coming again from pure Fermi-surface effects, multiplied by an envelope which decays asymptotically like $1/z^2$. For $R \to \infty$ [Fig. 6(a)] the correlation function becomes that of the one-impurity

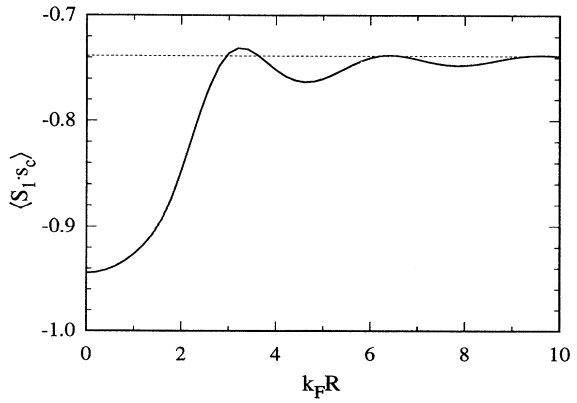

FIG. 5. Correlation function between one impurity spin and the total conduction spin. Parameters: J=0, B=1, Γ = 0.1, T_K = 0.001. The dotted line represents the $R \to \infty$ limit.

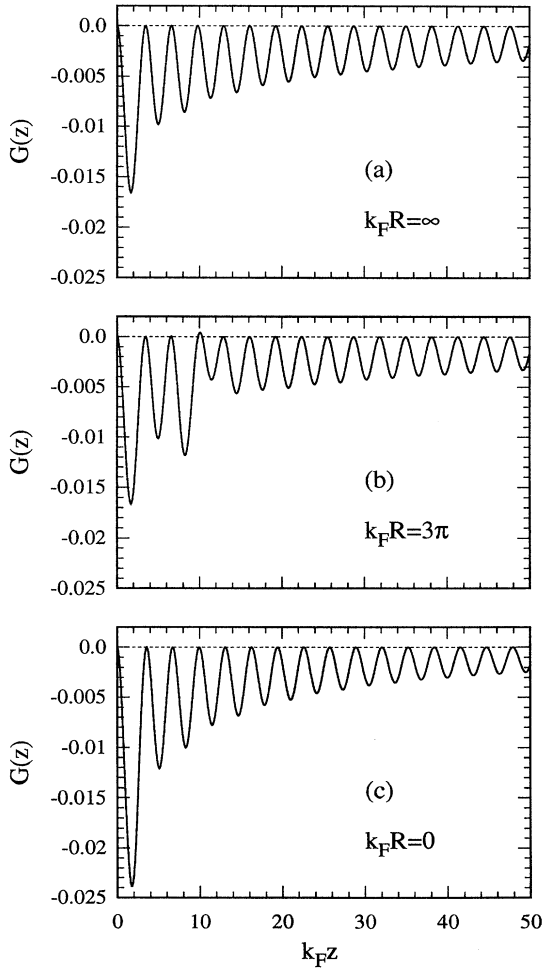

FIG. 6. Correlation function $G(z) = 4\pi z^2 \langle \mathbf{S}_1 \cdot \mathbf{s}(\rho = 0, z) \rangle$ between one impurity spin and the conduction spin density along the line connecting the two impurities. Parameters: $J = 0$, $B = 5$, $\Gamma = 0.1$, $T_K = 0.01$.

problem, which is given by $G(z) = -3\pi z^2 |\sum_{\mathbf{k}} a_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}}|^2$ [$a_{\mathbf{k}}$ is the coefficient of state (a) in Fig. 3(a)] and therefore is always negative. $G(z)$ is normalized according to the sum rule $\int_0^\infty G(z)\,dz = -(3/4)n_f$: this has been verified numerically. It has also been verified that about 70% of the sum rule is recovered if the upper limit of the integral is taken to be $\zeta = v_F/T_K$ ($k_F\zeta \simeq 500$ with the parameters of Fig. 6):[39] this can be taken as a working definition of the extension of the screening cloud in the one-impurity problem. It is gratifying that the description of the screening cloud within the simple variational wave function to lowest order is in very good agreement with that obtained by more elaborate methods.[39]

When the two impurities are at a distance $R = 3\pi/k_F$, it can be seen from Fig. 6(b) that the behavior of the single-impurity correlation is modified only for $z \simeq R \pm 1/k_F$. This can be understood again from the partial-wave argument: far from the second impurity, the two screening holes do not feel each other, and the single-impurity correlation is essentially unchanged.

For zero interimpurity distance [Fig. 6(c)], the correlation $G(z)$ resembles that of one impurity, but with a faster decay, i.e., a smaller characteristic length. This is related to the enhanced binding energy: for $R = 0$, the correlation length becomes $\zeta = v_F/\delta_-$ and is exponentially smaller than for $R \to \infty$. However since for $R = 0$ only one of the two holes occupies the screening orbital, while the second one is in a plane-wave state with an infinite characteristic length, we expect that only one-half of the total impurity spin is compensated in a finite region around the two impurities. In fact by evaluating $\int_0^L G(z)\,dz$ for $L \gg \zeta$ we find a result close to $-1/2$, which is the characteristic value for a spin-1 partially compensated by a spin 1/2. Since the second hole does not dynamically contribute to screening, we expect the susceptibility to diverge for $R \to 0$: this is confirmed by the numerical results (see Ref. 34).

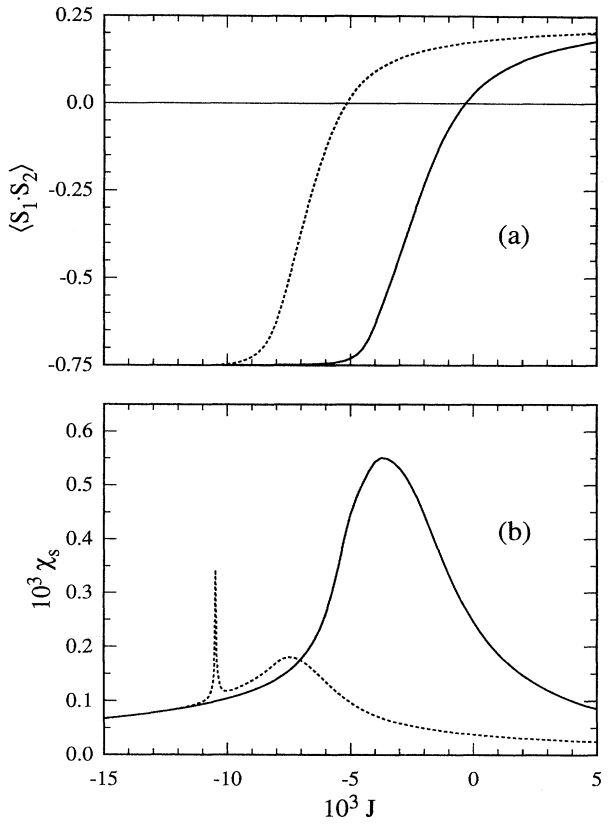

FIG. 7. (a) Spin correlation function $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle$ and (b) staggered susceptibility as a function of magnetic coupling, at a fixed distance $k_F R = 4.5$ (solid lines), $k_F R = 1.5$ (dotted lines). Other parameters: $B = 1$, $\Gamma = 0.1$, $T_K = 0.001$.

IV. EFFECT OF MAGNETIC INTERACTION

In this section we study the effect of including a magnetic interaction term $-J\mathbf{S}_1\cdot\mathbf{S}_2$ in the lowest-order calculation. Such a term simulates the effect of electron-hole excitations, as well as other contributions to the magnetic interaction not included in the model, like the one coming from local Heisenberg exchange between f and conduction spins. It is of particular interest to determine whether and under which conditions a phase transition occurs as J is varied.

In Fig. 7 we show the correlation function $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle$ and the staggered susceptibility χ_s as a function of magnetic coupling, for two fixed values of the distance. The results for $k_F R = 4.5$ (solid curves) are representative of the behavior for $R > R_c$: physical properties are a smooth function of the ratio J/T_K. Correlations between impurity spins are ferromagnetic for $J \gg T_K$ and antiferromagnetic for $J \ll -T_K$. A peak of the staggered susceptibility occurs when the antiferromagnetic coupling J is a few times the Kondo temperature. This peak originates from two competing factors. Starting from $J = 0$ and decreasing J, the gap between the $S = 0$ and the $S = 1$ states decreases, which first gives an increase of the susceptibility. However for $J \ll -T_K$ the lowest state is close to having $S_{\text{imp}} = 0$ in both subspaces $S = 0$ and $S = 1$, the two ground states differing only by the conduction electron quantum numbers: thus the matrix element of $S_{1z} - S_{2z}$ decreases, and makes the susceptibility tend to zero for $J \ll -T_K$. The solid curves in Fig. 7 are very similar to those calculated in a two-site "molecular" model,[37] showing that they do not depend in an essential way on the continuous nature of the conduction electron spectrum.

It was first shown by Jones, Varma, and Wilkins[20] using the numerical renormalization group method that for the particle-hole symmetric Kondo Hamiltonian a critical point with diverging staggered susceptibility occurs for an antiferromagnetic coupling $J \simeq -2T_K$. The existence of a critical point has been recently proved using the methods of conformal field theory.[28] Moreover it has been shown that potential scattering with different values in the two parity channels removes the divergence.[24,25] We do not insist on this point, which is discussed in detail in the literature.[23–25,28] We just remark that our model is not particle-hole symmetric, and that the An-

derson model does contain potential scattering with different values in the two parity channels: thus the smooth behavior we find for χ_s is in agreement with the results of Refs. 23–25, and 28. In the framework of the variational method, obtaining the divergence of χ_s would require the decoupling of even and odd parts of the Hilbert space, as shown by Yanagisawa.[26] This decoupling only occurs for $R = 0$ (see below).

For distances $R < R_c$, we expect that the relevant energy scale will be the enhanced binding energy δ_- (see Appendix B), and that the magnetic interaction term will play an important role only for $J < -\delta_-$. This is confirmed by the dotted curves in Fig. 7, which show that the interimpurity correlations remain ferromagnetic for couplings $J > -\delta_-$ [$\delta_- \simeq 9 \times 10^{-3}$ with the parameters of Fig. 7: see also Fig. 4(a)]. An additional sharp peak is also seen in the curve for χ_s. This additional peak, which for $R \neq 0$ is not a divergence, originates from an anticrossing of states in the $S = 0$ subspace. This can be understood from the limiting case $R = 0$: as shown in Appendix B, for $R = 0$ triplet and singlet impurity states are decoupled, and a crossing between these two states occurs at a value $J \simeq -\delta_-$. Thus the two peaks in the dotted curve of Fig. 7(b) merge into one and become a divergence of χ_s for zero distance.

In the periodic Anderson model, a second-order transition to an ordered state is expected at a critical value of $|J|/T_K$, whereby the system enters a reduced-moment phase which gradually evolves into the full-moment ordered state as $|J|/T_K$ is increased.[41,42] Thus the peaks of Fig. 7(b) can be seen as remnants of a phase transition, which, however, can only be reproduced in a lattice of impurities. A phase transition is also obtained for the two-impurity model in the $N_f \to \infty$ limit.[21] The fact that this transition disappears for $N_f = 2$ agrees with the arguments given about the possible effects of $1/N_f$ fluctuations.[21,23,25]

V. FINITE-TEMPERATURE PROPERTIES

Within the lowest-order variational basis ($0ab$), we can calculate finite-temperature properties by taking all eigenstates resulting from the generalized eigenvalue equations in the subspaces with total spin $S = 0$, 1, and 2 and performing standard thermodynamics. By this procedure, apart from the numerical approximation due to the discretization of the continuum, we are neglecting the effect of electronic excitations above the Fermi level.

The effect of electron-hole excitations can be judged from Fig. 8, where we compare $T\chi(T)$ for the one-impurity problem [in the basis ($0a$) of Fig. 3(a)] with the known Bethe-Ansatz solution.[43] The quantity $T\chi(T)$ can be interpreted as the square of the impurity magnetic moment. The impurity moment is screened at temperatures below T_K and vanishes for $T \to 0$. The slow transition of the exact solution becomes more rapid in our approximate calculation, as a result of neglecting the electron-hole pairs. Still, the qualitative behavior of the susceptibility is reproduced, which makes us believe that the main physics of the two-impurity system is also qualitatively described in this approach. However our approach must be limited to temperatures $T < |E_f|$: for $T \gg |E_f|$, by treating the impurity thermodynamics in the grand-canonical ensemble the impurity occupation is expected to be $n_f = N_f/(N_f + 1)$, whereas in the lowest-order variational basis ($0a$) of Fig. 3(a) the impurity occupation at high temperature is unity, and oscillates between zero and one when more variational states are included.

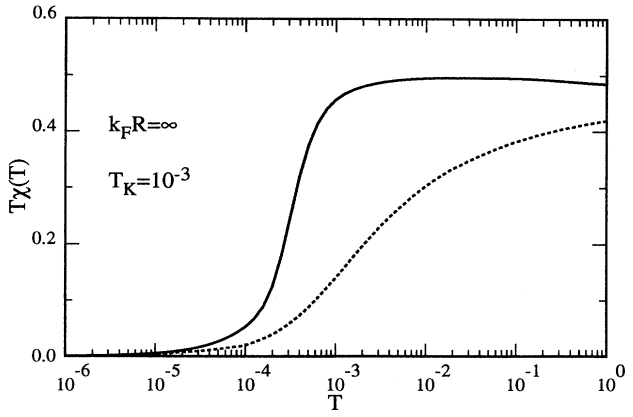

FIG. 8. Impurity susceptibility times temperature for the one-impurity problem. Parameters: $B = 1$, $\Gamma = 0.1$, $T_K = 0.001$. Dotted line: Bethe-Ansatz solution (Ref. 43).

In Fig. 9 we show the correlation $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle$ and the

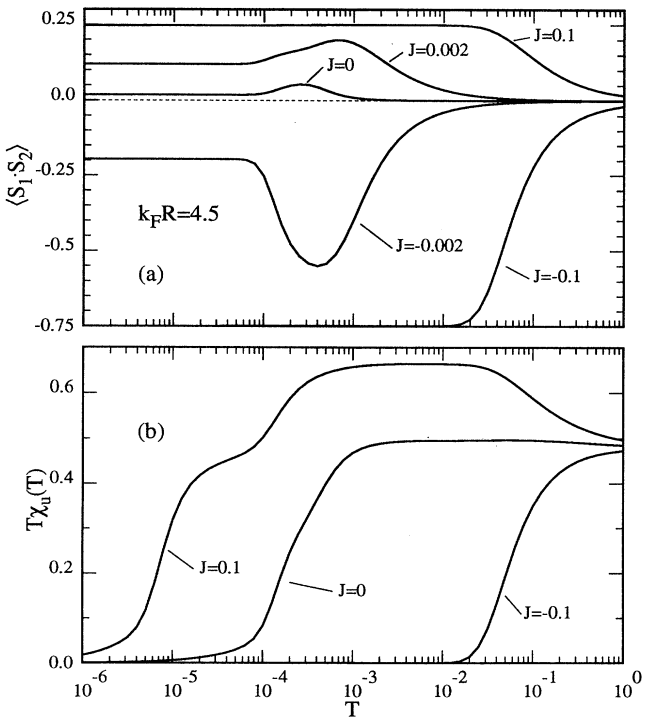

FIG. 9. (a) Correlation $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle$ and (b) uniform impurity susceptibility times temperature, at a fixed distance $k_FR = 4.5$. Other parameters: $B = 1$, $\Gamma = 0.1$, $T_K = 0.001$.

quantity $T\chi_u(T)$ for the two-impurity problem at a fixed distance $R > R_c$. In Fig. 9(a), magnetic correlations first develop according to the value of the magnetic coupling as the temperature is lowered down to $T \sim T_K$, where they stop growing and go over to the low-temperature value. If $|J| \gg T_K$, low-temperature correlations are fully ferro- or antiferromagnetic, whereas they have intermediate values when $|J| \sim T_K$. For $|J| \ll T_K$ magnetic correlations are always small. The low-temperature values are those of Fig. 7(a). The above picture is essentially identical to that resulting from quantum Monte Carlo simulations.[18] The peaks in Fig. 9(a) are probably spurious, and reflect the too rapid screening of the impurity moment shown in Fig. 8.

In Fig. 9(b), for $J = 0$, there is little interaction between the two impurities, and the behavior is similar to the one-impurity case. For antiferromagnetic (AFM) coupling $J \ll -T_K$, the impurity spins lock in a nonmagnetic singlet at $T \sim -J$, following a pure RKKY behavior, and no Kondo effect occurs. For a ferromagnetic coupling $J \gg T_K$, the impurity spins first lock in a triplet at $T \sim J$, with $T\chi_u(T) \simeq 2/3$. For lower temperatures, a two-stage Kondo effect occurs:[9] first only one-half of the total impurity spin is compensated, leading to a plateau $T\chi_u(T) \simeq 4/9$, and then this remaining moment is further screened, with a vanishing moment for $T \to 0$. These results are very similar to those predicted in Ref. 9, and show that for $R > R_c$ the two-impurity system is correctly described by scaling theory. We note that the two-stage compensation could not be observed in Monte Carlo simulations,[18] due to the difficulty of achieving extreme limits of the parameters. On the other hand, the present method is well suited to resolving quite different energy scales, due to the particular choice of the basis functions used for discretizing the continuum (Appendix A).

In Fig. 10 we show the magnetic correlation and susceptibility for a distance $R < R_c$. It can be seen that the relevant energy scale is now the enhanced binding energy δ_- ($\simeq 10^{-2}$: see Fig. 4). Magnetic correlations develop down to $T > \delta_-$. Low-temperature correlations are ferromagnetic for both $J \gg \delta_-$ and $|J| \ll \delta_-$, and become antiferromagnetic only when $J \ll -\delta_-$. For the susceptibility, when $J = 0$, there is still a semiquenched two-impurity regime for temperatures $T < \delta_-$, indicating that the two impurities form a ferromagnetic complex even in the absence of the indirect f-f interaction. The lower screening temperature is smaller than for $R > R_c$, and eventually vanishes as $R \to 0$, since the lowest gap also tends to zero (see Fig. 4). For $J \gg \delta_-$ the two-stage Kondo effect occurs, with the lowest screening temperature being about 10^{-12}. The semiquenched two-impurity regime is suppressed only for antiferromagnetic couplings $J \ll -\delta_-$.

In summary, for $R > R_c$ the present results confirm that the behavior of the two-impurity system depends on the ratio J/T_K. For $R < R_c$, the new scale given by the enhanced binding energy δ_- is found to be relevant also for finite-temperature properties. In the limit $R \to 0$, for small or ferromagnetic J, the lowest of the screening temperatures tends to zero, reflecting the fact that half

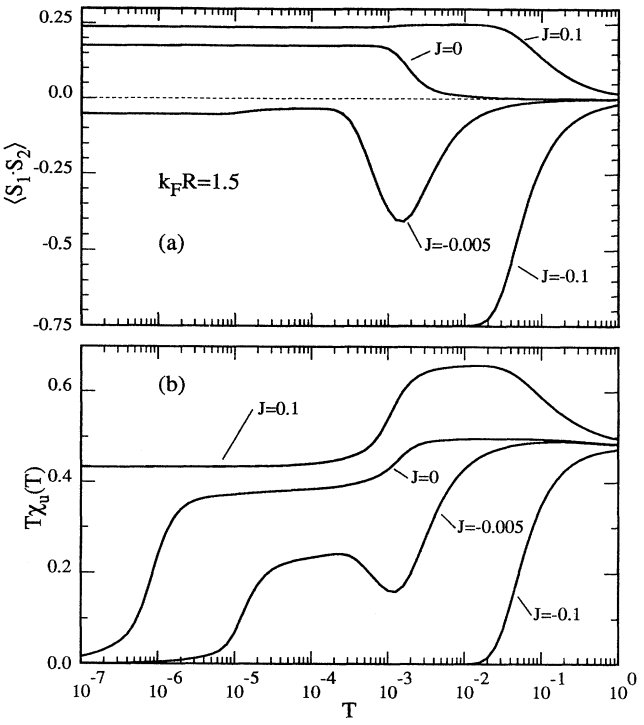

FIG. 10. As in Fig. 9, for a fixed distance $k_F R = 1.5$.

of the impurity moment remains uncompensated at low T.

VI. EFFECT OF ELECTRON-HOLE EXCITATIONS

The effect of electron-hole excitations can be studied first in the one-impurity problem.[33] In the nonmagnetic basis of Fig. 3(a), the lowest-order calculation corresponds to the basis $(0a)$, and electron-hole excitations are included in the basis $(0ac)$. The ground-state energy in the basis $(0ac)$, measured from the energy of the filled Fermi sea, is close to

$$E = E_f + \Delta E_f - T_K^*, \tag{16}$$

where the f-level position E_f is shifted by the negative quantity

$$\Delta E_f \simeq -\sum_{\mathbf{k}} \frac{\theta(\epsilon_{\mathbf{k}} - \epsilon_F)|V_{\mathbf{k}}|^2}{\epsilon_{\mathbf{k}} - E_f} = -\frac{\Gamma}{\pi} \ln\left(\frac{B' - E_f}{-E_f}\right) \tag{17}$$

and the triplet-singlet splitting T_K^* is given by

$$T_K^* \simeq B \exp\left(\frac{\pi(E_f + \Delta E_f)}{2\Gamma}\right). \tag{18}$$

Formula (17) also follows from second-order perturbation theory. Both expressions (17) and (18) involve a renormalized f-level energy $E_f^* = E_f + \Delta E_f$. Thus the effect of electron-hole excitations in the one-impurity problem

is basically to renormalize the f-level position.

In the two-impurity problem, the effect of electron-hole excitations can be analyzed along similar lines. In the basis of Fig. 1, let us take states $(0ab)$ as the zeroth-order subspace. States $(cdef)$ can be eliminated in degenerate fourth-order perturbation theory: i.e., in the subspace $(0ab)$ an effective Hamiltonian can be defined whose matrix elements $\tilde{H}_{ij}$ are given by

$$\tilde{H}_{ij} = H_{ij} + \sum_l \frac{H_{il}H_{lj}}{E_i - E_l} + \sum_{lmn} \frac{H_{il}H_{lm}H_{mn}H_{nj}}{(E_i - E_l)(E_i - E_m)(E_i - E_n)}, \quad (19)$$

where the indexes lmn run over states $(cdef)$. States (cd) can be eliminated in second order, yielding a renormalized f-level energy $E_f + \Delta E_f$. States (ef) can be eliminated in fourth order. Apart from spin-independent terms, they produce a magnetic interaction $-J\mathbf{S}_1 \cdot \mathbf{S}_2$.[44] The magnetic coupling J can be split into two parts. The contribution coming from the path (bde) describes a polarization of the Fermi sea, and will be called RKKY in the following: it is given by

$$J_{\mathrm{RKKY}} = 4 \sum_{\mathbf{k}\mathbf{k}'} |V_{\mathbf{k}}|^2 |V_{\mathbf{k}'}|^2 \frac{\theta(\epsilon_{\mathrm{F}} - \epsilon_k)\theta(\epsilon_{k'} - \epsilon_{\mathrm{F}})}{(\epsilon_{k'} - \epsilon_k)(\epsilon_{k'} - E_f)^2} \times \cos[(\mathbf{k} - \mathbf{k}') \cdot \mathbf{R}]. \quad (20)$$

The contribution coming from path (bdf) is nonzero even if the band is empty, and for this reason will be referred to as *superexchange*:

$$J_{\mathrm{SE}} = -2 \sum_{\mathbf{k}\mathbf{k}'} |V_{\mathbf{k}}|^2 |V_{\mathbf{k}'}|^2 \frac{\theta(\epsilon_k - \epsilon_{\mathrm{F}})\theta(\epsilon_{k'} - \epsilon_{\mathrm{F}})}{(\epsilon_k - E_f)(\epsilon_{k'} - E_f)} \times \left(\frac{1}{\epsilon_k - E_f} + \frac{1}{\epsilon_{k'} - E_f} \right) \cos[(\mathbf{k} - \mathbf{k}') \cdot \mathbf{R}]. \quad (21)$$

The two couplings are plotted in Fig. 11 as a function of distance. It can be seen that the RKKY term is mostly ferromagnetic, whereas the superexchange contribution is mostly antiferromagnetic.[45] If Brillouin-Wigner instead of Schrödinger-Rayleigh perturbation theory is performed [i.e., if the energy E_i is replaced by the eigenvalue E in Eq. (19)], the expressions for the magnetic couplings have to be evaluated at the renormalized f-level energy E_f^*.

In Fig. 12 we show the two lowest energies and the ground-state correlation function in the variational calculations with the bases $(0ab)$, $(0abc)$, and $(0abcd)$. It can be seen that the qualitative features of the lowest-order calculation are retained when electron-hole excitations are included. States (c) have a rather minor effect, since they couple only to state (a) which has little weight in the lowest-order ground state. Inclusion of states (d) has two effects: (i) the energy is shifted to negative values by a quantity close to $2\Delta E_f$, and (ii) the scale of the curves is reduced, corresponding to a renormalization of E_f in the exponent of the characteristic energy. The ground-state correlation functions for the three variational bases are seen to be close to one another. Thus when states (c) and (d) are included, the physics of the lowest-order calculation with a renormalized f-level energy is recovered.

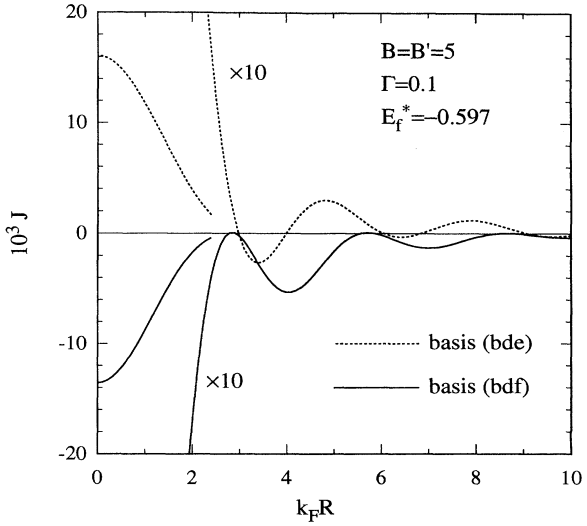

FIG. 11. RKKY (dotted line) and superexchange (solid line) magnetic couplings evaluated in fourth-order perturbation theory.

In Fig. 13 we show the energy and correlation function in the variational basis $(0abcdf)$ for two different values of the upper cutoff B'. In the limit $R \to \infty$, the basis $(0abcdf)$ factorizes into the product of the one-impurity basis $(0ac)$ for each impurity: we have verified that the energy in the $R \to \infty$ limit corresponds to twice the energy of the one-impurity problem in the basis $(0ac)$. State (e), which is very cumbersome to treat, has not been included. Thus only the superexchange part of the magnetic coupling is generated, leading to antiferromagnetic correlations at zero distance when the upper cutoff B' is sufficiently large [Fig. 13(d)]. However this behavior will be modified when state (e) is included. The value of the correlation function at zero distance can be derived as follows. For $R = 0$ even and odd impurity levels are decoupled, and the total impurity spin $\mathbf{S}_{\mathrm{imp}} = \mathbf{S}_1 + \mathbf{S}_2$ becomes a conserved quantity. Thus when states (e) and (f) are included, the ground-state correlation remains ferromagnetic unless $J < -\delta^*$, where δ^* is the (positive) singlet-triplet splitting in the basis $(0abcd)$ and $J = J_{\mathrm{RKKY}} + J_{\mathrm{SE}}$ is the total magnetic coupling. Usually the RKKY and superexchange contributions are of the same size, unless the conduction electron concentration is very small: in this limit, the sum over occupied states in Eq. (20) leads to a vanishing RKKY term.

Note that in the two-impurity Kondo model, correlations at $R = 0$ are always ferromagnetic. The reason is that the superexchange part of the magnetic interaction is not contained in the Kondo Hamiltonian, and is only recovered when the Schrieffer-Wolff transformation is carried out to higher order.[44,45] Thus the possibility of having zero-distance antiferromagnetic correlations be-

tween the impurities is characteristic of the Anderson model. It would be interesting to verify this prediction by renormalization group calculations on the two-impurity Anderson model in the limit of a small conduction electron concentration.

The results of Fig. 13 bear some resemblance to those obtained with a slave-boson technique in Ref. 16, where it is found that zero-distance correlations can be ferro- or antiferromagnetic according to the value of the parameter $q = Q/N_f$ which implements the occupation constraint (see, e.g., Fig. 14 of Ref. 16). However in the original Anderson model there is no free parameter q, and it is not clear what different values of q physically mean.

It is of particular interest to establish to which extent the results in the full basis can be reproduced by a lowest-order calculation with renormalized parameters. A comparison between the two calculations is done in Ref. 46,

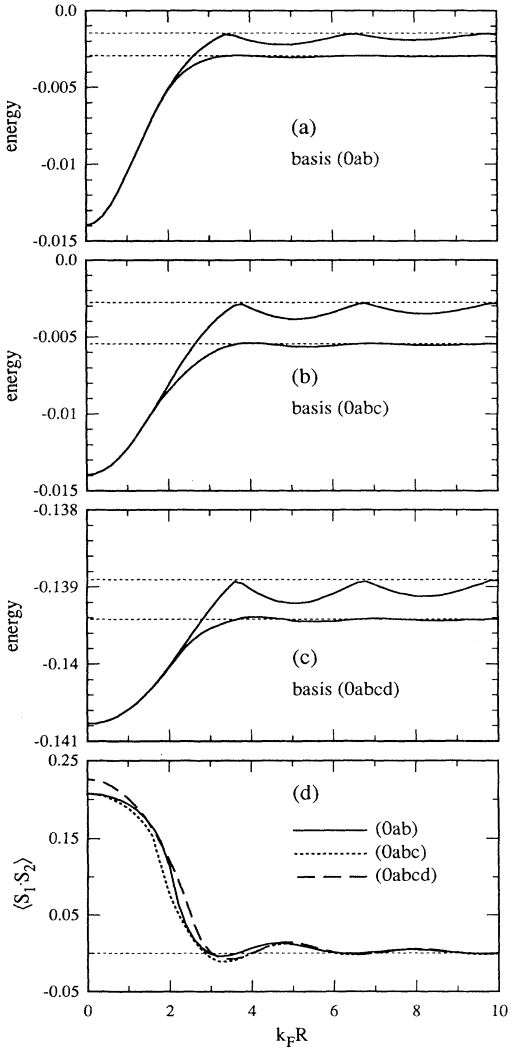

FIG. 12. (a)–(c) Energies of the two lowest states in different bases; the dotted lines represent the $R \to \infty$ limit. (d) Ground-state correlation function. Parameters: $B = B' = 5$, $E_f = -0.5$, $\Gamma = 0.1$.

with the following results: for a distance $R > R_c$, the results in the basis $(0abcdf)$ are close to the results in the basis $(0ab)$, provided the renormalized f-level position E_f^* is used and a magnetic interaction $-J_{\rm SE}(E_f^*)\mathbf{S}_1 \cdot \mathbf{S}_2$ is included in the lowest-order calculation. For $0 < R < R_c$, the two calculations agree only qualitatively. This might indicate that the magnetic coupling itself is renormalized by the collective Kondo effect. It has been shown by Cox[41] that for $k_F^{-1} < R < \zeta$ the RKKY interaction is not modified by the Kondo effect: however it is not clear what happens for $R < (k_F)^{-1} \sim R_c$.

VII. DISCUSSION AND CONCLUSIONS

The present study indicates that two effects can drive a magnetic interaction between two Anderson impurities: First, there is the interference between screening clouds, which is already described in the lowest-order basis $(0ab)$ and therefore is an effect of order $1/N_f$. For large distances, this effect modifies the single-impurity correlation function only in a spatial region of order $(k_F)^{-1}$ around the second impurity. For $R < R_c \sim 2.5/k_F$, one can no longer speak of independent screening clouds: for $R \to 0$, a collective Kondo effect occurs with the formation of an impurity spin triplet and an exponentially increased binding energy. Second, there is the fourth-order interaction, which is an effect of order $1/N_f^2$ and requires electron-hole excitations to be generated. The two effects can be distinguished by the spatial dependence: for the fourth-order interaction, the position of the nodes depends on the band structure via both the lower and upper cutoffs. Also, the fourth-order interaction can lead to both ferro- or antiferromagnetic correlations for $R \to 0$, according to the relative contributions of the RKKY and superexchange parts and the value of the enhanced binding energy.

For $R > R_c$ the interference between screening clouds is relatively weak, and the only important coupling between the impurities comes from the fourth-order interaction. The physics depends smoothly on the ratio J/T_K, with no phase transitions as the magnetic coupling is varied. In this regime, the effect of electron-hole excitations is mainly to renormalize the f-level energy E_f and to add a magnetic coupling $-J\mathbf{S}_1 \cdot \mathbf{S}_2$. At finite temperature, the results of scaling theory[9] and of quantum Monte Carlo simulations[18] are recovered: magnetic correlations grow down to temperatures $T \sim T_K$, where they go over to the low-temperature value. A two-stage Kondo effect occurs for $J \gg T_K$.

For $R < R_c$, an exponential increase of the binding energy occurs: the new characteristic energy δ_- becomes the relevant scale for both zero-temperature and finite-temperature properties. When electron-hole excitations are included, the magnetic interaction now competes with this new characteristic energy. For zero distance, the two impurities form a ferromagnetic complex, which is only partially compensated by conduction electrons at low temperature. Thus the lowest screening temperature in the two-stage Kondo effect vanishes for $R \to 0$.

It is interesting to compare the properties of the two-impurity model with those of the Anderson lattice. The

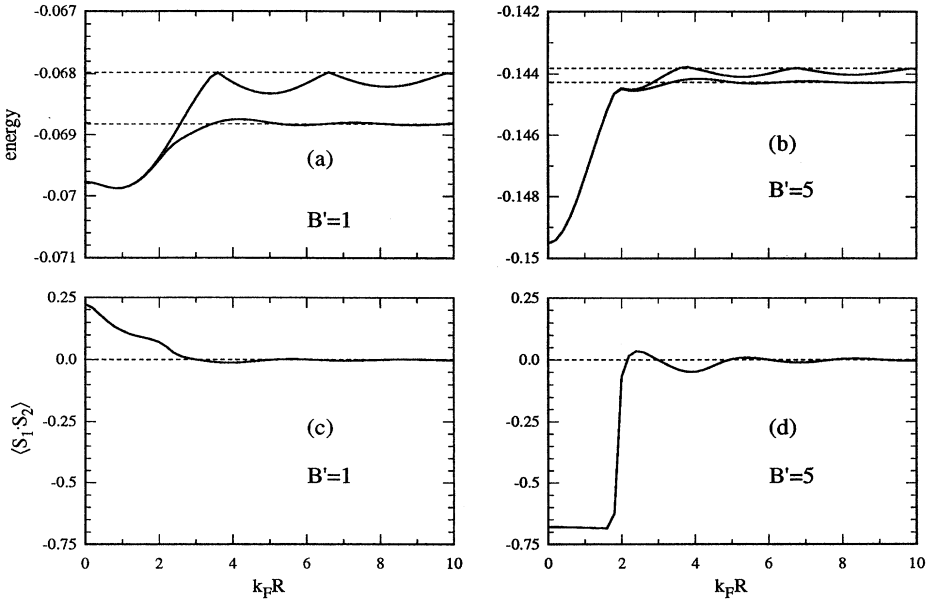

FIG. 13. (a) and (b) Energies of the two lowest states and (c) and (d) ground-state correlation function in the basis (0*abcdf*), for two different values of the upper cutoff B'. Other parameters: $B = 5$, $E_f = -0.5$, $\Gamma = 0.1$.

periodic Anderson model shows short-range antiferromagnetic correlations close to half-filling.[47–49] The reason can be stated as follows: since the Kondo effect involves conduction electrons in an energy shell of order T_K around the Fermi level, in a concentrated system there are not enough conduction electrons to screen all localized spins,[50] which therefore must compensate each other via short-range antiferromagnetic correlations. This "exhaustion" effect[50] is missing in any model with a finite number of impurities against an infinite number of conduction electrons. Thus it is no real surprise that the two-impurity model is unable to reproduce the antiferromagnetic correlations of the Anderson lattice close to half-filling. A more meaningful correspondence might be between the two-impurity model at short distance and the Kondo-lattice model with two conduction electrons.[51] Still, the indication that strong interference between screening clouds is limited to distances $R \sim (k_F)^{-1}$ suggests that the Anderson lattice might be adequately treated by a cluster Gutzwiller approximation.[52]

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APPENDIX A: DISCRETIZATION OF CONTINUOUS SPECTRUM

In this appendix we outline the technique used to solve the Schrödinger equation corresponding to the Hamiltonian (1) in the variational basis (3)–(11). In previous higher-order calculations on the one-impurity problem,[35,53] a logarithmic discretization of the energy spectrum was used, and the lowest eigenstates were found by the Chebyshev or the Lanczos method. Here we follow a different route.

The general idea of the procedure is as follows. Let the wave function for a total spin $S = 0$ be expanded as

$$\psi = a_0\psi_0 + \sum_{i\mathbf{k}} a_i(\mathbf{k})\psi^{(a)}_{i\mathbf{k}} + \sum_{\mathbf{k}_1\mathbf{k}_2}{}' [b^{(S_{\rm imp}=1)}(\mathbf{k}_1\mathbf{k}_2)\psi^{(b)}_{\mathbf{k}_1\mathbf{k}_2} + b^{(S_{\rm imp}=0)}(\mathbf{k}_1\mathbf{k}_2)\phi^{(b)}_{\mathbf{k}_1\mathbf{k}_2}] + \cdots \quad \text{(A1)}$$

[Note that $\sum'_{\mathbf{k}_1\mathbf{k}_2}$ is restricted to half of the values $(\mathbf{k}_1, \mathbf{k}_2)$.] Due to cylindrical symmetry around the axis connecting the two impurities it can be shown that the coefficient $a_1(\mathbf{k})$ has the form

$$a_1(\mathbf{k}) = V_{\mathbf{k}}[a_0(\epsilon) + a_1(\epsilon)e^{ik_zR}], \quad \text{(A2)}$$

where $a_0(\epsilon)$ and $a_1(\epsilon)$ depend only on energy (below the Fermi level $\epsilon_F \equiv 0$). These coefficients are expanded in a nonorthogonal basis consisting of N_α functions

$$h_l(\epsilon) = \frac{V_\epsilon}{\epsilon - \alpha_l}, \qquad l = 1, \ldots, N_<. \quad \text{(A3)}$$

This choice is motived by the single-impurity solution,[33] in which the ground state is given by only one basis function $h_l(\epsilon)$, provided α is chosen to be the Kondo temperature (given by $T_K \simeq B\exp[\pi E_f/(2\Gamma)]$ in the lowest-order basis $(0a)$ of Fig. 3(a)). By choosing the parameters $\alpha_1, \alpha_2, \ldots, \alpha_{N_<}$ in geometrical progression around T_K, we discretize the continuum in a particularly efficient way. For the dependence on wave vectors corresponding to energies above the Fermi level, we introduce in a similar way nonorthogonal basis functions:

$$g_m(E) = \frac{V_E}{E + \beta_m}, \qquad m = 1, \ldots, N_>. \quad \text{(A4)}$$

The choice of the parameters β_m is less critical: while the typical energy scale for holes is T_K, the typical energy scale for electrons is $|E_f|$, as can be seen, e.g., from Eq. (17). A number of parameters $N_< = 6$–10, $N_> = 2$ is found to be sufficient for numerical accuracy, as shown by convergence tests in the one-impurity case; qualitative trends are obtained even with $N_< = 4$. The overlap and Hamiltonian matrix elements within the variational basis, with the discretization of the continuum implied by the basis functions (A3) and (A4), can be expressed in terms of a small number of integrals which can be evaluated analytically in terms of the sine and cosine integral. The Schrödinger equation in the subspace (3)–(11) is thus transformed into a generalized eigenvalue problem with a small dimension (~100–500). This is solved numerically in all subspaces with given total spin, yielding all eigenvalues and eigenvectors and allowing one to calculate the partition function and the thermodynamic quantities at finite temperature. This is a distinct feature of the present method. Another advantage of the technique is that good qualitative trends can be obtained with small matrices and low computational effort: this is due to the fact that the basis functions (A3) and (A4) give a very good representation of the hole and electron wave functions. For comparison, the usual discretization procedure[35,53] corresponds to choosing the basis functions $h_l(\epsilon)$, $g_m(E)$ to be δ functions with discretized energies in logarithmic scale. This choice leads to a standard eigenvalue problem, but with much larger matrices.

APPENDIX B: SCHRÖDINGER EQUATION IN LOWEST-ORDER BASIS

In the lowest-order basis $(0ab)$, integral equations for the expansion coefficients can be derived by the "folding" technique.[33] In this appendix we derive such equations and discuss their solutions in the limiting cases $R \to \infty$ and $R \to 0$.

The Schrödinger equation is written as

$$H\psi = (E_0 + 2E_f + \Delta E)\psi, \tag{B1}$$

where E_0 is the energy of the filled Fermi sea: the energy ΔE is thus referred to the state $f_1^\dagger f_2^\dagger \psi_0$ with both impurities occupied. For the ground state, the positive quantity $-\Delta E$ can be interpreted as a binding energy. The off-diagonal matrix elements of the Hamiltonian (1) among the lowest-order basis states (3)–(6) are [the two impurities are assumed to be at $\mathbf{R}_1 = (0,0,0)$ and $\mathbf{R}_2 = (0,0,R)$]

$$\langle \psi_0 | H | \psi^{(a)}_{i\mathbf{k}} \rangle = \sqrt{2} V^*_{\mathbf{k}}, \tag{B2}$$

$$\langle \psi^{(a)}_{1m\mathbf{k}} | H | \psi^{(b)}_{\mathbf{k}_1\mathbf{k}_2} \rangle = -\sqrt{\frac{3}{2}} [\delta_{\mathbf{k}\mathbf{k}_1} V^*_{\mathbf{k}_2} e^{-ik_{2z}R} - \delta_{\mathbf{k}\mathbf{k}_2} V^*_{\mathbf{k}_1} e^{-ik_{1z}R}], \tag{B3}$$

$$\langle \psi^{(a)}_{2\mathbf{k}} | H | \psi^{(b)}_{\mathbf{k}_1\mathbf{k}_2} \rangle = -\sqrt{\frac{3}{2}} [\delta_{\mathbf{k}\mathbf{k}_2} V^*_{\mathbf{k}_1} e^{-ik_{2z}R} - \delta_{\mathbf{k}\mathbf{k}_1} V^*_{\mathbf{k}_2} e^{-ik_{1z}R}], \tag{B4}$$

$$\langle \psi^{(a)}_{1\mathbf{k}} | H | \phi^{(b)}_{\mathbf{k}_1\mathbf{k}_2} \rangle = -\sqrt{\frac{1}{2}} [\delta_{\mathbf{k}\mathbf{k}_1} V^*_{\mathbf{k}_2} e^{-ik_{2z}R} + \delta_{\mathbf{k}\mathbf{k}_2} V^*_{\mathbf{k}_1} e^{-ik_{1z}R}], \tag{B5}$$

$$\langle \psi^{(a)}_{2\mathbf{k}} | H | \phi^{(b)}_{\mathbf{k}_1\mathbf{k}_2} \rangle = -\sqrt{\frac{1}{2}} [\delta_{\mathbf{k}\mathbf{k}_2} V^*_{\mathbf{k}_1} e^{-ik_{2z}R} + \delta_{\mathbf{k}\mathbf{k}_1} V^*_{\mathbf{k}_2} e^{-ik_{1z}R}]. \tag{B6}$$

Let the wave function for a total spin $S = 0$ be expanded as in Eq. (A1). The Schrödinger equation (B1), with the matrix elements (B2)–(B6), gives rise to linear equations for the expansion coefficients. We express the coefficients $b^{(S_{\rm imp}=1)}$, $b^{(S_{\rm imp}=0)}$ in terms of $a_i(\mathbf{k})$, and redefine $a_i(\mathbf{k}) = V_{\mathbf{k}} \tilde{a}_i(\mathbf{k})$. After some algebra, we obtain the following equations:

$$(-2E_f - \Delta E) a_0 + \sqrt{2} \sum_{\mathbf{k}} |V_{\mathbf{k}}|^2 [\tilde{a}_1(\mathbf{k}) + \tilde{a}_2(\mathbf{k})] = 0, \tag{B7}$$

$$\sqrt{2} a_0 + (-E_f - \epsilon_k - \Delta E)\tilde{a}_1(\mathbf{k}) + \frac{3}{2} \sum_{\mathbf{k}'} |V_{\mathbf{k}'}|^2 \frac{\tilde{a}_1(\mathbf{k}) + \tilde{a}_2(\mathbf{k}') - [\tilde{a}_1(\mathbf{k}') + \tilde{a}_2(\mathbf{k})] e^{i(k_z - k'_z)R}}{\epsilon_k + \epsilon_{k'} + \Delta E + \frac{J}{4}}$$

$$+ \frac{1}{2} \sum_{\mathbf{k}'} |V_{\mathbf{k}'}|^2 \frac{\tilde{a}_1(\mathbf{k}) + \tilde{a}_2(\mathbf{k}') + [\tilde{a}_1(\mathbf{k}') + \tilde{a}_2(\mathbf{k})] e^{i(k_z - k'_z)R}}{\epsilon_k + \epsilon_{k'} + \Delta E - \frac{3J}{4}} = 0, \tag{B8}$$

$$\sqrt{2} a_0 + (-E_f - \epsilon_k - \Delta E)\tilde{a}_2(\mathbf{k}) + \frac{3}{2} \sum_{\mathbf{k}'} |V_{\mathbf{k}'}|^2 \frac{\tilde{a}_2(\mathbf{k}) + \tilde{a}_1(\mathbf{k}') - [\tilde{a}_2(\mathbf{k}') + \tilde{a}_1(\mathbf{k})] e^{-i(k_z - k'_z)R}}{\epsilon_k + \epsilon_{k'} + \Delta E + \frac{J}{4}}$$

$$+ \frac{1}{2} \sum_{\mathbf{k}'} |V_{\mathbf{k}'}|^2 \frac{\tilde{a}_2(\mathbf{k}) + \tilde{a}_1(\mathbf{k}') + [\tilde{a}_2(\mathbf{k}') + \tilde{a}_1(\mathbf{k})] e^{-i(k_z - k'_z)R}}{\epsilon_k + \epsilon_{k'} + \Delta E - \frac{3J}{4}} = 0. \tag{B9}$$

These equations embody all numerical results of Secs. III–V. We have not been able to find an analytical solution for the ground state, except in the limiting cases discussed below.

In the limit $R \to \infty$, the terms with the phase factor in (B8) and (B9) can be dropped. For $J = 0$, a solution of the nonlinear equations is given by the following ansatz (see also Ref. 29):

$$\tilde{a}_1(\mathbf{k}) = \tilde{a}_2(\mathbf{k}) = \frac{\sqrt{2}a_0}{\epsilon_k + \frac{\Delta E}{2}}. \tag{B10}$$

By substituting in (B7)–(B9), the following secular equation is obtained:

$$E_f + \frac{\Delta E}{2} = 2\frac{\Gamma}{\pi}\int_{-B}^{0} \frac{d\epsilon}{\epsilon + \frac{\Delta E}{2}}. \tag{B11}$$

The solution is clearly $\Delta E = -2T_K$, where $T_K \simeq B\exp[\pi E_f/(2\Gamma)]$ is the Kondo temperature in the one-impurity problem to lowest order. Thus the ansatz (B10) describes the product of two independent Kondo impurities.

We now consider the case $R \to 0$. In this limit, the coefficients $\tilde{a}_i(\mathbf{k})$ have spherical symmetry. We look for solutions of the form

$$\tilde{a}_1(k) = \pm\tilde{a}_2(k) = \delta_{\epsilon_k \bar{\epsilon}}, \tag{B12}$$

where $\bar{\epsilon}$ is a band energy which can be taken arbitrarily close to the Fermi level. The physical meaning of the ansatz (B12) is that the hole in state (a) of Fig. 1 [as well as one of the two holes in state (b)] is in a plane-wave state; the spectrum is continuous. For the even state it can be seen from the matrix elements (B3) and (B4) that the coefficient $b^{(S_{\rm imp}=1)} = 0$: thus in state (b) of Fig. 1 only state (6) is present, and the two impurity spins are in a singlet linear combination. Similarly, the odd state corresponds to a triplet combination of the impurity spins. The separation between triplet and singlet impurity states holds only for $R = 0$. In Eqs. (B8) and (B9), we can drop the term $\sqrt{2}a_0$ and the integral terms $\tilde{a}_i(\mathbf{k}')$, which are negligible compared to the δ function. The following algebraic equations are then obtained:

$$E_f + \epsilon + \Delta E = \frac{\Gamma}{\pi}\int_{-B}^{0} \frac{d\epsilon}{\epsilon + \epsilon' + \Delta E - \frac{3J}{4}} \quad \text{(even)}, \tag{B13}$$

$$E_f + \epsilon + \Delta E = \frac{3\Gamma}{\pi}\int_{-B}^{0} \frac{d\epsilon}{\epsilon + \epsilon' + \Delta E + \frac{J}{4}} \quad \text{(odd)}. \tag{B14}$$

The solutions are

$$\Delta E = -\epsilon + \frac{3J}{4} - \delta_+, \tag{B15}$$

$$\delta_+ \simeq B\exp\left(\frac{\pi(E_f + \frac{3J}{4})}{\Gamma}\right) \quad \text{(even)},$$

$$\Delta E = -\epsilon - \frac{J}{4} - \delta_-, \quad \delta_- \simeq B\exp\left(\frac{\pi(E_f - \frac{J}{4})}{3\Gamma}\right) \quad \text{(odd)}. \tag{B16}$$

For $J = 0$, the ground state is the odd (triplet) level, and the binding energy δ_- is exponentially larger than the single-impurity Kondo temperature: this can be interpreted as a collective Kondo effect. The even (singlet) state can become the ground state if the magnetic coupling J is antiferromagnetic and sufficiently large. Assuming $|J| \ll \Gamma$ and $\delta_+ \ll \delta_-$, the ground state is a triplet for $J > -\delta_-$, and becomes a singlet for $J < -\delta_-$, with a crossing between these two states as J is varied.

APPENDIX C: SCHRÖDINGER EQUATION IN SPIN-1/2 BASIS

Working with an odd number of electrons, and therefore with half-integer values of the total spin, the variational basis excluding electron-hole excitations corresponds to that of Fig. 2(b). The basis states with total spin $S = 1/2$ and $S_z = 1/2$ are given by

$$\psi_i^{(a)} = f_{i\uparrow}^\dagger \psi_0, \tag{C1}$$

$$\psi_{\mathbf{k}}^{(b)} = \frac{1}{\sqrt{6}}[f_{1\uparrow}^\dagger f_{2\uparrow}^\dagger c_{\mathbf{k}\uparrow} + (f_{1\uparrow}^\dagger f_{2\downarrow}^\dagger + f_{1\downarrow}^\dagger f_{2\uparrow}^\dagger)c_{\mathbf{k}\downarrow}]\psi_0, \tag{C2}$$

$$\phi_{\mathbf{k}}^{(b)} = \frac{1}{\sqrt{2}}(f_{1\uparrow}^\dagger f_{2\downarrow}^\dagger - f_{1\downarrow}^\dagger f_{2\uparrow}^\dagger)c_{\mathbf{k}\downarrow}\psi_0. \tag{C3}$$

We expand the spin-1/2 wave function in the variational basis (C1)–(C3) and derive an equation for the expansion coefficients by the "folding" technique, as done in Appendix B. Separating into even and odd states of the whole systems, the following algebraic equations are obtained for the energy spectrum:

$$E_f + \Delta E = \frac{3\Gamma}{2\pi}\int_{-B}^{0} \frac{d\epsilon}{\epsilon + \frac{J}{4} + \Delta E}\left(1 \mp \frac{\sin(kR)}{kR}\right) + \frac{\Gamma}{2\pi}\int_{-B}^{0} \frac{d\epsilon}{\epsilon - \frac{3J}{4} + \Delta E}\left(1 \pm \frac{\sin(kR)}{kR}\right), \tag{C4}$$

where the upper (lower) sign corresponds to even (odd) states, respectively. For $R \to \infty$ the two equations become identical, and give (for $J = 0$) $\Delta E = -T_{\rm K} \simeq -B\exp[\pi E_f/(2\Gamma)]$. The binding energy for $R \to \infty$ in the spin-1/2 basis is only one-half of the correct value given by Eq. (B11). This is due to the fact that only one hole is present in the state with both impurities occupied [state (b) of Fig. 2(b)]: thus the independent impurity limit is not properly described in the basis with an odd number of electrons.

For $R \to 0$, it can be shown (as in Appendix B) that even states correspond to an impurity singlet, while odd states correspond to an impurity triplet. The corresponding ground-state energies are

$$\Delta E = \frac{3J}{4} - \delta_+, \quad \delta_+ \simeq B\exp\left(\frac{\pi(E_f + \frac{3J}{4})}{\Gamma}\right) \quad \text{(even)}, \tag{C5}$$

$$\Delta E = -\frac{J}{4} - \delta_-, \quad \delta_- \simeq B \exp\left(\frac{\pi(E_f - \frac{J}{4})}{3\Gamma}\right) \quad \text{(odd)}. \tag{C6}$$

Comparing with Eqs. (B15) and (B16), we see that the positive energy $-\epsilon$ of the additional hole is not present in the spin-1/2 basis. However the physics is similar: for $J = 0$, the ground state is the odd (impurity-triplet) state, and a crossing between singlet and triplet states occurs as J is varied. Thus we can say that for $R \to 0$ the spin-1/2 basis provides an equivalent description of the lowest-order ground state. The correlation between f and conduction spins for $R = 0$ is $\langle \mathbf{S}_1 \cdot \mathbf{s}_c \rangle = -n_f/2$ in the spin-1/2 basis, compared to $\langle \mathbf{S}_1 \cdot \mathbf{s}_c \rangle = -n_f$ in the spin-0 basis. The difference between the two results comes from the additional plane-wave hole in the spin-0 basis: its spin is polarized oppositely to the impurity triplet, but since it is in a delocalized state it cannot be associated to a Kondo screening of the impurity spins.

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[1] J. Rossat-Mignod *et al.*, J. Magn. Magn. Mater. **76&77**, 376 (1988); J.-L. Jacoud, Ph.D. thesis, Université J. Fourier-Grenoble I, 1991 (unpublished).

[2] J.-M. Mignot *et al.*, J. Magn. Magn. Mater. **76&77**, 97 (1988).

[3] S. Quezel *et al.*, J. Magn. Magn. Mater. **76&77**, 403 (1988).

[4] J. K. Kjems and C. Broholm, J. Magn. Magn. Mater. **76&77**, 371 (1988); G. Aeppli *et al.*, *ibid.* **76&77**, 385 (1988).

[5] See, e.g., P. Fulde, J. Keller, and G. Zwicknagl, in *Solid State Physics*, edited by H. Ehrenreich and D. Turnbull (Academic, London, 1988), Vol. 41, p. 1.

[6] We reserve the term "RKKY" (Ruderman-Kittel-Kasuya-Yosida) interaction for a particular contribution to the magnetic coupling (see Sec. VI).

[7] S. Alexander and P. W. Anderson, Phys. Rev. **133**, A1594 (1964).

[8] K. Matho and M. T. Béal-Monod, Phys. Rev. B **5**, 1899 (1972); J. Phys. F **3**, 136 (1973); **4**, 848 (1974).

[9] C. Jayaprakash, H. R. Krishna-murthy, and J. W. Wilkins, Phys. Rev. Lett. **47**, 737 (1981).

[10] M. Lavagna and M. Cyrot, Solid State Commun. **55**, 555 (1985).

[11] M. Lavagna, J. Magn. Magn. Mater. **47&48**, 360 (1985).

[12] J. W. Rasul, J. Magn. Magn. Mater. **47&48**, 364 (1985).

[13] H. Suhl, Phys. Rev. Lett. **55**, 2999 (1985).

[14] C. Zhou and T. K. Lee, J. Magn. Magn. Mater. **63&64**, 248 (1987).

[15] V. Zlatić and D. Šokčević, Solid State Commun. **63**, 889 (1987).

[16] P. Coleman, Phys. Rev. B **35**, 5072 (1987).

[17] B. A. Jones and C. M. Varma, J. Magn. Magn. Mater. **63&64**, 251 (1987); Phys. Rev. Lett. **58**, 843 (1987); **62**, 1702 (1989); Phys. Rev. B **40**, 324 (1989).

[18] R. M. Fye, J. E. Hirsch, and D. J. Scalapino, Phys. Rev. B **35**, 4901 (1987); R. M. Fye and J. E. Hirsch, *ibid.* **40**, 4780 (1989).

[19] K. Matho and C. Marcenat, J. Phys. (Paris) Colloq. **49**, C8-717 (1988).

[20] B. A. Jones, C. M. Varma, and J. W. Wilkins, Phys. Rev. Lett. **61**, 125 (1988).

[21] B. A. Jones, B. G. Kotliar, and A. J. Millis, Phys. Rev. B **39**, 3415 (1989).

[22] J. W. Rasul and P. Schlottmann, Phys. Rev. Lett. **62**, 1701 (1989).

[23] A. J. Millis, B. G. Kotliar, and B. A. Jones, in *Field Theoretic Methods in Condensed Matter Physics*, edited by Z. Tesanovic (Addison-Wesley, Redwood City, 1990), p. 159.

[24] O. Sakai, Y. Shimizu, and T. Kasuya, Solid State Commun. **75**, 81 (1990); O. Sakai and Y. Shimizu, J. Phys. Soc. Jpn. **61**, 2333 (1992); **61**, 2348 (1992).

[25] B. A. Jones, Physica B **171**, 53 (1991).

[26] T. Yanagisawa, J. Phys. Soc. Jpn. **60**, 29 (1991); **60**, 3449 (1991).

[27] T. Saso, Phys. Rev. B **44**, 450 (1991); T. Saso and H. Kato, Prog. Theor. Phys. **87**, 331 (1992).

[28] I. Affleck and A. W. W. Ludwig, Phys. Rev. Lett. **68**, 1046 (1992).

[29] O. Gunnarson, T.C. Li, and G. Zwicknagl (unpublished).

[30] K. G. Wilson, Rev. Mod. Phys. **47**, 773 (1975).

[31] H. R. Krishna-Murthy, J. W. Wilkins, and K. G. Wilson, Phys. Rev. B **21**, 1003 (1980); **21**, 1044 (1980).

[32] C. M. Varma and Y. Yafet, Phys. Rev. B **13**, 2950 (1976).

[33] O. Gunnarson and K. Schönhammer, Phys. Rev. B **28**, 4315 (1983).

[34] L. C. Andreani and H. Beck, Solid State Commun. **79**, 17 (1991); J. Magn. Magn. Mater. **108**, 53 (1992).

[35] O. Gunnarson and K. Schönhammer, Phys. Rev. B **31**, 4815 (1985).

[36] In the nonmagnetic basis, a variational expansion to all orders has been worked out by S. Inagaki, Prog. Theor. Phys. **62**, 1441 (1979). A similar calculation for the magnetic basis shows that the binding energy of the ground state is identical for the two bases.

[37] L. C. Andreani and H. Beck, Solid State Commun. **77**, 635 (1991).

[38] D. M. Newns and N. Read, Adv. Phys. **36**, 799 (1987).

[39] H. Ishii, J. Low Temp. Phys. **32**, 457 (1978); J. E. Gubernatis, J. E. HIrsch, and D. J. Scalapino, Phys. Rev. B **35**, 8478 (1987).

[40] G. Chen and N. Giordano, Phys. Rev. Lett. **66**, 209 (1991).

[41] D. L. Cox, Phys. Rev. B **35**, 4561 (1987).

[42] T. Yamamoto and F. Ohkawa, J. Phys. Soc. Jpn. **57**, 3562 (1988).

[43] N. Andrei, K. Furuya, and J. H. Lowenstein, Rev. Mod. Phys. **55**, 331 (1983).

[44] See, e.g., J. M. Wills and B. R. Cooper, Phys. Rev. B **36**, 3809 (1987).

[45] Starting from the Kondo Hamiltonian, i.e., neglecting higher-order terms in the Schrieffer-Wolff transformation, the RKKY interaction is found to have similar amplitudes in the ferro- and antiferromagnetic parts, and the superexchange contribution is absent. See also Ref. 44.

[46] L. C. Andreani and H. Beck, J. Appl. Phys. **73**, 6628 (1993).

[47] K. Ueda, J. Phys. Soc. Jpn. **58**, 3465 (1989).

[48] P. Fazekas and E. Müller-Hartmann, Z. Phys. B **85**, 285 (1991).

[49] P. Santini, L. C. Andreani, and H. Beck, Phys. Rev. B **47**, 1130 (1993).

[50]P. Nozières, Ann. Phys. (Paris) **10**, 19 (1985).
[51]M. Sigrist, K. Ueda, and H. Tsunetsugu, Phys. Rev. B **46**, 175 (1992).
[52]P. Fazekas, Phys. Scr. **T29**, 125 (1989).
[53]O. Gunnarson and K. Schönhammer, in *Handbook on the Physics and Chemistry of Rare Earths*, edited by K. A. Gschneidner, Jr., L. Eyring, and S. Hüfner (Elsevier, Amsterdam, 1987), Vol. 10, p. 103.