Interaction between Kondo impurities in a quantum corral

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We calculate the spectral densities for two impurities inside an elliptical quantum corral, using exact diagonalization in the relevant Hilbert subspace and embedding into the rest of the system. For one impurity, the space and energy dependence of the change in differential conductance $\Delta dI/dV$ observed in the quantum mirage experiment is reproduced. In presence of another impurity $\Delta dI/dV$ is very sensitive to the hybridization between impurity and bulk. The impurities are correlated ferromagnetically between them. A hopping $\gtrsim 0.15$ eV between impurities destroys the Kondo resonance.

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I. INTRODUCTION

In recent years, the manipulation of single atoms on top of a surface using scanning tunneling microscopy (STM) was made possible,[1] and quantum corrals have been assembled by depositing a closed line of atoms or molecules on noble metal surfaces.[2–4] The local conduction spectral density of states $\rho_c(r,\omega)$, measured by differential conductance dI/dV reveals patterns that remind us of the wave functions of two-dimensional noninteracting electrons under the corresponding confinement potential. In a recent experiment, a Co atom has been placed at a focus of an elliptic quantum corral, and the corresponding Kondo feature is observed not only at that position, but also at the other focus, where a ''mirage'' is formed as a consequence of the quantum interference.[4] Variants of this experiment involving several impurities (Co atoms) and eventually mirages inside the corral are being performed, opening new possibilities in nanotechnology.[5] For example, for two impurities at given positions inside a circular corral of adequate radius, two independent mirages are observed, suggesting the possibility of a simultaneous transmission of information to remote places. Also, when two impurities are placed next to each other, the signature of the Kondo effect disappears and reappears again for a cluster of three impurities. For one impurity, the main features of the observed space and voltage dependence of dI/dV have been reproduced by several theories.[6–11] However, they have severe limitations. Since in Refs. 6–8 the density of states per spin at the impurity $\rho_d(\omega)$ is assumed rather than calculated, these theories cannot account for the interaction between impurities. In Ref. 9 the Kondo effect is absent, and perturbation theory in the Coulomb repulsion U (Refs. 10 and 11) is restricted to small values of U.

The aim of the present work is to present a many-body theory of the quantum mirage which reproduces the experimental results for the case of one impurity and gives reliable predictions when more than one impurity is inside the corral. We calculate dI/dV and several correlation functions. In addition, we show that experiments with two impurities can elucidate the role of the direct hybridization between the impurity and the bulk V_b. Scattering theories[3,6,7] obtained agreement with experiment assuming that the resonant level width due to hybridization with bulk states δ_b is as large as that due to the surface δ_s. On the other hand, the rapid decay of the hybridization matrix elements with distance and similar or larger density of s and p states at the surface[12] suggests that δ_b is negligible and the experiment for one impurity can also be explained if $V_b=0$.[10,11] A calculation of δ_b has not been made yet. A recent experiment suggests that V_b is more important than V_s based on the rapid decay in the amplitude of the dip in dI/dV as the STM tip is moved away from a Co impurity.[13] However, the interpretation, based on a model developed by Plihal and Gadzuk,[14] assumes a flat jellium model for the conduction states at the surface. If the s and p electrons of Co were included in the model, one would expect a bump in the local conduction density of states at the impurity site which should increase the amplitude of the resonance there. The role of V_b is not only crucial for a correct theory of the mirage experiment, but also for a general understanding of the interaction between metallic surfaces and adsorbates. Since actually δ_b was introduced as a phenomenological parameter which takes into account the electrons lost in the scattering process,[3,6,7] one expects that if $\delta_b=\delta_s$, the interaction between impurities is roughly a fourth of that for $V_b=0$ if the same total width $\delta_b+\delta_s$ is kept.

We obtain the ground state of the Anderson model in a cluster which contains one or two impurities and the relevant conduction states inside a hard wall ellipse using the Lanczos method. These states are then mixed with bulk states using an embedding method.[15] This embedding is essential to describe the low-energy physics.[16] Since the average separation between the relevant conduction states $d\sim 100$ meV (Refs. 8 and 10) is much larger than the Kondo temperature $T_K \sim 5$ meV,[4] a Kondo peak at the Fermi level ϵ_F is absent in the finite system.[10,11,17] This is confirmed by our calculations. In addition, if the energy scale for embedding t is much smaller than d, a Kondo peak is present at ϵ_F, but with an exponentially small width $\sim 2T_K$. In any case the experimental line shape for dI/dV cannot be reproduced for small t.

The model and the embedding approximation are described in Sec. II. Section III contains the results. Section IV is a summary.

II. MODEL AND APPROXIMATION

The Hamiltonian can be written as

$$H=\sum_{j\sigma}\ \varepsilon_j c^{\dagger}_{j\sigma}c_{j\sigma}+E_d\sum_{i\sigma}\ d^{\dagger}_{i\sigma}d_{i\sigma}+U\sum_{i}\ d^{\dagger}_{i\uparrow}d_{i\uparrow}d^{\dagger}_{i\downarrow}d_{i\downarrow}$$

$$+\sum_{ij\sigma}\ V[\varphi_j(R_i)d^{\dagger}_{i\sigma}c_{j\sigma}+\text{H.c.}]+H'. \qquad (1)$$

Here $c^{\dagger}_{j\sigma}$ creates an electron on the jth conduction eigenstate (in order of increasing energy) of a hard-wall elliptic corral with wave function $\varphi_j(r)$ (Ref. 18) and $d^{\dagger}_{i\sigma}$ is the corresponding operator for the impurity at site R_i. The hybridization of these states with bulk states of the same symmetry is described by H'. We assume that each of the impurity and conduction states mixes with a different continuum of bulk states:

$$H'\cong t\sum_{j\sigma}\ (c^{\dagger}_{j\sigma}b_{j\sigma}+\text{H.c.})+V_b\sum_{i\sigma}\ (d^{\dagger}_{i\sigma}b_{i\sigma}+\text{H.c.}). \qquad (2)$$

The $b_{l\sigma}$ represent bulk states for which we take a constant unperturbed density of 0.05 states/eV, similar to the density of bulk s and p states at ϵ_F.[12] Approximation (2) is justified by a comparison of the noninteracting Green functions for hard-wall corrals and more realistic boundary potentials.[11,19]

The dressed matrix **G** describing the one-particle Green function is calculated by solving the Dyson equation $\mathbf{G}=\mathbf{g}+\mathbf{g}H'\mathbf{G}$, where **g** is the corresponding matrix for $H'=0$.[15] This equation represents an infinite sum of particular diagrams in perturbation theory in H' (the chain approximation[20]). The diagonal matrix elements of **g** are calculated using the recursion technique combined with the Lanczos method. Off-diagonal matrix elements are calculated from diagonal elements of hybrid states, involving sum and difference of basis states. The resulting **G** is exact not only for $H'=0$ (isolated corral), but also for the infinite system in the uncorrelated case $U=0$. This shows that the method is able to take into account adequately both strong interactions at short distances and itineracy at small energy scales. The interplay between both is essential to the physics of the Kondo effect. A similar approximate Dyson equation in systems out of equilibrium has been used by Meir and Wingreen to extend the Landauer formula to interacting systems.[21] However, they do not attempt to solve the many-body problem.

Previous studies suggest that the approximation is good when the matrix elements of the many-body self-energy between states of the bath is small. This is the case here, because the bath is far from the impurities, and experimentally it is clear that the spectral density of the conduction states out of the corral is practically not altered by the addition of one impurity. One would expect that a rough criterium for the validity of the approximation in the description of the Kondo effect is that the size of the exactly solved part should be smaller or of the order of the screening length $\xi\sim\hbar v_F/T_K$, where T_K is the Kondo temperature and v_F is the Fermi velocity. In practice, even when ξ is 10 times larger than the size of the system, the resulting value of the impurity spectral density at the Fermi energy $\rho_d(\epsilon_F)$ practically coincides with the exact value, known from Friedel's sum rule in cases in which the unperturbed conduction density of states is nearly a constant around ϵ_F.[22,23] We have verified this for the whole functional dependence of $\rho_d(\epsilon_F)$ with the occupation at an impurity site, embedded in a linear chain. For much larger ξ, the approximation loses its quantitative validity. In the mirage experiment $\xi\sim 800$ Å and the size of the ellipse is ~ 140 Å. These arguments and comparison of our results with those of other approximations[10,11] indicate that the approximation is quantitatively valid for the parameters relevant for the experiment.

The $\varphi_j(r)$ are obtained as described elsewhere.[10] We choose the ellipse with eccentricity $e=1/2$ and size such that the state $j=42$ lies at ϵ_F.[4] The change in dI/dV ($\Delta dI/dV$) after an impurity is placed inside the corral is determined by the conduction states which lie near ϵ_F and have a strong amplitude $|\varphi_j(R_i)|$ at the impurity position. For R_i at one focus they are $j=32$, 35, 42, and 51.[10] We have also included $j=24$ and 62, although this inclusion leads to negligible changes in the results. We took the impurity parameters $E_d=-1$ eV and $U=3$ eV used before by Újsághy *et al.*[24] We first consider the case $V_b=0$ and one impurity at the left focus $[R_i=(-0.5a,0)]$. The value $V=0.04$ eV was chosen to lead to the observed width of $\Delta dI/dV$. This corresponds to a hopping $V_s=1.12$ eV between an impurity and a surface atom below it, if a tight-binding model were used to describe the surface.[9,11] The remaining parameter t controls the amplitude of the mirage at the right focus.

III. RESULTS

In Fig. 1(a) we represent the resulting impurity spectral density $\rho_d(\omega)$ for two values of t. A clear Kondo peak is obtained and for $t\gtrsim 0.3$ eV its width is very weakly dependent on t. Instead, for $t\to 0$, the peak splits into two very narrow peaks out of ϵ_F, in agreement with previous studies.[10,11,17] We note that in this limit there is also a peak at ϵ_F with very small spectral weight which corresponds to a depressed Kondo effect: as long as there is a finite density of unperturded conduction states at the Fermi energy ρ_0, one expects a Kondo peak at the Fermi energy. However, since the relevant energy scale T_K decreases exponentially with decreasing ρ_0, the spectral weight of this peak also vanishes when $t\to 0$ or if the temperature is increased above T_K. Since, for $T_K\to 0$, ξ diverges, our approximation (as well as previous ones[10,11,17]) are unable to describe this central peak. Instead, recent results using Wilson's renormalization group were able to describe correctly the structure with three peaks in a system with rotational symmetry in two dimensions.[25] In any case, the regime with split peaks does not correspond to the mirage experiments.

In contrast to $\rho_d(\omega)$, the magnitude of the change in the conduction density $\Delta\rho_c(r,\omega)$ at the empty focus ($r=-R_i$) is quite sensitive to $t\gtrsim 0.3$ eV: as t increases, the width of the conduction states increases, the weight of the states 32, 35, and 51 (odd under the reflection through the minor axis of the ellipse σ) at ϵ_F increases and the depression of $\rho_c(-R_i,\omega)$ decreases as a consequence of the negative inter-

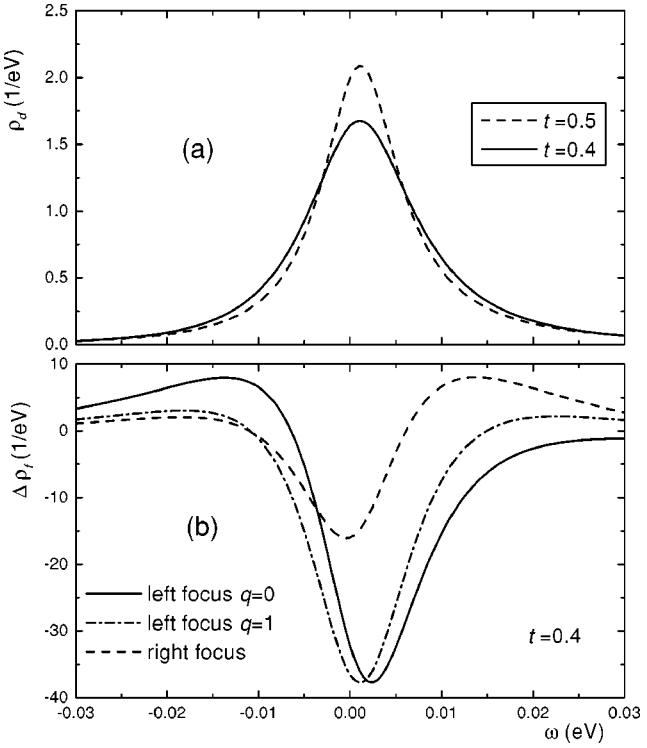

FIG. 1. (a) Impurity spectral density as a function of energy for two values of t. (b) Change in the density of the mixed state f_σ [Eq. (3)] at the impurity site (left focus) for two values of q and at the other focus for $t=0.4$ eV.

ference of these states with the even state 42.[10] The differential conductance dI/dV at zero temperature is proportional to the density ρ_f of the state[26]

$$f_\sigma(r)=\sum_j \varphi_j(r)c_{j\sigma}+qd_{j\sigma}. \tag{3}$$

Here q is related to Fano's interference parameter and represents the effect of a direct tunneling from the tip to the impurity. Therefore, it is relevant only very near the impurity. For $q=0$, $\rho_f(r,\omega)=\rho_c(r,\omega)$. In Fig. 1(b) we represent the effect of adding the impurity on $\rho_f(\pm R_i,\omega)$ ($\Delta\rho_f \sim \Delta dI/dV$). At the impurity site R_i, $\Delta\rho_c(r,\omega)$ is asymmetric and smaller at the right of the valley. This is a consequence of the asymmetry of the hybridization around ϵ_F [$|\varphi_{51}(R_i)|>|\varphi_{35}(R_i)|$]. A symmetric line shape, as observed in the experimental $\Delta dI/dV$, is restored for $q\sim 1$. The effect of this q is consistent with the fact that on a clean surface, $\Delta dI/dV$ is *larger* at the right of the peak. Another nice fact is that the minimum of $\Delta\rho_f$ for $q=1$ lies at the experimental position 1 meV. At the right focus ($r=-R_i$) we obtain a similar valley, although slightly asymmetric and shifted to the left. Increasing t from 0.4 to 0.5, the magnitude of this valley is strongly reduced (its minimum is shifted above -5/eV) but its shape and width is retained. At the impurity position there are no significant changes.

The space dependence of $\Delta\rho_f$ for $q=0$ is represented in Fig. 2. As in the experimental $\Delta dI/dV$, the main features of $|\varphi_{42}(r)|^2$, attenuated at the right focus, are displayed. Thus,

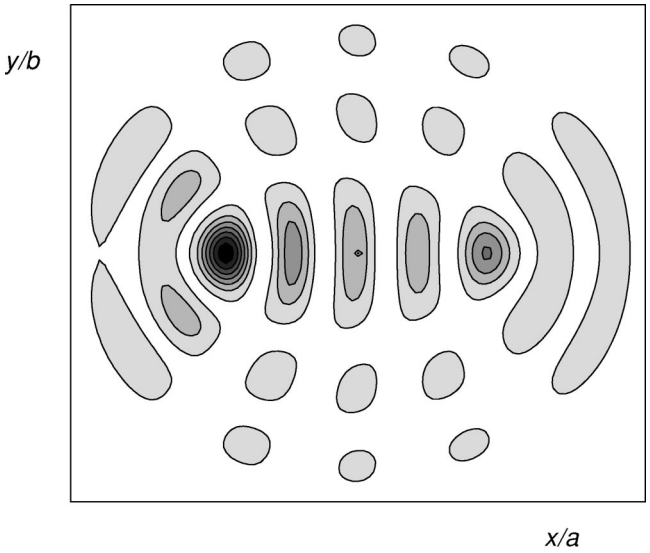

FIG. 2. Contour plot of $\Delta\rho_c(r,\omega)$ for $t=0.4$ eV and $\omega=10$ meV.

the theory reproduces the space and energy dependence of $\Delta dI/dV$ observed in the experiment.[4] All results so far agree semiquantitatively with perturbative calculations.[10,11] To see how the results change if $\delta_b\cong\delta_s$ is assumed, we have reduced V by a factor $\sqrt{2}$. This should reduce δ_s by a factor 2. Increasing V_b from zero to 1.2 eV, the original width of ρ_d is restored. The intensity is reduced by a factor ~ 2 (due to the strong energy dependence of δ_s). $\Delta\rho_c$ turns out to be ~ 4 times smaller. The additional factor 2 can be understood from the fact that the change in conduction electron Green function is proportional to $V^2G_d(\omega)$, where $G_d(\omega)$ is the impurity Green function.[10] Except for these factors, the results are surprisingly similar to the previous ones. Some of them will be displayed in Fig. 4.

We now turn to the case of two impurities, one at each focus, for $V_b=0$. The spectral density for one of these impurities is represented in Fig. 3(a). Comparison with the previous case (Fig. 1) shows that the peak around ϵ_F broadens (by a factor ~ 1.5), loses intensity, and shifts to lower energies. In addition, another very narrow peak appears ~ 13 meV below ϵ_F. An analysis of the energy dependence of the density of the individual conduction states shows that the broad peak around ϵ_F is due to hybridization with states even under σ (mainly 42), while the narrow peak reflects the hybridization of the impurity states with odd states (mainly 51). The effect of the second impurity on ρ_d is stronger than that on dI/dV. This is due to the effect of the unperturbed Green functions of the conduction states and is also present in the one impurity case.[10] Nevertheless, a broadening of the depression should be observed in $\Delta dI/dV$ and seems in qualitative agreement with recent experiments.[5] The space dependence is similar to that for one impurity (Fig. 2) but it is, of course, even under σ and not attenuated at the right focus.

Qualitatively, the shape of ρ_d can be understood looking at the noninteracting case $U=0$, $E_d\sim\epsilon_F$. In this case, for one impurity, the Kondo peak is replaced by a Lorentzian

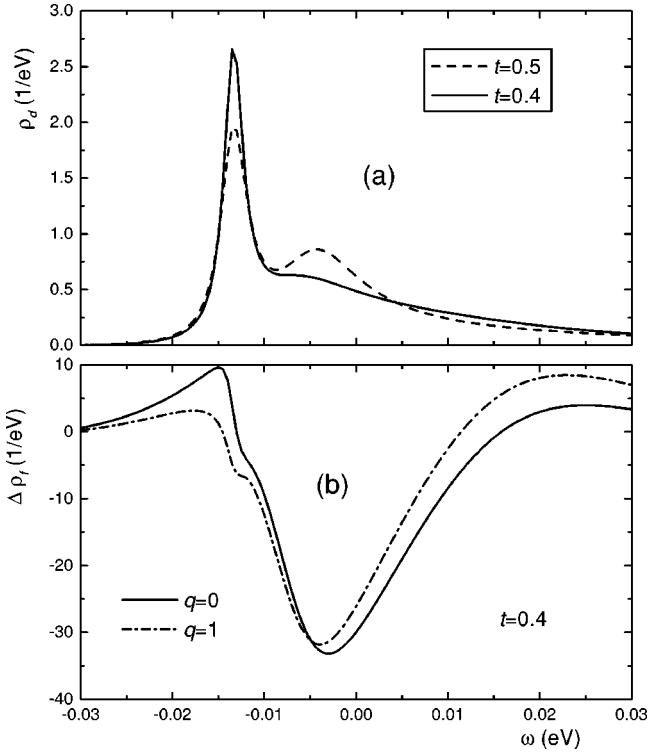

FIG. 3. (a) Impurity spectral density for one impurity at each focus and two values of t. (b) Change in the density of the mixed state f_σ after addition of both impurities [Eq. (3)], at one impurity site for two values of q. Parameters are $V=0.04$ eV, $V_b=0$, and $t=0.4$ eV.

near ϵ_F. For two impurities, a change of basis of the d orbitals to $e_\sigma=(d_{1\sigma}+d_{2\sigma})/\sqrt{2}$, $o_\sigma=(d_{1\sigma}-d_{2\sigma})/\sqrt{2}$, separates the problem into those corresponding to even and odd states under σ. The even state hybridizes mainly with conduction state 42 to form a resonance near ϵ_F, roughly twice wider than for one impurity due to the larger effective hybridization. Instead, the odd state o_σ is displaced towards lower energies due to hybridization with state 51 that lies above ϵ_F (the hybridization with other odd states like 32 and 35 is smaller). The interactions modify the quantitative details of this picture. However, it remains qualitatively valid, as indicated by the above-mentioned energy distribution of the different conduction states.

To gain insight into the nature of the ground state, we have also calculated spin-spin correlation functions for $t=0$. A reliable method to include H' in these calculations has not been developed yet. For one impurity we obtain $\langle \mathbf{S}_i \cdot \mathbf{s}_{42}\rangle = -0.73$, where $\mathbf{S}_i$ is the spin of the impurity i and $\mathbf{s}_j$ is the spin of the conduction state j. This value is close to the minimum possible one $-3/4$. For $j\neq 42$, $\langle \mathbf{S}_i\cdot \mathbf{s}_j\rangle$ are very small. Inclusion of H' should increase these correlations and decrease $\langle \mathbf{S}_i\cdot \mathbf{s}_{42}\rangle$ by a few percent. The space dependence of $\langle \mathbf{S}_i\cdot \mathbf{s}(r)\rangle$, where $\mathbf{s}(r)$ the conduction spin at position r follows closely $|\varphi_{42}(r)|^2$. For two impurities we find $\langle \mathbf{S}_i\cdot \mathbf{s}_{42}\rangle = -0.47$ and $\langle \mathbf{S}_1\cdot \mathbf{S}_2\rangle = 0.21$. In the limit of large U, one expects that the main features of the spin dynamics for $V_b=0$ are described by the Hamiltonian $H_0=J(\mathbf{S}_1+\mathbf{S}_2)\cdot \mathbf{s}_{42}$, where $J>0$ is the Kondo coupling. The ground state of this

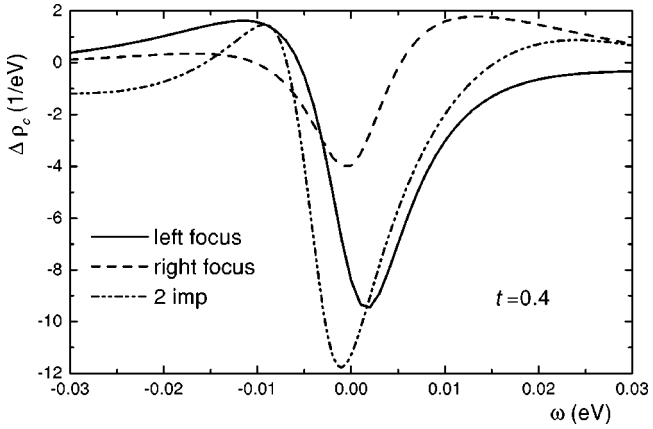

FIG. 4. $\Delta\rho_c(r,\omega)$ as a function of ω for the case of one impurity at the left focus (solid and dashed lines) or one impurity at each focus (dash–double-dotted line). Parameters are $V=0.04$ eV/$\sqrt{2}$, $V_b=1.2$ eV, and $t=0.4$ eV.

Hamiltonian is a doublet in which the impurity spins are correlated ferromagnetically between them ($\langle \mathbf{S}_1\cdot \mathbf{S}_2\rangle = 1/4$) and antiferromagnetically with state 42 ($\langle \mathbf{S}_i\cdot \mathbf{s}_{42}\rangle = -1/2$). These values are near to those we find. The effect of the hybridization of state 42 with bulk states can be modeled by a tight-binding Hamiltonian in terms of Wilson's orbitals. H_0 is the strong-coupling fixed point of Wilson's renormalization group. An analysis of the stability of this fixed point using perturbation theory as in Ref. 27 leads to the conclusion that the ground state is a doublet for $V_b=0$. However, we expect that as soon as $V_b\neq 0$, the doublet is screened at a very low temperature. The RKKY interaction between impurities is several orders of magnitude smaller than J and can be neglected.

For the set of parameters corresponding to $\delta_b\cong\delta_s$, $\rho_d(\omega)$ is much more similar to the one-impurity case, although a structure reminiscent of a splitting is also present near its maximum. In contrast to the case of $V_b=0$, when a second impurity is added, the depression in $\Delta dI/dV$ at one impurity site R_i increases and its width is roughly the same (see Fig. 4). Comparison with results when t is increased from 0.4 eV to $t=0.5$ eV (not shown) suggests that when $\delta_b\cong\delta_s$, $\Delta dI/dV$ at $\pm R_i$ for two impurities is roughly the sum of the results at R_i and $-R_i$ for one impurity. This is what one would expect if the interaction is small enough.

Coming back to the case $V_b=0$, we have also verified that qualitatively similar features in $\Delta dI/dV$ are obtained at one focus, if one impurity is placed there and the second impurity is put at another extremum of $\varphi_{42}(r)$, like $(0.22a,0)$ in Cartesian coordinates with the origin at the center of the ellipse (instead of placing it at the other focus). In this case, the spectral densities at $(0.22a,0)$ have some additional structure due to an important admixture of the state 41.[28] In contrast, if both impurities are placed close to the same focus and near each other, a moderate hopping $t\sim 0.15$ eV or larger between them is sufficient to destroy the Kondo resonance. In particular $\Delta dI/dV$ becomes flat and featureless near ϵ_F. This has been experimentally observed.[5] The phenomenological theories[6,7] would predict approximately an additive effect.

IV. SUMMARY

We have studied the spectral density for impurities inside a quantum corral, using a many-body approach which treats exactly the correlations in the impurities and their hybridization with the relevant conduction states at the surface and treats approximately the hybridization with bulk states. The method gives also the exact result in absence of interactions. We have reproduced the main features of the mirage experiment for one impurity inside the corral. For two impurities inside the corral, the differential conductance is very sensitive to the ratio V_s/V_b. For the parameters of the experiment, the spins of both impurities are antiferromagnetically coupled with the conduction electrons and ferromagnetically correlated between them, provided they are placed sufficiently far apart, so that the hopping between them can be neglected. If this hopping is larger than 0.15 eV, there is a tendency to form a singlet state between both impurity spins and the Kondo resonance disappears. To our knowledge, this is the first theory which is able to describe the line shape of the differential conductance when more than one Kondo impurity is inside the quantum corral. The theory with the same set of parameters should describe the differential conductance for other corral shapes or positions of the Fermi energy.

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