Conductance dip in the Kondo regime of linear arrays of quantum dots

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(Received 18 August 2003; revised manuscript received 5 April 2004; published 7 July 2004)

Using exact diagonalization of small clusters and Dyson equation embedding techniques, the conductance G of linear arrays of quantum dots is investigated. The Hubbard interaction induces Kondo peaks at low temperatures for an odd number of dots N and a filling of one particle per dot. Remarkably, for $N=3,5,\ldots$ the Kondo peak is split in half by a deep minimum, and the conductance vanishes at the gate voltage that induces particle-hole symmetry in the system. Tentative explanations for this unusual effect are proposed, including an interference process between two channels contributing to G, with one more and one less particle than the exactly solved cluster ground state. The Hubbard interaction and fermionic statistics of electrons also appear to be important to understand this phenomenon. Although most of the calculations used a particle-hole symmetric Hamiltonian and formalism, results also presented here show that the conductance dip exists even when this symmetry is broken. The conductance cancellation effect obtained using numerical techniques is potentially interesting, and other many-body techniques should be used to confirm its existence.

DOI: 10.1103/PhysRevB.70.035402 PACS number(s): 73.63.Kv, 73.23.−b, 73.21.La, 75.75.+a

I. INTRODUCTION

The possibility of destructive interference between two or more wave functions is among the most remarkable phenomena predicted by quantum mechanics. The effect can be observed when electronic beams are split and then brought together after traveling paths of different lengths, or in a Aharonov-Bohm (AB) geometry—such as a ring—where two equal-length paths nevertheless can carry different phase factors in the presence of a magnetic flux. Recent advances in nanotechnology have made possible the fabrication of quantum dots[1]—analogous to artificial atoms or molecules—where these effects can be tested. In fact, the AB effect was recently observed using a quantum dot embedded in a ring in the Coulomb blockade regime.[2] Another example of conductance cancellations are the well-known Fano resonances[3] that occur when charge can circulate through two paths: one with a discrete level and the other with a continuum of states. Many physical realizations of Fano resonances are known. For example, when an atom is deposited on a metallic surface, a scanning tunneling microscope (STM) tip probes transmission to the tip either through the atom or directly from the surface, leading to current cancellations.[4] In addition, theoretical studies predict that Fano resonances should appear in "T-shaped" geometries where an active dot–connected to left and right electrodes–is also side connected to another dot.[5] A similar conductance cancellation has been predicted using double quantum-dot molecules attached to leads[6] and in a 2×2 quantum-dot array.[7] All these cancellations are caused by destructive interference among two different paths between conductors. Related cases correspond to multiple-level dots with noninteracting electrons,[8] which can also be rephrased as a many-dot problem connected to leads in ring-like geometries, leading naturally to conductance cancellations.

It is the purpose of this paper to report an unexpected conductance cancellation found in linear arrays of N quantum dots ($N=3,5,\ldots$), in the approximation of one level per dot, and at a filling of one electron per dot. These arrays do not have any obvious real-space paths that may lead to explicit AB or Fano interferences to rationalize the conductance zeros found here—all electrons travel through the same chain—and in this respect the interference is exotic. In addition, the reported cancellations occur only in the presence of Coulomb interactions, and in the previously believed to be well-understood Kondo regime.[9] In fact, *the Kondo peaks for $N=3,5,\ldots$ are here found to be split in half* at the gate voltage that induces particle-hole symmetry, a curious effect that may be observable experimentally at very low temperatures. Although transport through many quantum dots[10] or STM-engineered atomic systems[11] has received considerable attention in recent years, experiments using 3 dots or atoms have not been sufficiently accurate to address the effect found in this paper.

Note that conductance dips have also been observed experimentally and theoretically at high magnetic fields in a two-level single dot.[12,13] This effect was ascribed to transitions between total spin $S=1$ and $S=0$ dot states, a situation that does not seem to apply to our case with an odd number of electrons in the ground state.[14]

The paper is organized as follows. In Sec. VI, the Hamiltonian and many-body technique are described. In Sec. III, the main results are presented, with emphasis on the conductance cancellation for an odd number of dots. The case of an even number of dots is also described, and in this situation there is no cancellation. The dependence of the results with parameters in the model is presented in this section as well. In Sec. IV, results for 1, 4, and 5 dots are briefly described. In Sec. V, possible explanations of the conductance dip effect are presented. They include interference between conduction processes with one more and one less particle in the cluster, as well as mappings into systems with the T-shape geometry that are known to lead to interference. In Sec. IV, conclusions are presented.

Throughout the paper it is emphasized that confirmation of our results using other techniques is important. Although the numerical studies presented later do not seem to be se-

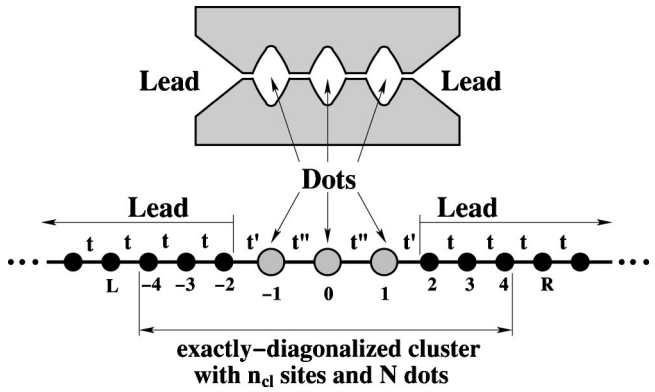

FIG. 1. Schematic geometry and hopping amplitudes of the quantum-dot linear array studied here. The exactly solved cluster—with $n_{cl}=9$ sites and $N=3$ dots in this example—includes some sites of the leads.

verely affected by size effects, size dependences are sometimes very subtle. Thus, further work is needed to confirm the exotic conductance dip found here numerically. If this confirmation occurs, the effect unveiled in the present investigations—an unexpected quantum interference process in linear chains of dots—should be searched for experimentally. The effort should be carried out at sufficiently low temperatures such that the dip structure becomes visible.

II. MODEL AND TECHNIQUE

Keeping one level per dot, the Hamiltonian for our N-dot system coupled to leads is $H=H_{\rm dots}+H_{\rm leads}+H_{\rm int}$, where

$$H_{\rm dots}=-t''\sum_{i\sigma}(c^{\dagger}_{i\sigma}c_{i+1\sigma}+{\rm H.c.})+U\sum_{i}n_{i\uparrow}n_{i\downarrow} \qquad (1)$$

represents the electronic hopping and Hubbard interaction in the dots subsystem (i labels the dots) using a standard notation. A gate voltage $V_g\Sigma_{i\sigma}n_{i\sigma}$ of equal strength for the N dots is also included. The term $H_{\rm leads}$ represents the noninteracting electrons in the leads, with a nearest-neighbors hopping amplitude t, while $H_{\rm int}$ is the hopping from the ideal leads to the dots and its amplitude is t'. Figure 1 illustrates the geometry used in the study and conventions followed. The Hamiltonian discussed here becomes particle-hole symmetric for the case $V_g=-U/2$, precisely the gate voltage needed for the conductance cancellation reported below. However, in Sec. III C other less symmetric models were studied as well, and the zero in the conductance survives. Thus, the dip reported in this paper does not seem to originate from a highly symmetric Hamiltonian but its origin is more robust.

The zero-temperature, $T=0$, Green function $G_{LR}(\omega)$ to transfer charge from sites L to R (Fig. 1) can be obtained by an exact-diagonalization (Lanczos) solution[15] of a cluster with $n_{\rm cl}$ sites containing the N dots. The exact information about the cluster under study is supplemented by an embedding procedure between the leads, already discussed in previous literature.[16,17] To reproduce the one-dot Kondo effect it is crucial that the exactly solved cluster contains also a small portion of the lead,[17] assumed also in a linear arrangement for simplicity. The cluster size $n_{\rm cl}$ is chosen such that $n_{\rm cl}=N+2n_{\rm odd}$, where $n_{\rm odd}=1,3,5,\ldots$. As discussed before,[17] with this convention the portion of the leads in the cluster contains a zero-energy state that induces the Kondo effect already at the cluster level, reducing finite-size effects. The rest of the contacts is incorporated using the Dyson equation $\hat{G}=\hat{g}+\hat{g}\hat{t}\hat{G}$, where $\hat{g}$ is the exactly known Green function matrix of the cluster, $\hat{G}$ is the dressed Green-function matrix across the cluster from L to R, and $\hat{t}$ is the matrix of hopping elements connecting the cluster and leads. In the present study, the total z component of the spin is either $1/2$ or $-1/2$ for an odd number of sites in the exactly solved cluster. To respect particle-hole symmetry at every step in the calculation, the cluster ground-state is here taken as the sum (divided by $\sqrt{2}$) of the ground states of the subspaces with total spin z-component $1/2$ and $-1/2$. This leads to Green functions for the "up" and "down" spins that are identical. Other conventions, discussed in the Appendix, lead to qualitatively similar results regarding the presence of internal structure in the conductance Kondo peak.

To consider charge fluctuations, the cluster Green functions $\hat{g}_m$ for m and $m+1$ electrons are combined. The mixed Green function $\hat{g}$ is written as $\hat{g}=(1-p)\hat{g}_m+p\ \ \hat{g}_{m+1}$. With the dressed Green function $\hat{G}$ from the Dyson equation, the total cluster charge is obtained as $Q=-1/\pi\int_{-\infty}^{E_F}\Sigma_j\,{\rm Im}\,G_{jj}(\omega)$ (the sum in j runs over the cluster sites and E_F is the Fermi energy, assumed 0 in the numerical calculations discussed later). On the other hand, the charge at the cluster in the mixed $(m/m+1)$ state is $q=(1-p)m+p(m+1)$ and, then, p can be found self-consistently to satisfy $Q=q$ (in the region emphasized in the next section, with a G cancellation, $q\sim n_{\rm cl}$). Finally, using the Keldish formalism the conductance G is written as[17] $G=(e/h)^2t^2|G_{LR}(E_F)|^2[\rho_{\rm leads}(E_F)]^2$. The leads density-of-states (DOS) is $\rho_{\rm leads}(\omega)$, assumed here to be a semicircle from $-2t$ to $2t$ (the results are weakly dependent on this assumption).

As the Wick's theorem breaks down in the presence of interactions this method is not the exact solution of the problem, and it is only a good aproximation. However, we want to remark that, due the local nature of the many-body interactions of the system, if we could consider a cluster larger than the Kondo cloud all the long-range many-body correlation will be properly treated, and the properties calculated within the cluster must represent the correct physics of the system analyzed. In particular, the conductance evaluated under these circumstances will be basically the exact solution of the problem. However, we can not always achieve these large clusters due to the limitations in the number of sites we can diagonalize exactly. For this reason, we use the Dyson equation to try to correct this constrains in the number of sites considered. From previous calculations[16,17] it is known that even for small clusters the results are usually qualitatively correct.

Previous studies showed that this formalism—combination of exact diagonalization and embedding—is sufficiently powerful to reproduce the Kondo effect in electronic transport across one dot,[17,18] and for this reason there is no *a priori* reason why it would fail for more dots. Nev-

ertheless, to be cautious in our discussion later statements are included to alert the reader on possible subtle size effects that could alter our conclusions. As already mentioned, in the Appendix alternative conventions to our choice of spin quantum numbers for the exactly solved cluster ground state are also discussed. These alternative conventions also lead to dips in the conductance Kondo peak, as in the results presented in the following sections. Although more work is needed to confirm the existence of the conductance dip reported later, the numerical results appear to be sufficiently robust that the effect could even be observed experimentally at very low temperatures.

III. RESULTS

A. Conductance dip for an odd number of dots

The technique described in the previous paragraph was applied here to the case of $N>1$ quantum dots forming a linear array. Our original motivation was the study of transport in the regime of large t'' where N odd (even) would lead to a quantum-dot subsystem with spin $1/2(0)$ and, as a consequence, the presence (absence) of the Kondo effect as indeed occurs. However, studies at intermediate couplings and hoppings regimes led to surprises. The most unexpected result of the present effort is shown in Fig. 2(a) where the conductance across 3 dots is shown for V_g near $-U/2$ (inducing one electron per dot), at relatively small t''. The shape of the broad peak (without the dip) resembles previous Kondo-like results for one dot.[17] Following standard arguments, this Kondo effect is obtained when the state of N (odd) electrons carrying a net spin couples to the leads.[9,17] However, the peak is found to be split in half by an unexpected zero in the conductance at exactly $V_g=-U/2$. This cancellation is absent at $U=0$, where $G/(e^2/h)=1$ at $V_g=0$ since the exactly solved cluster has a zero-energy state aligned with the leads Fermi energy (assumed at 0). As U increases, Coulomb blockade and Kondo peaks are generated, but the latter is always split by a zero at $V_g=-U/2$. As a consequence, the effect appears to originate in correlation effects induced by a nonzero U. Our study for increasing N suggests that the effect is present for any odd N, while for N even [2 as example, Fig. 2(b)] there is no conductance cancellation (the two peaks in Fig. 2(b) are related to the Kondo splitting—without a zero—of double quantum dots, previously discussed).[17,19,20] The t'' dependence shown in Figs. 2(c)–2(f) suggests that there is an intermediate hopping range where the zero conductance effect could be observed,[21] while both at very small and large t'', its experimental observation will be difficult.

The conductance cancellation Fig. 2(a) is unexpected since there are no obvious real-space multiple paths that can lead to interference. Electrons here travel through a one-dimensional geometry. Note also that one level per dot is kept in our analysis, and cancellations as in Ref. 8 are not obviously present.

To gain insight on the origin of the reported phenomenon, Fig. 3 shows the real (Re) and imaginary (Im) components of the *cluster* Green function from one extreme of the cluster to

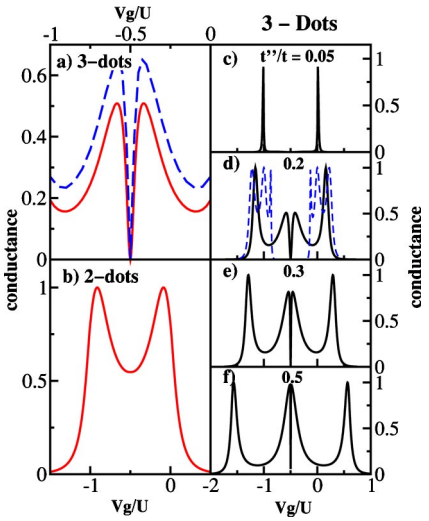

FIG. 2. Conductance (in units of e^2/h) across an array of quantum dots vs V_g/U, illustrating the cancellation reported in this paper. The couplings are $U/t=1$ and $t'/t=0.3$ (a) corresponds to $N=3$ dots, at $t''/t=0.2$. The solid (dashed) lines corresponds to an exactly solved cluster of $n_{cl}=5$ (9) sites. The size dependence suggests that this effect will survive the bulk limit. (b) is for 2 dots ($n_{cl}=4$), same t''/t as in (a). (c)–(f) are results in a wider range of V_g/U and varying t''. For very small t'', (c), the central dot is virtually decoupled and no Kondo effect is observed in the scale used. With increasing t'' a central peak is found, always split as in (a). Applying the method outlined in the text to a cluster that only has the dots (no extra lead sites), and then incorporating the effect of the leads through the Dyson equation, the Kondo peak is effectively eliminated (the exactly solved cluster does not have states near the leads Fermi energy). By this procedure, just the Coulomb blockade peaks are found, roughly representing the high-temperature solution of the problem. This result is shown with dashed lines in (d) for completeness.

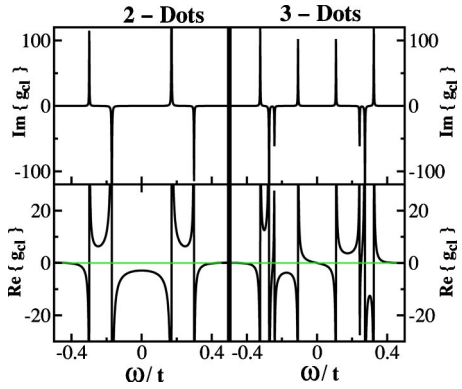

FIG. 3. Real and imaginary parts of the cluster Green function g_{cl} (from the first to the last site of the cluster) used to calculate G through the Dyson equation. ω is in units of t. Shown are exact results for $N=2$ dots ($n_{cl}=4$ cluster) and $N=3$ dots ($n_{cl}=5$ cluster). The couplings are as in Fig. 2(a). Note that for 3 dots the real part vanishes at $\omega=0$, while for 2 dots it is finite. The different behavior under $\omega\rightarrow-\omega$ for odd and even number of dots causes the cancellation of the conductance of the former, discussed in the text.

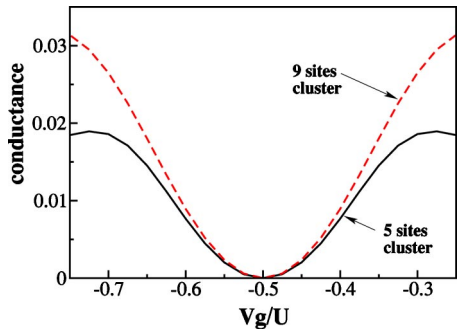

FIG. 4. Conductance at $U=1$, $t=1$, and $t'/t=0.3$, as used in Fig. 2(a), and for $t''/t=0.075$. Results for 3 dots and cluster sizes n_{cl} of 5 and 9 sites are indicated. The maximum in the conductance does not seem to move toward $V_g/U=-0.5$ as n_{cl} grows, suggesting that the dip will survive the bulk limit.

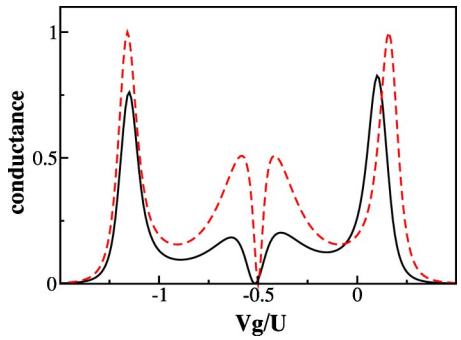

FIG. 5. Conductance for the 3-dot system, with 5 sites in the exactly solved cluster (solid line). In this figure the on-site Hubbard U couplings, as well as the on-site energies ϵ, of the three interacting sites are given random values of amplitude $0.01t$ in addition to the uniform values used in Fig. 2 (namely $U=1$ and $\epsilon=0$). The hopping amplitudes t' and t'' are also varied as follows: from the left lead to the first dot t' is 0.3 (in units of t), the next hopping amplitude is $t''=0.2$, then $t''=0.12$, and finally $t'=0.35$ for the connection between the last dot and the right lead. It is observed that the vanishing of the conductance still occurs although with a small shift in its position. For comparison, the result of Fig. 2(a) in the particle-hole symmetric case is also shown (dashed line).

the other (denoted g_{cl}), for 2 and 3 dots. The overall conductance emerges from the behavior of g_{cl} at $\omega=0$, in the embedding procedure. Clearly, the results for 2 and 3 dots have different symmetry properties under $\omega\rightarrow-\omega$: while for 2 dots $\mathrm{Re}(g_{\mathrm{cl}})$ is even, for 3 dots it is odd generating a zero at $\omega=0$. Since both imaginary parts cancel at $\omega=0$, then $\mathrm{Re}(g_{\mathrm{cl}})$ and $\mathrm{Im}(g_{\mathrm{cl}})$ are zero (Re nonzero) for odd (even) number of dots (this rule was verified numerically beyond the 2- and 3-dots example shown). If $g_{\mathrm{cl}}=0$, the Dyson-equation embedding procedure cannot generate a nonzero conductance. If $U\rightarrow 0$, the two peaks closest to $\omega=0$ in Fig. 3 (right upper panel) merge and the cancellation does not occur.

B. Analysis of size effects

An important aspect of the methodology discussed here, and in previous literature, involves the exact solution of a cluster followed by an embedding procedure. From the cluster size dependence it is possible to infer whether a particular feature under study will survive the bulk limit or not. Unfortunately, the CPU time rapidly grows with the cluster size since the cluster Green functions at all distances are needed for the Dyson equations, and each Green function is calculated with approximately one hundred steps in the continued-fraction procedure.[15] This limits our detailed study of the conductance dip to clusters with 5 and 9 sites (while a few values of the gate voltage can still be investigated using 13 sites). In Fig. 4, results for $n_{\mathrm{cl}}=5$ and 9 are presented at a small value of t''. This small hopping was used to amplify the region where the dip dominates [as t''/t increases, the dip width is reduced as shown in Figs. 2(c)–2(f)]. The results in the figure show that the dip *survives* the increase of the cluster size, and the maximum in the conductance actually is located even further away from $V_g/U=-0.5$ as the n_{cl} grows. While this is not a definite proof, it is strongly suggestive that the conductance dip is not an artifact of the many-body procedure and cluster size used, but it may be a real effect present in the bulk. Nevertheless, it is desirable to have independent tests of our results using other many-body methods to fully confirm our conclusions. Recently, the method used here has already been tested under a variety of circumstances, and it has been shown to be qualitatively reliable.[18]

C. Survival of the dip reducing the symmetries of the Hamiltonian

In real quantums dots, the electron-hole symmetry of the Hamiltonian used in previous sections cannot be achieved since the Fermi level lies just a small fraction of electron volts above the bottom of the conduction band. However, it is always possible to find a gate potential where the main levels involved—V_g and V_g+U—are symmetrically located around E_F. Since all the energy scales important for the Kondo effect (U and t') are of the order of milli-electron volts[22] these levels are very close of E_F, achieving an approximate electron-hole symmetry.

In addition to the previous argument, it is possible to repeat the calculations presented before for cases where the particle-hole symmetry is not present. This can be achieved, for instance, by merely adding small random components to the on-site Hubbard energies and, in addition, introducing small site energies. To further break symmetries of the problem, the hopping t' from the 3-dot region to the rest can also be made different on the right and the left, and even the two internal dot-dot hopping amplitudes t'' can be made different as well. One representative result of this study is shown in Fig. 5. It is interesting to observe that the dip in the conductance survives the breaking of symmetries in the model. As a consequence, the effect appears to be robust and independent of fine details in the analysis.

IV. RESULTS FOR NUMBER OF DOTS 1, 4, AND 5

The case of one dot is special. If a n_{cl} cluster with an odd number of sites (e.g., $+-o-+$) is solved exactly, the degeneracy between $n_{\mathrm{cl}}-1$, n_{cl}, and $n_{\mathrm{cl}}+1$ *remains* even for nonzero U. This is an accidental degeneracy that avoids the dip splitting of the Kondo peak found with 3 or more (odd) dots.

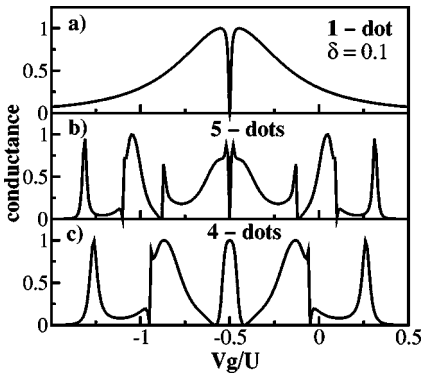

FIG. 6. (a) $G/(e^2/h)$ vs V_g/U for 1 dot, $t'/t=0.3$, introducing on-site energies $\pm\delta=0.1$ (see text). (b)–(c) are results for clusters with 5 and 4 dots, showing a rich structure. Parameters are as in Fig. 2(a). The case of 4 dots presents cancellations similar to those of an odd number of dots, although not at $V_g=-U/2$.

However, by simply adding on-site energies δ and $-\delta$ at the first and last sites of the cluster, the accidental degeneracy at $U\neq 0$ is removed and now a conductance cancellation occurs as in the other cases [Fig. 6(a)].[23] The dip phenomenon appears to be general and robust.

Our study also extended beyond the 2- and 3-dot cases. For example, Fig. 6(b) illustrates results obtained for 5 dots (7-site cluster). Here, once again, $G=0$ at $V_g=-U/2$. In addition, a rich structure if observed at higher frequencies with multiple conductance cancellations that resemble Fano resonances. Their origin is similar to those discussed for 3 dots and emerge from cancellations between "competing" poles at close distance in the Green function. Even 4 dots [Fig. 6(c)] shows a highly nontrivial structure, also with cancellations although away from $V_g=-U/2$. The richness unveiled in the conductance properties of linear-dot chains once unbiased accurate many-body techniques are used is remarkable. In the next section, the dip at $V_g=-U/2$ is tentatively explained, leaving for future work the understanding of the many other conductance dips that appear for *both* even and odd $N\leqslant 3$.

V. POSSIBLE EXPLANATIONS OF CONDUCTANCE CANCELLATION

A. Interference between states with $n_{\rm cl}\pm 1$ particles

The results of the previous paragraph suggest that simple symmetry arguments involving just two states of the entire Hilbert space—those closest to $\omega=0$—should be sufficient to understand the effect. With this in mind, consider the $n_{\rm cl}$-site-cluster Green function of interest expanded in the basis of Hamiltonian eigenstates as

$$g_{\rm cl}(\omega)=\sum_l \frac{\langle 0,n_{\rm cl}|c_1|l,n_{\rm cl}+1\rangle\langle l,n_{\rm cl}+1|c^\dagger_{n_{\rm cl}}|0,n_{\rm cl}\rangle}{\omega+E_l-E_0+i\epsilon} + \sum_m \frac{\langle 0,n_{\rm cl}|c^\dagger_{n_{\rm cl}}|m,n_{\rm cl}-1\rangle\langle m,n_{\rm cl}-1|c_1|0,n_{\rm cl}\rangle}{\omega+E_0-E_m+i\epsilon}, \tag{2}$$

where $\epsilon\to 0$ (10^{-7} in practice, and 10^{-2} for the DOS). In $|j,n\rangle$, j labels eigenstates of the Hamiltonian of n particles and eigenenergy E_j. The ground state for the cluster with $n_{\rm cl}$ particles is $|0,n_{\rm cl}\rangle$ with an eigenenergy E_0. The Hubbard Hamiltonian is particle-hole (p-h) symmetric if $V_g=-U/2$, where the energy spectrum of the particles is equal to the spectrum of holes. For this gate potential, the ground state of the cluster has a number of particles $n_{\rm cl}$ equal to the number of sites. Note also that the number of holes for this case is equal to the number of particles. The explicit p-h transformation is $c^\dagger_{l\sigma}\to(-1)^l c_{l\sigma}$. The empty state is mapped into the fully occupied state. It can be shown that

$$\langle 0,n_{\rm cl}|c_1|l,n_{\rm cl}+1\rangle\to(-1)^p\langle m,n_{\rm cl}-1|c_1|0,n_{\rm cl}\rangle, \tag{3}$$

for $n_{\rm cl}=2p+1$ or $n_{\rm cl}=2p$, with $p=$integer. To prove the last statement we have to consider that the ground state (for $V_g=-U/2$) does not change under the p−h transformation and that the vector $|l,n_{\rm cl}+1\rangle$ is transformed into other $|m,n_{\rm cl}-1\rangle$ eigenstate of the Hamiltonian with the same energy ($E_l=E_m$). The sign $(-1)^p$ came from the anticonmutation relations used to move the creation/destruction operators to their correct locations after the transformation. In addition, following similar considerations as for the previous matrix element, it can be shown

$$\langle l,n_{\rm cl}+1|c^\dagger_{n_{\rm cl}}|0,n_{\rm cl}\rangle\to(-1)^r\langle 0,n_{\rm cl}|c^\dagger_{n_{\rm cl}}|m,n_{\rm cl}-1\rangle, \tag{4}$$

where $r=p$ if $n_{\rm cl}=2p+1$, and $r=p+1$ if $n_{\rm cl}=2p$. Isolating a pair of states $|l,n_{\rm cl}+1\rangle$ and $|m,n_{\rm cl}-1\rangle$ connected by the p-h transformation—namely with equal energies relative to E_0 (i.e., $E_0-E_l=E_0-E_m$)—this leads to a simple contribution to $g_{\rm cl}(\omega)$ of the form

$$\frac{AB}{(\omega+\omega_l+i\epsilon)}\pm\frac{AB}{(\omega-\omega_l+i\epsilon)}, \tag{5}$$

where A,B are numbers (matrix elements where the p−h transformation was applied) and $\omega_l=E_l-E_0$, assumed nonzero. The +(−) sign corresponds to an *odd (even)* number $n_{\rm cl}$ of cluster sites. Clearly, for $n_{\rm cl}=$odd, Re$[g_{\rm cl}(\omega)]$ is odd under $\omega\to-\omega$, and, thus, it cancels at $\omega=0$. For the other case, $n_{\rm cl}=$even, there is no cancellation since the real part is even. Since the embedding process cannot generate a nonzero conductance if the cluster has a vanishing Green function, then the overall conductance is zero for $V_g=-U/2$ and $n_{\rm cl}$ odd.

The proof of the results of the previous paragraph has been mainly computational, using the entire Hilbert space for small values of $n_{\rm cl}$. However, a simpler qualitative understanding can be obtained for example considering $n_{\rm cl}=3$ and using $(|\uparrow\downarrow\uparrow\rangle+|\downarrow\uparrow\downarrow\rangle)/\sqrt{2}$ as a simplified $n_{\rm cl}$-particle ground-state $|0,n_{\rm cl}\rangle$. For $|l,n_{\rm cl}+1\rangle$, $c^\dagger_{-1,\uparrow}|0,n_{\rm cl}\rangle$ can be used, and $c_{-1,\downarrow}|0,n_{\rm cl}\rangle$ for $|l,n_{\rm cl}-1\rangle$. For these simplified states, it can be easily shown that $|l,n_{\rm cl}+1\rangle$ transforms under p−h to $|l,n_{\rm cl}-1\rangle$ for $n_{\rm cl}=$odd, and to $-|l,n_{\rm cl}-1\rangle$ for $n_{\rm cl}=$even. After simple algebra, recalling that the matrix elements are real, and being careful with the signs arising from fermionic anticommutations, the p-h transforms of the matrix elements are found, completing the proof. This $n_{\rm cl}=3$ derivation can easily be extended to arbitrary $n_{\rm cl}$.

The previous explanation of the anomalous zero conductance emphasizes the competition, and eventual interference,

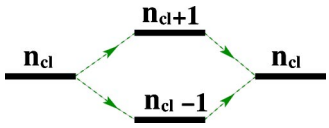

FIG. 7. The two "paths" that lead to the conductance cancellation involve intermediate states of $n_{cl}+1$ and $n_{cl}-1$ electrons.

between two states that contribute to the cluster Green function. The key aspect is the relative sign of the matrix elements for the two poles, which leads to interference for an odd number of cluster sites. Let us discuss these aspects more intuitively, and also explain why at $U=0$ the effect is not present. Consider as example a 5-site cluster with 3 dots (schematically +-o-o-o+, o=dot, +=lead site). At $U=0$ this cluster, and any cluster with a total number of sites odd and Hamiltonian Eq. (1), has a zero energy eigenvalue. This implies a *degeneracy* between the lowest-energy states with 4, 5, and 6 particles (or $n_{cl}-1$, n_{cl}, $n_{cl}+1$ particles for an n_{cl} (odd) cluster) since populating the zero-energy state has no energy cost. With the Fermi energy of the metal at 0 as well, there is a direct channel for conductance through the dots and no cancellation. However, when U is switched on, the degeneracy is removed since there is a penalization for having a site with two electrons (directly related to an empty site by p-h symmetry). The doubly occupied site, inevitable for $n_{cl}+1$ electrons on n_{cl} sites, is located with more probability outside the set of N dots, i.e., in the lead segments included in the exactly solved cluster. This produces a finite but small splitting ΔE, substantially smaller than U. As U increases, a Kondo peak is formed at $V_g=-U/2$, as previously discussed,[17] but with a dip of width ΔE in the middle. Note that for n_{cl} even, there is no zero in the cluster and no dip in the conductance. However, states approach zero energy as n_{cl} (even) increases and eventually as $n_{cl}\to\infty$ a common limit of zero conductance for both n_{cl} odd and even is expected.

The G cancellation arises from the U-induced splitting of the $n_{cl}+1$ and $n_{cl}-1$ states from the n_{cl} ground state. More intuitively, for charge to transport through a cluster or molecule there are two basic processes, that here interfere. In one case an electron first jump to the cluster, leading to $n_{cl}+1$ particles inside, and then an electron exits. In the other case, first an electron leaves the cluster [i.e, $(n_{cl}-1)$ electrons in the cluster intermediate state] and then another gets in. These two intermediate states corresponds to two "paths" in a quantum-mechanical formulation, and they do not need actual different real-space trajectories to interfere with one another (Fig. 7).

B. Two-paths interference in a one-dimensional multidot system

An alternative explanation of the conductance-cancellation effect described in this paper is the following. The n_{cl}-site cluster, with n_{cl} odd, has reflexion symmetry around the central dot (here denoted by 0). This suggests a change of basis defined by $d_{\alpha i\sigma}=(c_{i\sigma}+c_{-i\sigma})/\sqrt{2}$ and $d_{\beta i\sigma}=(c_{i\sigma}-c_{-i\sigma})/\sqrt{2}$, where the sites $i=1,2,\ldots$ $(-1,-2,\ldots)$ are on the right (left) of the central dot, which is left invariant by

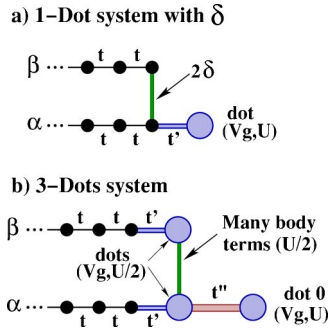

FIG. 8. Illustration of the transformation to the α-β basis described in the text. (a) corresponds to 1 dot with diagonal energies $\pm\delta$ in the sites next to the dot. (b) corresponds to 3 dots.

this transformation. It can be shown that for just one dot, $N=1$, the system in the new basis is equivalent to one-dot at the end of a semi-infinite chain coupled to the α band, and decoupled from a β band [as sketched in Fig. 8(a), for $\delta=0$]. This geometry corresponds to a one-channel Kondo problem, with a concomitant peak in electronic transport, plus an uncoupled noninteractive channel.

We want to remark that for N larger than 1 (or for $N=1$ but with nonzero δ) the previous uncoupled channel is now interacting with the other portion of the system. This fact creates an important difference between $N=1$ and $N>1$. In the case of one dot the system is transformed into one impurity coupled to one (symmetric combination) band while the other band (antisymmetric combination) is totally decoupled. If $N>1$ both bands (the symmetric and the antisymmetric) are coupled through many-body terms to the impurities showing that this system is similar to a two-channel Kondo problem.

In the new basis, the Green function used to calculate the conductance can be written as $G_{LR}(\omega)=1/2[G_{\alpha\alpha}(\omega)-G_{\beta\beta}(\omega)]$. Then, an interference in the conductance occurs when $G_{\alpha\alpha}(E_F)=G_{\beta\beta}(E_F)$ or when both are zero. At this point, it is important to emphasize that the Green function $G_{\alpha\beta}$ (which carries the information about the interference between α and β) does not participate of the transmission probability (G_{LR}). However, the interference could be present also in the diagonal Green functions $G_{\alpha\alpha}$ and $G_{\beta\beta}$.

As discussed in Sec. IV, consider now a diagonal energy δ at site $i=+1$ and $-\delta$ at $i=-1$ (i.e., immediately to the right and left of the active dot). Transforming the operators, the previously decoupled bands α and β are now effectively connected by a hopping term of strength 2δ [Fig. 8(a)]. In this representation, it is easy to visualize a possible interference between processes involving the direct hopping $\alpha\to\beta$ and those where jumping to and from the dot is part of the path. This abstract-space representation establishes a connection with the real-space T-geometry interference previously discussed.[5]

For $N>1$ the results are not as conclusive, but still suggestive. Consider as an example $U=0$ and $N=3$. In this case, the two channels α and β, each supplemented by one dot, decouple from one another. The central dot is coupled to the α channel [Fig. 8(b)]. At $U\neq 0$ a many-body coupling proportional to $U/2$ links the two channels. This coupling—too

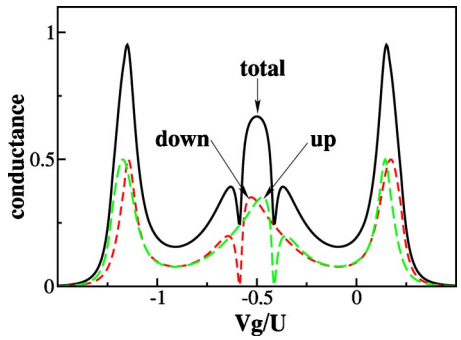

FIG. 9. Conductance vs gate voltage calculated using a 5 sites (3 dots) cluster state with total spin z component equal to $1/2$ (as opposed to the equal-weight $1/2$ and $-1/2$ used in the rest of the paper). Shown with dashed lines are the dressed conductances (divided by 2) for the up and down channels, each showing a zero at values of the gate voltage close to $-0.5U$. The solid line is the sum. In the sum, two dips can be observed. Although the result is quantitatively different using one convention or the other for the spin of the cluster state, the fact that the Kondo peak has internal structure in the form of dips is qualitatively the same in both cases.

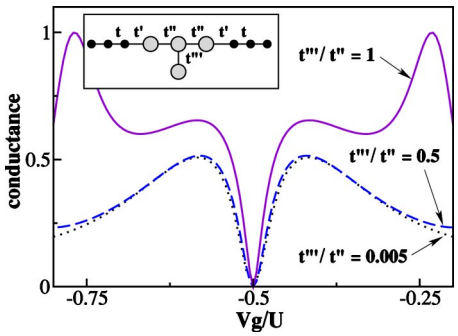

FIG. 10. Conductance vs gate potential for the T-geometry system (shown in the inset) proposed to avoid the ground-state degeneracy at $V_g/U=-0.5$. The parameters U, t, t', and t'' are the same as in Fig. 2(a). The point line corresponds to results at $t'''/t''=0.005$, the dashed line at $t'''/t''=0.5$, and the solid line at $t'''/t''=1$. The dip is present in all cases.

cumbersome to write it here explicitly—contains "spin-flip" contributions between α and β, density-density interactions, and even a two-electron hopping term. The T geometry appears once again, suggesting possible interferences, but now with an $\alpha \rightarrow \beta$ effective "hopping" which is very complicated. Nevertheless, this is sufficiently illustrative since for N even none of the two channels α-β have an extra dot attached, and the entire system is effectively linear with no obvious sources of interference, as indeed observed numerically. Then, *N odd and even are fundamentally different in this representation*, with the odd having possible sources of interference. Note that this analysis focuses on the gate voltage $V_g=-U/2$. The study of previous sections has shown that conductance cancellations occurs for 4 dots as well, although at different values of V_g. The study of the origin of these cancellations is left for future work.

VI. CONCLUSIONS

Using numerical techniques, in this paper it has been argued that the conductance Kondo peak of an odd $N=3,5\ldots$ number of quantum dots forming a linear array presents nontrivial internal structure in the form of a dip. The calculation has passed many tests, but the authors acknowledge that the reported result is quite unexpected and for this reason other theoretical techniques should be employed to test our predictions. If the present results are confirmed in the near future, the search for the "Kondo dip" in experiments should be carried out. The experimental observation of the conductance dip reported here may require considerable effort. Realizations of the linear-array geometry using atoms and employing STM techniques to measure conductances are difficult. For instance, atoms attract, and three of them on a metallic surface tend to form triangles rather than chains.[24] In addition, finite temperature effects will likely tend to fill the dip in G, and temperatures even lower than usually employed will be needed to see the effect. At present, the characteristic energy regulating the width of the dip is still unknown since the method used in the paper works only at zero temperature. In spite of these caveats, the interference discussed here is sufficiently novel and interesting that its experimental confirmation and theoretical extension to other types of arrays should be actively pursued.

ACKNOWLEDGMENTS

This work was supported by the NSF Grant Nos. DMR-0303348 and DMR-0122523. Conversations with Y. Meir, E. Anda, J. Vergés, G. Chiappe, S. Ulloa, L. Glazman, and S. Hershfield are gratefully acknowledged.

APPENDIX: RESULTS USING OTHER CONVENTIONS

As discussed in Sec. II, the state representing the cluster with an odd number of sites (and dots) used in this effort is the equal-weight sum of the states with total z component of spin, $S^z_{\rm tot}$, equal to $1/2$ and $-1/2$. By this procedure the particle-hole symmetry is respected at every step in the calculation. However, other conventions have been used in recent literature. For example, related work in Ref. 18 considers only the cluster state with $S^z_{\rm tot}=1/2$. With this convention the cluster Green functions for spins $1/2$ and $-1/2$ are different (although their sum is independent of the relative weights of the two states). If these up and down Green functions are independently dressed through the Dyson formalism, conductances for the up and down channels are obtained. Individually, *each of these conductances contains a zero* quite similar to the results shown in the bulk of the present paper. However, the location of the zero is different for the two channels, slightly shifted left and right from $V_g/U=-0.5$ (see Fig. 9) due to the breaking of the particle-hole symmetry. When the two conductances are added (and dividing by 2), the zeros are no longer present since the up and down contributions have the cancellation at different gate voltages. However, even accepting this symmetry-breaking alternative convention to carry out the calculation, two dips are clearly found in the overall result, as also shown

in Fig. 9. It is expected that the two procedures (with and without explicit particle-hole symmetry in the calculation) will lead to the same result in the bulk limit, and only further work can clarify which convention is the best given the inevitable size constraints of the present numerical technique.

Finally, to avoid the cluster ground-state ambiguity problem an alternative geometry sketched in the inset of Fig. 10 can be used. In this system, one extra dot is laterally coupled to the central dot with a hopping amplitude t'''. Clearly, when $t''' \to 0$ this system is equivalent to the 3 dots system described in the bulk of the paper. For $V_g/U=-0.5$ and one particle per site in the cluster, the extra dot adds one electron to the system studied before giving an $S^z_{\rm tot}=0$ for the (nondegenerate) ground state. This trick eliminates the up and down degeneracy at all finite values of t''' (while at $t'''=0$, the degeneracy is recovered). Repeating the calculation as in Fig. 2(a), the conductance for the system once again presents a symmetric dip for all the values of t''' investigated, even including the very small t''' regime where the extra dot and linear array are nearly decoupled. Then, once again it is concluded that different procedures to carry out the calculations lead all to the same qualitative conclusions. Both Figs. 9 and 10 show that the main point of the present paper remains the same irrespective of the convention: The Kondo peak of quantum-dot arrays with an odd number of dots appears to have internal structure in the form of dips as the gate voltage is varied.

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