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Kondo regimes in a three-dots quantum gate

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The transport properties of a linear structure of three quantum dots, with the central one connected to leads, are studied using the logarithmic discretization embedded cluster approximation. It is shown that the side dot spins can be ferromagnetically (F) or antiferromagnetically (AF) correlated between them, depending on the charge at the central dot. The system possesses a regime of coexistence of a two stage Kondo effect and the F phase. Ferromagnetism destroys the Kondo ground state when the system is driven to the molecular regime by increasing the interdot interaction above the largest Kondo temperature. Instead, an AF ground state does not compete with the Kondo regime. This remarkable behavior indicates that the measurement of the conductance can be an efficient readout procedure when the system operates as a quantum gate.

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Three-dot structure. Quantum dots (QDs) were theoretically proposed as ideal components to construct quantum gate devices.[1,2] The proposal was based on the flexibility to change in a continuous way its couplings and charge by manipulating the potentials that define the QD. Recently, transport properties of two dot systems have been theoretically studied.[3–8] It was shown experimentally that a controlled operation of long-time relaxation double dot spins was possible.[9–11] The manipulation of the gate voltage[10] allows us to control the dots charge and also the tunnel barrier between them, modifying their exchange interaction and the physics of the system. An efficient and reliable process to read out the spin configuration is the additional requirement for this structure to operate as a quantum gate.

Although less studied, three-dot structures have also received some attention.[12–16] Depending on the topology, it has been possible to investigate the two stage Kondo and Dicke effects, and the properties derived from a non-Fermi-liquid behavior in a triangular configuration.[17] However, the interplay between the Kondo effect and the various exchange interactions among the spins was disregarded. In particular this is the case of the structure of three QDs, two side localized [side QD (SQD)], one at one side (1), and other at the opposite side (2) of a central one [central QD (CQD)], which is connected with them and connected in turn to leads (L).[12] This system is capable of functioning as a quantum gate. This possibility is based on the fact that the spin-spin correlation between SQDs can be tuned by changing the charge state of the central dot by means of a gate potential. It has been suggested that a polyoxometalate molecule could be a materialization of this structure.[12] In the cotunneling regime a peak in the differential conductance is expected to show up at values of the gate potential at CQD, which depends on whether the spins of the SQD are ferromagnetically (F) or antiferromagnetically (AF) correlated between them. This transport measurement was proposed to read out that information.[12]

The aim of this Rapid Communication is to analyze the three-dot system in Fig. 1. This configuration is topologically similar to that proposed and studied in the weakly interacting regime, in Ref. 12. Here, we investigate the much richer physics that this system possesses in the strongly interacting regime, when there is an interplay between the spin-spin correlations among dots and various Kondo-like ground states. As regard to the computing gate capability of this structure, we analyze its transport properties and conclude that the Kondo regime is a fundamental tool to read out the information contained in the SQDs, i.e., whether they are F or AF correlated.

Hamiltonian. The system is described by an Anderson-like Hamiltonian that reads as

$$\hat{H}_M = \sum_{i=c,1,2;\sigma} \epsilon_i c_{i\sigma}^{\dagger} c_{i\sigma} + \sum_{i=1,2;\sigma} t'' c_{i\sigma}^{\dagger} c_{c\sigma} + \sum_{i=c,1,2} U_i n_{i\uparrow} n_{i\downarrow} + \sum_{\sigma} t' (c_{c\sigma}^{\dagger} c_{L1\sigma} + c_{c\sigma}^{\dagger} c_{L2\sigma}) + J\mathbf{S}_1 \cdot \mathbf{S}_2 + \text{c.c.},$$

where the operator $c_{i\sigma}^{\dagger}$ creates an electron at site $i=c,1,2$ with spin σ and $n_{i\sigma}$ is the number operator. We assume the diagonal energies of the SQDs to be $\epsilon_1=\epsilon_2=\epsilon_0$, and $U_1=U_2=U_c=U_0$ for the on-site Coulomb repulsion. The parameter t'' is the hopping probability from SQD to the CQD. Finally, $\epsilon_0=-U_0/2$ ensures that a charge close to one electron will occupy each SQD. The energy of the CQD is $\epsilon_c=V_g$, where V_g is the gate potential. J is an exchange pa-

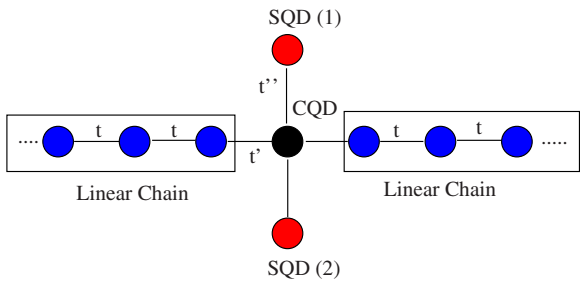

FIG. 1. (Color online) The linear three-dots structure investigated in this work. Leads are approximated by one-dimensional chains.

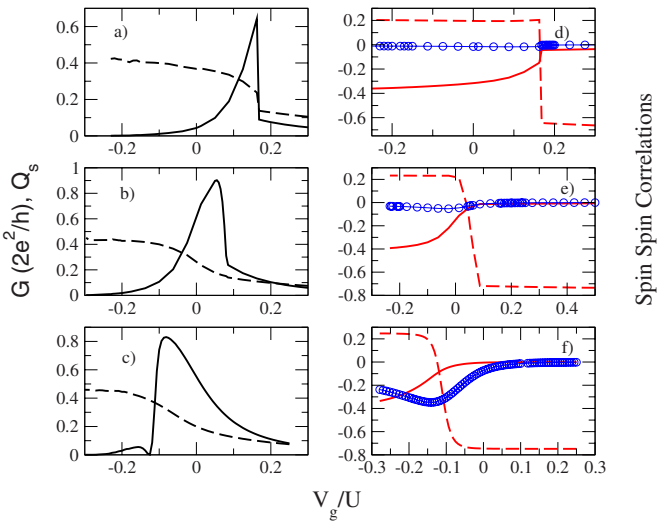

FIG. 2. (Color online) Left panels: conductance (continuous line) and charge (broken line) versus gate voltage V_g. Right panels: spin-spin correlations versus gate voltage V_g; $\mathbf{S}_1\cdot\mathbf{S}_2$ (broken line), $\mathbf{S}_\mathbf{c}\cdot\mathbf{S}_\mathbf{L}$ (continuous line), and $\mathbf{S}_\mathbf{c}\cdot\mathbf{S}_\mathbf{L}$ (circles). The results correspond to [(a) and (d)] $t''=0.4$, [(b) and (e)] 0.2, and [(c) and (f)] 0.05; $J=0$, $U_0=2$, and $t'=0.3$.

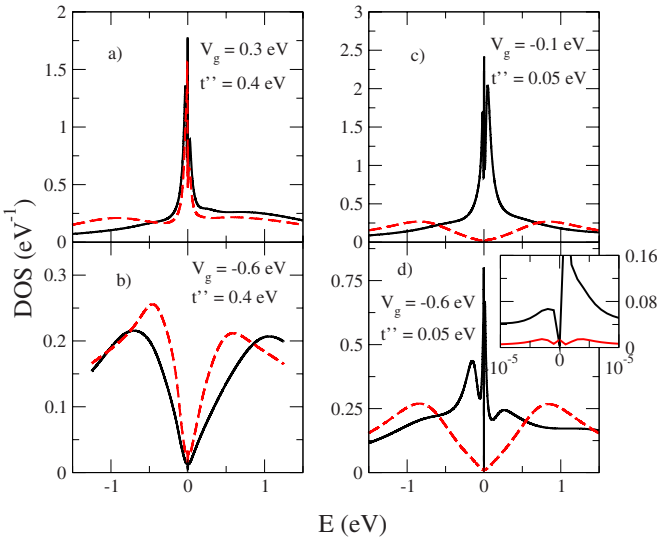

FIG. 3. (Color online) LDOS at the central dot (black lines) and the side dots (red lines) for $t''=0.4$ (left panels) and 0.05 (right panels). The rest of the parameters are given in the figures or in the main text. The inset shows the LDOS at a smaller scale.

rameter between S_1 and S_2 (upper and lower spins) used to stabilize the AF phase, as explained below. Sites $L1$ and $L2$ are the first sites of one-dimensional chains that represent the metallic leads. They are connected with t' to the central dot and due to the symmetry their spin operator is denoted by S_L indifferently. The Fermi level of the system is chosen as the zero of energy. We solve it by applying the logarithmic discretization embedded cluster approximation algorithm,[18] so we logarithmically discretize the lead Hamiltonian $H_L=\Sigma_{i,\sigma}t_{i,\lambda}c^\dagger_{i\sigma}c_{i+1\sigma}+\text{c.c.}$, where $t_{i,\lambda}=t(1+1/\lambda^2)/(2\lambda^{|i|-1})$ with t being the hopping probability in the leads. The discretization parameter λ is modified until size effects are eliminated, which guarantees a reliable description of the properties at the Fermi level.[18] The values of all the parameters are given in units of t.

Isolated three-dot structure. A calculation of the ground state of an isolated three-dot structure with $J=0$ shows that, with one electron at each SQD and none at the CQD, the side spins are AF correlated, while with roughly one electron at each dot, the correlation is F. This behavior persists when the central dot is connected to leads, as shown in Figs. 2(d)–2(f), which depict the spin-spin correlation of the side dots as a function of V_g. It should be noted that to stabilize the AF configuration, when the central dot is filled, a finite J is required.

Charging the CQD then triggers a transition from AF correlated SQDs (called AF configuration) to F correlated SQDs, which in turn are AF correlated with the CQD. We call the last the F configuration. The F configuration shows three regimes:

(i) *Kondo effect in SQDs*. The first regime occurs for $V_g>0$ and $t''>$ or $\sim t'$, when charge begins to enter into the CQD. At this point correlations between SQDs change from AF to F see [Figs. 2(d) and 2(e)]. Thereafter a peak with a maximum close to $2e^2/h$ (a characteristic of the Kondo effect) at positive values of V_g develops [see Figs. 2(a) and 2(b)]. This occurs because, in this case, the central dot is out of resonance ($V_g>0$) and has a small charge, so that effects of local repulsion in it can be neglected. This allows fourth-order spin flipping processes, between the lateral and the central dots, which are characteristic of the Kondo effect.[19,20] Spin-spin correlations between the CQD and the SQDs are AF [see Figs. 2(d) and 2(e)], and a peak at the Fermi level in the local density of states (LDOS) of the lateral dots raises up [see Fig. 3(a)]. Both are signatures of the Kondo effect, which in this regime provides the only open conduction channel, through the SQDs.

(ii) *Molecular regime*. When $V_g<0$ and $t''>t'$ the system enters into the molecular regime. The Kondo effect associated with the SQD disappears because the local Coulomb repulsion at the central dot increases, preventing the fourth-order process necessary for the Kondo resonance to show up. In this regime correlation between the lateral and central dots is large and antiferromagnetic [see Figs. 2(d) and 2(e)] and the LDOS shows a large dip instead of a Kondo resonance [Fig. 3(b)]. The spin correlations between the conduction electrons and the central dot are zero [see Figs. 2(d) and 2(e)] indicating that this dot is also outside the Kondo regime. In this F regime the molecular structure of the three dots competes with the Kondo regime of the CQD. To understand this competition it is convenient to realize that, for the central dot to be in the Kondo regime, a flipping of its spin cannot change the energy.[19,20] In the present case, the most important contribution to the ground state of an isolated three-dot structure $|1,c,2\rangle$ is given by $|F\rangle=2|\uparrow,\downarrow,\uparrow\rangle-|\downarrow,\uparrow,\uparrow\rangle-|\uparrow,\uparrow,\downarrow\rangle$. Flipping the central dot spin creates a state that has a finite projection on excited high-energy states of the three-dot system. This gives rise to a competition between ferromagnetism of the external dot spins and the Kondo regime of the CQD, which has a Kondo temperature T_{k1}. Then, if $t''>T_{k1}$ and $-U<V_g<0$, the system is driven out of the

Kondo regime and, thus, the conductance is almost zero and weakly dependent on temperature.

(iii) *Two stage Kondo regime*. The F state and the Kondo effect coexist when the system is no longer in the molecular regime, $t'' < T_{k1}$. In this case the transition from AF to F configuration of the SQDs occurs for $V_g < 0$ [see Fig. 2(f)]. Before this transition occurs, SQDs are AF correlated and the conductance follows the evolution corresponding to the CQD going through resonance in the Kondo regime [see Fig. 2(c)]. As seen in Fig. 2(f), there is an AF correlation between CQD and the leads and a sharp peak at the LDOS [Fig. 3(c)]. Once the transition from AF to F configuration of SQD spins occurs, the ground state shows all the features corresponding to a two stage Kondo regime. The conductance drops to zero as V_g is lowered [see Fig. 2(c)] and a Kondo-Fano resonance at the Fermi energy shows up in the LDOS at the central dot [see Fig. 3(d)]. The LDOS is characterized by an external width given by $T_{k1}(\sim 0.1)$, the largest Kondo temperature, and an internal antiresonance of width T_{k2} [see the inset of Fig. 3(d)]. This regime is the result of a Kondo-like AF spin-spin correlations between the SQDs and the heavy fermion system constituted by the CQD spin Kondo correlated with the conduction spins of the leads. This can be concluded from an inspection of Fig. 2(f), where the various spin-spin correlations are presented. Note the AF correlations that develop between the CQD and SQDs and also between the CQD and the leads. As the side dots provide Fano-type interference channels for the electrons, the conductance is zero around $V_g = -U/2$. This phenomenon is highly temperature dependent. Increasing the temperature above T_{k2}, a very small energy indeed[21] eliminates the antiresonance of the Kondo peak in the LDOS at the central dot and consequently transforms an insulator into a conducting system.

Side dot coupled AF. To analyze the AF spin configuration we introduce in the Hamiltonian an antiferromagnetic interaction, $J > 0$, between the side dot spins. This is only a necessary mathematical artifact because when the central dot is charged, the SQD spin-spin correlation is ferromagnetic, so J is necessary to stabilize the AF phase. The conductance depends marginally on the value of J provided it is small, although large enough to stabilize the AF ground state (see below). In this case the spin configuration does not compete with the Kondo regime. This can be understood realizing that the greatest contribution to the AF ground state of a system of three dots corresponds to the wave function $|\mathrm{AF}\rangle = |\uparrow,\uparrow,\downarrow\rangle - |\downarrow,\uparrow,\uparrow\rangle$. Flipping of the CQD spin creates a state that has the same energy as the original one, permitting us to construct a standard fourth-order perturbation theory that gives rise to the Kondo regime. Therefore, the conductance, spin correlations, and LDOS correspond to CQD going through resonance in the Kondo regime when its gate voltage is modified [see Figs. 4(a)–4(c)]. The SQDs have a negligible LDOS at the Fermi level and the absence of correlations with CQD confirms that SQDs do not play any role in this case.

Quantum gate operation. Let us discuss now how the Kondo regime may be used to read out the information contained in the SQDs. It was proposed in Ref. 12 to read the total spin S_0 of the two side dots by measuring the conductance through the central dot in the cotunneling regime. The

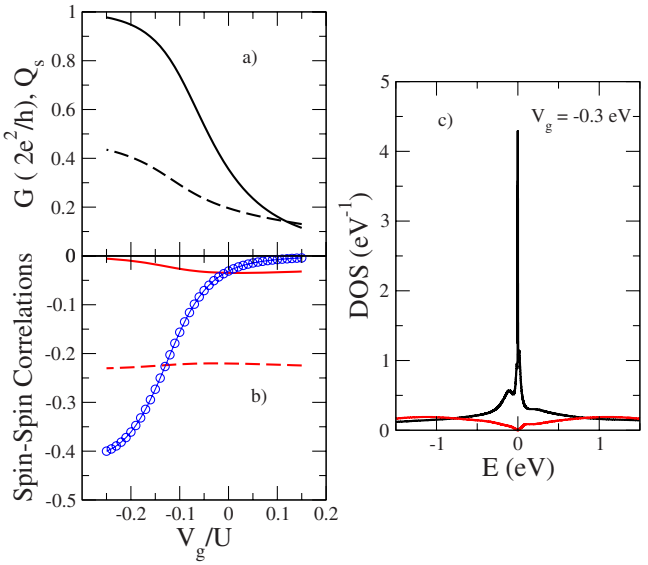

FIG. 4. (Color online) (a) Conductance (continuous line) and charge (broken line) versus gate voltage V_g. (b) Spin-spin correlations versus gate voltage V_g: $S_u^z S_l^z$ (broken line), $\mathbf{S_l}\cdot\mathbf{S_c}$ (continuous line), and $\mathbf{S_c}\cdot\mathbf{S_L}$ (circles). (c) LDOS (in eV^{-1}) at the central dot (black lines) and the lateral dots (red lines) The results correspond to $t''=0.4$, $J=0.4$, $U_0=2$, and $t'=0.3$.

conductance shows a peak at a value of the gate potential, which depends on whether the SQD spin correlation is F or AF. It is due to the energy difference between F and AF configurations; $\sim t''^2/U$. The different gate potential at which the peak occurs allows us to differentiate the two configurations. Keeping this difference noticeable requires the peak widening, due to the coupling to the leads $(\sim t'^2/t)$, to be weak enough. Then, the readout process needs substantially smaller values of t' than those necessary for the quantum gate operation.[12] This complicates the performance of the device as the connection to the leads should be changed during the quantum gate operation.[12] To avoid this difficulty we propose the system to operate in the molecular regime for small negative V_g $(|V_g| < U)$ and $t'' \sim t'$. These values of the model parameters guarantee that the structure appropriately behaves as a quantum gate, as discussed below. Due to the large differences between the F and AF configuration conductances for these parameter values [see Figs. 2(a) and 4(a)], a transport measurement permits us to distinguish between these two configurations without changing the value of t'.

Understanding how this system may operate as a quantum gate requires a full time-dependent study. However, equilibrium stationary studies are reliable in this case because the processes taking place in the system are controlled by very different time scales. The charge enters or comes out from the dot at a rate given by the tunneling time $\tau_t \sim |V_g|/t'^2$. After this process has taken place, the spins interact during the gate time τ_g that is on the order of U/t''^2. The entrance of charge from the leads into the three-dot system is a stochastic event that could perturb the quantum gate performance. This can be studied calculating the overlap of the result of a perfect performance of the gate and the real performance ("gate fidelity"). It can be shown[12] that fidelity increases when the

connection of the central dot to the leads is increased, such that $\tau_t < \tau_g$,[12] a condition that is compatible with our choice of model parameters. In order to perform a quantum gate operation it is necessary to read the configurations of the SQD spins (F or AF). If the original state was ferromagnetic, the Kondo regime is absent and the process of measuring the conductance does not change this configuration. Transport requires an electron in the central dot, which then mediates ferromagnetic correlation. The conductance in this situation is close to zero. However, if the state to be read were AF, measuring the conductance would introduce a charge into the central dot, which would tend to modify the AF configuration. As antiferromagnetism is compatible with the Kondo effect, although it was not originally present when the central dot was empty, it will appear after a characteristic time τ_K on the order of the inverse of a tenth of T_k: $\tau_K \sim 1/(10\sqrt{(t'^2U/t)e^{-|V_g||V_g+U|t/(2t'^2U)}})$.[22] This satisfies $\tau_K < \tau_t$ for negative values of V_g not very far from the Fermi energy. For example, taking, $t'=0.3$, $t''=0.4$, $U=2$, and $V_g=-0.4$, we are clearly within the Kondo regime (see Fig. 4) and the results are $\tau_K \sim 1$, $\tau_t \sim 4$, and $\tau_g \sim 12$. Without mattering how the AF configuration was obtained, within this time scales, the conductance can be studied supposing a system in equilibrium with an electron in the central dot in Kondo regime and, therefore, having a large conductance.

We have studied the three-dot system shown in Fig. 1. This structure possesses a two stage Kondo ground state coexisting with a F phase when the hopping probability from the lateral to the central dots is smaller than that from the central dot to the leads. Increasing the former destroys the Kondo effect driving the system into a ferromagnetic molecular regime. However, when the ground state is AF there is a coexistence with the Kondo regime. As the spin configuration of the external dots depends on the charge at the central one, which can be manipulated by a gate voltage, the system is a good candidate to be used as a quantum computing gate device. We studied its transport properties and concluded that the readout process requires the system to be in the Kondo regime.

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[1] A. Barenco, C. H. Bennett, R. Cleve, D. P. DiVincenzo, N. Margolus, P. Shor, T. Sleator, J. A. Smolin, and H. Weinfurter, Phys. Rev. A **52**, 3457 (1995).
[2] D. Loss and D. P. DiVincenzo, Phys. Rev. A **57**, 120 (1998).
[3] W. G. van der Wiel, S. De Franceschi, J. M. Elzerman, T. Fujisawa, S. Tarucha, and L. P. Kouwenhoven, Rev. Mod. Phys. **75**, 1 (2002).
[4] C. A. Büsser, E. V. Anda, A. L. Lima, M. A. Davidovich, and G. Chiappe, Phys. Rev. B **62**, 9907 (2000).
[5] J. M. Aguiar-Hualde, G. Chiappe, and E. Louis, Phys. Rev. B **76**, 085314 (2007).
[6] P. A. Orellana, G. A. Lara, and E. V. Anda, Phys. Rev. B **65**, 155317 (2002).
[7] G. A. Lara, P. A. Orellana, and E. V. Anda, Phys. Rev. B **78**, 045323 (2008).
[8] P. A. Orellana, G. A. Lara, and E. V. Anda, Phys. Rev. B **74**, 193315 (2006).
[9] G. Burkard, D. Loss, and D. P. DiVincenzo, Phys. Rev. B **59**, 2070 (1999).
[10] J. R. Petta, A. C. Johnson, J. M. Taylor, E. A. Laird, A. Yacoby, M. D. Lukin, C. M. Marcus, M. P. Hanson, and A. C. Gossard, Science **309**, 2180 (2005).
[11] F. H. L. Koppens, C. Buizert, K. J. Tielrooij, I. T. Vink, K. C. Nowack, T. Meunier, L. P. Kouwenhoven, and L. M. K. Vandersypen, Nature (London) **442**, 766 (2006).
[12] J. Lehmann, A. Gaita-Ariño, E. Coronado, and D. Loss, Nat. Nanotechnol. **2**, 312 (2007).
[13] M. C. Rogge and R. J. Haug, Phys. Rev. B **77**, 193306 (2008).
[14] M. Hentschel, D. C. B. Valente, E. R. Mucciolo, and H. U. Baranger, Phys. Rev. B **76**, 235309 (2007).
[15] L. Gaudreau, S. A. Studenikin, A. S. Sachrajda, P. Zawadzki, A. Kam, J. Lapointe, M. Korkusinski, and P. Hawrylak, Phys. Rev. Lett. **97**, 036807 (2006).
[16] S. G. Schirmer, D. K. L. Oi, and A. D. Greentree, Phys. Rev. A **71**, 012325 (2005).
[17] K. Ingersent, A. W. W. Ludwig, and I. Affleck, Phys. Rev. Lett. **95**, 257204 (2005).
[18] E. V. Anda, G. Chiappe, C. A. Büsser, M. A. Davidovich, G. B. Martins, F. Heidrich-Meisner, and E. Dagotto, Phys. Rev. B **78**, 085308 (2008).
[19] D. Goldhaber-Gordon, H. Shtrikman, D. Mahalu, D. Abusch-Magder, U. Meirav, and M. A. Kastner, Nature (London) **391**, 156 (1998).
[20] T. A. Costi and C. Hewson, J. Phys.: Condens. Matter **6**, 2519 (1994).
[21] P. S. Cornaglia and D. R. Grempel, Phys. Rev. B **71**, 075305 (2005).
[22] P. Nordlander, M. Pustilnik, Y. Meir, N. S. Wingreen, and D. C. Langreth, Phys. Rev. Lett. **83**, 808 (1999).