Transport properties of strongly correlated electrons in quantum dots using a simple circuit model

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Numerical calculations are shown to reproduce the main results of recent experiments involving nonlocal spin control in nanostructures (N. J. Craig et al., Science 304, 565 (2004)). In particular, the splitting of the zero-bias-peak discovered experimentally is clearly observed in our studies. To understand these results, a simple “circuit model” is introduced and shown to provide a good qualitative description of the experiments. The main idea is that the splitting originates in a Fano anti-resonance, which is caused by having one quantum dot side-connected in relation to the current path. This scenario provides an explanation of Craig et al.’s results that is alternative to the RKKY proposal, which is here also addressed.

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The total Hamiltonian is

\[ t c_{i\sigma}^\dagger c_{i\sigma} + h.c. \]  

(3)

where \( c_{i\sigma}^\dagger \) (\( c_{i\sigma} \)) creates an electron at site \( i \) with spin \( \sigma \) in the left (right) lead. The CR is composed of one tight-binding site, unless otherwise stated. Site ‘0’ is the first site at the left (right) of QD1 (CR) in the left (right) lead. The total Hamiltonian is \( H = H_A + H_{\text{leads}} + H_{\text{d}} \). Note that for \( V_{g1} = V_{g2} = -U/2 \), the Hamiltonian is particle-hole symmetric. To calculate the conductance \( G \), using the Keldysh formalism \( \), accompanied by a suppression of the ZBA (for \( V \) dependent on \( g_2 \) values of \( \langle n_2 \rangle \)), essentially the same as if QD2 was not present. For higher values of \( g_2 \), the conductance through QD1 is present for all finite values of \( t'' \). By increasing \( t'' \) from 0.0 (red curves) to 0.1 (green), the ZBA is now split in two and \( \langle n_2 \rangle \) varies from 0.0 to 0.2. By increasing \( t'' \) further increases (0.2 (blue)), the dip becomes wider, the two side-peaks decrease and \( G \) still vanishes for \( \langle n_2 \rangle = 0.5 \) (one electron in QD2). Our calculations show that, if \( \langle n_2 \rangle \) varies around 0.5, the dip in \( G \) is present for all finite values of \( t'' \), with a width proportional to \( t'' \). Comparing the results in Figs. 3A and 3B of Craig et al. with Figs. 2c and 2b in this Letter, respectively, one notices a striking similarity: The splitting of the ZBA observed in the experimental results (their Fig. 3A), when the number of electrons in the control QD is odd and the coupling to the central region is increased, is very similar to the dip in \( G \) for all finite-\( t'' \) curves in Fig. 2c (as mentioned above, at finite temperatures, one expects that the dip in \( G \) will not reach zero). When the occupancy of QD2 is even (Fig. 3B in the experimental results) and Fig. 2b in this Letter), the \( G \) dependence on \( t'' \) is much less significant and the splitting of the ZBA does not occur.

What is the origin of these results? Below, it will be argued that a qualitative description of the results can be achieved by analyzing the two quantum dots through a so-called ‘circuit model’. This model starts with the conductance of each QD calculated separately, as independent elements of a circuit, and then the conductance of the ‘complete circuit’ is obtained by combining the conductances of the two elements connected in series. Fig. 3 describes schematically the steps involved in this approach. In Fig. 3a, the complete system formed by QD1 and QD2 (shown in Fig. 1b) is divided into two components. QD1 is modeled as a QD connected directly to left (L) and right (R) leads, while QD2 is modeled as a side-connected QD. Fig. 3b shows the respective conductances and occupancies for each independent element vs. gate voltage, and Fig. 3c represents the scattering processes (represented by transmission and reflection ampli-
of the same parameters as in Fig. 2. Although the quantities of QD1 will influence the charge occupancy of QD2, and being analyzed here, the variation of the gate potential will in turn this will influence the conductance through QD1.

FIG. 3: Schematic representation of the main ideas behind the “circuit model”. In (a), the system represented in Fig. 1b is divided into its constituent elements: QD1 is modeled as a QD connected in series with the leads and QD2 is modeled as a side-connected QD. The curves in (b) represent the conductance and occupancy of each separate circuit element vs. the applied gate potential. (c) Schematic representation of how the two individual elements are connected to form the final ‘circuit’: Incident and reflected wave amplitudes are represented in the right side of QD2 by black arrows. A transmitted wave through QD2 undergoes multiple reflections between the two quantum dots until it is finally transmitted past QD1. The superposition of all these processes results in the final conductance for the ‘circuit’.

The conductance and occupancy of each separate circuit element can be expressed as

\[ T = \frac{T_1 T_2}{1 - R_1 R_2} \]

where the transmittances \( T_1 \) and \( T_2 \) are proportional to the conductances for QD1 and QD2, as depicted in Fig. 3b, and \( R_{1(2)} = 1 - T_{1(2)} \) are the reflectances. To calculate \( T \), one needs to establish how \( T_2 \) depends on \( V_{g1} \). The natural way to do that is to use the dependence of \( \langle n_2 \rangle \) on \( V_{g1} \), as depicted in Fig. 2, and then use the relation between conductance and occupancy, as shown in the red curves in Fig. 3b. In other words, the functional relation can be expressed as \( T_2 = T_2(\langle n_2 \rangle(V_{g1})) \). It is not surprising that in a strongly correlated system like the one being analyzed here, the variation of the gate potential of QD1 will influence the charge occupancy of QD2, and in turn this will influence the conductance through QD1.

In Fig. 4, conductance results using Eq. (4) are shown for the same parameters as in Fig. 2. Although the quantitative agreement varies, there is good overall qualitative agreement. All the trends are correctly reproduced and some of the details are quite similar, such as for example the asymmetric shape of the curves at higher values of \( V_{g2} \) (−0.35 and −0.3) in Fig. 4a. It is important to notice that there are no adjustable parameters in the circuit model here presented. The only input necessary is \( \langle n_2 \rangle \) vs. \( V_{g1} \), which is obtained through a calculation for the complete system (values displayed for \( \langle n_2 \rangle \) in Fig. 2). The success of the circuit model implies that the dip in \( G \) arises from the Fano anti-resonance which cancels the conductance of QD2 (red solid curve in Fig. 3b). The Fano anti-resonance can be seen as a destructive interference process between two different trajectories an electron can take on its way to QD1: it can cross the CR without passing through QD2; or it can visit QD2, return to the CR and then proceed to QD1.

The similarities between the experimental results and our simulations suggest that our model and numerical technique have captured the essential physics of the experiments. However, these same experiments have also been explained using RKKY ideas. Can our numerical results be also understood in this alternative context? To try to answer this question, several calculations were performed with different parameter values and number of sites in the CR. In Fig. 5a, results for spin correlations between QD1 and QD2 (denoted \( S_1 \cdot S_2 \)) are presented for the same parameters used in Fig. 2c. At \( t'' = 0.0 \) (red curve) QD1 and QD2 are uncorrelated as expected. As \( t'' \) increases to 0.1 (green), and then 0.2 (blue), it is observed that in the region where \( G \) reaches its maximum value (see Fig. 2c), \( S_1 \cdot S_2 \) also assumes a maximum value and it is positive (ferromagnetic (FM)). For \( t'' > 0.2 \) (not shown), \( S_1 \cdot S_2 \) saturates and starts decreasing. The maximum of \( S_1 \cdot S_2 \), for all values of \( t'' \), decreases even further as the size of the central region increases (the results in Fig. 5a are for a CR with just one site). In addition, the sign of \( S_1 \cdot S_2 \) alternates as the size of the CR increases and the QDs move farther apart from each other. In Fig. 5b, results for the spin correlation between QD1 and its neighboring site in the CR (denoted \( S_1 \cdot S_3 \)) is shown for the same parameters as in Fig. 5a. \( S_1 \cdot S_3 \) is a rough measure of the Kondo correlation in QD1, having a direct connection with the ZBA in Fig. 2c. Indeed, for \( t'' = 0.0 \) (red) when \( G \) reaches the unitary limit, a robust antiferromagnetic (AF) corr-
relation develops between QD1 and its neighboring site in the CR. For $t'' = 0.1$ (green), despite the narrow dip in $G$, the side-peaks are still close to the unitary limit (see Fig. 2c) and $S_1 \cdot S_2$ is still strongly AF. However, for $t'' = 0.2$ (blue), both $G$ and $S_1 \cdot S_2$ are strongly suppressed, in qualitative agreement with a suppressed ZBA due to a weakened Kondo resonance.

The results thus far seem to indicate that the CR could be mediating a long range coupling between QD1 and QD2, with the characteristics of an RKKY interaction. However, the magnitude of the maximum value of $S_1 \cdot S_2$ (see scale in Figs. 5a-b) is too small to account for all the effects observed in the conductance in Fig. 2c. One possible way of increasing $S_1 \cdot S_2$ is by coupling QD1 more strongly to the CR than to the left lead. This was exactly the setup chosen in Ref. 3, where those authors performed the measurements with asymmetric couplings to the left ($\Gamma_L$) and right ($\Gamma_{CR}$) sides of QD1. In fact, the voltages applied to the gates in Fig. 1a were such that $\Gamma_{CR} \gg \Gamma_L$. In our model, this is equivalent to having an asymmetric $t^*$, with $t^*_{CR} \gg t^*_L$. An analysis of the results in this asymmetric regime indicates that the correlation between QD1 and QD2 does indeed increase. However, if one performs the calculations with the sites in the CR at a filling lower than one electron per site (half-filling), it is observed that $S_1 \cdot S_2$ is gradually suppressed as the electron filling falls to a more appropriate level to simulate the two-dimensional electron gas in the CR. Although one can argue that some of the dependence of the conductance of QD1 on the charge state of QD2 seen in Fig. 2 is associated to the correlations between the two dots, it is apparent that other effects are also present. This is dramatically exemplified by the fact that the cancellation of $G$ presented in Fig. 2c occurs for any finite value of $t''$, and of course for $t'' \approx 0$, one finds that $S_1 \cdot S_2 \approx 0$. The fact that the dip seen in the conductance in Fig. 2c is not dominantly caused by correlations between the dots can be made more clear by checking the results for the conductance as $U_1$ (Hubbard interaction in QD1) is reduced to zero. In Fig. 5c, results for $G$ are shown for 3 different values of $U_1$, for the same parameters as for the blue curve in Fig. 2c. As $U_1$ decreases from 0.4 (blue) to 0.2 (green), and then to 0.0 (red), the dip in the conductance remains, only becoming narrower, indicating that its origin is not associated with many-body interactions, but more likely with cancellations typical of $T$-geometries that occur even in the non-interacting limit.

In summary, the numerical results qualitatively reproduce the main aspects of important recent experiments involving nonlocal spin control in nanostructures. The main result is that the splitting observed in the ZBA is caused by a cancellation in the conductance due to destructive interference. This so-called Fano anti-resonance has its origin in one of the dots being side-connected to the current’s path. A simple ‘circuit model’ qualitatively reproduces the experiments and offers an alternative to a purely RKKY interpretation of the results, underscoring that a laboratory realization of the two-impurity Kondo system should avoid any geometry susceptible to a Fano anti-resonance.

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A full discussion of results will be presented in G. B. Martins et al., in preparation.