

# Transmission phase of quantum dots: Testing the role of population switching

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We propose a controlled experiment to clarify the role of “population switching,” i.e., filling of one level at the expense of another one, in causing phase lapses of the amplitude for electron transmission through nano-scale devices. Such lapses are generically observed in valleys between adjacent Coulomb-blockade peaks. The experiment involves two quantum dots embedded in the same arm of an Aharonov-Bohm interferometer. By varying independently their gate voltages, one can controllably induce population switchings in consecutive Coulomb-blockade valleys, and test whether the expected phase lapses follow.

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## I. INTRODUCTION

In experiments on the phase  $\phi$  of the transmission amplitude  $\mathcal{T}$  through a quantum dot (QD), the following striking pattern has been observed:<sup>1-3</sup> As a function of gate voltage  $V_g$ ,  $\phi$  increases (as expected) by  $\approx\pi$  over the width of a Coulomb-blockade peak for the conductance but then (unexpectedly) displays a sharp phase lapse (PL) of  $\approx-\pi$  in the adjacent Coulomb-blockade valley. The PL is found to occur in every conductance valley between two Coulomb-blockade peaks. No general consensus as to the mechanism underlying the PL has been reached yet in spite of determined theoretical efforts (see review 4). Here we propose a controlled experimental test to confirm or rule out one of the key mechanisms (“population switching”) considered in the literature. The present work consists of the first proposed setup in which one can tune the system in and out of the occurrence of a sequence of population switchings, and test whether this is accompanied by the appearance and disappearance of correlated PLs (the latter was not facilitated in the original setup of Refs. 1 and 2).

The need for some mechanism to induce PLs is seen as follows. We consider transmission through a QD that supports two orbital<sup>5</sup> levels  $i=1,2$ . The levels are coupled to single-channel leads ( $\alpha=R,L$  with  $R$  and  $L$  for right and left, respectively) by real<sup>7</sup> tunneling matrix elements  $t_{i,\alpha}$ . Depending on the value of  $s \equiv \prod_{i,\alpha} t_{i,\alpha}$ , we distinguish<sup>7</sup> two cases:  $s > 0$  and  $s < 0$ . PL is a manifestation of the vanishing of  $\mathcal{T}$ . We consider first the case of no electron-electron interaction at zero temperature. By the Friedel sum rule,<sup>8</sup> for symmetric dot-lead coupling, (i.e.,  $|t_{1L}|=|t_{1R}|, |t_{2L}|=|t_{2R}|$ ),  $\mathcal{T}$  is given by  $\exp[i\pi(n_1+n_2)]\sin[\pi(n_1 \pm n_2)]$ , where  $n_{1,2}$  are the populations of levels 1 and 2, respectively, and the sign is that of  $s$ . In the valley between two Coulomb-blockade peaks the lower (upper) level 1 (2) is almost full (empty), and for  $s > 0$   $\mathcal{T}$  vanishes there. For  $s < 0$  a PL occurs for  $n_1=n_2$  and that condition is not met in the valley. These statements, concerning both  $s > 0$  and  $s < 0$ , are expected, by continuity, to hold even in the presence of not too large deviations from left-right symmetry. In reality we expect the signs of the  $t_{i\alpha}$  to be random. Then, correlated sequences of PLs are not expected, cf. measurements on uncorrelated mesoscopic

QDs.<sup>2</sup> One faces a similar dilemma for interacting electrons since the Friedel sum rule is also valid<sup>9</sup> in that case. Thus explaining the occurrence of correlated sequences of PLs implies finding a mechanism by which a PL occurs for  $s < 0$ .

Population switching provides one such mechanism. It requires the populations  $n_1(V_g)$  and  $n_2(V_g)$  of the two levels to become equal,  $n_1(V_g^{(0)})=n_2(V_g^{(0)})$ , at some value  $V_g^{(0)}$  of  $V_g$  in the Coulomb-blockade valley and to switch [ $n_2(V_g) > n_1(V_g)$  for  $V_g > V_g^{(0)}$ ] as  $V_g$  is increased further.<sup>10</sup> The case  $s > 0$  is symmetric in  $n_1$  and  $n_2$ : PLs appear then irrespective of population switching, while for  $s < 0$  a population switching would produce a PL. Population switching has been considered in two somewhat different scenarios. The first, displayed and explained in Fig. 1, requires two sets of energy levels which respond differently to  $V_g$ , a set of “flat” and a set of “steep” levels with small and large slopes, respec-

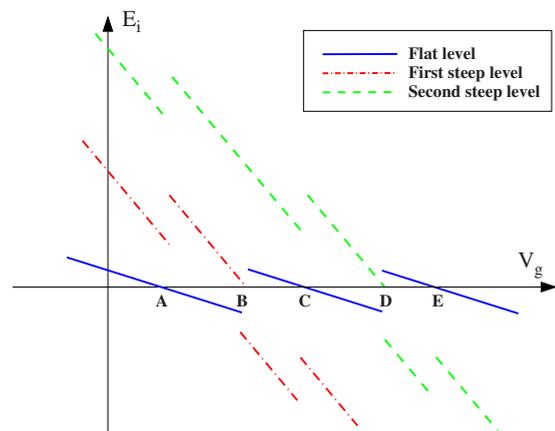


FIG. 1. (Color online) Scenario I (after Refs. 12 and 13): The renormalized (Hartree) energies of the “flat” and “steep” levels are schematically shown as functions of the applied gate voltage  $V_g$ . In our picture, population switching is discontinuous. As  $V_g$  increases, a flat level becomes populated at  $V_g=A$ . That increases the energy of the empty steep levels. At  $V_g=B$ , the lower steep level crosses the Fermi surface and becomes occupied, causing a depletion and a rise in energy of the flat level, and population switching. At  $V_g=C$ , the flat level is filled again, and the process repeats itself with the next steep level. We thus obtain a sequence of population switchings.

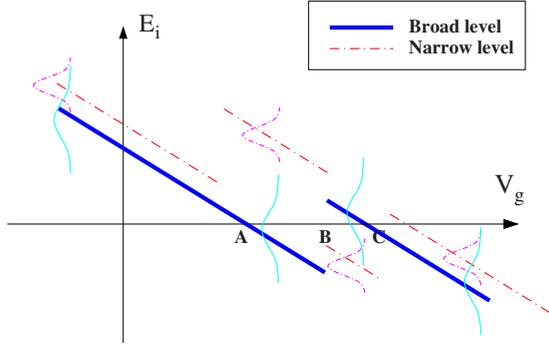


FIG. 2. (Color online) Scenario II (after Ref. 14): Renormalized level energies are schematically plotted as functions of the applied gate voltage  $V_g$ . Population switching are shown as discontinuous for simplicity. All levels have the same gate-voltage dependence; however, one of them is significantly broader and overlaps with one or more narrow levels. As the gate voltage is increased, the broad level is first (partially) filled (point A), pushing up the energy of the narrow one. At point B, however, it becomes favorable to populate the narrow level while depleting the broad one, which leads to population switching. As the gate voltage is further increased, the broad level begins to fill up again, and the process may repeat itself with another narrow level (not shown).

tively, the occupancy of which depends nonmonotonically on  $V_g$ .<sup>12,13</sup> In the second scenario (described in Fig. 2) a set of energy levels with identical slopes contains both broad and narrow levels.<sup>14</sup> In both scenarios, the interplay between tunneling and charging gives rise to population switching. These scenarios have been investigated within a mean-field approximation,<sup>11,15</sup> perturbative calculations,<sup>16</sup> the numerical renormalization-group approach for scenario II,<sup>17</sup> the density-matrix renormalization-group approach,<sup>18</sup> and the functional renormalization-group (FRG) approach.<sup>19</sup> Either scenario implies special requirements (e.g., commensurability of the spacings of the flat set and the steep set in scenario I or the presence of a generic ultrabroad level in scenario II).

In this paper we suggest a double-dot geometry to experimentally test the relation between PLs and population switchings in a controllable fashion. The configuration is detailed in Sec. II. We then describe our numerical method and present some typical results for the outcome of such an experiment in Sec. III. Our findings are summarized in Sec. IV.

## II. PROPOSED SETUP

Our proposed experimental setup is schematically shown in Fig. 3. By varying separately the gate voltages applied to each dot, and by adjusting the strengths of the dot-lead couplings, one can tune the levels in one dot independently of those in the other. This makes it possible to realize both the first and the second scenario mentioned above, as one can separately control both the gate-voltage coupling (scenario I) and the widths (scenario II) of the levels in the two QDs. Thus, the system can be tuned in and out of the conditions for observing a correlated sequence of PLs. In the sequel we focus attention on scenario I. The two sets of levels would be those in  $QD_1$  and in  $QD_2$ , respectively. With the help of our

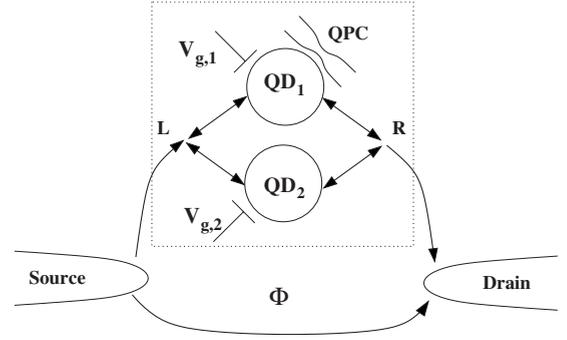


FIG. 3. Schematic view of the proposed setup. Two quantum dots ( $QD_1$  and  $QD_2$ ) are embedded into the same arm of an Aharonov-Bohm interferometer and are connected in parallel to a left ( $L$ ) and a right ( $R$ ) lead. Arrows denote possible tunneling processes. A quantum point contact (QPC) probes the changes in population of  $QD_1$ . Our analysis addresses the physical processes within the dotted box.

setup, it is possible to test experimentally the idea that PLs for  $s < 0$  come hand in hand with population switching.

To investigate the expected properties of our setup theoretically, we restrict ourselves to spin-polarized electrons and neglect both tunneling between the two dots, and the electron-electron interaction in the leads. The Hamiltonian consists of three parts,

$$\hat{H} = \hat{H}_D + \hat{H}_L + \hat{H}_T. \quad (1)$$

Here  $\hat{H}_D$  is the Hamiltonian for the dots,

$$\hat{H}_D = \sum_{i=1,2;j} \epsilon_{ij} \hat{a}_{ij}^\dagger \hat{a}_{ij} + \sum_{i=1,2} \frac{U_i}{2} \sum_{j \neq j'} \hat{n}_{ij} \hat{n}_{ij'} + U_{12} \sum_{j,j'} \hat{n}_{1j} \hat{n}_{2j'}, \quad (2)$$

$\hat{H}_L$  is the Hamiltonian for the leads,

$$\hat{H}_L = \sum_{\ell=L,R;k} \epsilon_{\ell,k} \hat{c}_{\ell,k}^\dagger \hat{c}_{\ell,k}, \quad (3)$$

and the dot-lead coupling is given by

$$\hat{H}_T = \sum_{\substack{i=1,2;j \\ \ell=L,R;k}} (t_{\ell,k}^{ij} \hat{a}_{ij}^\dagger \hat{c}_{\ell,k} + \text{H.c.}), \quad (4)$$

while  $\hat{a}_{ij}$  ( $\hat{c}_{\ell,k}$ ) are the Fermi operators of the  $j$ th level of the  $i$ th dot ( $k$ th mode of the  $\ell$ th lead, respectively),  $\hat{n}_{ij}$  are the number operators, and  $\epsilon_{ij} = \epsilon_{ij}^{(0)} - eV_{g,i}$  are the single-particle energies modified by the gate voltage. The intradot and interdot charging energies are denoted by  $U_i$  and  $U_{12}$ , respectively. We assume a constant density of states in the leads with a band width that exceeds all other energy scales. The real tunneling matrix elements  $t_{\ell,k}^{ij}$  are taken to be independent of  $k$ .

For scenario I it would be best to make  $QD_1$  so small that only one of its levels plays an active role and functions as the flat level in Fig. 1. The levels in  $QD_2$  are steep and must be well separated to avoid population switching among them.<sup>11,14,19,21</sup> The gate voltages on both QDs should be var-

ied simultaneously but not at the same pace so as to induce level crossings. For the gate voltages we write  $V_{g,1} = \alpha V_{g,2} + V_0$ , where  $0 \leq \alpha \leq 1$ .  $V_0$  is chosen so that the flat level gets filled before it encounters the first steep level. To estimate  $\alpha$  we observe that the change in  $V_{g,2}$  between adjacent crossings of two steep levels with the Fermi surface is roughly given by  $U_2 + \Delta_2$ ,  $\Delta_2$  being the mean level spacing in QD<sub>2</sub>. As  $V_{g,2}$  is changed, the flat level must not sink too deeply below the Fermi surface so that it can eventually get depleted due to the interdot interaction of strength  $U_{12}$ . That implies that as  $V_{g,2}$  changes by  $U_2 + \Delta_2$ ,  $V_{g,1}$  should change roughly by  $U_{12}$  so that  $\alpha \approx U_{12}/(U_2 + \Delta_2)$ . Too large a value of  $\alpha$  will take the flat level too far down to be depopulated while for too small a value it will not repopulate. In both these cases, PLs should occur at random, and the absence of a correlated sequence of PLs should be akin to the mesoscopic fluctuations of PLs observed in Ref. 2, while for intermediate values of  $\alpha$  we expect to see a sequence of consecutive PLs. Tuning of  $\alpha$  to a range which implies population switching (and consequently the occurrence of PLs) should be experimentally possible with the aid of the QPC (Fig. 3) (the latter is employed to detect the occurrence of population switching).

### III. TYPICAL RESULTS

Let us now turn to present the results expected from such an experiment. In the calculations we use the FRG which has recently been applied to similar systems.<sup>19,20</sup> Earlier calculations using that method have resulted in accuracy comparable to NRG, at least for zero temperature and when not more than two levels are close to each other.<sup>19</sup> These conditions are met in our case. FRG is based on a functional-integral formulation with an infrared cutoff. The cutoff dependence of the vertex functions is given in terms of an exact hierarchy of coupled nonlinear differential RG equations. For very large values of the cutoff all the modes of the system are excluded, and the vertex functions are given by the bare parameters of the Hamiltonian. In principle, the exact vertex functions could be found by integrating the FRG equations from that point to the limit where the cutoff tends to zero (in which case all the modes of the system are included). However, to make the computation feasible, some truncation scheme must be applied. Usually one neglects all vertices not present within the bare Hamiltonian, i.e., three-particle or higher vertex functions, as well as the energy dependence of the one- and two-particle vertex functions.<sup>19,20</sup> The resulting set of equations can then be solved numerically. From the (approximate) single-particle vertex functions the dots' single-particle Green's functions, the level occupations, the linear conductance, and the transmission phase are readily derived.

In Fig. 4 we give the results of a calculation on a typical set of parameters. In accordance with the discussion in Sec. II, we observe that a PL is obtained in every Coulomb-blockade valley only in the central panel where scenario I fully applies. Details of the population switching that occurs in the central panel near  $V_{g,2}/U_2 = 2.83$  in a conductance valley with  $s < 0$  are shown in Fig. 5. We observe that the popu-

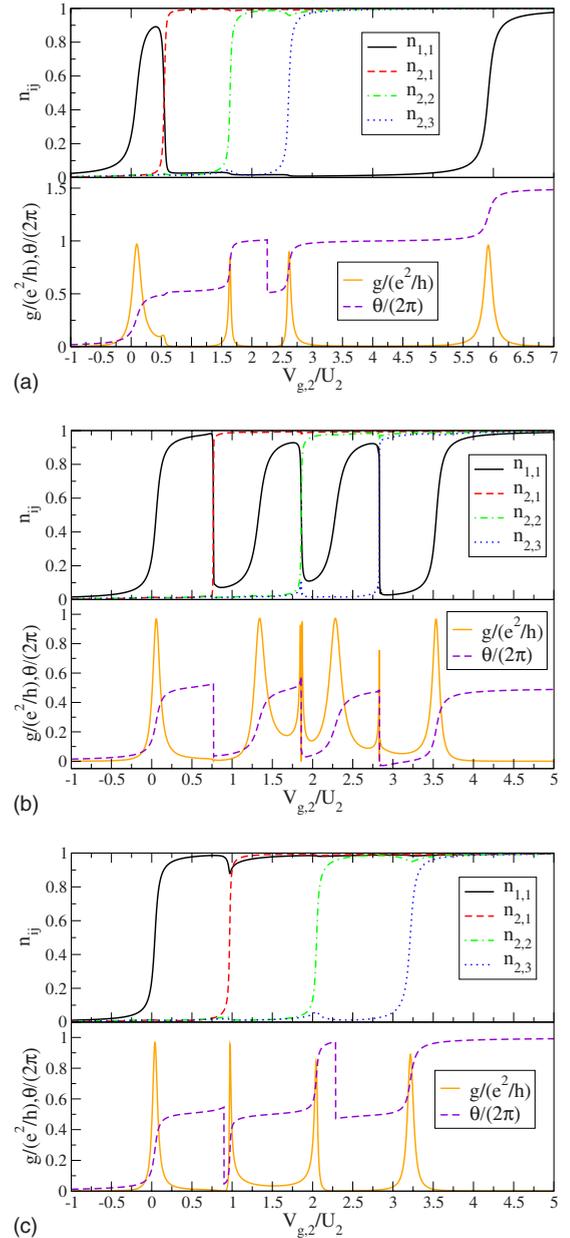


FIG. 4. (Color online) The upper part of each panel shows the population of the flat level ( $n_{1,1}$ ) and of three steep ones ( $n_{2,1}$ ,  $n_{2,2}$ , and  $n_{2,3}$ ); the lower part shows the dimensionless conductance and the transmission phase divided by  $2\pi$ , all versus the gate voltage  $V_{g,2}$  on QD<sub>2</sub>. The level energies (in units of  $U_2$ ) are 0, 0.3, 0.52, and 0.7, respectively, while their widths due to the coupling to the left (right) lead are 0.02 (0.03), 0.018 (0.01), 0.035 (0.016), 0.039 (0.021). All the tunneling matrix elements are positive, except  $t_{R,2}^{2,2}$  and  $t_{R,3}^{2,3}$ .  $U_{12} = 0.6U_2$ . The upper, central, and lower panel correspond to  $\alpha = 0.3, 0.5 [=U_{12}/(U_2 + \Delta_2)]$ , and 0.7, respectively.

lation switching is continuous, albeit very steep. The scale of the switching is given by an exponentially small<sup>20</sup> orbital Kondo temperature<sup>21</sup>

$$\Delta V_{g,2} \sim T_K = \frac{\sqrt{U_{12}(\Gamma_1 + \Gamma_2)}}{\pi} \exp\left[\frac{\pi E_0(U_{12} + \epsilon_0)}{2U_{12}(\Gamma_1 - \Gamma_2)} \ln\left(\frac{\Gamma_1}{\Gamma_2}\right)\right]$$

(this expression acquires a more complicated form when right-left symmetry is not maintained). Here  $\Gamma_{1,2}$  are the

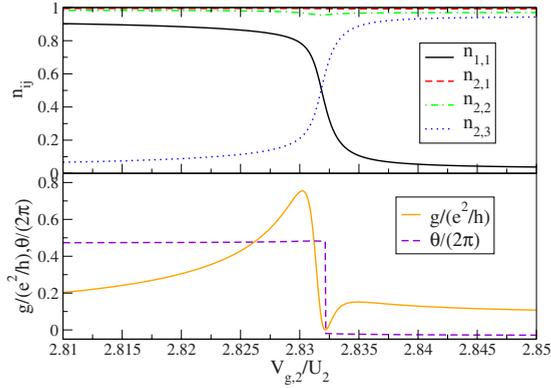


FIG. 5. (Color online) Details of one of the peaks due to population switching ( $s < 0$ ) in the central panel of Fig. 4.

widths of the two levels that switch population, and  $E_0$  is the average of their positions at the point of population switching. As expected, a PL occurs in the vicinity of the point of level crossing. It is accompanied by two very narrow conductance peaks. The appearance of these sharp “correlation-induced resonances”<sup>20</sup> is easily explained in the case of left-right symmetry. Then, according to the Friedel sum rule, the conductance is given by  $g = (e^2/h) \sin^2[\pi(n_1 - n_2)]$  for  $s < 0$ , and is maximal when  $|n_1 - n_2| = 1/2$ . Since at the population crossing point  $n_1 = n_2$  while far from it either  $n_1 = 1$  and  $n_2 = 0$  or  $n_1 = 0$  and  $n_2 = 1$ , conductance peaks should occur on both sides of the population crossing point. By continuity, the argument probably applies at least qualitatively also for nonsymmetric cases if the asymmetry is not too large, as our numerical data indicates, although we have no analytic deri-

vation in this case. The width of the peaks is again given by the orbital Kondo temperature. We expect the peaks to disappear for temperatures higher than that scale.<sup>19</sup> Similar sharp peaks are seen at the PL near  $V_{g,2}/U_2 = 1.86$  in the central panel of Fig. 4 but not at the PL near  $V_{g,2}/U_2 = 0.77$  because there we have  $s > 0$ .

#### IV. CONCLUSIONS

In summary, we propose an experiment to test the role played by population switching for phase lapses (PLs) of the transmission amplitude through a nanoscale device. In a system of two coupled quantum dots with gate voltages  $V_{g,1}$  and  $V_{g,2}$ , we expect sequences of PLs to occur in consecutive conductance valleys only for intermediate values of  $\alpha = (V_{g,1} - V_0)/V_{g,2}$ . The associated population switching can be measured by coupling QD<sub>1</sub> to a quantum point contact. Further structures due to correlation-induced resonances should emerge below the Kondo temperature and provide an even more detailed test of population switching. While the present analysis has been focused on scenario I, very similar phenomena are expected for scenario II.

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