Transmission phase of a quantum dot: Testing the role of population switching

Moshe Goldstein,1 Richard Berkovits,1 Yuval Gefen,2 and Hans A. Weidenmüller3

1The Minerva Center, Department of Physics, Bar-Ilan University, Ramat-Gan 52900, Israel
2Department of Condensed Matter Physics, The Weizmann Institute of Science, Rehovot 76100, Israel
3Max–Planck–Institut für Kernphysik, D-69120 Heidelberg, Germany

We propose a controlled experiment to clarify the physical mechanism causing phase lapses of the transmission amplitude for electron transmission through nanoscale 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. It offers a decisive test of “population switching”, one of the leading contenders for an explanation of the phenomenon.

PACS numbers: 73.23.-b, 73.63.Kv, 73.23.Hk

In experiments on the phase $\phi$ of the transmission amplitude $T$ through a quantum dot (QD), the following striking pattern has been observed [1, 2, 3]: 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 the reviews [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 need for some mechanism to induce PLs is seen as follows. We consider transmission through a QD that supports two orbital levels $i = 1, 2$. These levels are coupled to single–channel leads ($\alpha = R, L$ with $R, L$ for right, left, respectively) by real tunneling matrix elements $t_{i,\alpha}$. Depending on the value of $s = \prod_{i,\alpha} t_{i,\alpha}$, we distinguish two cases: $s > 0$ and $s < 0$. PL is a manifestation of the vanishing of $T$. We consider first the case of no electron–electron interaction at zero temperature. By the Friedel sum rule, $\mathcal{T}$ 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. 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 [2]. One faces a similar dilemma for interacting electrons since the Friedel sum rule is also valid 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 [11]. 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 (large) slopes, respectively, the occupancy of which depends non–monotonically on $V_g$ [13, 14]. In the second scenario (not displayed) a set of energy levels with identical slopes contains both broad and narrow levels [15]. In both scenarios, the interplay between tunneling and charging gives rise to population switching. These scenarios have been investigated within a mean–field approximation, perturbative calculations, the numerical renormalization–group approach for scenario I and the density–matrix renormalization–group approach and the functional renormalization–group (FRG) approach. 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 ultra–broad level in scenario II). In the sequel we focus attention on the more easily realizable scenario I.

Our proposed experimental setup to test the idea of population switching is schematically shown in Fig. 2. 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, and to tune in and out of the conditions for observing a correlated sequence of PLs. For scenario I, the two sets of levels are those in QD1 and in QD2, respectively. With the help of our 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.
the changes in population of QD tunneling processes. A quantum point contact (QPC) probes to a left (L) and a right (R) lead. Arrows denote possible Aharonov–Bohm interferometer and are connected in parallel dots (QD)

\[ \text{FIG. 2: Schematic view of the proposed setup. Two quantum dots (QD}_1 \text{ and QD}_2 \text{ are embedded into the same arm of an Aharonov–Bohm interferometer and are connected in parallel to a left (L) and a right (R) lead. Arrows denote possible tunneling processes. A quantum point contact (QPC) probes the changes in population of QD}_1. \text{ Our analysis addresses the physical processes within the dotted box.} \]

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,

\[ \hat{H} = \hat{H}_D + \hat{H}_L + \hat{H}_T. \]  

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

\[ \hat{H}_D = \sum_{i=1,2; j} \epsilon_{ij} \hat{a}^\dagger_{ij} \hat{a}_{ij} + \sum_{i=1,2} U_i \sum_{j \neq j'} \hat{n}_{ij} \hat{n}_{ij'} + U_{12} \sum_{j \neq j'} \hat{n}_{1j} \hat{n}_{2j'}, \]  

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

\[ \hat{H}_L = \sum_{\ell=L,R; k} \epsilon_{\ell,k} \hat{c}^\dagger_{\ell,k} \hat{c}_{\ell,k}, \]  

and the dot–lead coupling is given by

\[ \hat{H}_T = \sum_{i=1,2; j; \ell=L,R; k} t_{ij}^{\ell} \hat{a}^\dagger_{i,j} \hat{c}_{\ell,k} + \text{H.c.} \]  

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.

In the calculations we use the FRG which has recently been applied to similar systems \[20, 21\]. 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 \[20\]. These conditions are met in our case. FRG is based on a functional integral formulation with an infra–red 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 \[20, 21\]. The resulting set of equations can then be solved numerically. From the (approximate) single–particle vertex functions the dots’ single–particle Green functions, the level occupations, the linear conductance, and the transmission phase are readily derived.
For scenario I we assume in the calculation that QD$_1$ is so small that only one of its levels plays an active role and functions as the flat level in Fig. I. The levels in QD$_2$ are steep and must be well separated to avoid population switching amongst them, see Refs. [12,13,24,22]. We vary the gate voltages on both QDs 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 of $V_{g,2}$ 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$_2$. 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 inter–dot 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. 2 (The latter is employed to detect the occurrence of population switching).

This picture is supported by typical results of our calculations shown in Fig. 3. We observe that we obtain a PL 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. 4. We observe that the population switching is continuous, albeit very steep. According to Refs. [22], the scale of the switching is given by an exponentially small orbital Kondo temperature $\Delta V_{g,2} \sim T_K = \sqrt{U_{12}(1+\gamma_2)} / \pi \exp \left[ \frac{\pi E_0(U_{12}+\gamma_2)}{2U_{12}(1+\gamma_2)} \ln(T_2) \right]$ [8]. Here $\gamma_1,2$ are the 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” [21] is easily explained in the case of left–right symmetry and probably applies at least qualitatively also for non–symmetric cases. 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 cross-
ing point. 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. Similar sharp peaks are seen at the PL near $V_{g,2}/U_2 = 1.86$ in the central panel of Fig. 3 but not at the PL near $V_{g,2}/U_2 = 0.77$, because there we have $s > 0$.

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$_1$ 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.

We thank D.I. Golosov, Y. Oreg and J. von Delft for useful discussions. M.G. is supported by the Adams Foundation Program of the Israel Academy of Sciences and Humanities. Financial support from the Israel Science Foundation (Grants 569/07, 715/08), Schwerpunkt Spintronics SPP 1285, the German-Israeli Foundation (GIF) and the Minerva Foundation is gratefully acknowledged.

[1] R. Schuster, E. Buks, M. Heiblum, D. Mahalu, V. Umansky, and H. Shtrikman, Nature 385, 417 (1997).

[2] M. Avinun-Kalish, M. Heiblum, O. Zarchin, D. Mahalu, and V. Umansky, Nature 436, 529 (2005).

[3] K. Kobayashi, H. Aikawa, S. Katsumoto, and Y. Iye, Phys. Rev. Lett. 88 256806 (2002); Phys. Rev. B 68 235304 (2003).

[4] G. Hackenbroich, Phys. Rep. 343, 463 (2001); A. Aharony and S. Katsymoto (eds.) Focus on Interference in Mesoscopic Systems, New J. Phys. 9 111-125 (2007).

[5] Y. Gefen, in Strongly Correlated Fermions and Bosons in Low-Dimensional Disordered Systems eds. I.V. Lerner, B.L. Altshuler, V.I. Fal'ko, and T. Giamarchi (Kluwer, Dordrecht, 2002); and references therein.

[6] In the present discussion we neglect the spin degrees of freedom. We do not expect that these will modify our analysis in any qualitative way.

[7] D.R. Stewart, D. Sprinzak, C.M. Marcus, C.I. Duruöz, and J.S. Harris Jr., Science 278, 1784 (1997).

[8] A. Silva, Y. Oreg, and Y. Gefen, Phys. Rev. B 66, 195316 (2002).

[9] Here we assume symmetric dot-lead coupling, $|t_{1L}| = |t_{1R}|, |t_{2L}| = |t_{2R}|$. We expect similar results in the case of left-right asymmetry.

[10] S. Datta and W. Tian, Phys. Rev. B 55, R1914 (1997).

[11] D. Langreth, Phys. Rev. 150, 516 (1966).

[12] Population switching is central to the two mechanisms described in Ref. [12].

[13] D.I. Golosov and Y. Gefen, Phys. Rev. B 74, 205316 (2006); New J. Phys. 9, 120 (2007).

[14] G. Hackenbroich, W. D. Heiss, and H.A. Weidenmüller, Phys. Rev. Lett. 79, 127 (1997).

[15] R. Baltin, Y. Gefen, G. Hackenbroich, and H.A. Weidenmueller, Eur. Phys. J. B 10, 119 (1999).

[16] P.G. Silvestrov and Y. Imry, Phys. Rev. Lett. 85, 2565 (2000).

[17] M. Goldstein and R. Berkovits, New J. Phys. 9, 118 (2007).

[18] J. König and Y. Gefen Phys. Rev. B 71, 201308(R) (2005); B. Kubala, Y. Gefen, J. König, and J. von Delft, unpublished.

[19] M. Sindel, A. Silva, Y. Oreg, and J. von Delft, Phys. Rev. B 72, 125316 (2005).

[20] R. Berkovits, F. von Oppen, and Y. Gefen, Phys. Rev. Lett. 94, 076802 (2005).

[21] C. Karrasch, T. Hecht, A. Weichselbaum, Y. Oreg, J. von Delft, and V. Meden, Phys. Rev. Lett. 98, 186802 (2007); C. Karrasch, T. Hecht, A. Weichselbaum, J. von Delft, Y. Oreg, and V. Meden, New J. Phys. 9, 123 (2007).

[22] V. Meden and F. Marquardt, Phys. Rev. Lett. 96, 146801 (2006); C. Karrasch, T. Enss, and V. Meden, Phys. Rev. B 73, 235337 (2006).

[23] P.G. Silvestrov and Y. Imry, Phys. Rev. B 75, 115335 (2007); V. Kashcheyevs, A. Schiller, A. Aharony, and O. Entin-Wohlman, Phys. Rev. B 75, 115313 (2007); H.W. Lee and S. Kim, Phys. Rev. Lett. 98, 186805 (2007).