Spin effects and transport in quantum dots with overlapping resonances

P. G. Silvestrov[1,2,3] and Y. Imry[2]

[1]*Budker Institute of Nuclear Physics, 630090 Novosibirsk, Russia*
[2]*Weizmann Institute of Science, Rehovot 76100, Israel*
[3]*Instituut-Lorentz, Universiteit Leiden, P.O. Box 9506, 2300 RA Leiden, The Netherlands*

The role of spin is investigated in the transport through a quantum dot with two overlapping resonances [one having a width larger than the level separation and the other very narrow, cf. Silvestrov and Imry, Phys. Rev. Lett. **85**, 2565 (2000)]. For a series of consecutive charging resonances, one electron from the leads populates one and the same broad level in the dot. Moreover, there is the tendency to occupy the same level also by the second electron within the same resonance. This second electron is taken from the narrow levels in the dot. The narrow levels are populated (and broad level is depopulated) via sharp rearrangements of the electronic configuration in the Coulomb blockade valleys. Possible experimental manifestations of this scenario are considered. Among these there are sharp features in the valleys and in the mixed-valence regime and an unusual Kondo effect.

I. INTRODUCTION

In this paper, we consider the transmission through a multilevel quantum dot[1] having only one broad level well coupled to the leads. Such a model has been suggested in Ref. 2 in order to provide an explanation for the behavior of the transmission phase through a quantum dot observed in the experiment (Ref. 3). Within that model, electrons are transferred from the leads to the broad level in the quantum dot within the charging peaks, and are then transferred to and "stored" in the narrow levels via sharp transitions in between peaks. Thus, the charging (or conductance) peaks are very similar to each other, in the behaviors of both the conductance and the transmission phase. In the present paper, we treat the effects associated with the spin degeneracy of the levels for such quantum dots (QD's).

Many of the sharp rearrangements of the electronic configuration in the QD, which we will consider, take place due to spin or are sufficiently modified compared to the spinless case to make the discussion of spin rather interesting. The strong coupling of one level to the leads, leads now to the tendency to have this "valence" level either doubly occupied or completely empty. However, the total number of electrons in the dot may change only by one at any charging resonance. In particular, the resolution of this formal contradiction leads to prediction of singular behavior of the conductance just at the top of charging resonance.

The peculiar temperature (bias) dependence of the Kondo effect,[4–6] which takes place in the transport through the quantum dot with nonzero spin, may facilitate the experimental verification of our predictions. Moreover, in the experiments (see, e.g., Refs. 7–9) designed to observe the Kondo effect, in order to measure the conductance in the Coulomb blockade valley the dot is strongly coupled to the leads. Thus, it may naturally happen that the widths of some accidentally close levels will exceed the interlevel energy difference. However, the new effects that we consider in this paper either take place in the mixed-valence regime, or

should be seen already at the temperature sufficiently higher than the Kondo temperature.

In general, we consider the situation when the transport through the quantum dot has well-defined resonance structure with pronounced peaks and Coulomb blockade valleys. However, the coupling to the leads of the single broad level is already strong enough to change the usual formation of the many-electron ground state of the dot via the consecutive occupation of single particle levels. The energetics of such a system is described in the following section. In Sec. III, we consider the conductance of such a quantum dot in the limit of vanishing width of all narrow "spectator" levels. In Sec. IV, we investigate the smearing of the sharp features of the conductance predicted in Sec. III due to the finite temperature or width of narrow level. Following the experimental tendency for miniaturization of the QD's, we mainly consider only a two-level dot (with one narrow level and one having the width exceeding the interlevel energy spacing). However, in Sec. V, we consider the effect of spin for the transport in the quantum dot having many narrow and one broad level with $\Gamma \gg \Delta$ (with Γ being the width of the broad level and Δ the interlevel spacing). Discussion and conclusions are given in Sec. VI.

II. THE GROUND STATE ENERGY

To model the quantum dot, we use the tunneling Hamiltonian in the constant interaction (U) approximation

$$H = \sum_i \varepsilon_i a_i^+ a_i + U \sum_{i<j} a_i^+ a_i a_j^+ a_j + \sum_k \varepsilon^L(k) b_k^{L+} b_k^L$$

$$+ \sum_{k,j} [t_j^L a_j^+ b_k^L + \text{H.c.}] + L \leftrightarrow R. \quad (1)$$

Here, a and $b^{L(R)}$ are the annihilation operators for the electrons in the dot and in the left(right) lead, respectively. We will use $\varepsilon(k) = k^2/2m - E_F$ and will not introduce any k dependence of the tunneling matrix elements t_j. All summa-

tions in Eq. (1) include also the summation over spin. Only one level ε_1 is well coupled to the leads, having the width

$$\Gamma \equiv \Gamma_1 = 2\pi \sum_{i=L,R} |t_1^i|^2 dn^i/d\varepsilon > \Delta. \qquad (2)$$

We take $\Gamma \ll U$. Since we have in mind the experiments with really very small quantum dots, let us consider only two levels in the dot (e.g., having accidentally close energies). The generalization to many narrow levels will be considered in Sec. V. We assume that coupling between the dot and the gate electrode is pure capacitive. Then, the levels flow uniformly with the gate voltage $d\varepsilon_i/dV = \text{const}$ and without a loss of generality we may put

$$\varepsilon_1 = -V, \quad \varepsilon_2 = -V + \Delta. \qquad (3)$$

There are four charging resonances of the conductance $G(V)$ at $V \approx 0$, U, $2U$, and $3U$ (see for the review on the Coulomb blockade in quantum dots, e.g., Ref. 10).

Our first aim will be to find the ground state of the system (1) at different values of V. In the limit $\Gamma_2 \to 0$, the number of electrons on level 2 is a good quantum number. Let us denote by $E^{(0)}$, $E^{(1)}$, and $E^{(2)}$ the total energy of the lowest state of the quantum dot interacting with the leads, with the narrow level populated by, respectively, 0, 1, and 2 electrons [more precisely, $E^{(i)}$ is defined as the eigenenergy of the Hamiltonian (1) minus the trivial energy of the electrons in the leads $\Sigma \varepsilon(k)$]. The functions $E^{(i)}(V)$ evolve smoothly with the gate voltage and the (averaged) occupation number of the broad level 1 also changes continuously. For example, the branch $E^{(0)}$ corresponds to an empty level 1 at $V<0$, singly occupied at $0<V<U$ and doubly occupied at $U<V$. For $t_2^{L,R} = 0$ the functions $E^{(i)}$ may cross at some values of V, which, in particular, may lead to a sharp change of ground state.

With the use of perturbation theory in $t_1^{L,R}$, it is easy to find $E^{(i)}$ far from the charging peaks. Below the first resonance (at $V \ll -\Gamma$) the true ground state is evidently $E^{(0)}$. However, already here the virtual jumps of the electrons from the wire to level 1 give rise to the correction

$$E^{(0)} = 2\sum_{k<k_F} \frac{|t^{L,R}|^2}{\varepsilon(k) - \varepsilon_1} = \frac{-\Gamma}{\pi} \ln\left(\frac{4E_F}{\varepsilon_1}\right), \qquad (4)$$

$$E^{(1)} \approx \varepsilon_2, \quad E^{(2)} \approx 2\varepsilon_2 + U.$$

The overall factor 2 in $E^{(0)}$ accounts for the spin. It is clear that $E^{(0)}$ in this region lies significantly below $E^{(1)}$ and $E^{(2)}$ ($E^{(0)}$ is the true ground state). The factor of 4 in the argument of the logarithm, is specific to the dispersion of the conduction electrons we took. It does not appear in the physical results.

When the (increasing) voltage crosses the region $|V| \sim \Gamma$, the dot is charged by the first electron. However, this electron may stay in the dot on the level 1 (described by $E^{(0)}$) or on the level 2 ($E^{(1)}$). Depending on what level is occupied, the perturbation theory gives in this range of V
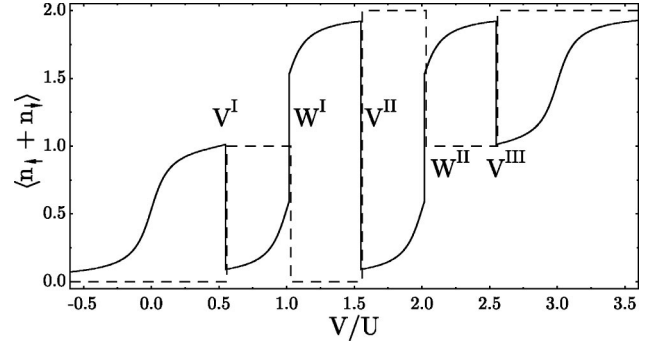

FIG. 1. Schematic drawing of the averaged occupation number $\langle n_\uparrow + n_\downarrow \rangle$ for the broad level 1 (solid) and narrow level 2 (dashed). The gate voltage V is measured in units of the charging energy U. The charging resonances are at $V/U \approx 0,1,2,3$.

$$E^{(0)} = \varepsilon_1 - \frac{\Gamma}{2\pi} \left\{ \ln\left(\frac{4E_F}{|\varepsilon_1|}\right) + \ln\left(\frac{4E_F}{\varepsilon_1 + U}\right) \right\}, \qquad (5)$$

$$E^{(1)} = \varepsilon_2 - \frac{\Gamma}{\pi} \ln\left(\frac{4E_F}{\varepsilon_1 + U}\right), \quad E^{(2)} \approx 2\varepsilon_2 + U.$$

The first logarithm in $E^{(0)}$ accounts for the virtual jumps of an electron from the level 1 in the dot to the wire. The other logarithms correspond to virtually adding the second electron to the dot (having $\varepsilon_1 + U$ instead of ε_1 in the denominator). The two levels $E^{(0)}$ and $E^{(1)}$ cross at a gate voltage given by[2]

$$V = V^I = \frac{U}{\exp\{-2\pi\Delta/\Gamma\} + 1}. \qquad (6)$$

This result is valid for both signs of Δ. For $\Gamma \gg |\Delta|$, Eq. (6) reduces to $\varepsilon_1 \approx -U/2$. At $V = V^I$ the electron in the dot jumps from the broad level to the narrow one.[2] We will describe the consequences of such a "jump" for the transmission below.

In the second valley, $U < V < 2U$ the dot is charged already by two electrons, which may populate the two doubly degenerate levels in the dot in different ways. Thus,

$$E^{(0)} = 2\varepsilon_1 + U - \frac{\Gamma}{\pi} \ln\left(\frac{4E_F}{|\varepsilon_1 + U|}\right), \qquad (7)$$

$$E^{(1)} = \varepsilon_1 + \varepsilon_2 + U - \frac{\Gamma}{2\pi} \left\{ \ln\left(\frac{4E_F}{|\varepsilon_1 + U|}\right) + \ln\left(\frac{4E_F}{\varepsilon_1 + 2U}\right) \right\},$$

$$E^{(2)} = 2\varepsilon_2 + U - \frac{\Gamma}{\pi} \ln\left(\frac{4E_F}{\varepsilon_1 + 2U}\right).$$

First of all, we see that just after the charging peak, at $V > U$ the true ground state is $E^{(0)}$. This is in contrast with the situation at $V<U$, where the ground state was $E^{(1)}$ (5). Thus, we may conclude, that within the resonance not only is one electron gradually transmitted from the wire to the level 1 in the dot, but also a second electron is taken from the narrow level 2 to the broad one 1 (see Fig. 1). In the limit $\Gamma_2 \to 0$ this second "transfer" is abrupt and takes place at some $V = W^I \approx U$ (we remind the reader that we consider only the ground-

state energy in this section and, therefore, $T \equiv 0$). This prediction of the possibility to have sharp features within the charging resonance is probably the main result of this paper.

All three energies (7) cross at the same value of gate voltage [c.f., (6)]

$$V^{II} = U + \frac{U}{\exp\{-2\pi\Delta/\Gamma\}+1} \qquad (8)$$

and the true ground state becomes $E^{(2)}$. Now already two electrons jump together from the broad level to the narrow one.

At $V > V^{II}$ (8) the occupation of the quantum dot proceeds in a fashion that is almost symmetric under particle-hole replacement. At the third peak the third electron is added to the dot. Were the branch $E^{(2)}$ the stable one, this would have been the uncoupled electron at the level 1. However, $E^{(2)}$ and $E^{(1)}$ cross at the top of the third peak (at $V = W^{II} = W^{I} + U$) and the ground state for the first half of last valley has a single unpaired electron at the narrow level. Finally, at

$$V^{III} = 2U + \frac{U}{\exp\{-2\pi\Delta/\Gamma\}+1} \qquad (9)$$

$E^{(2)}$ and $E^{(1)}$ cross and the broad level became singly occupied again. The fourth peak ($V \approx 3U$) completes the charging of two levels in the quantum dot by four electrons.

To summarize the discussion of this section, we show schematically in Fig. 1 the averaged occupation numbers of our two levels $\langle n_{1\uparrow} + n_{1\downarrow} \rangle$ and $\langle n_{2\uparrow} + n_{2\downarrow} \rangle$. The four charging resonances correspond to $V/U \approx 0$, 1, 2, and 3. One may see on the figure many abrupt changes in the population of both broad and narrow levels. Unfortunately, the averaged occupation number of the given level is not measured directly in the typical experiments, with the quantum dots. In order to make the connection with possible experiments, we consider in the following sections the transport properties of the quantum dot described by the Hamiltonian Eq. (1).

III. CONDUCTANCE, LEADING ORDER

The zero-bias conductance G of our two-level quantum dot is shown schematically in Fig. 2. In the limit of "invisible" level 2 ($\Gamma_2 \to 0$), we may introduce three conductances $G^{(0,1,2)}$ corresponding to empty, singly and doubly occupied narrow level (corresponding to the three "ground-state" energies $E^{(0,1,2)}$ of the previous section). The role of electrons at the level 2 reduces in this case to simply raising the current-transmitting level 1 via the Coulomb repulsion. Thus,

$$G^{(0)}(V) = G^{(1)}(V+U) = G^{(2)}(V+2U). \qquad (10)$$

We have shown schematically the function $G^{(0)}$ on the same Fig. 2 (slightly offset vertically). In the limit $\Gamma_2 \ll \Gamma_1$ the curve for two-level dot is obtained simply by cutting and horizontally shifting the parts of the curve for single-level dot, in agreement with Eq. (10), as shown in the figure. Thus, the relations Eq. (10) allow one to describe the singular behavior of the conductance even without the explicit calculation of $G^{(0)}$. This result is particularly useful at low tempera-
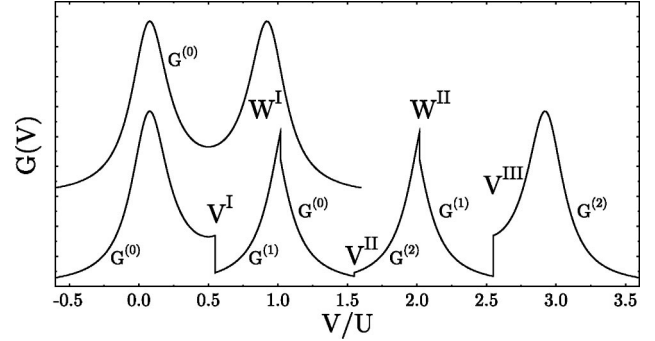

FIG. 2. The gate-voltage dependence (schematic) of the conductance G. The upper curve shows $G^{(0)}$ in the case of only one (broad) level in the quantum dot (vertically offset for clarity). The lower curve depicts the conductance given by different $G^{(n)}$ in various regimes. Sharp features at two peaks and three valleys are seen.

tures close to the charging resonances and in the Kondo valleys, where simple analytical formulas are not available.

Simple analytical expressions for the conductance may be found by means of perturbation theory only far from the resonances. In particular, below the first resonance ($V<0$) and above the second ($V>U$) one has for $G^{(0)}$

$$G^{(0)} = 2G_Q \frac{\Gamma_L \Gamma_R}{\varepsilon^2} \quad \text{and} \quad G^{(0)} = 2G_Q \frac{\Gamma_L \Gamma_R}{(\varepsilon+U)^2}. \qquad (11)$$

Here, $G_Q = e^2/h$. Because of Eq. (11) being valid only far from the resonance, there is no need to distinguish between ε_1 and ε_2. The first formula here accounts for the virtual jump of the electron (with any spin orientation) from the left lead first to the dot and then to the right lead. For $V>U$, first one of the two electrons jumps from the dot to the right lead, then another electron from the left lead fills in its place in the quantum dot.

In the valley $0<V<U$ one electron stays at the level 1 in the dot. Let it have, e.g., a spin up $\uparrow$. (The total current is evidently the "average" of two equal currents for the dot up $\uparrow$ and the dot down $\downarrow$.) We calculate the current via the transmission of electrons from the left to the right lead. There are two contributions to the spin-conserving current: either an electron with spin down $\downarrow$ goes from the left lead to the dot and then to the right lead (energy denominator $\varepsilon + U$), or the $\uparrow$ electron from the quantum dot goes to the right lead (energy denominator ε) and then a $\uparrow$ electron jumps to the dot from the left lead. The *probabilities* of these two processes should be added. Then, there are two spin-flip processes, whose total current should be added to the spin conserving one above: either a $\downarrow$ electron goes from the left lead to the dot [energy denominator $-(\varepsilon+U)$] and then the $\uparrow$ electron goes to the right lead, or the $\uparrow$ electron goes to the right lead first (energy denominator ε) and then the $\downarrow$ electron goes from the left lead to the dot. The amplitudes for these two last contributions, which simply accounts for the two different intermediate states, has to be added. Thus, the total conductance is given by

$$G^{(0)} = G_Q \Gamma_L \Gamma_R \left[\left(\frac{1}{\varepsilon} - \frac{1}{\varepsilon + U} \right)^2 + \frac{1}{\varepsilon^2} + \frac{1}{(\varepsilon + U)^2} \right]. \quad (12)$$

The quantum dot in the regime described by Eq. (12) contains one electron on the broad level 1. Effective antiferromagnetic interaction of this electron with the electrons in the lead conduction bands, leads to a strong enhancement of conductance at low temperature. This is the Kondo effect in quantum dots.[4-6] With the use of Schrieffer-Wolf transformation, one easily maps the Anderson impurity model Hamiltonian [Eq. (1) with only one level] onto the Kondo Hamiltonian (see, e.g., Ref. 11). Far from the resonances the Kondo corrections to Eq. (12) are of the relative order $\sim \ln(T^{-1})\Gamma/U$, where T is a (small) temperature. At $T \approx T_K = (U\Gamma/2)^{1/2} \exp[\pi \varepsilon_d(\varepsilon_d + U)/2\Gamma U]$ the renormalized antiferromagnetic coupling diverges and the conductance reaches the unitarity limit $G \approx G_Q$. Explicit calculation of G in this regime may be done only by means of numerical renormalization group. Still even in this extreme case Eq. (10) allows for qualitative description of singular behavior of G.

Two kinds of sharp features are seen in Fig. 2. First, there are a cusp and a jump at the peaks W^I, where the curve $G^{(1)}$ is replaced by $G^{(0)}$ and W^{II}, where $G^{(2)}$ is replaced by $G^{(1)}$. Accurate analytical description of $G(V)$ in this mixed-valence regime is possible only at $T \gg \Gamma$. (Although at such a high temperature the singularity becomes smeared out, see the next section.) The jump vanishes for $\Delta \ll \Gamma$, but the pronounced cusp survives even for $\Delta = 0$.

Besides that, there are three jumps in the valleys. The values of the conductance at $V = V^I \pm 0$ ($V^{III} \mp 0$) are (assuming $\Delta \ll \Gamma$)

$$G \approx 48 G_Q \frac{\Gamma_L \Gamma_R}{U^2} \quad \text{and} \quad G \approx 16 G_Q \frac{\Gamma_L \Gamma_R}{U^2}. \quad (13)$$

The contribution from the spin-flip processes for $V < V^I$ is twice that from the elastic processes. Therefore, the conductance drops near $V = V^I$ by a factor of 3. At $V = V^{II}$ the two electrons jump from the broad to narrow level. The discontinuity at V^{II}, which follows from the small difference in the probability of the electronlike and holelike processes, vanishes for $\Delta \ll \Gamma$ (restoration of particle-hole symmetry at $\Delta = 0$).

In this paper, we consider mainly the zero-bias effects. The finite bias conductance G_b may also be found easily, assuming that the same model Eq. (1) describes the quantum dot at finite bias (see, however,[12] for a discussion of self-consistent screening, strictly valid for small bias only). In the limit $\Gamma_{12}, \Gamma_2 = 0$, the differential conductance G_b acquires a cusp at the bias voltage V_b coinciding with the energy difference between the lowest and first excited state for the corresponding valley. This singularity should be seen as two lines inside the Coulomb blockade diamond relatively close to the zero-bias diagonal ($V_b \ll U$) crossing correspondingly at the gate voltage $V = V^I, V^{II}, V^{III}$. Namely, this is $V_b = \pm |E^{(0)} - E^{(1)}|$ for the first valley, $V_b = \pm |E^{(2)} - E^{(1)}|$ for the third valley, and $V_b = \pm |E^{(0)} - E^{(1)}| = \pm |E^{(2)} - E^{(1)}|$ for
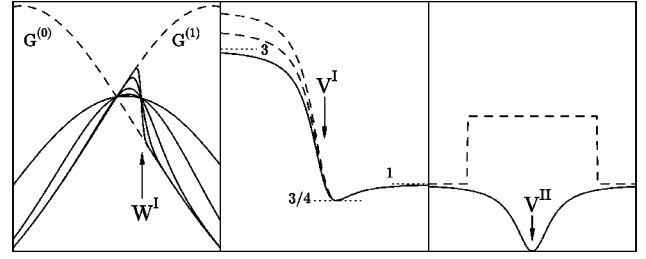

FIG. 3. The fine structure of the sharp features of $G(V)$ seen in Fig. 3. *Left*: The smearing of the second peak due to the finite temperature T at few values of T. Dashed lines are the conductances for the dot staying in the state (0) or (1). *Middle*: $G(V)$ at the middle of the first valley $V \approx V^I$, without the Kondo effect (solid) and with Kondo effect included for two different temperatures [Eq. (18)]. The numbers 1,3/4,3 show the relative magnitude of the current to the left and right of the transition and at the minimum at $V = V^I + \gamma/\sqrt{3}$. *Right*: Conductance at the middle of the second valley $V \approx V^{II}$ for the pure model Eq. (3) (solid) and with the exchange interaction Eq. (21) added (dashed). The scales are the same for middle and right figures.

the second valley. The explicit calculation of $G_b(V_b)$ may be done with the use of standard master equation techniques.

IV. RESOLVING SHARP FEATURES

So far, we have considered only the case of an "invisible" second level in the dot $t_2^{L,R} \equiv 0$. However, even in this limit the sharp features shown on Fig. 2 should be smoothed due to the finite temperature. We show this smoothening for the cusp+jump at $V = W^I$ on the left panel of Fig. 3. The corresponding analytic expression

$$G = \frac{G^{(1)} \exp\{-E^{(1)}/T\} + G^{(0)} \exp\{-E^{(0)}/T\}}{\exp\{-E^{(1)}/T\} + \exp\{-E^{(0)}/T\}} \quad (14)$$

accounts simply for a different probability of thermal populations of the states $E^{(1)}$ and $E^{(0)}$ of the dot. The same formula describes the jump of the conductance in the middle of the left ($V \approx V^I$) valley. Here, the smoothed conductance has a form of a Fermi function $\{\exp[(E^{(0)} - E^{(1)})/T] + 1\}^{-1}$.

The crossings of energy levels $E^{(i)}$ both at the peaks (W^i) and in the valleys (V^i) become "avoided" due to the finite coupling $t_2^{L,R}$ of the level 2 to the leads. This effect determines the smearing of the conductance at very low temperatures. Unfortunately, we do not have a simple way to take into account the coupling of the narrow level in the mixed-valence regime at $V \approx W^{I,II}$. On the other hand, taking the second coupling into account at the valley, turns out to be relatively easy.[13] Consider, for example, the first crossing at $V \approx V^I$ (6). First, in a way analogous to Eq. (2) one may introduce the width of the second level Γ_2 and the interlevel width Γ_{12} (defined as $\Gamma_{12} = 2\pi \Sigma_{i=L,R} t_1^i t_2^{i*} dn^i/d\varepsilon$). In the first valley, there is (almost) always one electron in the dot either on the level 1, or on the level 2. Hence, we may introduce the effective single-particle Hamiltonian, account-

ing also for the coupling to the leads. A simple calculation in the second order of perturbation theory gives for the elements of this Hamiltonian,

$$H_{11} = -\frac{\Gamma_1}{2\pi}\ln\left(\frac{\varepsilon+U}{|\varepsilon|}\right), \quad H_{22} = \Delta - \frac{\Gamma_2}{2\pi}\ln\left(\frac{\varepsilon+U}{|\varepsilon|}\right),$$
$$(15)$$

$$H_{12} = -\frac{\Gamma_{12}}{2\pi}\ln\left(\frac{\varepsilon+U}{|\varepsilon|}\right) = H_{21}^*.$$

In particular, here H_{11} and H_{22} are nothing more than the renormalized single-particle energies ε_1 and ε_2 given by the first two formulas in Eq. (5) (with Γ_2 included) minus a proper constant (see also Refs. 19,20). Moreover, the small Γ_2 may be omitted in the Eq. (15). Only Γ_{12} is important, since it is responsible for the mixing. We expect also that $\Gamma_{12} \sim \sqrt{\Gamma_1\Gamma_2} \gg \Gamma_2$. Close to $V = V^I$, the logarithms in Eq. (15) may be expanded in series. Now by simple diagonalization of the 2×2 matrix one finds the closest level splitting δE and the width γ (in gate voltage) of the avoided crossing.

$$\delta E = 2\Delta\frac{\Gamma_{12}}{\Gamma}; \quad \gamma = \frac{\Gamma_{12}\Delta}{\Gamma^2}\pi U \sim \frac{\Delta}{\Gamma}\sqrt{\frac{\Gamma_2}{\Gamma_1}}U. \quad (16)$$

The temperature is taken to be small compared to δE.

In the leading-order coupling to the leads of the two levels found after diagonalization of the 2×2 Hamiltonian (15) is simply determined by the amplitude of the broad level 1 in the corresponding wave function ($\delta V = V - V^I$)

$$t_{\pm}^{L,R} = t_1^{L,R}\sqrt{\frac{1}{2}\left(1\pm\frac{\delta V}{\sqrt{\delta V^2+\gamma^2}}\right)}. \quad (17)$$

The calculation of the conductance with this V-dependent coupling analogous to the derivation of Eq. (12) gives

$$G = 2G_0\frac{\Gamma_L\Gamma_R}{(U/2)^2}\left[1 - \frac{\delta V}{\sqrt{\delta V^2+\gamma^2}} + \frac{\delta V^2}{\delta V^2+\gamma^2}\right.$$
$$\left. + \left(1 - \frac{\delta V}{\sqrt{\delta V^2+\gamma^2}}\right)^3\frac{3\Gamma}{4\pi U}\ln\left(\frac{U}{T}\right)\right]. \quad (18)$$

This result is illustrated in the central part of Fig. 2. The first line in Eq. (18) is the result of the calculation in the leading order of perturbation theory, interpolating between the limiting values (13) at $\delta V \ll -\gamma$ and $\delta V \gg \gamma$. In addition to the smearing of the step at $V \approx V^I$ the conductance Eq. (18) acquires a narrow minimum at $\delta V = \gamma/\sqrt{3}$.

The last term in Eq. (18) is the (first) Kondo correction. The Kondo effect is present to the left of the drop of G (where the electron stays on the broad level) and vanishes (became proportional to $\sim\Gamma_2^3$) to the right of that drop. Calculation of this low-temperature Kondo correction is straightforward. The factor $(1 - \delta V/\sqrt{\delta V^2+\gamma^2})^3$ accounts for the renormalized coupling of spin to the leads (17). As

usually this presence of the Kondo correction only at $V < V^I$ may be easily checked by applying the small bias $V_b > T$.

The same effective Hamiltonian (15) describes the electronic configuration of the quantum dot in the second valley. In this case, one simply has always two electrons with opposite spins occupying one of the two levels in the dot. The coupling of these two levels to the leads changes rapidly at $V - V^{II} \sim \gamma$. Since we always have a zero total spin, $S = 0$, here, there is no Kondo effect. The transmission amplitude includes two competing contributions, electronlike and holelike, which lead to the vanishing of the conductance at $V = V^{II}$ (see Fig. 3, right frame)

$$G \sim \frac{(V - V^{II})^2}{(V - V^{II})^2 + \gamma^2}. \quad (19)$$

This formula is valid for $\Delta \ll \Gamma$, but G has a node for $\Delta \sim \Gamma$ as well.

In the constant interaction model, Eq. (1), the transition at the second valley is a triple crossing $E^{(0)} = E^{(1)} = E^{(2)}$. This degeneracy is easily lifted if, e.g., in addition, to the direct Coulomb interaction (1) one introduces the exchange interaction of the usual form

$$H_{exchange} = J\sum_{\sigma,\sigma'}a_{1,\sigma}^+a_{2,\sigma}a_{2,\sigma'}^+a_{1,\sigma'}. \quad (20)$$

As long as J is sufficiently small ($J \ll \Gamma$) the level crossing at $V = V^{II}$ will be splitted into two close crossings with a spin 1 ground state of the quantum dot in between. The conductance in the three parts of the valley is now proportional to

$$\frac{2}{(\varepsilon+U)^2}; \quad (21)$$

$$\frac{1}{(\varepsilon+U)^2} + \frac{1}{(\varepsilon+2U)^2} + \frac{1}{2}\left(\frac{1}{\varepsilon+U} - \frac{1}{\varepsilon+2U}\right)^2;$$

$$\frac{2}{(\varepsilon+2U)^2}.$$

The derivation of this result essentially repeats the proof of Eqs. (11),(12). The second expression in (21) corresponds to the transmission through the dot having total spin $S = 1$. Although only one of the two electrons constituting this $S = 1$ is visible (i.e., well coupled to the leads) the spin conservation within transition leads to a factor 1/2 in the spin-flip contribution. Since in Eq. (21), we describe the states with different spin, the crossing of the eigenstates is not avoided and the transitions are abrupt (at low T). Due to Eq. (21) the current is enhanced around the transition in the second valley. The Kondo effect (at $S = 1$) leads to a further increase of the transmission. The interesting physics of the Kondo effect at the triplet-singlet transition was investigated recently both experimentally[15] and theoretically.[16–18]

V. TRANSMISSION THROUGH
A MULTILEVEL DOT ($\Gamma \gg \Delta$)

It is generally believed that the Coulomb blockade in multilevel quantum dot may be seen only if the connection of the dot to the leads is weak enough. Namely, one expects the parameters of the dot to be chosen to satisfy the inequality

$$\Gamma \ll \Delta < U, \tag{22}$$

where Γ, Δ, and U are the typical width, the level spacing and the charging energy. Just in order to fulfill this condition and still to have a larger Γ, very small quantum dots with large Δ were prepared for the Kondo experiments.[7–9] However, in the case when only one level in the dot has an anomalously large width, the inequality (22) may be weakened to[2]

$$\Delta \ll \Gamma < U, \tag{23}$$

where Γ is the width of single anomalously broad level. Still $\Gamma_i \ll \Delta$ for all other levels. Such rare dominant levels are common for integrable dots and for dots with the mixed (partly regular and partly chaotic) classical dynamics. *Thus, instead of miniaturization of the quantum dot, one may try to look for the new physics by making the dot more clean and symmetric.*[21]

The model (23) with spinless electrons was used in Ref. 2 in order to explain the transmission phase behavior observed in the double-slit experiment of Ref. 3. Here, we briefly discuss the modification of the same scenario due to the spin.

In general for $\Gamma \gg \Delta$, charging of the quantum dot for a large series of resonances resembles that for adding of the second and third electron into the two-level dot considered in the previous sections. In the case of large Γ the electron taken to the dot from the leads within the charging resonance always occupies the broad level (even if there are empty narrow levels with smaller single-particle energies). This effect may be understood by introducing the $\sim \Gamma$ logarithmic correction to the single-particle energies in the dot arising due to the coupling to the leads [see Eq. (15)]. Due to the spin degeneracy of the single-particle levels a larger gain in energy is achieved, if after the charging resonance the broad level becomes occupied by two electrons. Since only one external electron may be added to the dot at the resonance, the second electron is taken to the broad level from the narrow one (of course, if there is such electron with close enough energy). This fast rearrangement of the electronic configuration within the resonance leads to a new structure of the conductance peaks (see two central peaks on Fig. 2). In the middle of the valley both two electrons from the broad level jumps to the narrow level (again if there is such an empty close level). However, this double jump corresponds to the triple level crossing of the states of the quantum dot (7) and may be easily splitted into two jumps by going beyond the constant interaction model (Fig. 3, right).

In Ref. 2 it was found that for $\Gamma \gg \Delta$ the transmission phase ϕ through the quantum dot increases by π through each charging peak and sharply decreases by π in $(2\Gamma / \pi \Delta) \ln(U/\Gamma)$ valleys. In the limit of vanishing width of all the narrow levels the function $\phi(V)$ may be constructed simply from the function $\phi^{(0)}(V)$ describing the charging of single level. The procedure is similar to the way we found the conductance G from the single-level function $G^{(0)}(V)$ on Fig. 2 with the use of Eq. (10). In the spinless case, the function $\phi^{(0)}(V)$ is described by the Breit-Wigner formula. For the spin $S = 1/2$ (the Anderson impurity model) the $\phi^{(0)}(V)$ may be taken, e.g., from Ref. 14. Compared to the case of Ref. 2, the main new effect taking place due to spin is the sharp depopulation of the narrow level at the charging resonance. The phase at the peak now first increases smoothly from $\phi \approx 0$ to the value somewhat below $\pi/2$, then jumps up by some fraction of π and then continues the smooth increase towards $\phi \approx \pi$. The finite temperature tends to smear this three stage increase of phase. The plateau with $\phi \approx \pi/2$ at the Kondo valley predicted in Ref. 14 does not appear in the model (23). The crude behavior of the transmission phase remains the same as in Refs. 2 (and consistent with the experiment[3]). The phase increases by π at the resonance (although now the increase contains both smooth and abrupt component) and drops down abruptly close to the middle of the valley.

Thus, taking into account spin does not lead to a serious revision of the explanation[2] of the transmission phase behavior of the experiment of Ref. 3. The sequence of resonances accompanied by the $-\pi$ jumps in the valley is even doubled because of doubling of single-particle density of states due to spin. Other attempts to explain the same experiment may be found in Ref. 22. Although, none of the mechanisms presented so far is capable to explain by itself the observed phase behavior.

VI. CONCLUSIONS

In this paper, we have considered the effects of the spin on transport through a quantum dot having one level that is strongly coupled to the leads. If this coupling is strong enough, the coupled level will play an essential role for the energetics of the dot and it can change the distribution of electrons over the discrete single-particle levels. We introduced the model for multilevel quantum dot (1),(2) with one level having its Breit-Wigner width larger than the level spacing $\Gamma > \Delta$. For spinless electrons (and $\Gamma \gg \Delta$) the analogous model was investigated in our recent paper.[2] Here, we were mostly interested in the effect of spin for electronic transport. Following the experimental tendency towards miniaturization of the quantum dots, we also mainly considered the sequence of charging resonances corresponding to occupation of only two levels by four electrons.

The main effect taking place due to spin in our model is the fast change of electronic configuration close to the top of the charging resonance (in the mixed valence). Within this transition one of the electrons in the dot jumps from the narrow level to the well-coupled one.[23] The population of narrow levels in our model takes place in the Coulomb blockade valleys and also leads to the peculiar behavior of the conductance (Fig. 3).

Finally, due to a tendency to a double occupation(depopulation) of well-coupled levels, we predict the suppression of the usual (odd valley $S = 1/2$) Kondo effect for $\Gamma > \Delta$. On the other hand, the possibility to observe the sharp features in the mixed-valence regime, as well as $S = 1$ Kondo effect and singlet-triplet transitions in the valley, should partially compensate this drawback.

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