Ballistic weak localization in regular and chaotic quantum-electron billiards

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We report systematic numerical studies of the weak localization (WL) effect in ballistic quantum dots with nominally square geometry similar to that studied in the recent experiments of Bird *et al.* [Phys. Rev. B **52**, 14 336 (1995)]. Conductance through the dot is calculated within the Landauer formalism, where dot openings are modeled as quantum point contacts connected to reservoirs. We find that at sufficiently low temperature ballistic fluctuations due to coherent mode mixing inside the dot obscure any average features in magnetoresistance. As the temperature increases, conductance oscillations are smeared out and dot resistance is well described within the Ohmic addition of resistances of two independent quantum point contacts. We demonstrate, as the Ohmic behavior is established, that the shape of the WL peak of a square dot follows the unusual linear dependence predicted by semiclassical theory for geometries for which the corresponding classical dynamics is regular. With a greater number of propagating states in the leads, the agreement with the semiclassical linear behavior is improved. The physical reason for this is given. Effect of the rounding of dot corners and leads (which simulates the change of the potential with decreasing gate voltage in a real device) on magnetoconductance through the dot is investigated. We find that the magnetoconductance is quite robust to rounding of the leads, whereas a relatively small rounding of corners inside the dot is sufficient to destroy regular motion of electrons. This may explain a transition from the linear to the Lorentzian dependence of the WL peak (the latter, according to the semiclassical theory, is characteristic for chaotic billiards) which was detected in the experiment. We also discuss effects of the real potential inside the dot on the shape of the WL peak. [S0163-1829(96)02431-9]

I. INTRODUCTION

In artificial semiconductor billiards electron motion is ballistic at low temperatures and the billiard shape can be controlled by an applied gate voltage.[1–6] This has brought new attention to the problem of quantum chaos and its relation to the corresponding classical dynamics (for the review of quantum chaos see, for example, Ref. 7). For closed structures a signature of quantum chaos can be found in statistics of energy level spacings[7–10] and the existence of scarred eigenstates resembling the unstable periodic orbits of a classically chaotic system.[10,11] For open geometries, recent theoretical studies[12–14] predict a striking difference in statistics of the conductance fluctuations for structures, the classical dynamics of which is either chaotic or regular. In particular, the weak localization (WL) effect in ballistic cavities is shown to be sensitive to the shape of the cavity (chaotic vs regular) and can be used to probe quantum chaos in the regime of ballistic transport. The above effect for ballistic structures is an analog of the well-known weak localization effect for disordered samples (see, for example, Ref. 15 and references herein), where the constructive electron interference for time-reversed returning trajectories enhances the probability of coherent backscattering, thereby increasing the resistivity for zero magnetic field. Turning on the magnetic field lifts the time-reversal invariance, which decreases the probability for the electron to return to the point of departure and causes the negative magnetoresistivity. In ballistic cavities, electrons are scattered at the boundaries of the cavity rather than at impurities as in the case of disordered systems. The semiclassical theory of Baranger *et al.*[13] predicts different line shapes of the averaged magnetoresistance peak near $B=0$ for chaotic and regular geometries, the difference being attributed to the different classical distribution of the effective trajectories areas inside the cavities. In particular, for the chaotic cavities the average reflection coefficient, $\langle R(B)\rangle$, has the Lorentzian dependence on B of the form

$$\langle R(B)\rangle = R_0 + \Delta R/[1+(2B/\alpha\phi_0)^2], \tag{1}$$

whereas for regular cavities theory predicts unusual linear dependence,

$$R_0 - \langle R(B)\rangle \propto |B|. \tag{2}$$

In Eqs. (1), (2), R_0 stands for the average reflection coefficient in the absence of the weak localization effects, ΔR is the zero-field weak localization corrections to the reflection coefficient, $\phi_0 = h/e$ is the flux quantum, α is the inverse of the typical area S (times 2π) enclosed by the classical path. For the ergodic motion, the parameter $S=(2\pi\alpha)^{-1}$ can be roughly considered as the area of a cavity.

While dependencies (1), (2) have been experimentally confirmed for stadium-shaped and circular dots,[3] the classical dynamics of which is chaotic and regular, respectively, an interpretation of the experimental results for other geometries remains controversial and far from complete understanding. In particular, for the square billiards, the classical dynamics of which is regular, Chan *et al.*[4] reported the Lorentzian shape of the weak localization peak for the effective ensemble of the dots, whereas Bird *et al.*[6] observed striking transition from the Lorentzian to the linear peak for the *single* dot, as the width of the quantum point contacts (leads) connecting the dot to the reservoirs were narrowed. In addition, Eqs. (1), (2) are obtained in the semiclassical regime of electron dynamics with many propagating states in the leads when the distribution of incoming electrons is averaged over the wide (infinite) energy interval. In contrast, many experiments which are analyzed on the basis of Eqs. (1), (2) are performed on a *single* device in the *quantum* regime of very low temperature (up to $\sim$25 mK) with only a few modes (or even near a pinch-off regime), when the semiclassical approach is not well-justified and ballistic fluctuations, due to coherent mode mixing inside the dot, could obscure any average features in magnetoresistance.

Thus, existing ambiguity in explanation and interpretation of the experimental data motivates us for a detailed numerical study of the weak localization effect in the ballistic quantum dots with nominally square geometry. In the next section, we will investigate the temperature evolution of the WL peak, and we will find the condition when semiclassical predictions can be observed in the single dot. We will investigate effects of geometry on the shape of the WL peak, as well as discuss the role of the real smooth potential inside the dot. A comparison to the experiment is made in Sec. III. Section IV summarizes our main results.

II. RESULTS AND DISCUSSION

A schematic diagram of the structure under consideration is depicted in the inset of Fig. 1. Geometry and parameters of the dot are chosen to model the experimental setup of Bird *et al.*[6] To account for the effect of lead openings on electron scattering in real structures, we model junctions as quantum point contacts (QPC's) of a finite width connected to wide leads (reservoirs). Conductance through the dot at zero temperature is related to the transmission coefficient $\mathcal{T}=\mathrm{Tr}(\mathbf{tt}^{\dagger})$ via the two-terminal Landauer formula $G(\epsilon,0)=2e^2/h\mathcal{T}$, where $t_{\alpha,\beta}(\epsilon)=(\mathbf{t})_{\alpha,\beta}$ is the transmission amplitude from incoming state α to outgoing state β at energy ϵ.[15] Convolution of $G(\epsilon,0)$ with the derivative of the Fermi-Dirac distribution $f(E_F,T)$ gives us a conductance for finite temperature T,

$$G(E_F,T)=-\int d\epsilon G(\epsilon,0)\partial f(\epsilon-E_F,T)/\partial\epsilon.$$

We calculate matrix $\mathbf{t}$ on the basis of a hybrid recursive Green's-function technique,[16] specially adapted for wide or/and gradually changing geometries. This method is proved to be both numerically efficient and stable for solution of scattering problems with magnetic fields of arbitrary strength. We shall limit ourselves to the coherent regime of electron transport in the dot. Inelastic scattering (which destroys phase coherence at relatively high temperature) as well as the effects of soft impurity potential is beyond the scope of this work.

Figure 1 shows the magnetoconductance of the square dot for different temperatures T for one representative value of the QPC opening $w=50$ nm (this corresponds to $N=1-2$ propagating states in the QPC).[17,18] For the low temperatures, $T\lesssim 1$ K, ballistic fluctuations (BF's) due to coherent mode mixing inside the dot obscure any average features in magnetoresistance. Generally, the dependence $G=G(B)$ does not show any regular behavior, being strongly sensitive to the width of the QPC openings and temperature. Small variations in both w and T can cause significant changes in the corresponding magnetoresistance curves. As the temperature is increased, BF's are smeared out and the dependence $G=G(B)$ remains qualitatively the same when QPC openings vary in the range for which the number of propagating states is not changed. When the temperature is high enough ($T\gtrsim 2$ K for the structure under consideration), the WL peak reasonably well follows the linear dependence (2), which is characteristic for classically nonchaotic billiards, see Fig. 2.

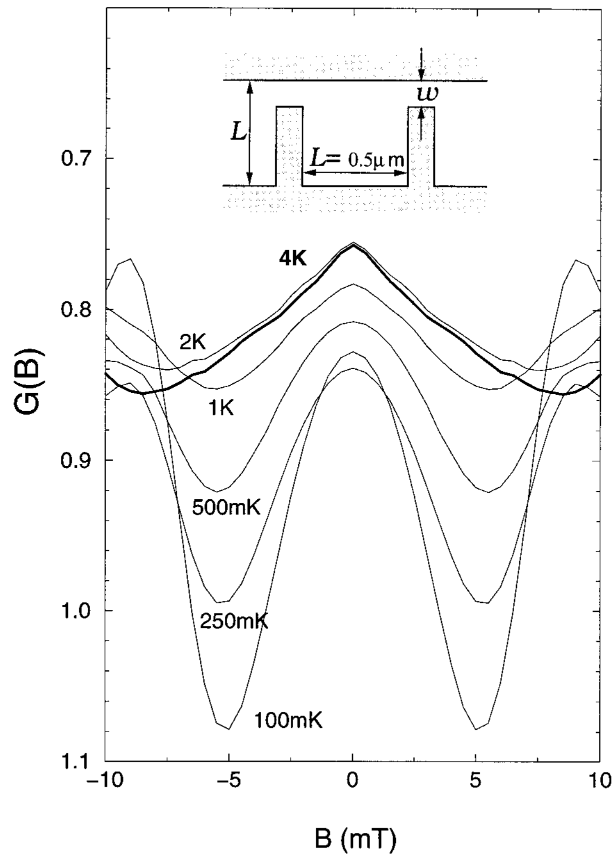

FIG. 1. Temperature evolution of the WL peak; sheet electron density $n_s=2.5\times10^{15}$ m^{-2}, QPC opening $w=50$ nm. Here, and in the following figures, the conductance G is in units of $2e^2/h$. At magnetic field of $B=10$ mT, the flux enclosed by the dot is equal to 0.6 h/e. Inset: a scematic geometry of the square quantum dot in a strip geometry. The potential V is zero in the wide leads, junctions and dot, infinite outside, and $V=10E_F$ in stubs defining the dot. The width of the stubs is 125 nm.

To find a condition when the semiclassical electron dynamics in the dot described by Eq. (1) takes over the quantum regime with BF's dominating the transport, we consider the dependence of the magnetoconductance on the QPC openings in more detail. Figure 3 shows dependencies $G=G(w)$ for some representative temperatures (magnetic field is restricted to zero). Dotted lines correspond to the conductance of the cavity calculated as an Ohmic addition of the resistances of the individual QPC's, which define the dot, $G^{-1}_{\mathrm{Ohmic}}=2G^{-1}_{\mathrm{QPC}}$. QPC's are assumed to be identical; their resistance, $R_{\mathrm{QPC}}=G^{-1}_{\mathrm{QPC}}$, is computed in the same strip geometry as that one depicted in the inset to Fig. 1. For low temperatures, $T\lesssim 1$ K, the total conductance deviates significantly from its Ohmic value, due to the strong mode mixing inside the dot. As the temperature is increased, conductance

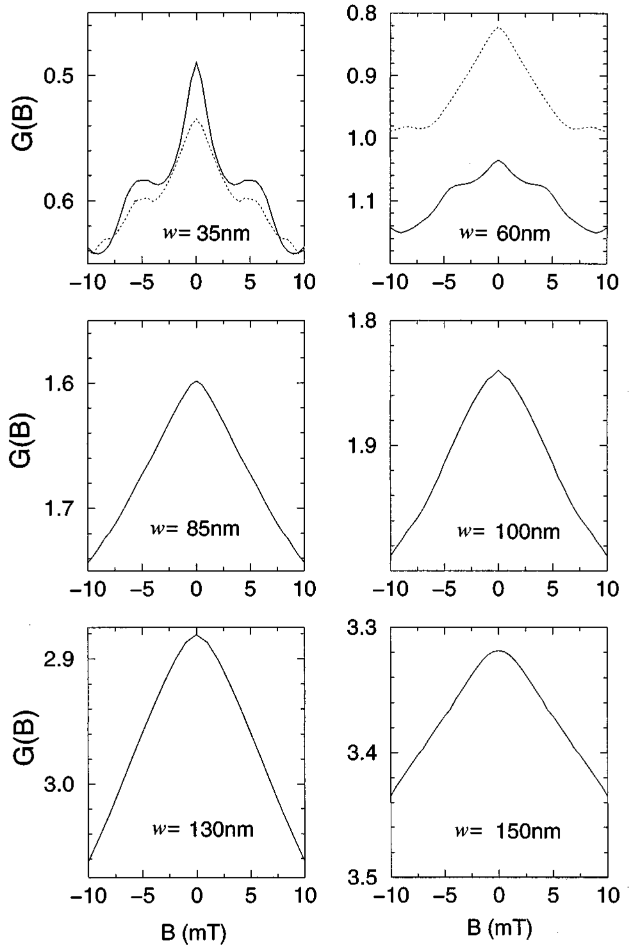

FIG. 2. Shape of the WL peak for the square dot for different values of the QPC opening w (solid lines); $T=4$ K. Dashed lines in the top panel: WL peak in the dot with QPC's of the same width (125 nm), but with slightly rounded openings, $r\approx 25$ nm; $n_s=2.5\times 10^{15}$ m^{-2}.

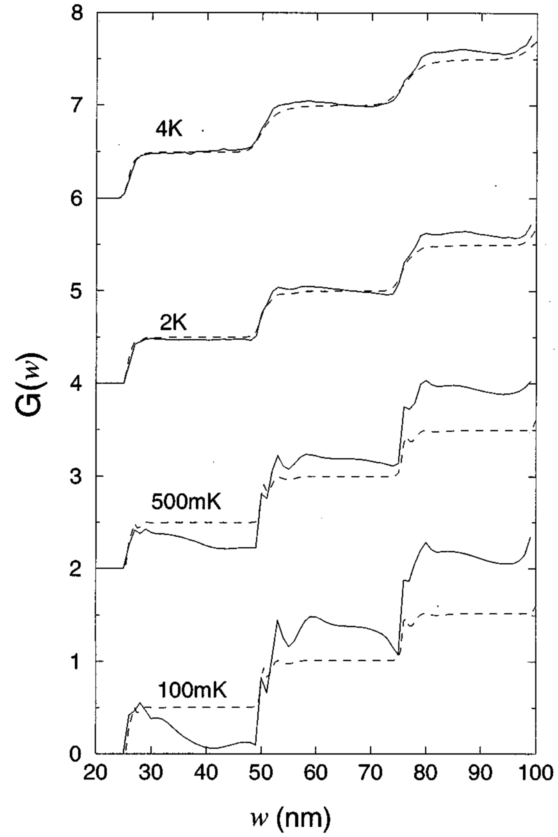

FIG. 3. Comparison between the magnetoconductance of the square dot (solid line) and the value $G^{-1}_{\mathrm{Ohmic}}=2G^{-1}_{\mathrm{QPC}}$ calculated as an Ohmic addition of the resistances of the individual QPC's which define the dot (dashed lines). The curves have been offset for clarity; $n_s=2.5\times 10^{15}$ m^{-2}; $B=0$.

fluctuations are averaged out and at $T\gtrsim 2$ K the dot conductance approaches its Ohmic value. The resistance of the two QPC's in a series defining a quantum dot has been studied in experiments of Kouwenhoven *et al.*,[19] where the Ohmic behavior had been found at temperatures as low as 0.6 K. We attribute this difference in the temperature to the effect of the smooth potential inside a real dot produced by the remote gates. Smoothing of the potential is an additional factor to the temperature smearing, which effectively makes the conductance fluctuations weaker. Note that many cavities are often designed in a way to avoid direct transmission from one lead to another.[1–4] We show by this example that corrections to the Ohmic behavior, due to the effect of the direct trajectories in the case of closed geometries, are negligible. This is in contrast to the *open* geometries in the four-terminal configuration, where direct transmission causes the nonadditivity of the QPC resistances.[20]

Now, comparing the results of our numerical calculations of the dependencies $G=G(B)$ for different parameters of w to the data shown in Fig. 3, we find, that *as the Ohmic behavior is established, the shape of the WL peak of a square dot follows the unusual linear dependence predicted by the semiclassical theory*[13] *for billiards for which the corresponding classical dynamics is regular*. This has an obvious physical explanation. Classically, the Ohmic addition of resistances implies that the electron velocity distribution in the dot is effectively randomized by multiple boundary reflections and averaging over a wide energy interval, due to effect of the finite temperature. Thus, the assumptions made in the derivation of Eqs. (1) and (2) (uniform distribution of scattering angles and averaging over the wide energy interval[13]) hold and the dot magnetoconductance follows its semiclassical predictions. Note, however, that sometimes the computed dependencies are not perfectly linear, and, therefore, an agreement between calculated dependencies and Eq. (2) should be taken as a tendency, rather than detailed quantitative correspondence. The discrepancy is especially pronounced for the case of $N\lesssim 2$ propagating states in the QPC's (when the semiclassical approximation is not well justified), where an overall linear increase of G can be modulated by oscillations. On the contrary, experimental curves exhibit well-defined linear behavior even when QPC's are close to the pinch-off regime.[6] Thus, the effect of a realistic smooth potential[21] should be seriously taken into account when comparing with experimental data. Simply modeling the potential profile variations of a real structure by rounding the QPC openings, we find that the above oscillations are strongly suppressed for $N=1$ and an almost perfect linear increase of magnetoconductance is recovered for the case of

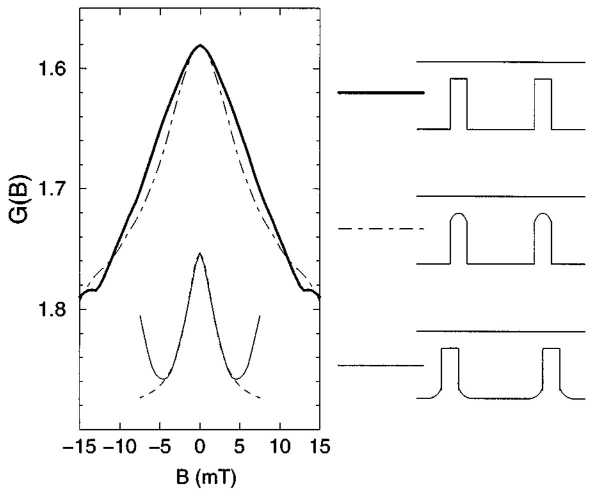

FIG. 4. Effects of the rounding of the dot corners and QPC openings on the shape of the WL peak; radius of the curvature, $R\approx 60$ nm. Dashed line is the Lorentzian fit. $n_s=2.5\times 10^{15}\ \mathrm{m}^{-2}$; $w=90$ nm; $T=4$ K.

$N=2$ (Fig. 2, upper left and right panels correspondingly). We attribute this to the *anticollimation* effect in QPC's with slightly rounded corners, leading to the more uniform angle distribution of electrons entering the dot. Indeed, with hard wall confinement, the energy of the electron in the jth eigenstate in the QPC's is $E=(\hbar^2/2m^*)k_F^2$, where $k_F^2=k_\parallel^{j\,2}+k_\perp^{j\,2}$, $k_\perp^j$ and $k_\parallel^j$ are the transverse and longitudinal wave numbers, and $k_\perp^j=\pi j/w$, with w the width of the QPC. The state with the transverse wave number $k_\perp^j$ inside the QPC is mostly coupled to outgoing modes in the dot with transverse wave numbers close to $k_\perp^j$.[22] From energy conservation, this implies that longitudinal wave numbers of outgoing states are close to $k_\parallel^j$. Thus, at the exit of the QPC, the angular distribution of the electrons is roughly confined to a cone with an opening angle $\beta\sim\tan^{-1}[k_\perp^j/k_\parallel^j]$. The smaller the subband index j is, the smaller the ratio $k_\perp^j/k_\parallel^j$ is, and, therefore, the more narrow the injection cone is. This implies that for a square corner geometry, the wide angular distribution (which is a necessary condition for the semiclassical approach to be justified) can be achieved only in the case of many occupied subbands. But if the QPC is *nonadiabatically* widened from the width w in the center to the width W on the exit (due to rounding of QPC openings), strong mode mixing occurs while an electron passes this region. As a result, the number of occupied subbands on the exit of the QPC with rounded corners, $\sim\mathrm{int}[k_F W/\pi]$, can be significantly higher than that for the case of abrupt square corners, $\sim\mathrm{int}[k_F w/\pi]$. This leads to a wider and more uniform angular distribution of injected electrons even for a low number of modes in the QPC's. Note that an opposite effect of electron collimation in a crossbar geometry with *adiabatically* tapered junctions plays the central role in the explanation of the observed quenching of the low-field Hall resistance.[23]

Now we shall find how the deformation of the shape of the dot affects the dynamics of electrons and, consequently, the shape of the WL peak. When the gate voltage is varied in the wide range, a real potential profile defining the dot can deviate quite significantly from the nominally square lithographic geometry of the gates. In Fig. 4, the magnetoconductance of the nominally square dot is compared to the conductance of the dot where, respectively, corners inside the dot and QPC openings are rounded, and the diameter of the circle defining the QPC shape is equal to the QPC width. We find that the dot conductance and consequently the shape of the WL peak is quite robust to the rounding of the QPC openings. (In fact, small rounding of the QPC's opening, as discussed above, improves the agreement with the semiclassical theory.) At the same time, the similar rounding of the corners inside the dot causes remarkable changes in magnetoconductance and the shape of the WL peak is transformed from the linear to the Lorentzian dependence. Fitting the WL peak to the Lorentzian (1) gives us the effective area $S=(2\pi\alpha)^{-1}\approx 0.16\ \mu\mathrm{m}^2$ which, in agreement with the semiclassical theory, is close to the geometrical area of the dot $S_{\mathrm{dot}}=0.25\ \mu\mathrm{m}^2$. According to the semiclassical theory, this is a clear indication of a transition from regular to chaotic motion inside the dot. To explain the striking difference in the effects of rounding of the dot corners and QPC openings on the character of the electron motion, one may speculate that rounding of the leads affects mostly electrons which bounce near the dot openings and which, therefore, are about to leave the dot. At the same time, most of the electrons, the trajectories of which are scrambled by rounding the inner corners remain inside and destroy the regular motion in the dot.

Note that the electrostatic confinement produced by the gates, in addition to the rounding of dot corners, causes a softening of the dot walls.[21] The latter, in contrast to the former, may induce the *opposite* effect of a transition from chaotic to regular dynamics.[24] Thus, the effect of a realistic potential is twofold: the rounding of the dot causes a transition to chaos, whereas soft walls tend to restore regular motion. This may explain why the linear dependence, Eq. (2), which is a signature of regular dynamics, has been detected in the experiment, despite the fact that even relatively small deviations from square geometry (which are inevitable in the real dots), cause, as demonstrated above, the transition to chaos in a model of infinite hard walls. Thus, to achieve a quantitative agreement with experimental data, one has to compute the magnetoconductance on the basis of self-consistent calculations for the potential profile. The work along this line is in progress and we plan to report these calculations in the near future.

To conclude this section, we briefly discuss the magnetoconductance of a dot of the same nominal geometry, but with different arrangements of the leads. In particular, we consider a cavity, which is formed by stubs connected to upper and lower gates, respectively, rather than to lower gate as in Fig. 1. The results (not displayed here) show that the WL peak, in this case, can be described neither by Eq. (1) nor by Eq. (2). Moreover, for some values of the QPC openings w the dependence $G=G(B)$ exhibits *positive* differential magnetoresistance. This reflects the fact that Eqs. (1), (2) have been derived neglecting the contribution from the ''off-diagonal'' terms in the semiclassical estimations of quantum corrections to $\langle R(B)\rangle$. In ballistic structures, in contrast to disordered samples, this term is not averaged out to zero, and for some geometries its contribution can be even dominant.[13] Thus, before applying Eqs. (1), (2) to the interpretation of experimental data for cavities of a particular geometry and arrangements of leads, detailed numerical simulations are rewarding.

III. COMPARISON TO EXPERIMENT

The results of the previous section set the condition when the semiclassical behavior, Eqs. (1), (2), can be observed in a *single* device. Namely, temperature has to be high enough for the Ohmic addition to be established in the dot resistance. However, the Ohmic addition is not necessary if magnetoconductance is measured for an ensemble of dots;[3,4] averaging over configuration plays a role similar to the temperature averaging.

Evolution of the WL peak of a single rectangular dot has been studied by Bird *et al.*[6] When the dot was near the pinch-off regime, the linear dependence (2) has been observed. As the gate voltage decreases (and the real potential deviates from its lithographically designed square shape), the transition to the Lorentzian dependence (1) occurs. On the basis of the numerical calculations of the Sec. II, this can be explained as the transition to chaos, due to scrambling electron trajectories *inside* the dot, rather that due to effects of the leads (as was initially suggested in Ref. 6). However, an alternative explanation, based on the fact that Ohmic behavior in the dot might not be established when the dot is relatively open, cannot be ruled out. Indeed, in the above experiment, the linear dependence (2) has been observed down to temperatures of 45 mK, when, according to our calculation, BF's obscure any average features in the conductance. In our opinion, this might indicate that the real electron temperature inside the dot is higher than that one of the base refrigerator, due to effect of Joule heating in the QPC regions. In fact, the observation made in Ref. 6 that both the shape and magnitude of the linear WL peak remain intact when the base temperature varies in the interval $\sim$45 to $\sim$500 mK, supports this view. The limit of $\sim 100-200$ mK was also found in experiments[25,26] on the temperature dependence of the dot conductance near the pinch-off regime. As the dot becomes more open, the resistance of the QPC's decreases, resulting in a decrease of the Joule heating.[26] This may bring the electron temperature in the dot close to its base value. As a result, the electron transport in a dot is no longer in the Ohmic regime, but is dominated by the BF's. This is illustrated in Fig. 1, where the shape of the WL peak at the temperatures lower that one when the Ohmic law is established can be reasonably well fit by the Lorentzian. But, in contrast to Eq. (1), this Lorentzian, being rather a fitting curve, does not carry any information concerning the character of electron motion in the dot and, therefore, cannot be taken as a signature of quantum chaos. Thus, additional experimental data on the temperature evolution of the WL peak in the regime when the dot is open are needed to support (or to rule out) this interpretation.

IV. CONCLUSION

In conclusion, the main findings of our work can be summarized as follows.

(i) Ballistic fluctuations due to coherent mode mixing dominate low-field transport in the dot at milli-Kelvin temperatures. As the temperature is increased and Ohmic behavior is established in the dot, the shape of the WL peak follows the linear dependence predicted by the semiclassical theory for regular electron billiards. This temperature sets a limit when the above predictions can be observed at *a single* device.

(ii) The shape of the WL peak is quite robust to the rounding of the QPC openings, whereas a relatively small rounding of the corners inside the dot is sufficient to destroy the regular motion of the electrons. This may explain a transition from the linear to the Lorentzian dependence of the WL peak (the latter is characteristic for chaotic billiards in the semiclassical picture), which was detected in the experiment. However, an alternative interpretation, based on the fact that Ohmic behavior in the dot might not be established when the dot is relatively open, cannot be ruled out.

(iii) The effect of the real smooth potential defining the dot has to be taken into account to achieve a quantitative agreement of the calculated magnetoconductance with experimental data. In particular, a small rounding of the QPC openings leads to an anticollimation effect (widening of the angular distribution of electrons entering the dot) which, for the low number of modes in the QPC, strongly improves the agreement with the semiclassical predictions.

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