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On additional conductance quantization and related effects of an electric field in 2D quantum point contacts

A.I. Onipko[a,*], L.I. Malysheva[a], Yu.A. Klimenko[b]

[a] *Bogolyubov Institute for Theoretical Physics, Kiev 252143, Ukraine*
[b] *Glushkov Institute of Cybernetics, Kiev 252207, Ukraine*

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Abstract

Influence of the electric field on the quantum point contact (QPC) differential conductance is studied in two cases of well-developed transmission spectrum of (a) step-like and (b) resonance character. These are exemplified by a symmetric rectangular constriction and double-bend constriction in two-dimensional electron gas. It is shown that an additional structure in the constriction–conductance dependence on the Fermi energy (referred sometimes as half integer quantization) reflects the specific field distribution in the contact region at moderate fields and is washed out by nonlinear field effects produced by the potential variation inside the contact. To study field effects, we suggest an analytical expression for the transmission probability, which includes as particular cases two models used previously to confirm and to reject the possibility of the QPC conductance quantization by value e^2/h. We also briefly discuss the case of resonance doubling accompanied by two-times decrease of the resonance intensity, representing another example of transformations in the QPC conductance, which have the same origin.

1. Introduction

The current carried by ballistic electrons confined in a two-dimensional (2D) infinite wire is quantized as a function of the Fermi energy. The current quantization is due to the fact that each propagating electron state associated with a subband (or mode) of the transverse quantization contributes $2e^2/h$ to the wire conductance [1]. In practice, this effect reveals itself, in particular, in the current through narrow (of the order of the Fermi wave length) constrictions in the two-dimensional electron gas (2DEG) [2, 3]. However, since such a constriction or quantum point contact (QPC) bears a little resemblance of an ideal 2D wire, the manifestation of the QPC conductance quantization is far from just observing steps in the conductance versus Fermi energy dependence, denoted hereinafter by $g(E_F)$. The constriction shape [4], impurities and other QPC irregularities [5, 6], the temperature [7] considerably affects the QPC ballistic conductance in the scale $2e^2/h$. Electric field effects are among those inevitably present in measurements of the QPC conductance. The role of the former factors extensively discussed in a number of papers seems to be understood fairly well. With regard to the electric field effect, there still exist serious contradictions in theoretical predictions. In particular, some calculations claim that electric field produces additional steps in the g versus E_F dependence [8–11], while the others reject the existence of the definite structure similar to quantization in scales other than $2e^2/h$ [12].

* Corresponding author.

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It should be emphasized that above-mentioned contradicting conclusions were obtained under different assumptions concerning the applied potential distribution in QPC. Therefore, it remains unclear what is decisive for the presence or absence of the "additional quantization effect".

In this work, the total voltage drop V is assumed to be a combination of an abrupt change in V at the ends of a rectangular constriction in 2DEG (non-adiabatic QPC model) supplemented by its linear variation inside the constriction, so that previous models [11, 12], which diverge in their predictions, are included as particular cases. This enable us to confirm that both results were correct within the postulated models. It will be shown that, on the one hand, an additional structure, which to an extent resembles the half-integer conductance quantization, indeed may appear in the $g(E_F)$ dependence. But, on the other hand, since the particular form of this additional structure is strongly influenced by the magnitude and distribution of the applied voltage (under certain conditions it does not at all appear), the new steps distinguished in $g(E_F)$ dependence can hardly be referred as additional conductance quantization.

We also pay attention to peak doubling in the conductance spectrum. This effect has the same origin as the appearance of additional steps in the conductance versus Fermi energy dependence. Such a possibility is demonstrated by calculations of the conductance for a QPC shaped as a double bend constriction in 2DEG, which has been already realized experimentally and is suitable therefore for verification of the predicted effect.

2. Basic relations

We start our discussion with the Landauer formula for the QPC conductance at zero temperature:

$$g = \frac{\partial}{\partial eV}\int_{U(E_F^0-(1-\beta)eV)}^{E_F^0+\beta eV} T(\varepsilon, V)\,d\varepsilon$$
$$= \beta T(E_F^0+\beta eV) + (1-\beta)T(E_F^0+(1-\beta)eV)$$
$$+ \int_{U(E_F^0-(1-\beta)eV)}^{E_F^0+\beta eV} \frac{\partial}{\partial eV} T(\varepsilon, V)\,d\varepsilon\,, \qquad (1)$$

where $U(x) = x$ (0) for $x \geqslant 0$ (< 0), E_F^0 is the Fermi energy in the absence of the source–drain electric potential difference $eV \geqslant 0$, and $T(\varepsilon, V)$ denotes the through QPC transmission coefficient.

Eq. (1) implies that the current carriers are at equilibrium on both sides of the contact, where the electrochemical potential is shifted (in comparison with the zero voltage case) by $+\beta eV$ ($0 \leqslant \beta \leqslant 1$) and $-(1-\beta)eV$ in the source and drain reservoirs, respectively. For a symmetric QPC, in which case the transmission coefficient is independent of the applied potential sign, $T(\varepsilon, V) = T(\varepsilon, -V)$, one has from Eq. (1) for small biases, $eV/E_F^0 \ll 1$,

$$g_{(V\to 0)} = \beta T_0(E_F^0 + \beta eV)$$
$$+ (1-\beta)T_0(E_F^0 - (1-\beta)eV) + 0(eV/E_F^0), \quad (2)$$

where $T_0(\varepsilon) \equiv T(\varepsilon, 0)$.

Note that in an idealized case of $\beta = \frac{1}{2}$ and $T_0(E_j < E_F^0 < E_{j+1}) = j$, where E_j is the energy of the jth propagating mode opening in an unbiased QPC, the linear-response QPC conductance is, in accordance with Eq. (2), a quantity that takes half integer values only (with the accuracy to corrections $\sim eV/E_F^0$). This is the result of Glasman and Khaetskii [8].

First, we consider the QPC model shown in Fig. 1(a), which represents a particular realization of the wide–narrow–wide (WNW) structure (Fig. 1(c)) with infinite width of wide parts and constriction parameters expressed in the lattice site numbers denoted hereinafter by N (width) and N_1 (length). The dynamics of a free electron in the given lattice is supposed to be determined by the electron transfer energy L ($L < 0$) between the nearest lattice sites. In other words, the 1s tight-binding model is used to describe electron propagation through the constriction.

Strictly speaking, the electron potential energy profile inside the contact must be found self-consistently by solving the Schrödinger and the Poison equations. Instead, it is assumed to be constant on both sides of the constriction and to vary inside it in the following way: it is equal to βV_{in} on the border sites labeled by 1 in Fig. 1(c) and falls linearly up to the value $-(1-\beta)V_{in}$ on the sites labeled by N_1.

For the model just specified the transmission coefficient is usually found by means of numerical

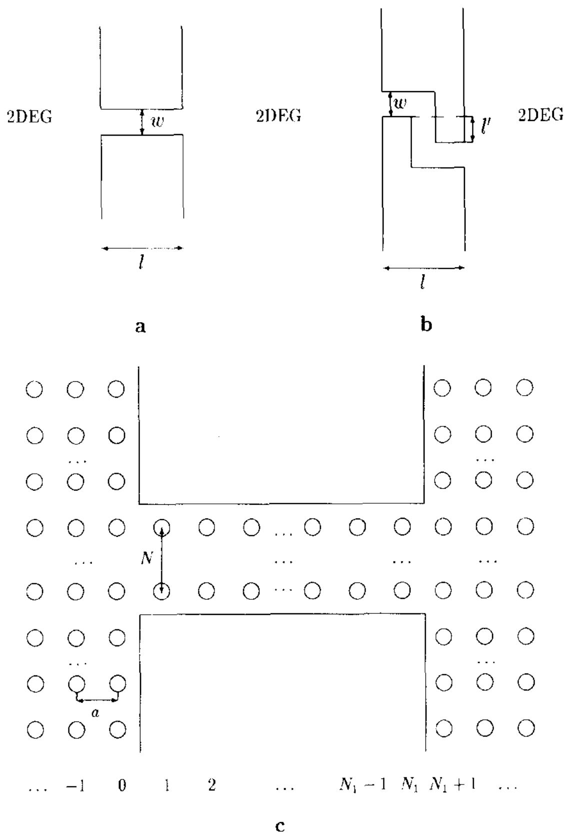

Fig. 1. Models of rectangular (**a**) and double-bend (**b**) constrictions in the two-dimensional electron gas (dashed areas are inaccessible for electrons). Lattice model of wide–narrow–wide configuration **c** includes model **a** as a particular case. The interrelation between the continuous and discrete parameters of constrictions **a** and **c** is given by $l = (N_1 - 1)a$ and $w = (N+1)a$, where a is the lattice constant.

solution of the corresponding scattering problem. However, the theory can be also advanced to nearly exact analytical expression for $T(\varepsilon, V)$. For the case $V = 0$, such an expression has been recently found [13]. The generalization of the formalism suggested in the cited paper to the case of an arbitrary bias is straightforward and, therefore, omitting details we present here only the final result for the transmission coefficient (the electron energy ε and the potential difference eV are in units $2|L|$):

$$T(\varepsilon, V) = 4\sum_{j=1}^{N} \frac{\Re(A_j^+)\Re(A_j^-)(\tilde{G}^j_{N_1,1})^2}{|(\tilde{G}^j_{1,1} - \varepsilon^j_{+V} - iA_j^+)(\tilde{G}^j_{N_1,N_1} - \varepsilon^j_{-V} - iA_j^-) - [(\tilde{G}^j_{N_1,1}]^2|^2}, \tag{3}$$

where the quantities $A_j^{\pm} = (2/\pi^2)k_{\text{th}}\sin^2(k_{\text{th}}j)\times[\Re(A_j(\varepsilon_{\pm V})) + i\Im(A_j(\varepsilon_{\pm V}))]$,

$$\Re(A_j(\varepsilon)) = \int_0^{\arccos(1-\varepsilon)} \mathrm{d}x \frac{\sqrt{1-(2-\cos x-\varepsilon)^2}}{(\cos x - \cos k_{\text{th}}j)^2} \times \begin{cases} \sin^2(\frac{\pi x}{2k_{\text{th}}}), & \text{even } j, \\ \cos^2(\frac{\pi x}{2k_{\text{th}}}), & \text{odd } j, \end{cases}$$

$$\Im(A_j(\varepsilon)) = \int_{\arccos(1-\varepsilon)}^{\pi} \mathrm{d}x \frac{\sqrt{(2-\cos x-\varepsilon)^2-1}}{(\cos x - \cos k_{\text{th}}j)^2} \times \begin{cases} \sin^2(\frac{\pi x}{2k_{\text{th}}}), & \text{even } j, \\ \cos^2(\frac{\pi x}{2k_{\text{th}}}), & \text{odd } j, \end{cases}$$

appear due to nonorthogonality of the basis functions which describe the transverse electron motion in wide and narrow parts of the WNW structure, the notation $\tilde{G}^j_{n,n'}$ represents a certain combination of one-dimensional Green functions which describe the longitudinal electron motion in a biased constriction with N_1 sites in length, namely,

$$[J_{\nu_j}(z)Y_{\nu_j+1-N_1}(z) - Y_{\nu_j}(z)J_{\nu_j+1-N_1}(z)]\tilde{G}^j_{n,n'}(\varepsilon, V_{\text{in}}) = \begin{cases} J_{\nu_j}(z)Y_{\nu_j-N_1}(z) - Y_{\nu_j}(z)J_{\nu_j-N_1}(z), & n = n' = 1, \\ J_{\nu_j+1}(z)Y_{\nu_j+1-N_1}(z) & \\ \quad - Y_{\nu_j+1}(z)J_{\nu_j+1-N_1}(z), & n = n' = N_1, \\ 2/(\pi z), & n = 1(N_1),\ n' = N_1(1), \end{cases}$$

and also the following abbreviations are used $k_{\text{th}} = \pi/(N+1)$, $\varepsilon^j_{\pm V} = 2 - \cos(k_{\text{th}}j) - \varepsilon_{\pm V}$, $\varepsilon_{+V} \equiv \varepsilon + (1-\beta)eV$, $\varepsilon_{-V} \equiv \varepsilon - \beta eV$, $z = (N_1 - 1)/eV_{\text{in}}$, $\nu_j = (2 - \cos(k_{\text{th}}j) - \varepsilon + \beta eV_{\text{in}})z$, $J_\nu(z)$, $Y_\nu(z)$ – the Bessel functions of the first and second order, respectively.

Eq. (3) has proved to be in excellent agreement with results of exact calculations. To an extent this is not surprising since the reservoir- and constriction-mode mixing is mostly taken into account in overlapping integrals $A_j^{\pm}$, and exactly found Green functions include contribution coming from all modes referred to an unbiased constriction. Note that for the symmetric QPC structure β should be set equal to $\frac{1}{2}$ (and this value was used in all calculations presented here). However, it is useful to have a possibility for quick evaluation of field-asymmetry effects by varying the value of β. For this reason Eq. (3) has been derived for arbitrary values of this parameter.

As mentioned above, some models previously studied in the effective mass approximation are included in the present one as particular cases. The corresponding results can be restored by using Eq. (3) with sufficiently large N, precisely, in the continuum limit: $k_{th} \to 0$, $a(N+1) = \text{const}$, where a is the lattice constant. In this limit, the relationship between the discrete and continuous parameters of the constriction is as follows: $a(N+1) = w$ – the constriction width and $a(N_1 - 1) = l$ – the constriction length, see Fig. 1. If we set $\beta = 0$ and $V = V_{in}$, the electron potential profile coincides with that assumed by Castaño and Kirczenow [12]. By setting $V_{in} = 0$ we arrive at the model of an abrupt electric potential drop at the entrance and exit of the constriction considered by Hongqi Xu [11].

We are aware of only one analytical expression for the through constriction transmission coefficient obtained so far and worth mentioning here. This is an expression suggested by Szafer and Stone [14]. Formally, it follows from Eq. (3) in the continuum limit at $V = 0$, but differs in the definition of the overlapping integrals A_j. As a consequence, Eq. (3) describes the transmission spectrum with high precision, whereas its analogue in Ref. [14] does this with noticeable deviations from exact results (for more detailed discussion of this point see Ref. [13]).

We now turn to the QPC model shown in Fig. 1(b). The zero-field transmission coefficient for this type of constriction can be expressed in terms of solutions of the scattering problem for a single rectangular bend with one end connected to semi-infinite 2DEG reservoir [15]. The problem is considerably simplified by the restriction to the energy interval of the one-mode propagation. Furthermore, we assume that the source and the drain leads have the length l, which is longer than the distance between the two bends l', see Fig. 1(b). Since we are primarily interested in the electric field effects and not in the precise form of the transmission spectrum, we may neglect to pay strict attention to the fine structure originated from the interference in the source and drain leads. In this case, an envelope of the QPC transmission spectrum follows the double bend transmission spectrum, which has been already discussed in detail [15]. It has been shown that specific features of this spectrum for energies below the second mode opening are accurately reproduced by

$$T_0(\varepsilon_F) = \frac{T_{sb}^2(\varepsilon_F)}{(1 - R_{sb}(\varepsilon_F))^2 + 4R_{sb}(\varepsilon_F)\sin^2[\varphi(q) + \pi q l'/w]}, \tag{4}$$

where $q = \sqrt{\varepsilon_F - 1}$, ε_F is the Fermi energy in units of $\varepsilon_{th} = \hbar^2\pi^2/(2m^*w^2)$ the propagation threshold energy in the constriction, $m^* = \hbar^2/(2|L|a^2)$ is the electron effective mass, T_{sb} (R_{sb}) denotes the zero-field transmission (reflection) coefficient for an infinite wire with a single bend, and φ is the phase acquired by an electron in the connecting wire as a result of a single reflection from one of the bends.

The above-presented energy dependencies for the transmission coefficient through constrictions shaped as a rectangular channel (Fig. 1(a), Eq. (3)) and as a double bend channel (Fig. 1(b), Eq. (4)) are used below in the discussion of electric field effects in the QPC ballistic conductance.

3. Discussion

Long-dashed lines in Fig. 2 exemplify well-known structure of the linear-response conductance calculated at negligible fields ($g_{(V\to 0)} \approx T_0(\varepsilon_F)$, $eV \ll \varepsilon_F$) plotted here for reference. It has the form of a staircase with the resonance structure superimposed. Note that one should speak about QPC conductance quantization effect with some precaution since the step shape varies with ε_F and l/w. Nevertheless, with certain accuracy the QPC conductance is quantized and for definiteness we consider the first peak in any plateau of g as its beginning. With the reference to these points, the structure of nonlinear conductance plotted for the case $V_{in} = 0$ (solid lines) associates with the appearance of an additional conductance quantization. Indeed, each increase in $g(\varepsilon_F)$ by 1 is preceded by an increase equal to $\frac{1}{2}$. Similar transformations in $g(\varepsilon_F)$

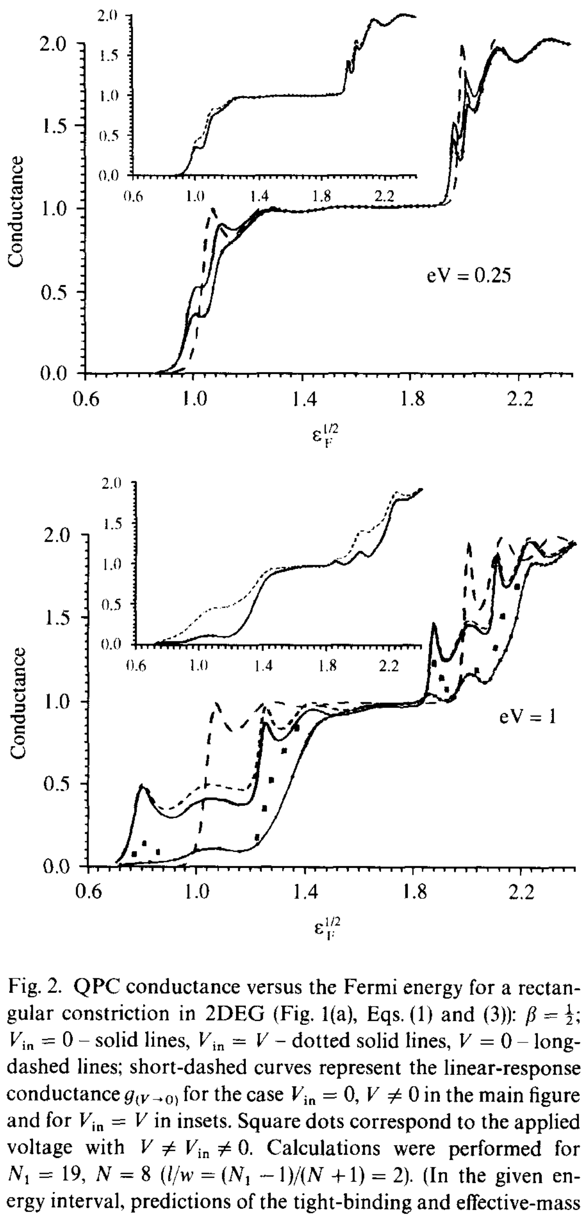

Fig. 2. QPC conductance versus the Fermi energy for a rectangular constriction in 2DEG (Fig. 1(a), Eqs. (1) and (3)): $\beta = \frac{1}{2}$; $V_{in} = 0$ – solid lines, $V_{in} = V$ – dotted solid lines, $V = 0$ – long-dashed lines; short-dashed curves represent the linear-response conductance $g_{(V\to 0)}$ for the case $V_{in} = 0$, $V \neq 0$ in the main figure and for $V_{in} = V$ in insets. Square dots correspond to the applied voltage with $V \neq V_{in} \neq 0$. Calculations were performed for $N_1 = 19$, $N = 8$ ($l/w = (N_1 - 1)/(N+1) = 2$). (In the given energy interval, predictions of the tight-binding and effective-mass models are undistinguished.) Values of the Fermi energy ε_F and source–drain electric potential difference eV are in units of the through channel propagation threshold energy $\varepsilon_{th} = \hbar^2\pi^2/(2m^*w^2)$.

are produced by the electric field at other values of QPC parameters, voltages, and also at nonzero but low enough temperatures [11]. Field effects in the case $V = V_{in}$ (solid dotted lines) are essentially in contrast, especially for higher voltages. We see that even at smallest values of V, when the appearance of new "steps" becomes pronounced, the additional structure by no means can be regarded as half-quantization of the conductance. Moreover, while at $eV = 0.25$ this structure is well distinguished, it is about to be washed out by rather moderate fields ($eV = 1$), at which nonlinear field effects come into play, as one can see from the comparison of the linear-response (short-dashed lines) and nonlinear conductance represented in insets. Naturally, the combined voltage drop at the contact boundaries and inside it produces an intermediate effect indicated by square dots. It is noteworthy that in the case $V = V_{in}$ and $\beta = 0$, there is no structure in $g(\varepsilon_F)$ which would resemble additional quantization, as it has been stated in Ref. [12].

Thus, it can be concluded that the "effect" of the additional quantization is, in fact, rather the matter of conductance–spectrum structure transformations produced by the electric field and strongly dependent on its particular distribution in the contact region. The favorable conditions for the appearance of a structure similar to conductance quantization are symmetric QPC realizations and the absence or weakness of the field inside the contact. Remarkably, in experiments of Patel et al. [9], where "half-quantization effect" has been observed, the QPC structure was rather symmetric.

Fig. 3 displays typical transformations produced by the electric field in the linear-response conductance of a constriction shaped as a double bend. The curves represented in this figure were obtained by the exact (numerical) solution of the scattering problem for a double-bend wire, but in the region of the fundamental mode propagation, $1 \leqslant \varepsilon_F \leqslant 4$ they are undistinguished from those calculated by using Eq. (4).

Calculations have been performed for $l'/w = 4$, in which case in the region of the single-mode propagation ($\varepsilon_F \leqslant 4$) there exist eight interference resonances [15]. Besides, two lowest resonances (not resolved) originate from quasi-bound states which are present in this structure. The narrow energy interval of resonance tunneling ($\varepsilon_F < 1$) is not well defined in the approximation (4) and, therefore, this region is described in Fig. 3 rather schematically, than precisely. For the rest, the $g(\varepsilon_F > 1)$ curves calculated for $eV = +0$, 0.05, 0.1 reliably reproduce characteristic transformations

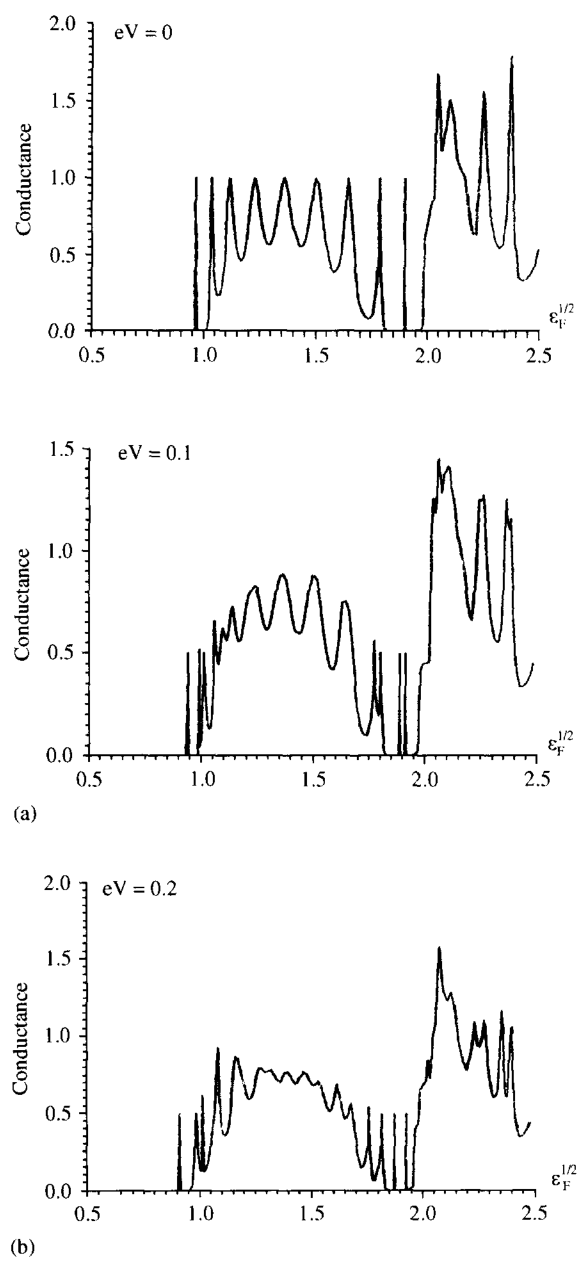

Fig. 3. Transformations of the linear-response conductance (Eq. (2)) under the influence of the applied voltage in the case of a constriction shaped as a double bend (Fig. 1(b)). Values of $eV = 0$ (physical limit), 0.1, and 0.2 are in units ε_{th}.

of the conductance in response to the applied voltage increase. The nonlinear field effects for indicated values of V are negligible. As seen from Fig. 3, with the voltage increase narrow resonances are doubling. In accordance with Eq. (2), this effect is accompanied by the two-times reduction of the resonance intensity. So, if the resonance width observed in the linear-response conductance is smaller or comparable with eV energy, the number of resonances, which appear in the dependence $g_{(V\to 0)}(\varepsilon_F)$, might be substantially different from that predicted for the QPC transmission spectrum and be varied by changes in the applied potential. It should be emphasized that doubling of resonances just pointed out is not the splitting effect in its true sense (as, e.g., the Stark effect).

In conclusion, the dependence of the QPC differential conductance on the applied voltage is studied with an account to the voltage drop at the boundaries and inside the contact region. The field distribution assumed includes as particular cases two models used previously to confirm and to reject the possibility of the QPC conductance quantization by a value e^2/h. The results presented make this long term dispute seemed to be settled. It is also shown that in appropriately shaped constrictions, one can observe resonance doubling accompanied by two-times decrease of the resonance intensity. The latter effect (produced by the electric field in the linear-response QPC conductance) has the same origin as the appearance of additional steps. An analytical expression for the transmission probability through a biased channel is suggested for the first time.

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