Pseudo Proton transfer via very short 3D tech

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We do not present a brief calculation of the electrical conductance of a two-dimensional quantum point contact (2D QPC). The QPC is modelled as a planar configuration in which two ideally conductive leads are isolated from one another by a straight line, with the exception of a constriction (a 'window' of a given lateral width $2a$) through which they are short-circuited. The leads are considered as reservoirs of a 2D strongly degenerate electron gas at $T = 0$. The Fermi wavelength is assumed to be of the same order of magnitude as $2a$. We distinguish between the self-conductance of the QPC, when the resistance of the leads is neglected, and the conductance of the configuration 'QPC plus leads taken as resistors'. (In measurements, the conductance of the leads cannot be separated from the self-conductance of the QPC.) We show that the plots of the dependence of conductance of the 2D QPC on the test momentum manifest curved steps exhibiting well-defined spikes.

I. INTRODUCTION

The new transfering of electrons through two-dimensional (2D) quantum point contacts (QPCs) has been a topic attracting much attention during the past two decades. A breakthrough came in 1989 when two groups of investigators [1, 2] published results of precise low-temperature measurements of the conductance of 2D QPCs formed in GaAs/AlAs heterostructures. These measurements corroborated the phenomenon of the conductance quantization which was previously predicted theoretically. The statistics of the conduction electrons in such heterostructures as those described in [1, 2] is the same as in a 2D metal. In metals, as is well known, the theory of the electric conduction at low temperatures may rely on the zero-temperature approximation. Correspondingly, we may use the concept of the Fermi energy $E_{\rm F}$ and the Fermi momentum $\hbar k_{\rm F} = h/\lambda_{\rm F}$ calculated for $T = 0$. The zero-temperature approximation allows us to calculate the conductance of the QPC in a purely *quantum-mechanical* manner, without any necessity to solve a kinetic equation.

The theory of QPCs may be viewed as a special subject of the theory of quantum transport in mesoscopic structures. (Cf. e.g. the monograph [3]. We recommend also the review [4] where early references to the topic of the present paper can be found. An up to date information about great potentialities of the point contact spectroscopy can be found in the monograph [5].) Since 1988, many theorists began to discuss various particular problems related to the quantization of the conductance of 2D QPCs (cf. e.g. [6-16]). Some papers provided an extensive and elaborated analysis [11,16]. Notwithstanding, we do feel that there is one detail in the theory of QPCs which was not, as far as we know, scrutinized in the literature yet and we want to focus attention especially on it. We have in mind the singular behavior of the dependence of the *self-conductance* of an ideal QPC on the variable $k_{\rm F}$. We will denote the self-conductance of the QPC as $\Gamma_{\rm self}$. Here, to avoid any misunderstanding, we deem it necessary to emphasize that when one measures the conductance of a point contact, one measures actually the conductance of a system consisting of the point contact itself plus its environment, but not the self-conductance $\Gamma_{\rm self}$ separately. Indeed, let $R_{\rm self}$ and $R_{\rm env}$ be the intrinsic resistance of the QPC and the resistance of the environment of the QPC, respectively. Viewing these resistances as resistances in series, we may define (approximately) the total resistance of the QPC as the sum $R_{\rm pc} = R_{\rm self} + R_{\rm env}$. Correspondingly, for the conductance $\Gamma_{\rm pc} = 1/R_{\rm pc}$, we may write

$$\Gamma_{\rm pc} = \frac{\Gamma_{\rm self}\Gamma_{\rm env}}{\Gamma_{\rm self} + \Gamma_{\rm env}} \tag{1}$$

where $\Gamma_{\rm self} = 1/R_{\rm self}$ and $\Gamma_{\rm env} = 1/R_{\rm env}$. Thus, although we can predict the existence of singularities in the dependence of $\Gamma_{\rm self}$ on $k_{\rm F}$, they are absent in the dependence of $\Gamma_{\rm pc}$ on $k_{\rm F}$. This is because the value of $\Gamma_{\rm env}$ is always finite and $\Gamma_{\rm pc} \to \Gamma_{\rm env}$ if $\Gamma_{\rm self} \to \infty$. Only if we take formally $\Gamma_{\rm env} \to \infty$, we obtain $\Gamma_{\rm pc} \to \Gamma_{\rm self}$.

Let $a > 0$ be a quantity characterizing the lateral size of the QPC. (We will use a as the contact half-width.) We say that the QPC is *ideal* if all stochastic influences − such as fluctuations due to the non-zero temperature and geometric roughness of boundaries − may be ignored. It is convenient to use the dimensionless variable

$$u = k_{\rm F} a \tag{2}$$

instead of $k_{\rm F}$ and to employ the value

$$\Gamma_{\rm q} = 2e^2/h \tag{3}$$

(meaning the conductance quantum [3]) in the role of a conductance unit. Then we focus attention on the dimensionless quantities

$$F = \Gamma_{\rm pc}/\Gamma_{\rm q}\,, \quad F_{\rm self} = \Gamma_{\rm self}/\Gamma_{\rm q}\,, \quad \eta = \Gamma_{\rm env}/\Gamma_{\rm q} \tag{4}$$

When speaking of spectra of QPCs, we have in mind the dependence of the conductance $\Gamma_{\rm pc}$ on $k_{\rm F}$ with fixed

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values of $\Gamma_{\rm env} > 0$. Correspondingly, according to definitions (4), the spectrum of a QPC is defined by the function $F = F(u,\eta)$ of the variable $u > 0$ with a fixed value of the parameter $\eta > 0$. We will calculate $F_{\rm self}$ in the so-called 'ballistic approximation'. This means that $F_{\rm self}$ is η-independent. Both $F_{\rm self}(u)$ and $F(u,\eta)$ are step-like functions of the variable u. The coordinates of the edges of the steps in the $F_{\rm self}$ vs. u and F vs. u plots are $u_n = \pi n/2\,, \quad n = 1, 2, \ldots$ This manifests the phenomenon of the conductance quantization. The constancy of the width $u_{n+1} - u_n = \pi/2$ of the steps of the functions $F_{\rm self}(u)$ and $F(u,\eta)$ is characteristic especially of 2D QPCs. In the case of 3D QPCs, the widths of the steps differ from step to step in an apparently irregular way [17].

Since the intrinsic conductance (self-conductance) of the 2D QPC behaves singularly if u approaches from the right the points $u = u_n$, the steps in the $F_{\rm self}$ vs. u plot have to be considerably curved. Nevertheless, according to the measurements [1, 2], the steps in the dependence of the conductance $\Gamma_{\rm pc}$ of the 2D QPCs on $k_{\rm F}$ should look like horizontal plateaus. We have a simple explanation of these plateau-like form of the steps: it represents the limiting shape of the function $F(u,\eta)$ if the values of the parameter η are small. The main objective of the present paper is right to discuss whether and when it is possible to approximate the steps as plateaus.

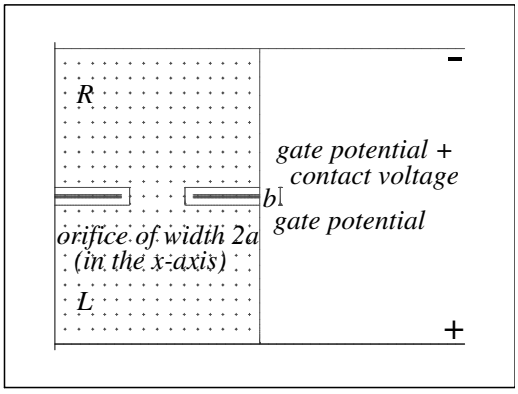

FIG. 1: Scheme of a 2D quantum point contact. The vertical axis is the y-axis. The doted region is a degenerate semiconductor. The bold horizontal lines located in the x-axis and separated by the gap of width $2a$ represent the gate. The gate is considered as a good conductor isolated from the semiconductor neighborhood and adjustable to a variable voltage $U_{\rm G}$.

We will deal with the model of the QPC whose scheme is shown in Fig. 1. Two 2D reservoirs of electrons are separated by a straight-line screen. The interval $(0, 2a)$ of the coordinate x corresponds to a window in the screen. On the flanks of the window, i.e. for $x < 0$ and $x > 2a$, the screen is opaque for the electrons. We assume that the reservoirs play the role of metallic leads. Both the leads are perfectly coalesced with one another through the window. Thus the window represents a perfect electrical contact between the leads. Let b be the thickness of the screen. We assume that $2a$ and b are nanoscaled quantities and that $b \ll 2a$. The leads are considered as rectangles with the widths L_x and L_y. (The distance between the electrodes is $2L_y$.) As the y-axis is the current axis, we have on purpose denoted the lower and upper lead in Fig. 1 as L and R, respectively. (Realizing Fig. 1 rotated by 90 degrees, L and R is the left and right lead, given by $y < 0$ and $y > 0$, respectively.) If an electric current flows across the window suggested in Fig. 1, the potential of L differs from the potential of R. Let the potential of the left lead be $\varphi_{\rm L} = 0$. Then the gate potential is $\varphi_{\rm G} = U_{\rm G}$ and the potential of the right lead is $\varphi_{\rm R} = U_{\rm G} + U$. The role of the gate potential is to control the value of the variable $k_{\rm F}a$. Clearly, the dependence of the intrinsic conductance of the QPC $\Gamma_{\rm self}$ on $k_{\rm F}a$ is directly related to the dependence of the current I (or rather of the derivative $\partial I/\partial U_{\rm G}$) on the gate voltage $U_{\rm G}$.

II. INTEGRAL FORMULA FOR THE INTRINSIC CONDUCTANCE OF 2D POINT CONTACTS

The 2D electron gas is a concept relevant to semiconductor nanolayers. We consider a direct-gap semiconductor with the isotropic dispersion function $E(\mathbf{k}) = \hbar^2 k^2/(2m)$ of the conduction band. The parameter $m > 0$ is the effective mass of the conduction electrons. In the effective-mass approximation, $-\hbar^2\nabla^2/(2m)$ is the 'kinetic-energy operator' of the one-electron hamiltonian $\hat{H}(\mathbf{r})$ corresponding to the conduction band of the semiconductor. We consider a nanolayer of the semiconductor parallel with the plane (x, y) and define the 'potential-energy operator' $V_\perp(z)$ of the hamiltonian $\hat{H}(\mathbf{r})$. We assume that $V_\perp(z)$ represents a potential-energy well whose perpendicular profile is invariant along any direction parallel with the nanolayer. In this well, the motion of each conduction electrons is perpendicularly quantized, i.e. the hamiltonian $\hat{H}(\mathbf{r})$ allows discrete eigen-energies $\mathcal{E}_n$ in the z-direction. If the well is sufficiently narrow, the distance between the basic eigen-energy $\mathcal{E}_0$ and the first excited eigen-energy $\mathcal{E}_1$ may be relatively large. Then, at low temperatures, almost all conduction electrons have their 'perpendicular kinetic energy' fixed to $\mathcal{E}_0$ and we may speak of a 2D electron gas. We will consider this gas at the zero temperature, $T = 0$.

The 3D wave function of each conduction electron may be written as $\psi^{\rm 3D}(\mathbf{r}) = \psi_0^{\rm 1D}(z)\,\psi^{\rm 2D}(x,y)$, where $\psi_0^{\rm 1D}(z)$ is the 1D eigen-function corresponding to $\mathcal{E}_0$. The function $\psi^{\rm 2D}(x,y)$ is the solution of the Schrödinger equation with the 2D hamiltonian

$$\hat{H}_{\rm 2D}(x,y) \;\equiv\; \hat{H}(\mathbf{r}) + \frac{\hbar^2}{2m}\,\frac{\partial^2}{\partial z^2} \;-\; V_\perp(z) \;\equiv$$

$$-\,\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) \;+\; V_\parallel(x,y)$$

We define the potential energy $V_\parallel(x,y)$ in the form $V_\parallel(x,y) = V_\mathrm{b}\,[\Theta(y) - \Theta(y-b)]\,[1 - \Theta(x) + \Theta(x-2a)]$. Here $\Theta(x)$ is the unit step function defined for real x and equal to unity if $x > 0$ and to zero if $x < 0$. We assume that the value of $b > 0$ is very small while the value of $V_\mathrm{b} > 0$ is very large. In the limiting case when $b \to 0$ and when $V_\mathrm{b} b \to \infty$, we say that the potential energy $V_\parallel(x,y)$ defines an ideal 2D QPC. Evidently, the condition $V_\mathrm{b} b \to \infty$ means that the x-axis represents an impenetrable screen for the conduction electrons, with the exception of the gap of width $2a$ where the potential energy is equal to zero. We interpret the regions L and R as 'massive' 2D leads. In the thermodynamic equilibrium, the electron gas in both the leads has the Fermi energy $E_\mathrm{F}^{(0)} = \hbar^2 k_\mathrm{F}^2/(2m) + \mathcal{E}_0$. The density n_2D of the conduction electrons in the leads is a constant. The Fermi momentum $\hbar k_\mathrm{F}$ corresponding to the zero-temperature equilibrium Fermi energy $E_\mathrm{F}^{(0)}$ is proportional to the square root of n_2D: $k_\mathrm{F} = \sqrt{2\pi n_\mathrm{2D}}$.

Our objective is to study the non-equilibrium scenario when a voltage U is applied on the point contact. From now on, we will leave out the superfix '2D' in $\psi^\mathrm{2D}(x,y)$. With $b \to 0$, we write the 2D wave function as

$$\psi(x,y) = \begin{cases} \psi_\mathrm{L}(x,y) & \text{for} \quad y < 0 \\ \psi_\mathrm{R}(x,y) & \text{for} \quad y > 0 \end{cases}$$

If $U \neq 0$, we have to take into account that the Fermi energy of the rear side of the screen, $E_\mathrm{F}^{+0} = E_\mathrm{F}$, differs from that of the frontal side of the screen, $E_\mathrm{F}^{-0} = E_\mathrm{F} + eU$. We assume that $eU > 0$ is a small value. According to Ohm's law, the voltage U is proportional to the electric current I flowing (perpendicularly) through the point contact. Inversely, we write the relationship

$$I = \Gamma_\mathrm{self} U \tag{5}$$

(Equation (5) corresponds to Ohm's law.) We assume that when calculating the quantity Γ_self, we need not consider electron collisions inside the leads. Of course, these collisions determine the value of Γ_env, cf. formula (1).

If an electron travels towards the screen with a given (group) velocity from the left at an angle of incidence θ_0 ($-\pi/2 < \theta_0 < \pi/2$), we consider the plane wave

$$\psi_0(x,y) = \exp[\mathrm{i}(k_{0x}x + k_{0y}y)] = \exp[\mathrm{i}k(x\sin\theta_0 + y\cos\theta_0)]$$

for $y < 0$. We have to solve the equations

$$\partial^2\psi_\mathrm{L,R}(x,y)/\partial x^2 + \partial^2\psi_\mathrm{L,R}(x,y)/\partial y^2 + k^2\psi_\mathrm{L,R}(x,y) = 0$$

(L for $y < 0$, R for $y > 0$) with respect to the boundary conditions

$$\left.\begin{matrix}\psi_\mathrm{L}(x,-0) \\ \psi_\mathrm{R}(x,+0)\end{matrix}\right\} = 0 \quad \text{for} \quad x < 0 \quad \text{and} \quad \text{for} \quad x > 2a$$

The wave function $\psi(x,y)$ is a superposition of plane waves $\exp(\mathrm{i}\mathbf{k}.\mathbf{r})$ with wave vectors $\mathbf{k} = (k_x, k_y, 0)$ differing by directions but not by absolute values. Clearly, $k^2 = k_x^2 + k_y^2 = k_{0x}^2 + k_{0y}^2$ and

$$k_y = \begin{cases} \mp\sqrt{k^2 - k_x^2} = \mp\sqrt{k_{0x}^2 + k_{0y}^2 - k_x^2} & \text{if} \quad |k_x| < k \\ \pm\mathrm{i}\sqrt{k_x^2 - k^2} = \pm\mathrm{i}\sqrt{k_x^2 - k_{0x}^2 - k_{0y}^2} & \text{if} \quad |k_x| > k \end{cases} \tag{6}$$

(The upper sign in definition (6) is valid for $y < 0$, the lower sign for $y > 0$.)

Let us now focus attention on a stripe $\mathcal{S}_\epsilon$ parallel with the x-axis and defined by inequalities $-\epsilon < y < \epsilon$ in the (x,y)-plane. We assume that $\epsilon > 0$ is a small parameter.

We define the integer N by the inequalities $\pi N/2 < ka$, $\pi(N+1)/2 \geq ka$. Then we write the wave function in the lower half of the stripe $\mathcal{S}_\epsilon$ (i.e. for $y < 0$) in the form

$$\psi_\mathrm{L}(x,y) = \exp[\,\mathrm{i}k(x\sin\theta_0 + y\cos\theta_0)]$$
$$+ \sum_{n=1}^{N} \sin\left(\frac{\pi n x}{2a}\right) \exp\left[-\mathrm{i}\left(k^2 - \frac{\pi^2 n^2}{4a^2}\right)^{1/2} y\right] R_n(\theta_0)$$
$$+ \sum_{n=N+1}^{\infty} \sin\left(\frac{\pi n x}{2a}\right) \exp\left[\left(\frac{\pi^2 n^2}{4a^2} - k^2\right)^{1/2} y\right] R_n(\theta_0) \tag{7}$$

This series becomes accurate if $\epsilon \to +0$. Similarly we can write the wave function in the upper half of $\mathcal{S}_\epsilon$ (i.e. for $y > 0$):

$$\psi_\mathrm{R}(x,y) =$$
$$\sum_{n=1}^{N} \sin\left(\frac{\pi n x}{2a}\right) \exp\left[\mathrm{i}\left(k^2 - \frac{\pi^2 n^2}{4a^2}\right)^{1/2} y\right] T_n(\theta_0)$$
$$+ \sum_{n=N+1}^{\infty} \sin\left(\frac{\pi n x}{2a}\right) \exp\left[-\left(\frac{\pi^2 n^2}{4a^2} - k^2\right)^{1/2} y\right] T_n(\theta_0) \tag{8}$$

The second sums (running from $N+1$ to infinity) in series (7) and (8) correspond to evanescent waves. They do not contribute to the conductance of the point contact. According to quantum mechanics, the one-electron contribution to the current density in the window of the screen is given by the formula

$$j_y^{(1)}(x|\theta_0)\big|_{y=+0} =$$
$$\mathrm{i}\,\frac{\hbar e}{2m}\left[\psi_\mathrm{R}(x,y)\,\frac{\partial\psi_\mathrm{R}^*(x,y)}{\partial y} - \psi_\mathrm{R}^*(x,y)\,\frac{\psi_\mathrm{R}(x,y)}{\partial y}\right]_{y=+0}$$

When employing series (8), we obtain the sum

$$j_y^{(1)}(x|\theta_0)\big|_{y=+0} =$$
$$\frac{\hbar e}{m}\sum_{n=1}^{N}\left(k^2 - \frac{\pi^2 n^2}{4a^2}\right)^{1/2} \sin^2\left(\frac{\pi n x}{2a}\right) |T_n(\theta_0|^2$$

Hence,

$$I^{(1)}(\theta_0) = \int_0^{2a} \mathrm{d}x\, j_y^{(1)}(x|\theta_0)\big|_{y=+0} =$$

$$\frac{\hbar e}{m}\sum_{n=1}^{N}(k^2a^2-\pi^2n^2/4)^{1/2}\,|T_n(\theta_0)|^2 \tag{9}$$

The coefficients $T_n(\theta_0)$ follow from the continuity of the wave function $\psi(x,y)$ and of its derivative $\partial\psi(x,y)/\partial y$ on the interval $(0,2a)$ of the x-axis. For $k>\pi n/(2a)$, the Fourier analysis gives the solution

$$T_n(\theta_0)=\left[1\,+\,\frac{ka\sin\theta_0}{(k^2a^2-\pi^2n^2/4)^{1/2}}\right]\mathcal{I}_n(\theta_0) \tag{10}$$

where

$$\mathcal{I}_n(\theta_0)=\frac{1}{2a}\int_0^{2a}\mathrm{d}x\,\exp(\mathrm{i}kx\sin\theta_0)\sin\left(\frac{\pi nx}{2a}\right)=$$

$$\frac{\pi n}{4}\,\frac{1-(-1)^n\exp(2\mathrm{i}ka\sin\theta_0)}{\pi^2n^2/4-k^2a^2\sin^2\theta_0}$$

After a straightforward calculation, we obtain the squares

$$|\mathcal{I}_{2p-1}(\theta_0)|^2=$$

$$\frac{\pi^2(2p-1)^2}{4[\pi^2(2p-1)^2/4-k^2a^2\sin^2\theta_0]^2}\,\cos^2(ka\sin\theta_0) \tag{11a}$$

and

$$|\mathcal{I}_{2p}(\theta_0)|^2=$$

$$\frac{\pi^2p^2}{[\pi^2p^2/4-k^2a^2\sin^2\theta_0]^2}\,\sin^2(ka\sin\theta_0)\,, \tag{11b}$$

with $p=1,2,\ldots$ As is seen,

$$|\mathcal{I}_n(-\theta_0)|^2=|\mathcal{I}_n(\theta_0)|^2 \tag{12}$$

Let us now consider incident wave vectors with absolute values $\sqrt{k_{0x}^2+k_{0y}^2}$ lying in the interval $(k_\mathrm{F},k_\mathrm{F}+\Delta_\mathrm{F})$, $\Delta k_\mathrm{F}\approx meU/(\hbar^2k_\mathrm{F})$. (Recall that U is the voltage between the frontal and rear side of the screen and $eU>0$.) In the small area defined in the plane (k_x,k_y) of the **k**-space by the intervals $(k_\mathrm{F},k_\mathrm{F}+\Delta_\mathrm{F})$ and $(\theta_0,\theta_0+\mathrm{d}\theta_0)$, there are $2k_\mathrm{F}\Delta k_\mathrm{F}\mathrm{d}\theta_0/(2\pi)^2$ electrons per unit area of the frontal (i.e. left) lead. Therefore the total amount of the charge flowing per second through the point contact is given by the integral

$$I=U\,\frac{me}{2\pi^2\hbar^2}\int_{-\pi/2}^{\pi/2}\mathrm{d}\theta_0\,I^{(1)}(\theta_0)\big|_{k=k_\mathrm{F}} \tag{13}$$

We have to distinguish between two cases: *i*. $k_\mathrm{F}a<\pi/2$ and *ii*. $k_\mathrm{F}a>\pi/2$. The first case is simple:

$$\Gamma_\mathrm{self}=0\quad\text{if}\quad k_\mathrm{F}a<\pi/2 \tag{14}$$

According to equation (14), the self-conductance of the QPC is equal to zero if the lateral width $2a$ of the window is smaller than the half of the Fermi wavelength $\lambda_\mathrm{F}=2\pi/k_\mathrm{F}$. The proper topic of the present paper concerns the second case. When putting equations (9), (10), (11a), (11b), (12) and (13) together, we can easily obtain, for $k_\mathrm{F}a>\pi/2$, the formula

$$\frac{\Gamma_\mathrm{self}(u)}{\Gamma_\mathrm{q}}=\frac{1}{\pi}\sum_{n=1}^{N}\int_0^{\pi/2}\mathrm{d}\theta_0\left[(u^2-\pi^2n^2/4)^{1/2}\right.$$

$$\left.+\,\frac{u^2\sin^2\theta_0}{(u^2-\pi^2n^2/4)^{1/2}}\right]|\mathcal{I}_n(\theta_0)|^2\big|_u \tag{15}$$

where Γ_q is given by equation (3). The squares $|\mathcal{I}_n(\theta_0)|^2\big|_u$ are functions of the variable u defined by equation (2).

III. CONDUCTANCE QUANTIZATION

A. Self-conductance of the QPC

The function $F_\mathrm{self}(u)=\Gamma_\mathrm{self}(u)/\Gamma_\mathrm{q}$ is piecewise continuous, exhibiting discontinuities at discrete values u_n of u, $u_n=\pi n/2$, $n=1,2,\ldots$ For the Nth step of the $\Gamma_\mathrm{self}(u)$ vs. u plot, we write $\Gamma_{\mathrm{self},N}(u)\equiv\Gamma_\mathrm{self}(u)$ if $u_N<u<u_{N+1}$. Then

$$\Gamma_\mathrm{self}(u)=\sum_{N=1}^{\infty}\Gamma_{\mathrm{self},N}(u)[\Theta(u-u_N)-\Theta(u-u_{N+1})] \tag{16}$$

The function $\Gamma_{\mathrm{self},N}(u)$ in equation (16) is equal to the sum

$$\Gamma_{\mathrm{self},N}(u)=\Gamma_\mathrm{q}\sum_{n=1}^{N}\mathcal{G}_n(u) \tag{17}$$

where $\mathcal{G}_n(u)$ is given, according to equation (15), by the integral

$$\mathcal{G}_n(u)=$$

$$\frac{1}{\pi}\int_0^{\pi/2}\mathrm{d}\theta_0\left[(u^2-u_n^2)^{1/2}+\frac{u^2\sin^2\theta_0}{(u^2-u_n^2)^{1/2}}\right]|\mathcal{I}_n(\theta_0)|^2\big|_u \tag{18}$$

defined for $u>u_n$.

After inserting expressions (11a) and (11b) here, we obtain (for $p=1,2,\ldots$) the functions

$$\mathcal{G}_{2p-1}(u)=\frac{u_{2p-1}^2}{\pi}\int_0^{\pi/2}\mathrm{d}\theta_0\left[(u^2-u_{2p-1}^2)^{1/2}\right.$$

$$\left.+\,\frac{u^2\sin^2\theta_0}{(u^2-u_{2p-1}^2)^{1/2}}\right]\left[\frac{\cos(u\sin\theta_0)}{u^2\sin^2\theta_0-u_{2p-1}^2}\right]^2 \tag{19a}$$

and

$$\mathcal{G}_{2p}(u)=\frac{u_{2p}^2}{\pi}\int_0^{\pi/2}\mathrm{d}\theta_0\left[(u^2-u_{2p}^2)^{1/2}\right.$$

$$+\frac{u^2\sin^2\theta_0}{(u^2-u_{2p}^2)^{1/2}}\Bigg]\left[\frac{\sin(u\sin\theta_0)}{u^2\sin^2\theta_0-u_{2p}^2}\right]^2 \qquad (19b)$$

Unless u is equal to one of the edges of the steps, the sub-integral functions in integrals (19a) and (19b) are finite since

$$\lim_{\xi\to u_{2p-1}}\left|\frac{\cos\xi}{\xi^2-u_{2p-1}^2}\right|=\frac{1}{(2p-1)\pi}$$

and

$$\lim_{\xi\to u_{2p}}\left|\frac{\sin\xi}{\xi^2-u_{2p}^2}\right|=\frac{1}{2p\,\pi}$$

There is probably no other way of calculating integrals (19a) and (19b) than a numerical integration.

We interpret the index n as the serial number of the *eigen-channels*. Having in mind the Nth step of the $\Gamma_{\rm self}$ vs. u plot, we say that N active eigen-channels contribute to the value of the conductance. This has been expressed explicitly by formula (17). Whenever the variable u crosses the rear side of a step, a new eigen-channel begins to take part in the transport of electrons across the point contact.

If $n=1,\ldots,N-1$, the functions $\mathcal{G}_n(u)$ behave on the interval (u_N,u_{N+1}) quite regularly. On the other hand, the case when $n=N$ is exceptional. Indeed, the function $\mathcal{G}_N(u)$ is singular if $u\to u_N$ from the right. The singularity is of the type $\sim(u^2-u_N^2)^{-1/2}\approx(2u_N)^{-1/2}(u-u_N)^{-1/2}$, as is seen from the second term of the sub-integral function in integral (18).

In the calculation of integrals (19a) and (19b), it is convenient to use the substitution $\sin\theta_0=t$ and introduce, for $P\geq 1$, the function

$$C_P(u,t)=$$

$$\frac{1}{\pi}\sum_{p=1}^{P}\left[(u^2-u_{2p-1}^2)^{1/2}+\frac{u^2t^2}{(u^2-u_{2p-1}^2)^{1/2}}\right]\frac{u_{2p-1}^2}{(u^2t^2-u_{2p-1}^2)^2}$$

defined for $u>u_{2P-1}$ and function

$$S_P(u,t)=$$

$$\frac{1}{\pi}\sum_{p=1}^{P}\left[(u^2-u_{2p}^2)^{1/2}+\frac{u^2t^2}{(u^2-u_{2p}^2)^{1/2}}\right]\frac{u_{2p}^2}{(u^2t^2-u_{2p}^2)^2}$$

defined for $u>u_{2P}$. Using the formal identities $C_0(u,t)\equiv 0$ and $S_0(u,t)\equiv 0$, we can write, for $P=1,2,\ldots$, the obvious recursive scheme

$$C_P(u,t)=C_{P-1}(u,t)+\Delta C_P(u,t)$$

with

$$\Delta C_P(u,t)=$$

$$\frac{1}{\pi}\left[(u^2-u_{2P-1}^2)^{1/2}+\frac{u^2t^2}{(u^2-u_{2P-1}^2)^{1/2}}\right]\frac{u_{2P-1}^2}{(u^2t^2-u_{2P-1}^2)^2}$$

for $u>u_{2P-1}$) and

$$S_P(u,t)=S_{P-1}(u,t)+\Delta S_P(u,t)$$

with

$$\Delta S_P(u,t)=$$

$$\frac{1}{\pi}\left[(u^2-u_{2P}^2)^{1/2}+\frac{u^2t^2}{(u^2-u_{2P}^2)^{1/2}}\right]\frac{u_{2P}^2}{(u^2t^2-u_{2P}^2)^2}$$

for $u>u_{2P}$.

We call $\Delta C_P(u,t)$ and $\Delta S_P(u,t)$ the *singular parts* of the functions $C_P(u,t)$ and $S_P(u,t)$, respectively. Correspondingly, having the Nth step in mind, we write

$$F_{{\rm self},N}(u)=\frac{\Gamma_{{\rm self},N}(u)}{\Gamma_{\rm q}}=F_{{\rm self},N}^{\rm reg}(u)+F_{{\rm self},N}^{\rm sing}(u) \qquad (20)$$

The regular and singular parts of expression (20) are calculated in the Appendix.

B. Conductance $\Gamma_{\rm pc}$ of the structure consisting of the QPC and of its leads

For the Nth step, when recalling equation (1) and definitions (4), we can readily write down the formula for the conductance $\Gamma_{{\rm pc},N}(u,\eta)$ respecting the conductance $\Gamma_{\rm env}$ of the leads to which the QPC is connected:

$$F_{{\rm pc},N}(u,\eta)=\frac{\Gamma_{{\rm pc},N}(u,\eta)}{\Gamma_{\rm q}}=\frac{F_{{\rm self},N}(u)\,\eta}{F_{{\rm self},N}(u)+\eta} \qquad (21)$$

We assume that the leads represent an n-type degenerate semiconductor, such as n-GaAs. If it were possible to imagine the leads as bulk materials (at $T=0$) with the concentration of ionized donors $5\times10^{15}\,{\rm cm}^{-3}$, we might consider the conduction electrons as a 3D degenerate gas with the same density, $n_{\rm 3D}\approx 5\times10^{15}\,{\rm cm}^{-3}$. However, we consider the electrons as a 2D gas, so we may regard the leads in a thin-layer realization, with a thickness $d\approx 10\,{\rm nm}$, say. Then the 2D density of the electrons is $n_{\rm 2D}=n_{\rm 3D}\,d\approx 5\times10^{9}{\rm cm}^{-2}$. The conductance $\Gamma_{\rm env}$ of the leads in the arrangement shown in Fig. 1 is

$$\Gamma_{\rm env}=\frac{e\mu_{\rm e}n_{\rm 2D}}{2}\,\frac{L_x}{L_y} \qquad (22)$$

As a possible value of the low-temperature mobility of the electrons in GaAs, we choose $\mu_{\rm e}=2\times10^5\,{\rm cm}^2/({\rm Vs})$. (This is a fairly high value of the low-temperature electron mobility in GaAs layers [18], although recently even mobilities in excess of $5\times10^6\,{\rm cm}^2/({\rm Vs})$ were reported [19]. The value of $\mu_{\rm e}$ is much dependent on technological conditions of preparing a GaAs layer on a suitable substrate.) When taking into account that $e=1.6\times10^{-19}\,{\rm C}$, we can readily verify that the factor $e\mu_{\rm e}n_{\rm 2D}/2$ in expression (22) is approximately equal to $8\times10^{-5}\,{\rm Ohm}^{-1}$. On the other hand, the conductance quantum $\Gamma_{\rm q}$ is equal to

$7.73 \times 10^{-5}\,\mathrm{Ohm}^{-1}$. Thus, in the example that we are discussing, Γ_{env} is roughly equal to Γ_{q}, i.e. η is approximately equal to unity, if $L_x = L_y$. We may then say that the leads are long if $L_y > L_x$ and short if $L_y < L_x$. It is instructive to put forward graphical presentation of the F_{pc} vs. u plots for several values of η. This is done in the next section.

IV. GRAPHICAL PRESENTATION OF RESULTS

Fig. 2 shows the quantization of the self-conductance of the 2D QPC under consideration. Near to the frontal edge of the Nth step, the function $\Gamma_N(u)/\Gamma_{\mathrm{q}}$ (defined for $u_N < u < u_{N+1}$) exhibits the singularity of the type $1/\sqrt{u-u_N}$. (The position of the frontal edge of the Nth step is $u_N = \pi N/2$.)

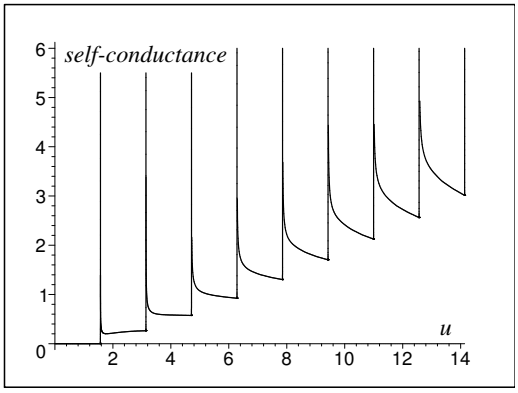

FIG. 2: Dependence of the self-conductance $\Gamma_{\mathrm{self}}/\Gamma_{\mathrm{q}}$ on the variable $u = k_{\mathrm{F}}a$.

Figs. 3-6 show the conductance steps for four finite values of η. As is seen, the maximum value of all functions (21) is equal to η. (The dotted horizontal lines in Figs. 3-6.) The spikes in Figs. 3-6, in contrast to Fig. 2, are not singular. (Let us recall that the function $F_{\mathrm{self}}(u) = \Gamma_{\mathrm{self}}(u,\eta)/\Gamma_{\mathrm{q}}$ depicted in Fig. 2 corresponds to the function $F_{\mathrm{pc}}(u,\eta) = \Gamma_{\mathrm{pc}}(u,\eta)/\Gamma_{\mathrm{q}}$ with $\eta \to \infty$.)

We define the height of the Nth step of the function $F_{\mathrm{pc}}(u,\eta)$ as the difference

$$(\Delta F_{\mathrm{pc}})_N = F_{\mathrm{pc}}(u_{N+1},\eta) - F_{\mathrm{pc}}(u_N,\eta) \qquad (23)$$

Clearly, if N increases, the steps converge asymptotically (from below) to the value η. This implies that the significance of the spikes of the steps becomes gradually weakened if $N \to \infty$, since the height of the steps defined by equation (23) tends to zero.

If we disregard the spikes, we may state that the steps in the $\Gamma_{\mathrm{pc}}(u,\eta)/\Gamma_{\mathrm{q}}$ vs. u plots look indeed like almost horizontal plateaus if the value of N is sufficiently high.

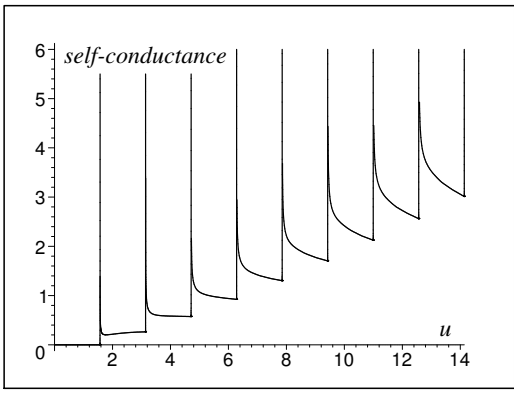

FIG. 3: Dependence of the conductance $\Gamma_{\mathrm{pc}}/\Gamma_{\mathrm{q}}$ on the variable u with $\eta = 5$.

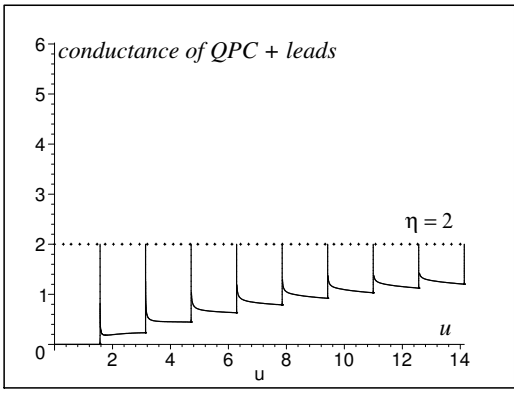

FIG. 4: Dependence of the conductance $\Gamma_{\mathrm{pc}}/\Gamma_{\mathrm{q}}$ on the variable u with $\eta = 2$.

V. CONCLUDING REMARKS

In general, any theoretical prediction of singularities, but also of finite spikes, in spectral curves evokes a concern of spectroscopists. In real situations, naturally, there are always stochastic reasons for a certain blurring of singularities and/or spikes. For instance, the eigenenergies in the ballistic theory in our derivation of the function $\Gamma_{\mathrm{self}}(u)$ have a natural width. Measurements of the conductance quantization should necessarily be performed at low temperatures but it is impossible to achieve the zero temperature. The electron-phonon collisions (which are inelastic) may cause the blurring of the eigen-energies, although these collisions may be rare at low temperatures. Besides, according to the quantum many-body theory [20], if the density of the electron gas is too low (and the low density is actually advisable for the manifestation of the conductance quantization), the electron-electron interaction results in the loss of accuracy in the use of the Fermi momentum $\hbar k_{\mathrm{F}}$. The electron-electron interaction, which does not lose its significance even if the temperature tends to zero, affects not

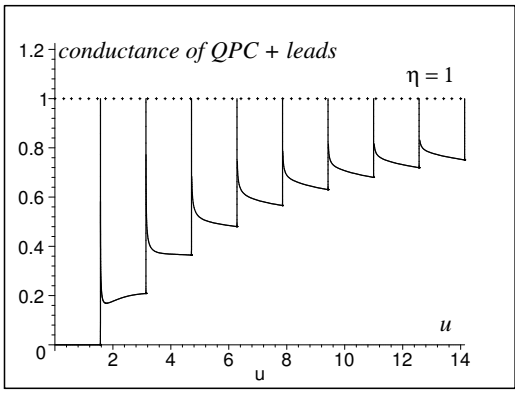

FIG. 5: Dependence of the conductance $\Gamma_{\rm pc}/\Gamma_{\rm q}$ on the variable u with $\eta = 1$.

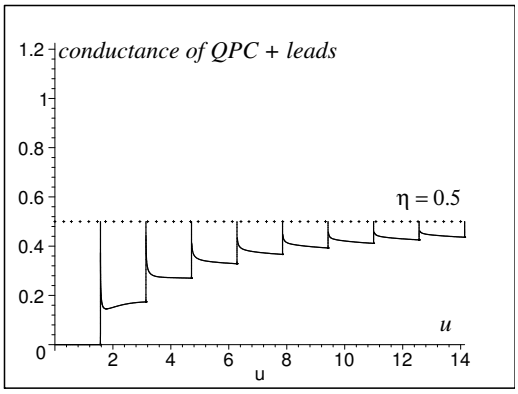

FIG. 6: Dependence of the conductance $\Gamma_{\rm pc}/\Gamma_{\rm q}$ on the variable u with $\eta = 0.5$.

only the blurring of the spikes but also some equalization of the values of the functions $\Gamma_{{\rm self},N}(u)$ and $\Gamma_{{\rm pc},N}(u)$.

Notwithstanding, we do admit that it may be possible to observe vestiges of the spikes as 'humps' in the dependence of the conductance $\Gamma_{\rm pc}$ on the variable $u = k_{\rm F}a$. In a sense, these vestiges may serve as markers of the conductance steps. Fortunately, there is some evidence supporting this idea. Experiments carried out with 3D QPCs [21] suggested persuasively the presence of humps at the frontal side of the steps in the dependence of $\Gamma_{\rm pc}$ on u, in concordance with what we have recently calculated [17]. (In 3D QPCs, we considered a circular window of radius a in a planar opaque screen.) Regrettably, no such humps have been observed with 2D QPCs yet.

What is the origin of the singularities suggested in Fig. 2? We believe it is the same as in the case of the well-known van Hove singularities derived for the quantum-mechanical density of states $g(E)$ [20]. The van Hove singularities of the type $g(E) \sim 1/\sqrt{E - E_n}$ (for $E > E_n$) are typical for the density of states of electrons in a magnetic field: the 3D motion of the electrons is quantized in the plane perpendicular to the magnetic field but not in the direction parallel with the magnetic field. In the problem concerning a QPC defined as an orifice in an opaque screen, the lateral motion of electrons (parallel to the screen) is quantized but the motion perpendicular to the screen is not.

A comment should be said about the Landauer-Büttiker formalism [3]. Our calculation of the self-conductance of the QPC corresponding to Fig. 1 is not in contradiction with the well known Landauer-Büttiker theory. According to this theory, the self-conductance should be expressed as the sum

$$\Gamma_{\rm self}/\Gamma_{\rm q} = \sum_{j,n}^{N} T_{j,n} \tag{24}$$

where $T_{j,n}$ is the transmission probability for an electron incident in the subband j and leaving the window of the screen in subband n. In our case, j is replaced by θ_0. (θ_0 may be considered as a continuous variable since when solving the Schrödinger equation, we have approximated the left lead as the half-plane $y < 0$, i.e. we have assumed that $L_x \to \infty$, $L_y \to \infty$, respecting a finite value of L_x/L_y.) In formula (24), the sum with respect to j is to be understood as the integral $(1/\pi)\int_0^{\pi/2} {\rm d}\theta_0 \ldots$, and

$$T_{j,n} \;\to\; \left[(u^2 - \pi^2 n^2/4)^{1/2} + \frac{u^2 \sin^2\theta_0}{(u^2 - \pi^2 n^2/4)^{1/2}}\right] |\mathcal{I}_n(\theta_0)|^2\big|_u \tag{25}$$

It is the second term in expression (25) which is responsible for the singular behavior of the self-conductance steps.

In this paper, we have demonstrated the conductance quantization using the model of a 2D point contact with $b = 0$ (Fig. 1). The geometry of the point contact in this model has been defined with one parameter only, the lateral width $2a$. If the profile of the window depicted in Fig. 1 is taken, in the (x, y)-plane, as a rectangle with the perpendicular width $b > 0$, a new phenomenon makes its appearance: the Schrödinger equation implies oscillations of the Fabry-Pèrot type in the y-direction [7]. To suppress these oscillations, Van Wees *et al.* [1] used a trapezoidal profile and other authors – cf. e.g. [14] – considered profiles of the window with arched sides. Quite generally, the width of the quantized steps in the function $\Gamma_{\rm pc}(u)$ with $u = k_{\rm F}a$ is a universal feature of point contacts with the given lateral width $2a$. However, the shape of the conductance steps is sensitive to the shape of the profile of the window. In this context we state that although the model of the 2D QPC with $b = 0$ was before treated by some other authors (cf. e.g. [6-10], [13], [18]), none of them mentioned the spikes, or humps, in the steps of the function $\Gamma_{\rm pc}(u)/\Gamma_{\rm q}$.

There are, of course, some particulars in the theory presented in the present paper that may call for a refinement. Namely, we employed the simplest possible approximation (which was also accepted by other authors) in which the conduction electrons were considered as an

ideal gas. Details of our results may undergo changes if a self-consistent many-body approach (in the style of a Thomas-Fermi theory, say [20]) is applied. To improve the calculation of the conductance of quantum point contacts in this sense is a difficult problem that we have left open yet.

Appendix A: Calculation of $\Gamma_{\mathrm{self},N}(u)/\Gamma_{\mathrm{q}}$

The objective of this Appendix is to indicate some technical details of our calculations that enabled us to present the functions $\Gamma_{\mathrm{self},N}(u)/\Gamma_{\mathrm{q}}$ in Fig. 2. Throughout this Appendix, we assume that $P \geq 1$.

The regular parts of the conductance are defined as

$$\Gamma^{\mathrm{reg}}_{\mathrm{self},2P-1}(u)/\Gamma_{\mathrm{q}} = \int_0^1 \frac{\mathrm{d}t}{\sqrt{1-t^2}} \left[\cos^2(ut) C_{P-1}(u,t) \right.$$

$$\left. + \sin^2(ut) S_{P-1}(u,t) \right], \quad u_{2P-1} < u < u_{2P}$$

and

$$\Gamma^{\mathrm{reg}}_{\mathrm{self},2P}(u)/\Gamma_{\mathrm{q}} = \int_0^1 \frac{\mathrm{d}t}{\sqrt{1-t^2}} \left[\cos^2(ut) C_{P}(u,t) \right.$$

$$\left. + \sin^2(ut) S_{P-1}(u,t) \right], \quad u_{2P} < u < u_{2P+1}$$

Clearly, $\Gamma^{\mathrm{reg}}_1(u) \equiv 0$.

Fig. 7 shows the regular functions defined by the above integrals. As is seen, the plots of these functions in the intervals $(u_N, u_{N+1})/2$ do not differ much from straight lines. Anticipating this fact, we divided each interval (u_N, u_{N+1}) into four subintervals. The end coordinates $\{u_{N,j}\}$ of these subintervals were chosen as $u_{N,j} = u_N + (j/4)(u_{N+1} - u_N)$, $j = 0, 1, \ldots, 4$. For each step, we calculated the values $\Gamma^{\mathrm{reg}}_{\mathrm{self},N}(u_{N,j})/\Gamma_{\mathrm{q}}$ with the aid of programs involved in MAPLE 8. Fig. 7 represents actually the result of the piecewise interpolation of $\Gamma^{\mathrm{reg}}_{\mathrm{self},N}(u)/\Gamma_{\mathrm{q}}$ by means of the spline command with first-order polynomials. (This means that the neighboring points $(u_{N,j}, \Gamma^{\mathrm{reg}}_N(u_{N,j})/\Gamma_{\mathrm{q}})$ in the 2D plot of the Nth step were connected by straight lines. The fact that each step in Fig. 7 is depicted as a broken line is hardly apparent.) The computing time for the implementation of the plot shown in Fig. 3 with Pentium AMD Athlon(tm) (64 Processor, 3000+, RAM 1GB) and with the 2D graphics of MAPLE 8 was about 1.5 minutes.

Fig. 8 shows the singular functions $\Gamma^{\mathrm{sing}}_{\mathrm{self},N}(u)/\Gamma_{\mathrm{q}}$, $N = 1, 2, \ldots$ These functions are responsible for the spikes shown in Fig. 2. The function plotted in Fig. 2 is the sum of the functions plotted in Figs. 7 and 8. (The axes in Figs. 2, 7 and 8 have been equally scaled.) In the subwavelength case when $0 < k_{\mathrm{F}} a < \pi/2$ (which means that $N = 0$), we have simply to respect that $\Gamma^{\mathrm{reg}}_{\mathrm{self},0}(u) \equiv 0$ and $\Gamma^{\mathrm{sing}}_{\mathrm{self},0}(u) \equiv 0$.

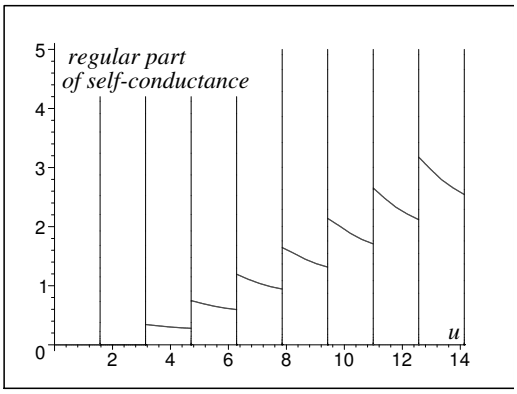

FIG. 7: Plot of the regular parts $\Gamma^{\mathrm{reg}}_{\mathrm{self},N}(u)/\Gamma_{\mathrm{q}}$ of the functions $\Gamma_{\mathrm{self},N}(u)/\Gamma_{\mathrm{q}}$ for the first eight steps, $N = 1, \ldots, 8$.

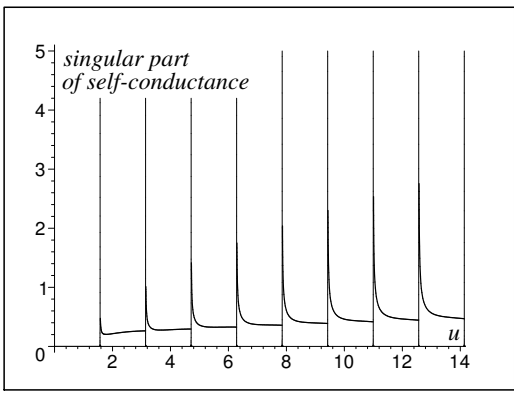

FIG. 8: Plot of the singular parts $\Gamma^{\mathrm{sing}}_{\mathrm{self},N}(u)/\Gamma_{\mathrm{q}}$ of the functions $\Gamma_{\mathrm{self},N}(u)/\Gamma_{\mathrm{q}}$ for the first eight steps, $N = 1, \ldots, 8$.

The singular parts of the conductance are defined as

$$\Gamma^{\mathrm{sing}}_{\mathrm{self},2P-1}(u)/\Gamma_{\mathrm{q}} = \frac{u^2_{2P-1}}{\pi} \int_0^1 \frac{\mathrm{d}t}{\sqrt{1-t^2}} \frac{\cos^2(ut)}{(u^2t^2 - u^2_{2P-1})^2}$$

$$\times \left[(u^2 - u^2_{2P-1})^{1/2} + \frac{u^2t^2}{(u^2 - u^2_{2P-1})^{1/2}} \right], \quad u_{2P-1} < u < u_{2P}$$

and

$$\Gamma^{\mathrm{sing}}_{\mathrm{self},2P}(u)/\Gamma_{\mathrm{q}} = \frac{u^2_{2P}}{\pi} \int_0^1 \frac{\mathrm{d}t}{\sqrt{1-t^2}} \frac{\sin^2(ut)}{(u^2t^2 - u^2_{2P})^2}$$

$$\times \left[(u^2 - u^2_{2P})^{1/2} + \frac{u^2t^2}{(u^2 - u^2_{2P})^{1/2}} \right], \quad u_{2P} < u < u_{2P+1}$$

Acknowledgments

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References

[1] van Wees BJ, van Houten H, Beenakker CWJ, Williamson JG, Kouwenhoven LP, van der Marel D, Foxon CT. Quantized conductance of point contacts in a two-dimensional electron gas. Physical Review Letters 1988; 60: 848-850.

[2] Wharam DA, Thornton TJ, Newbury R, Pepper M, Ahmed H, Frost JEF, Hasko DG, Peacock DC, Ritchie DA, Jones GAC. One-dimensional transport and the quantization of the ballistic resistance. Journal of Physics C 1988; 21: L 209-L 214.

[3] Datta S. Electronic transport in mesoscopic systems. Cambridge: University Press 1995.

[4] Beenakker CWJ, van Houten H. Quantum transport in semiconductor nanostructures. Solid State Physics 1991; 44: 1-228.

[5] Naidyuk YG, Yanson IK. Point-contact spectroscopy. New York: Springer 2005.

[6] Haanappel EG, van der Marel D. Conductance oscillations in two-dimensional Sharvin point contacts. Physical Review B 1988; 39: 5 484-5 487.

[7] Kirczenow G. Resonant conduction in ballistic quantum channels. Physical Review B 1989; 39: 10 452-10 455.

[8] Szafer A, Stone AD. Theory of quantum conduction through a constriction. Physical Review Letters 1989; 62: 300-303.

[9] Avishai Y, Band YB. Ballistic electronic conductance of an orifice. Physical Review B 1989; 40: 12 535-12 538.

[10] Matulis A, Šegžda D. Quantum oscillations of point-contact conductance in a short-contact-constriction case. Journal of Physics - Condensed Matter 1989; 1: 2 289-2 292.

[11] Tekman E, Ciraci S. Ballistic transport through a quantum point contact - Elastic scattering by impurities. Physical Review B 1990; 42: 9 098-9 103.

[12] Tekman E, Ciraci S. Theoretical study of transport through a quantum point contact. Physical Review B 1991; 43: 7 145-7 169. (1991)

[13] Berggren KF, Ji ZL. Resonant tunneling via quantum bound-states in a classically unbound system of crossed narrow channels. Physical Review B 1990; 43: 4 760-4 764.

[14] Nikolić B, Allen PB. Electron transport through a circular constriction. Physical Review B 1999; 60: 3 963-3 969.

[15] Lal S, Rao S, Sen D. Conductance through contact barriers of a finite-length quantum wire. Physical Review B 2002; 65: 195 304 (1-20).

[16] Dacal LCO, Damião ÁJ, de Andrada e Silva EA. Physical Review B 2005; 71: 155 330 (1-6).

[17] Bezák V. Conductance quantization of an ideal Sharvin contact. Annals of Physics (New York) 2007; 322: 2 604-2 617.

[18] Milanova M, Terziyska P. Low-temperature liquid-phase epitaxy growth from Ga-As-Bi solution. Thin Solid Films 2006; 500: 15-18.

[19] Wagenhuber K, Tranitz HP, Reinwald M, Wegscheider W. Influence of manganese contamination on high-mobility GaAs/AlGaAs heterostructures. Applied Physics Letters 2004; 85: 1 190-1 192.

[20] March NH, Young WH, Sampanthar S. The many-body problem in quantum mechanics. Cambridge: University Press 1967.

[21] Nagaoka K, Yaginuma S, Nagao T, Nakayama T. Local electronic structure of a quantum point contact observed with STM. Physical Review B 2006; 74: 033 310 (1-4)