

Nonlinear conductance of a quantum contact containing single impurities

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The conductance of a quantum contact containing single point defects and a potential barrier is investigated theoretically. The dependence of the conductance G on the applied voltage U is obtained for the model of a quantum wire connecting massive banks. The comparative values of the different nonlinear contributions to the conductance due to the interference of electron waves scattered by defects and by defects and the barrier are analyzed. The latter contribution becomes dominant even at extremely small coefficients of reflection of electrons from the barrier. It is shown that the dependence of the transmission coefficient T_{12} on the electron energy E explains the experimentally observed suppression of oscillation of the conductance $G(U)$ when its absolute value is close to the single-quantum value $G_0 = 2e^2/h$. © 2004 American Institute of Physics. [DOI: 10.1063/1.1645168]

INTRODUCTION

The physical characteristics of conductors with mesoscopic dimensions, such as quantum contacts, wires, rings, and dots, for example, are extremely sensitive to the presence of single defects, which can substantially alter their properties and give rise to new effects that are absent in the pure, ballistic objects. Diverse defects inevitably arise in the preparation of conducting structures, and the study of their influence on the transport characteristics is important in connection with the intensive development of nanoelectronics. On the other hand, the introduction of a controlled number of impurities having definite properties into mesoscopic systems opens up the possibility of varying their kinetic coefficients. A study of the influence of individual impurities on transport properties in mesoscopic systems is also interesting from the standpoint of basic physics, since in that case the scattering of electrons (e.g., Kondo scattering) manifests itself in the most explicit form, unobscured by averaging over a large number of defects, so that detailed information can be obtained from it. These circumstances have attracted interest in the experimental and theoretical study of the properties of conductors of small size containing single defects.

One of the classes of mesoscopic conductors now being studied intensively is that of quantum ballistic contacts. Quantum contacts are microscopic constrictions or wires having diameters comparable to the electron de Broglie wavelength and connecting massive metallic “banks.” The conductance G (the first derivative of the current–voltage characteristic, $G = dI/dU$) of such systems is determined by the number N of transverse quantization levels of the electron energy with $\varepsilon_s < \varepsilon_F$ (ε_F is the Fermi energy, $s = 1, \dots, N$) or, as is often said, the number of quantum conducting modes. Each of those modes, according to the Landauer theory,^{1,2} contributes to G a single quantum $G_0 = 2e^2/h$, so that the total conductance $G = NG_0$. The value of N can be varied, for example, by varying the diameter d of the contact. Here the function $G(d)$ is a step function with a step equal to the quantum of conductance G_0 . This effect

was first obtained in necks created on the basis of a two-dimensional electron gas and was later observed in three-dimensional contacts of ordinary metals (see, e.g., the reviews^{3,4}). In real contacts the reflection of electrons can be taken into account with the aid of a transmission coefficient of the s th mode, $\tau_s \leq 1$, and the conductance in the Ohm’s law approximation ($U \rightarrow 0$) at low temperatures ($T \rightarrow 0$) is described by the Landauer–Buttiker formula^{1,2}

$$G = G_0 \sum_{s=1}^N \tau_s. \quad (1)$$

The difference of the coefficients τ_s from unity is due to both the shape of the contact and the scattering of electrons. Here if the conductance is determined by a small number of quantum modes, then the presence of single defects can lead to a substantial change in the conductance. A number of papers have been devoted to the theoretical study of this question.^{5–12} However, effects nonlinear in the voltage in quantum contacts have been little studied. At the same time, the small size of the contact and, hence, its large resistance make it possible to avoid heating effects at biases eU of the order of tenths of the Fermi energy, making it possible to study highly nonequilibrium electronic states.

The nonmonotonic dependence of the conductance of a quantum contact on the voltage U was first observed experimentally in Ref. 13. This effect was subsequently observed in the experiments of Ref. 14. It was conjectured in Ref. 13 that the cause of this nonmonotonicity might be interference of electron waves. The essence of this effect is as follows. An electron wave with wave vector k_s incident on the contact passes through it with a probability t_s or is reflected with a probability r_s . If a defect is located a distance z_i from the contact, the reflected wave after backscattering on it can return again to the contact. The two waves are coherent and interfere. The corresponding contribution of this process to the total transmission coefficient τ_s depends in an oscillatory manner on the relative phase shift $2k_s z_i$ between the two waves. Since the electron energy and, hence the wave vec-

tors k_s depend on the applied voltage U , varying the latter leads to a nonmonotonic dependence of the conductance $G(U)$. The influence of “dirty” banks on the nonlinear conductance $G(U)$ of ballistic contacts was examined theoretically in Refs. 14 and 15. The authors of Ref. 15 predicted that conductance fluctuations will be suppressed near the edges of the steps of the function $G(d)$, and this effect was subsequently observed experimentally.¹⁴ The study in Ref. 15 was based on a numerical simulation using definite values of the parameters, and for that reason its results cannot be used for analysis of concrete experimental data. In Ref. 14 the scattering-matrix formalism was used to obtain a quite general expression for the nonlinear conductance. Besides the scattering matrix for electrons in the contact the theory also took into account the scattering matrix for backscattering in the banks, and the total probability T_{12} of transmission of an electron from one bank of the contact to another was expressed in terms of the latter matrix. Because the concrete form of the scattering matrices in the formulas for the conductance which were obtained in Ref. 14 is indefinite, it is impossible to estimate the amplitude and characteristic periods of the nonmonotonocities of the function $G(U)$. At the same time, the probability that an electron will again be incident on the contact after scattering by an impurity located a sufficient distance from it at a point \mathbf{r}_i is small, of the order of the solid angle within which the contact is viewed from the point \mathbf{r}_i (Ref. 16). A more realistic situation, it seems, is the interference of electron waves reflected from defects within the contact or in the direct vicinity of it. In Ref. 5 the conductance of a long quantum contact (wire) containing single point defects was analyzed theoretically, and the nonlinear corrections oscillatory in the voltage were found. Such a model ignores one important fact—the finite probability of reflection of electrons even in a pure ballistic contact. Such reflection may be due, for example, to a mismatch of the Fermi velocities when different metals are brought into contact or to nonadiabaticity of the shape of the contact.

In this paper we consider the voltage dependence of the conductance of a quantum wire that contains single point defects (for which no averaging over their positions is done) and a potential barrier cutting across the wire. This model allows one to take into account both the reflection from the plane of the contact (which is described by the coefficient of reflection from the barrier) and also scattering on impurities. The relative simplicity of the model makes it possible to obtain exact analytical expressions describing the dependence of the conductance on the position of the defects.

MODEL AND CALCULATION OF THE TRANSMISSION COEFFICIENT OF ELECTRONS THROUGH THE CONTACT

Consider a contact in the form of a long, narrow channel having a length L much greater than its diameter $d=2R$. The edge of the channel is smoothly (on the scale of the Fermi wavelength λ_F) connected to massive metallic “banks” (the adiabatic approximation¹⁷), to which a voltage $eU \ll \varepsilon_F$ is applied (Fig. 1). These conditions permit one to neglect the reflection of electrons from the edges of the contact. At the center of the contact ($z=0$) is a potential barrier V , near

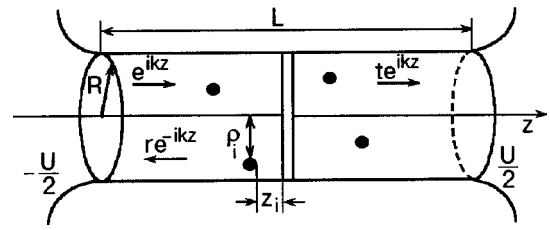


FIG. 1. Model of a quantum contact in the form of a channel of radius R connecting two massive “banks.” The barrier and the impurities inside the contact are shown schematically. The arrows indicate the direction of motion of the electrons coming into the contact, reflected by the barrier, and transmitted through it; ρ_i is the distance of the defect from the axis of the contact.

which, at the points \mathbf{r}_i , are found several point impurities. The single-electron Hamiltonian of this system is written in the form

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} + V \delta(z) + g \sum_i \delta(\mathbf{r} - \mathbf{r}_i), \quad (2)$$

where $\hat{\mathbf{p}}$ and m are the momentum operator and the effective mass of the electron, and g is the coupling constant of the electron with the impurities.

Calculation of the conductance of a mesoscopic channel (see, e.g., Ref. 18) reduces to determination of the scattering matrix $\hat{t}(E)$ as a function of the electron energy E . The most general expression for the electric current through the channel has the form

$$I = \frac{2e^2}{h} \int_{-\infty}^{\infty} dE T_{12}(E) \left[f_F \left(E + \frac{eU}{2} \right) - f_F \left(E - \frac{eU}{2} \right) \right], \quad (3)$$

$$T_{12} = \text{Tr}(\hat{t}^\dagger \hat{t}) = \sum_{ss'} T_{ss'} = \sum_{ss'} |t_{ss'}|^2, \quad (4)$$

where $T_{ss'}$ is the probability that an electron belonging to the quantum conducting mode of index s in the left bank of the contact will pass through it and belong to the mode with index s' in the right bank. The summation over s and s' in formula (4) is restricted by the condition $\varepsilon_{s(s')} < \varepsilon_F$. One can diagonalize the matrix $\hat{t}^\dagger \hat{t}$ and write the Landauer–Buttiker formula (1) in terms of its eigenvalues τ_s . At temperature $T \rightarrow 0$ the expression for the conductance takes the simple form

$$G = \frac{e^2}{h} \left[T_{12} \left(\varepsilon_F + \frac{eU}{2} \right) + T_{12} \left(\varepsilon_F - \frac{eU}{2} \right) \right]. \quad (5)$$

We note that at finite voltages U the conductance of a ballistic contact is determined by two fluxes of electrons moving in opposite directions, with energies differing by an amount eU .¹⁹ Accordingly, the energy of the transverse quantum modes for these groups of electrons also differ by eU . Therefore with increasing diameter of the contact the quantum mode becomes allowed for one direction of the wave vector first, viz., that with the lowest energy. As a result, the conductance jumps by $G_0/2$.^{20,21}

The probabilities $T_{ss'}$ can be expressed in terms of the advanced Green’s functions $G^+(\mathbf{r}, \mathbf{r}', E)$ of the electrons (see below). In the adiabatic approximation (far from the edges) the wave functions $\psi_\alpha(\mathbf{r})$ of the electrons in a ballistic chan-

nel in the absence of the barrier ($V=g=0$) can be written in the form

$$\psi_\alpha(r) = \frac{1}{\sqrt{L}} \psi_{\perp\beta}(\mathbf{R}) e^{ik_z z}, \quad (6)$$

where $\alpha=(\beta, k_z)$ is the complete set of quantum numbers, consisting of a set of two discrete numbers $\beta=(m, n)$ which specify the energy levels ε_β of the transverse quantization, and the continuous wave number k_z is the projection of the wave vector of the electron on the axis of the contact, $\psi_{\perp\beta}(\mathbf{R})$ is the component of the electron wave function perpendicular to the axis of the contact and can be chosen real, and $\mathbf{r}=(\mathbf{R}, z)$. Accordingly, the total energy of the electron is $\varepsilon_\alpha = \varepsilon_\beta + \hbar^2 k_z^2 / 2m$. The functions $\psi_{\perp\beta}(\mathbf{R})$ satisfy zero boundary conditions at the surface of the contact. In the numerical calculations presented below we have assumed for definiteness that the channel has a cylindrical shape. Then the wave functions and energy levels of the transverse quantization of the electrons in a ballistic channel ($L \rightarrow \infty$) without the impurities and barrier have the form

$$\psi_{\perp nm}(\rho, \varphi, z) = \frac{1}{\sqrt{\pi R^2} J_{m+1}(\gamma_{mn})} J_m\left(\gamma_{mn} \frac{\rho}{R}\right) e^{im\varphi};$$

$$\varepsilon_{nm} = \frac{\hbar^2 \gamma_{mn}^2}{2mR^2}. \quad (7)$$

Here we have used the cylindrical coordinates $\mathbf{r}=(\rho, \varphi, z)$; γ_{mn} is the n th zero of the Bessel function $J_m(x)$.

By factorizing the wave function (6), we can write $G^+(\mathbf{r}, \mathbf{r}', E)$ in the form of an expansion:

$$G^+(\mathbf{r}, \mathbf{r}', E) = \sum_{\beta\beta'} \psi_{\perp\beta}(\mathbf{R}) \psi_{\perp\beta'}(\mathbf{R}') G_{\beta\beta'}^+(z, z'). \quad (8)$$

In accordance with the results of Ref. 22, the transmission probabilities $T_{\beta\beta'}(E)$ are equal to

$$T_{\beta\beta'}(E) = \frac{\hbar^4}{m^2} k_\beta k_{\beta'} |G_{\beta\beta'}^+(z, z', E)|^2, \quad z \rightarrow -\infty, \quad z' \rightarrow +\infty, \quad (9)$$

where $k_\beta = \sqrt{2m(E - \varepsilon_\beta)}/\hbar$ is the electron wave vector corresponding to the quantized energy level ε_β . In formula (9) we have gone from the classification of electron modes according to index s [formulas (1) and (4)], for which the en-

ergies ε_s increase with that index, to a classification according to a set of discrete quantum numbers β .

The Green's function $G_b(\mathbf{r}, \mathbf{r}')$ in a channel with a potential barrier in the absence of impurities satisfies the equation

$$G_b(\mathbf{r}, \mathbf{r}') = G_0(\mathbf{r}, \mathbf{r}') + V \int d\mathbf{R}'' G_0(\mathbf{r}, \mathbf{R}'') G_b(\mathbf{R}'', \mathbf{r}')|_{z''=0}, \quad (10)$$

where

$$G_0^+(\mathbf{r}, \mathbf{r}') = \lim_{\eta \rightarrow 0} \sum_{\alpha} \frac{\psi_\alpha(\mathbf{R}) \psi_\alpha^*(\mathbf{R}')}{E - \varepsilon_\alpha - i\eta} \quad (11)$$

is the Green's function in the absence of impurities and the barrier. From Eq. (10) we find the coefficients of the expansion (9) of the function $G_b(\mathbf{r}, \mathbf{r}', E)$:

$$G_{b\beta\beta'}^+(z, z', E) = -\delta_{\beta\beta'} \frac{im}{\hbar^2 k_\beta} \{e^{ik_\beta |z' - z|} + r_\beta e^{ik_\beta (|z| + |z'|)}\}, \quad (12)$$

where the amplitude for reflection from the barrier, r_β , is equal to

$$r_\beta = -\frac{imV}{(\hbar^2 k_\beta + imV)} = -i|r_\beta| e^{i\varphi_\beta}. \quad (13)$$

The matrix $T_{\beta\beta'}$ from (9) can be written in the form $T_{\beta\beta'} = T_\beta^b \delta_{\beta\beta'}$, where T_β^b is expressed in terms of the amplitude of the transmitted wave $t_\beta = r_\beta + 1 = |t_\beta| e^{i\varphi_\beta}$:

$$T_\beta^b = |t_\beta|^2 = \left[1 + \left(\frac{mV}{\hbar^2 k_\beta}\right)^2\right]^{-1}. \quad (14)$$

In the presence of impurities the Green's function $G(\mathbf{r}, \mathbf{r}', E)$ that determines the transmission probability (9) must be found from the equation

$$G(\mathbf{r}, \mathbf{r}') = G_b(\mathbf{r}, \mathbf{r}') + g \sum_i G_b(\mathbf{r}, \mathbf{r}_i) G(\mathbf{r}_i, \mathbf{r}'). \quad (15)$$

Equation (15) can be solved exactly for any finite number of impurities i . For this it is necessary to write Eq. (15) at all the values $\mathbf{r}=\mathbf{r}_i$ and solve the system of i linear algebraic equations for the functions $G^+(\mathbf{r}_i, \mathbf{r}')$. As examples, let us solve Eq. (15) for one and two impurities.

For one impurity at the point \mathbf{r}_1 :

$$G^{(1)}(\mathbf{r}, \mathbf{r}') = G_b(\mathbf{r}, \mathbf{r}') + G_1(\mathbf{r}_1) G_b(\mathbf{r}, \mathbf{r}_1) G_b(\mathbf{r}_1, \mathbf{r}'). \quad (16)$$

For two impurities located at the points $\mathbf{r}=\mathbf{r}_{1,2}$:

$$G^{(2)}(\mathbf{r}, \mathbf{r}') = G_b(\mathbf{r}, \mathbf{r}') + \frac{G_1(\mathbf{r}_1) G_b(\mathbf{r}, \mathbf{r}_1) G_b(\mathbf{r}_1, \mathbf{r}') + G_1(\mathbf{r}_1) G_1(\mathbf{r}_2) G_b(\mathbf{r}_1, \mathbf{r}_2) G_b(\mathbf{r}, \mathbf{r}_1) G_b(\mathbf{r}_2, \mathbf{r}')}{1 - G_b(\mathbf{r}_2, \mathbf{r}_1) G_b(\mathbf{r}_1, \mathbf{r}_2) G_1(\mathbf{r}_1) G_1(\mathbf{r}_2)} + \frac{G_1(\mathbf{r}_2) G_b(\mathbf{r}, \mathbf{r}_2) G_b(\mathbf{r}_2, \mathbf{r}') + G_1(\mathbf{r}_1) G_1(\mathbf{r}_2) G_b(\mathbf{r}, \mathbf{r}_2) G_b(\mathbf{r}_2, \mathbf{r}_1) G_b(\mathbf{r}_1, \mathbf{r}')}{1 - G_b(\mathbf{r}_2, \mathbf{r}_1) G_b(\mathbf{r}_1, \mathbf{r}_2) G_1(\mathbf{r}_1) G_1(\mathbf{r}_2)}, \quad (17)$$

where $G_1(\mathbf{r}_i) = g/1 - gG_b(\mathbf{r}_i, \mathbf{r}_i)$.

For a rather large number of impurities the exact expression for the function $G(\mathbf{r}, \mathbf{r}')$ becomes extremely cumbersome. If it is assumed that the coupling constant g is small, the expression for the transmission probabilities (9) can be obtained with the use of the Born expansion in powers of g .

With accuracy to terms proportional to g^2 we obtain

$$T_{\beta\beta'} = T_\beta^b \delta_{\beta\beta'} + \Delta T_{1\beta\beta'} + \Delta T_{2\beta\beta'}. \quad (18)$$

The first-order correction is equal to

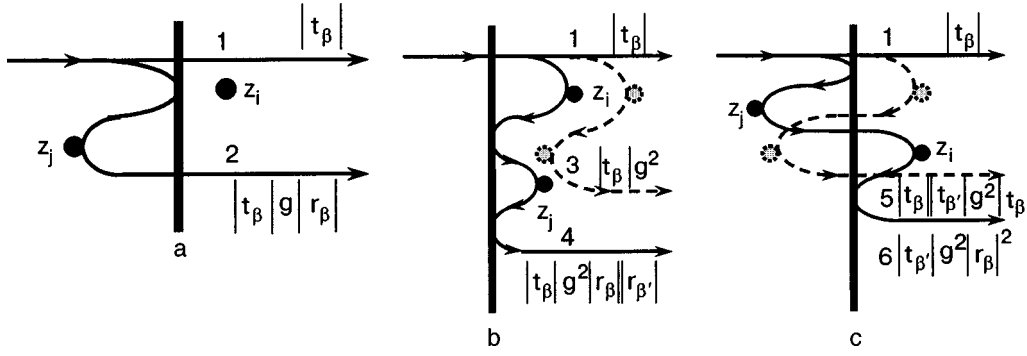


FIG. 2. Schematic illustration of some possible types of electron trajectories in a quantum channel with a barrier and impurities.

$$\Delta T_{1\beta\beta'} = -2\delta_{\beta\beta'} \left(\frac{m}{\hbar^2} \right) T_{\beta\beta}^b g \frac{1}{k_\beta} \sum_i A_{\beta\beta}^{(ii)} |r_\beta| \cos(2k_\beta z_i + \varphi_\beta), \quad (19)$$

where $A_{\beta\beta'}^{(ij)} = \psi_{\perp\beta}(\mathbf{R}_i) \psi_{\perp\beta'}(\mathbf{R}_j)$.

The form of the second-order correction $\Delta T_{2\beta\beta'}$ to the transmission coefficient depends on the position of the defects relative to the barrier. In the case when the impurities are located on different sides of the barrier, $\Delta T_{2\beta\beta'}$ is given by the formula ($z_i < 0, z_j > 0$)

$$\begin{aligned} \Delta T_{2\beta\beta'} = & - \left(\frac{gm}{\hbar^2} \right)^2 \frac{1}{k_\beta k_{\beta'}} [-2|t_{\beta'}||t_\beta| \sum_{i \neq j} A_{\beta'\beta'}^{(ij)} A_{\beta\beta}^{(ij)} \{-T_\beta^b \cos((k_\beta + k_{\beta'})(z_j - z_i) + \varphi_\beta + \varphi_{\beta'}) \\ & + |r_\beta|^2 \cos((k_\beta + k_{\beta'})(z_j - z_i) + 2\varphi_\beta) + |r_\beta||r_{\beta'}| \cos((k_\beta + k_{\beta'})(z_i + z_j))\} \\ & + T_\beta^b \sum_i A_{\beta\beta'}^{(ii)2} \{T_{\beta'}^b + 2|r_\beta| \sin(2k_\beta z_i + \varphi_\beta) + |r_\beta||r_{\beta'}| \cos(2(k_\beta + k_{\beta'})z_i + \varphi_\beta + \varphi_{\beta'})\}] \end{aligned} \quad (20)$$

or in the case when the impurities lie on one side of the barrier ($z_i < z_j$):

$$\begin{aligned} \Delta T_{2\beta\beta'} = & - \left(\frac{gm}{\hbar^2} \right)^2 \frac{1}{k_\beta k_{\beta'}} [-2T_\beta^b \sum_{i \neq j} A_{\beta'\beta'}^{(jj)} A_{\beta\beta}^{(ii)} \{-\cos((k_\beta + k_{\beta'})(z_j - z_i)) \\ & + 2|r_\beta||r_{\beta'}| \cos((k_\beta + k_{\beta'})(z_j + z_i) + \varphi_\beta + \varphi_{\beta'}) \\ & - 2|r_\beta| \sin(k_\beta(z_i + z_j) + k_{\beta'}(z_j - z_i) + \varphi_\beta) + |r_{\beta'}|^2 \cos((k_\beta + k_{\beta'})(z_i - z_j))\} \\ & + T_\beta^b \sum_i A_{\beta\beta'}^{(ii)} \{T_{\beta'}^b + 2|r_\beta| \sin(2k_\beta z_i + \varphi_\beta) - 2|r_\beta||r_{\beta'}| \cos(2(k_\beta + k_{\beta'})z_i + \varphi_\beta + \varphi_{\beta'})\}]. \end{aligned} \quad (21)$$

These formulas are valid when the value of the total energy of the electrons is not close in value to the energies ε_β of the quantum modes. If that is not the case (i.e., $k_\beta \rightarrow 0$), then the transmission coefficient must be calculated using the exact expression for the Green's function.

DISCUSSION OF THE RESULTS

When the reflection of electrons from a barrier in the contact is taken into account, the conductance becomes a complicated nonmonotonic function of the voltage. If the coupling constant g of an electron with the impurity is small, then the electron transmission probability $T_{\beta\beta'}$ in (18) can be obtained in the Born approximation for an arbitrary number of defects (15). In this case the terms in the probability $T_{\beta\beta'}$ (18) with an oscillatory dependence on energy have a clear physical meaning and can be explained in terms of electron trajectories. As we discussed in the Introduction, the pres-

ence of such terms is due to the interference of the electron wave passing through the contact without scattering (trajectory 1 in Fig. 2) and the electron waves reflected by the defects and barrier. As an example, Fig. 2 shows several possible electron trajectories. The first correction $\Delta T_{1\beta\beta'}$ (proportional to g) corresponds to the interference between the directly transmitted wave and the wave that undergoes one reflection from an impurity and one reflection from the barrier (trajectory 2 in Fig. 2a). The interference of the trajectories illustrated in Fig. 2b and 2c corresponds to a certain term in the second-order correction $\Delta T_{2\beta\beta'}$, while trajectories 3 and 5 contain two scatterings on impurities, and trajectories 4 and 6 also include two reflections from the barrier. The first and second terms in formula (21) are due to the interference between trajectories 1 and trajectories 3 and 4 in Fig. 2b, respectively. Figure 2c shows trajectories 5 and 6, the interference between each of which and trajectory 1 cor-

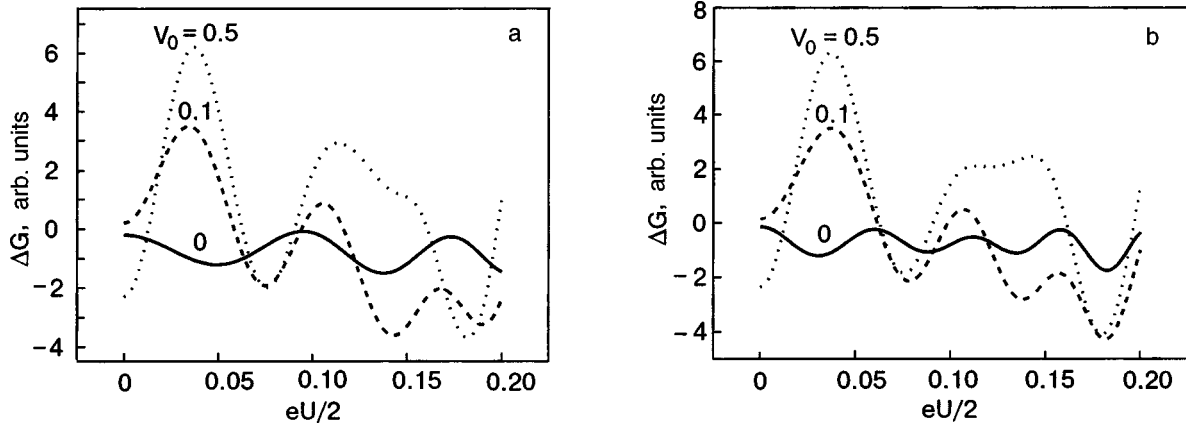


FIG. 3. Dependence of the conductance on $eU/2$ (in units of the Fermi energy) in the presence of two defects in the contact (impurities located on one side (a) and on different sides (b) of the barrier); $\rho_1 = \chi_F$, $\rho_2 = 1.5\chi_F$, $g_0 = 0.1$, $R = 3\chi_F$, $V_0 = mV/(\hbar^2 k_F)$, $g_0 = mg/(\pi R^2 \hbar^2 k_F)$.

responds to the first and second terms in formula (20). It is interesting to note that the conductance of the contact contains a term proportional to g , which is absent when impurity scattering processes are taken into account with the quantum analog of the collision integral, for example. Although this term vanishes after averaging over positions of a large number of impurities, in a mesoscopic contact with several defects and a barrier it can play a decisive role. The additional phase shift depends on the distance between impurities, their distribution relative to the barrier, the possible variation of the magnitude of the wave vector k_β (the index β of the quantum mode) in scattering on an impurity and also in the reflection of an electron from the barrier. We note that the interaction of an electron with the barrier in the framework of this model does not lead to mixing of the quantum modes. The contribution of the interference terms to the conductance depends substantially on the position of the impurities relative to the axis of the contact, \mathbf{R}_i , and is determined by the local density of states for the β th mode at the point \mathbf{R}_i : $\nu_\beta(\mathbf{R}_i, E) = m\psi_{\perp\beta}^2(\mathbf{R}_i)/(\hbar^2 k_\beta(E))$. Since the transverse wave functions $\psi_{\perp\beta}$ vanish at certain points, the scattering on impurities located near such points contributes little to the conductance of the β th mode. In particular, impurities on the surface do not influence the conductance.

Figure 3 shows the voltage-dependent part of the con-

ductance $\Delta G(U)$ for various values of the barrier potential V and for two impurities located on the same side or on different sides of the barrier (all the numerical calculations were done at zero temperature). These curves show that even at relatively small values of V the contribution corresponding to a single act of scattering on an impurity and reflection from the barrier becomes dominant. For comparison Fig. 4 shows the analogous dependence $\Delta G(U)$ calculated in second-order perturbation theory in the coupling constant g .

Figure 5 shows the dependence $\Delta G(U)$ for a single-mode channel $\beta = (0,1)$ at different values of its radius. At $R = 3\chi_F$ the energy of the quantum mode ε_{01} is quite far from the Fermi level ε_F , while for $R = 2.6\chi_F$ it is found near the Fermi level. These dependences clearly demonstrate suppression of the oscillations of $\Delta G(U)$ near the steps where the conductance jumps occur; this agrees with the experimental result of Ref. 14. In the framework of our model this decrease in the conductance oscillations has a natural physical explanation. The coefficient of transmission of an electron through the barrier, T_{01}^b (14), depends on the mode energy ε_β , which, according to formula (7), decreases with increasing radius R . When R approaches the value R_2 corresponding to the entry of the next mode with a higher energy ε_{11} in the channel, the coefficient T_{01}^b increases and the interference contribution due to reflection from the barrier is

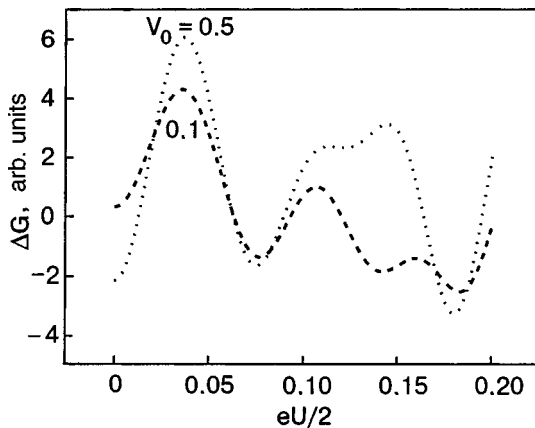


FIG. 4. Dependence of the conductance on $eU/2$ (in units of the Fermi energy) calculated in the linear approximation in the coupling constant g ; $\rho_1 = \chi_F$, $\rho_2 = 1.5\chi_F$, $g_0 = 0.1$, $R = 3\chi_F$.

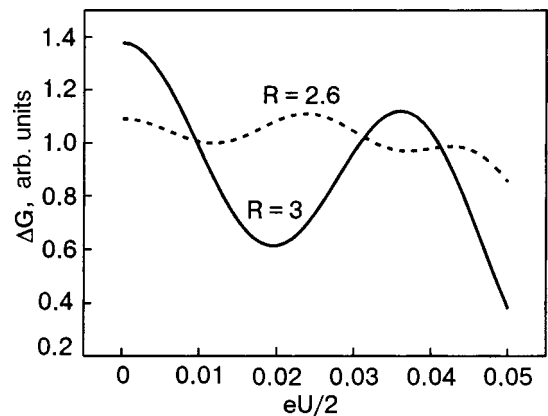


FIG. 5. Dependence on $eU/2$ (in units of the Fermi energy) of the conductance of a single-mode channel ($\beta = (0,1)$) for different values of the radius of the contact (the radius is indicated in units of χ_F); $g_0 = 0.1$, $V_0 = 0.1$.

minimum. The conductance oscillations are small near $R = R_2$ in the two-mode channel ($R > R_2$) as well, since $T_\beta^b \rightarrow 0$ for $E \rightarrow \varepsilon_\beta$, as can easily be seen from formula (14).

CONCLUSION

In this paper we have investigated theoretically the non-linear conductance $G(U)$ of a quantum channel containing single impurities and a barrier. It is shown that the additional phase shift of the wave function, which depends on the distances between impurities or between impurities and the barrier, leads to oscillations of the transmission probability of an electron through the contact as a function of the electron energy E . Upon reflection of the electron from the barrier or transmission through it, the electron wave function also acquires a certain phase $\varphi_\beta(E)$. Increasing the applied voltage U alters the energies of the incoming electrons, leading to a nonmonotonic dependence of $G(U)$. The function $G(U)$ is aperiodic (it cannot be represented by a finite number of Fourier harmonics with respect to the voltage U) because of the complicated dependence of the phase of the wave functions on the energy E . The amplitude of the nonmonotonicities of the conductance $G(U)$ is determined by the distribution of impurities relative to the axis of the contact. Impurities located at points where the local density of electron states for one of the quantum modes vanishes and impurities on the surface of the contact do not influence the contribution to the conductance from that mode. We have shown that the reflection of electrons from a barrier in the contact become the main cause of nonmonotonic behavior of $G(U)$ already at extremely small amplitudes of that reflection (the absolute value of the conductance is close to the value it has in a ballistic contact in the absence of a barrier). The results obtained provide evidence that the energy dependence of the probability of transmission of electrons through the barrier can account for the experimentally observed¹⁴ suppression of conductance oscillations of a single-mode contact having a diameter close to the value corresponding to the entry of the next quantum mode.

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