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The quantum conductance of ballistic microconstrictions in metals with an open Fermi surface

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It is shown that the conductance G of a quantum microconstriction in a metal with an open Fermi surface undergoes jumps e^2/h of the opposite sign as a function of the contact diameter. The negative jumps are a result of the limitation of the energy of the electron motion along the direction in which the Fermi surface is open. The point contact spectrum dG/dV of such a constriction has additional peaks at the bias eV where the maximum energy ε_{max} of the quantum subband is equal to the energies $\varepsilon_F \pm eV/2$ (ε_F is the Fermi energy).

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The quantum size effect in conductors was predicted theoretically by I. Lifshits and A. Kosevich in 1955 [1] and was found experimentally in thin films of metals and semiconductors (see, for example, [2]). In these studies, quasiclassical oscillations of the thermodynamic and kinetic properties were investigated, because of the limited range of the sample thicknesses d which were then accessible (as usual $d >> \lambda_F$, where λ_F is the Fermi wavelength). Advances in the modern technology of nanofabrication make it possible to realize the ultraquantum limit of the size effect in the conducting properties by using small ballistic contacts of a size comparable to the Fermi wavelength. The current I through such a microconstriction is governed by the currents of one-dimensional quantum subbands, each of which contribute to the conductance $G = dI/dV$ a value $G_0 = 2e^2/h$ (V is the voltage applied to the contact). As a result, the conductance G displays a step-like structure versus contact size. For «large» contacts ($d >> \lambda_F$) this structure turns in to quasiclassical oscillations. The conductance quantization effect was first observed in a model system in the two-dimensional (2D) electron gas formed at a GaAs–$Al_xGa_{1-x}As$ heterojunction [3,4]. The development of methods of scanning tunneling microscopy and mechanically controllable break junctions enables one to investigate the conductivity of ultrasmall (down to atomic size) contacts in real metals [5–8]. By using these methods the quantum steps of the conductance were observed in three-dimensional (3D) point contacts. In the simple metals (Na, Cu, Au) the conductance steps are rather similar to the conductance of 2D contacts [8–10]. But for metals with a more complicated electronic structure, such as Al and Pt, the size dependence of the conductance has a more irregular behavior, as compared to the simple metals [9]. In Al and Pt the first few conductance plateaus have positive slope. It signifies that the conductance decreases when the contact size increases. In some cases weakly expressed negative steps of the conductance have been observed [9]. One of the reasons for negative slope may be the resonances due to the electron reflection at the ends of the constriction [11].

The theory of electron transport in mesoscopic microconstrictions (see, e.g., [12]) explains the conductance quantization as being the result of the existence of discrete transverse electron states (modes). With increasing contact diameter new modes open up, and the conductance increases in a

sequence of steps of height G_0 [13]. At finite voltages, as a result of the splitting of the Fermi surface in the constriction by the applied bias eV [14,15], a steplike structure of the nonlinear conductance occurs at integer multiples of $G_0/2$, as function of the constriction width [16]. The new period of the quantum steps is caused by the difference of the maximum energy of electrons with different directions of the electron velocity $v_{\|}$ along the contact axis. With increasing contact width a new quantum mode opens up nonsimultaneously for electrons with the energy $\varepsilon_F + eV/2$ and the energy $\varepsilon_F - eV/2$. Each time, when a quantum mode opens up for one of the two directions of the vector $v_{\|} \lessgtr 0$, the conductance increases by $G_0/2$. If the bias eV is larger than the distances between the energy levels of quantum modes, it is possible to change the number of opened modes by changing the voltage V. In this case the conductance jumps in a sequence of steps of height $G_0/2$, as a function of the voltage V. This effect can be used for a spectroscopy of energy levels in quantum constrictions [17]. The conductance quantization in 3D point contacts of a metal with a spherical Fermi surface was considered in the theoretical papers [18,19]. It was found that for sufficiently long the constrictions conductance has the steplike dependence on the contact diameter. For the symmetric model of the contact, because the degeneracy of the electron energy with respect to one of discrete quantum numbers, the conductance has not only steps G_0 , but also steps $2G_0$ [18,19].

In a majority of real metals the Fermi surface is a complicated periodic surface, which continuously passes through the whole inverse lattices (open Fermi surface). The energy $\varepsilon_{\|}$ of the electron motion in the direction in which the Fermi surface is open is limited ($0 \le \varepsilon_{\|} \le \varepsilon_1$), and its maximum value ε_1 may be considerably smaller than the Fermi energy ε_F . That leads to phenomena such as, for example, the linear magnetoresistance of polycrystals [20] (Kapitsa effect [21]) or the oscillation of the resistance of single crystals as a function of the direction of the strong magnetic field [22], which are absent in conductors with a closed Fermi surface. The limitation of the electron velocity in some direction is most important in the «organic layered metals», the Fermi surface of which is a slightly «warped» cylinder [23].

In this paper we analyze the conductance of 3D quantum microconstriction in a metal with an open Fermi surface. It is shown that the conductance G may display not only steps G_0 but also negative steps $-G_0$, as a result of the limited width of quantum conducting subbands $\Delta\varepsilon = \varepsilon_{\max} - \varepsilon_{\min}$. The point contact spectrum (dG/dV) contains two series of maxima. One of them corresponds to the voltages $eV = \pm 2(\varepsilon_F - \varepsilon_{\min})$, as in 2D microconstrictions and 3D point contacts in metals with an isotropic Fermi surface [17]. The second series of maxima satisfies the condition $eV = \pm 2(\varepsilon_F - \varepsilon_{\max})$.

If the contact axis coincides with the axis of the open Fermi surface, for the participation of the nth quantum mode in the electrical current, not only must the minimum energy of the transverse mode $\varepsilon_{\min}(\mathbf{n})$ be smaller than $\varepsilon_F \pm eV/2$, but also $\varepsilon_{\max}(\mathbf{n}) \ge \varepsilon_F \pm eV/2$, where $\mathbf{n} = (n_1 , n_2)$ is the set of two transverse discrete quantum numbers, $\varepsilon_{\min}(\mathbf{n})$ and $\varepsilon_{\max}(\mathbf{n})$ are the minimum and maximum energies of the quantum subband, which is characterized by the set $\mathbf{n}$. As a result, with increasing contact diameter d, starting from the energy $\varepsilon_{\max}(\mathbf{n}, d) = \varepsilon_F \pm eV/2$, the nth mode does not contribute to the conductivity.

We consider a model of the microconstriction in the form of a long ballistic channel of length L and diameter $d << L$, which is smoothly (adiabatically [24]) connected with bulk metallic reservoirs. In the long ($L >> d$) ballistic channel the «duplicated» electron distribution function $f(\varepsilon)$ has the form [14,15]

$$f(\varepsilon) = f_F\left(\varepsilon + \frac{eV}{2}\,\mathrm{sign}\; v_z\right), \qquad (1)$$

where $f_F(\varepsilon)$ is the equilibrium Fermi distribution. The distribution function $f(\varepsilon)$ (1) is valid if the bias is small $eV << \sqrt{\varepsilon_F \delta\varepsilon}$ (where $\delta\varepsilon$ is the characteristic distance between quantum levels of the transverse motion). With this inequality, which we suppose is fulfilled, the distribution (1) satisfies the condition of the electroneutrality, and the electric field inside the channel is negligibly small.

The total current flowing through the contact can be described by a Landauer-type formula [25], which at finite voltages is given by

$$I = \frac{2e}{h}\sum_{\mathbf{n}}\int_{\varepsilon_{\min}}^{\varepsilon_{\max}} d\varepsilon\left[f_F\left(\varepsilon - \frac{eV}{2}\right) - f_F\left(\varepsilon + \frac{eV}{2}\right)\right]. \qquad (2)$$

The expression (2) has a clear physical meaning: The bias eV applied to the contact splits the Fermi surface of the injected electrons into the channel into two parts ($v_{\|} > 0$ and $v_{\|} < 0$) with maximum energies differing by eV. The net current inside the contact is determined by the contributions of these

two electron streams moving in opposite directions, with energies differing by the bias energy eV.

After the integration in Eq. (2) over the energy ε we obtain the following equation for the ballistic conductance:

$$G = \frac{dI}{dV} = \frac{1}{2} G_0 \sum_{\mathbf{n}} \left[f_F\left(\varepsilon_{\min} + \frac{eV}{2}\right) + \right.$$

$$\left. + f_F\left(\varepsilon_{\min} - \frac{eV}{2}\right) - f_F\left(\varepsilon_{\max} + \frac{eV}{2}\right) - f_F\left(\varepsilon_{\max} - \frac{eV}{2}\right) \right] . \quad (3)$$

At $V \to 0$ formula (3) describes the G_0 steps of the conductance as a function of the contact size:

$$G = G_0 \sum_{\mathbf{n}} [f_F(\varepsilon_{\min}) - f_F(\varepsilon_{\max})] . \quad (4)$$

Let us consider a «model metal» with the Fermi surface

$$\varepsilon(\mathbf{p}) = \varepsilon_0 (\mathbf{p}_\perp) + \varepsilon_1(\mathbf{p}_\perp) \cos\left(\frac{p_\parallel a}{\hbar}\right); \quad \varepsilon_1 < \varepsilon_0 , \quad (5)$$

where a is the separation between the atoms. The «warped» cylinder $\varepsilon(\mathbf{p})$ is an infinite surface in the direction $p_\parallel$ and in this direction passes through all cells of the reciprocal space. If the contact axis is parallel to the $p_\parallel$ axis, the transverse part ε_0 of the total energy is quantized $\varepsilon_0 = \varepsilon_0(\mathbf{n})$. But in the difference from the spherical Fermi surface, the widths of quasi-one-dimensional subbands have the limited value $\varepsilon_1(\mathbf{n})$. So, if the energy $\varepsilon_{\max}(\mathbf{n}) = \varepsilon_0(\mathbf{n}) + \varepsilon_1(\mathbf{n})$ is smaller than the Fermi energy ε_F, the subband below the Fermi level is completely filled and does not participate in the current. That results in the negative steps $-G_0$ under the condition $\varepsilon_{\max}(\mathbf{n}) = \varepsilon_F$. The Fig. 1 illustrates the conductance of a channel of square cross section as a function of the size d. For simplicity we used a model of the Fermi surface in which $\varepsilon_0 = \mathbf{p}_\perp^2/2m$ and $\varepsilon_1 = \text{const}$.

By changing the voltage eV we can change the number of open quantum modes for different directions of the electron velocity [17]. In a metal with a closed Fermi surface, if the bias is larger than the distances between energy levels, then as the voltage is increased, the number of quantum modes below the energy level $\varepsilon_F + eV/2$ increases (and each time the conductance increases by $G_0/2$), while the number of modes below the level $\varepsilon_F - eV/2$ decreases, and that leads to jumps $-G_0/2$. The peaks on the point-contact spectrum dG/dV are determined by the minimum energies of the transverse

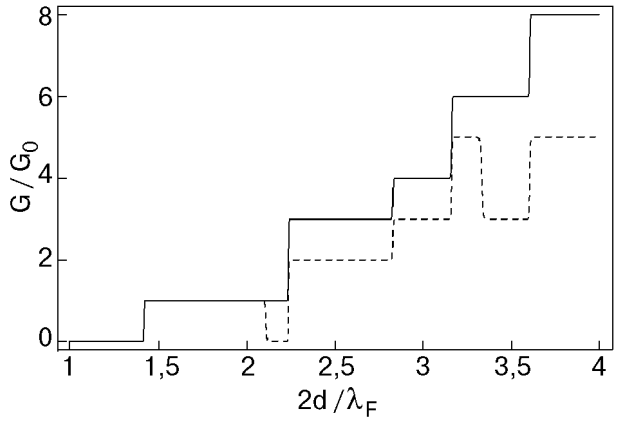

Fig. 1. Quantum steps of the conductance in the limit $V \to 0$. The solid line is for $\varepsilon_1 = 0.9\,\varepsilon_F$, the dashed line for $\varepsilon_1 = 0.55\,\varepsilon_F$; $T = 0.001\,\varepsilon_F$.

electron modes $\varepsilon_{\min}$ [17]. In the case of an open Fermi surface, increasing the bias leads not only to this but also to the opposite processes: at some voltages the maximum energies $\varepsilon_{\max}$ of the subbands go through the energy levels $\varepsilon_F \pm eV/2$, changing the conductance by values $\pm G_0/2$. As a result, the point-contact spectrum has two series of sharp peaks at energies $\varepsilon_F \pm eV/2 = \varepsilon_{\min}(\mathbf{n})$ and $\varepsilon_F \pm \pm eV/2 = \varepsilon_{\max}(\mathbf{n})$. Measuring of the distances between these peaks makes it possible to find not only the (minimal) energy of quantum modes in the constriction, but also the width of the quantum subbands and its dependence on the number of the mode. In Figs. 2, 3 the voltage dependence of the quantized conductance and the point contact spectrum of the same constriction are shown.

In the quasiclassical case, we can use the Poisson formula for the summation over discrete quantum numbers in Eq. (3). Using the method developed by Lifshits and Kosevich [1], we can write the conductance at zero temperature in the form

$$G = G_{\text{Sh}} + G_0 \frac{2}{\pi} \sum_{\mathbf{k},i} \sum_{\alpha=1}^{2} (-1)^\alpha \left[|\mathbf{k}|^{1/2} \, |\nabla\varepsilon(\mathbf{n}_{i,\alpha})| \times \right.$$

$$\left. \times |K_{i,\alpha}|^{1/2} \left(\mathbf{k} \frac{\partial \mathbf{n}_{i,\alpha}}{\partial \varepsilon} \right) \right]^{-1} \sin\left(2\pi \mathbf{k}\mathbf{n}_{i,\alpha} \pm \frac{\pi}{4}\right) \times$$

$$\times \cos \pi \mathbf{k} \frac{\partial \mathbf{n}_{i,\alpha}}{\partial \varepsilon} eV . \quad (6)$$

Here G_{Sh} is the Sharvin conductance [14]; the vector $\mathbf{k}$ is the aggregate of two positive integers k_1 and k_2; $\mathbf{n}_{i,1}$ are the coordinates of the points on the curve $\varepsilon_{\max}(\mathbf{n}) = \varepsilon_F$, and $\mathbf{n}_{i,2}$ are the coordinates of

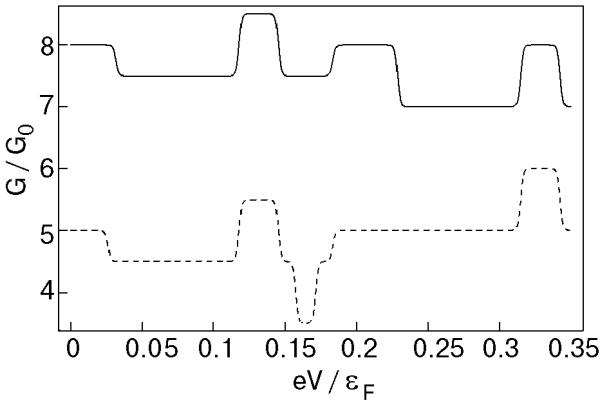

Fig. 2. The dependence of the conductance on the applied voltage. The solid line is for $\varepsilon_1 = 0.9\,\varepsilon_F$, the dashed line for $\varepsilon_1 = 0.5\,\varepsilon_F$; $T = 0.001\varepsilon_F$; $d = 1.95\,\lambda_F$.

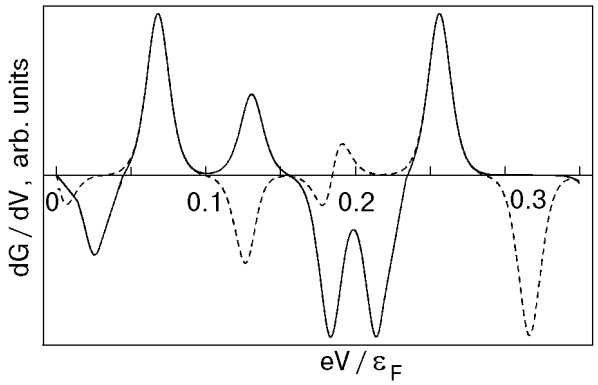

Fig. 3. The point contact spectrum of the microconstriction. The solid line is for $\varepsilon_1 = 0.9\,\varepsilon_F$, the dashed line for $\varepsilon_1 = 0.5\,\varepsilon_F$; $T = 0.005\,\varepsilon_F$; $d = 1.95\,\lambda_F$.

the points on the curve $\varepsilon_{\min}(\mathbf{n}) = \varepsilon_F$, at which the normal to these curves is parallel to the vector $\mathbf{k}$; $K_{i,\alpha}$ is the curvature of the curve $\varepsilon(\mathbf{n}) = \varepsilon_F$ at the points $\mathbf{n}_{i,\alpha}$. The sign before the phase $\pi/4$ is minus if at the point $\mathbf{n}_{i,\alpha}$ the convexity of the curve is directed in the direction of vector $\mathbf{k}$. In the opposite case, the sign before $\pi/4$ is plus. In Eq. (6) the summation is over $\mathbf{k} \neq 0$ and all points $\mathbf{n}_{i,\alpha}$ in the first quadrant. Hence, in the quasiclassical region the conductance oscillate as a function of the constriction diameter and the applied bias, and also depends on the maximum energy of electron motion along the constriction.

Thus the conductance of three-dimensional point contacts between metals with an open Fermi surface may display positive and negative steps $2e^2/h$ as a function of the contact diameter. The negative steps can be observed in the experimental geometry in which the contact axis is parallel to the direction in which the Fermi surface is open. The decreasing of the conductance is a result of the complete population of quantum subbands below the Fermi level. The negative steps of the quantum conductance in Al and Pt, which have an open Fermi surface, could be a result of this effect. Of course, the electronic structure of Al and Pt is very complicated, and electrical properties of these metals cannot be described by the simple model (5). The effect of the open part of the Fermi surface may be masked by the influence on the conductivity of other parts, and instead of negative jumps a negative slope of the conductance plateaus was observed in experiments [9]. Recently research on of the nonlinear quantum conductance has begun [26,27]. The ultrasmall size of a point contact makes it possible produce biases up to 1 V [26], which opens up the possibility of point-contact spectroscopy of quantum energy modes in three-dimensional contacts. An experimental investigation of point-contact spectra for different directions of the contact axis with respect to the crystallographic orientation of the sample to be studied could enable observation of the effects discussed theoretically in this paper, manifested in the voltage dependence of the conductance of quantum microconstrictions.

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