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The influence of single magnetic impurities on the conductance of quantum microconstrictions

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The nonlinear ballistic conductance of three-dimensional quantum microconstrictions, which contain a magnetic impurities, is investigated. The nonlinear part of the conductance, which is due to the interaction of electrons with magnetic impurities, is obtained. The analytical results have been analyzed numerically. It is shown that the intensity of the Kondo anomaly in the conductance as a function of the applied voltage depends on the diameter of the constriction and the positions of the impurities.

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The impurity-electron interaction in Kondo systems can be effectively studied by using point contacts (PCs). In the first measurements of the differential PC resistance $R(V)$ in metals with magnetic impurities the zero-bias Kondo anomaly was observed [1–3]. These experiments were explained by quasiclassical theory of Kondo effect in PCs [4]. It was shown that in the second-order Born approximation the magnetic impurity contribution to the PC resistance includes the logarithmic dependence $R(V) \sim \ln(V)$ for $eV >> T_K$ and saturation for $eV << T_K$ (T_K is the Kondo temperature, V is the voltage applied to the PC). In accordance with the theory [4], the nonlinear correction to the ballistic PC resistance is proportional to the contact diameter. But in the experiments [1–3] the size dependence of the PC current was not investigated due to the limited range of contact diameters accessible.

The development of the technique of mechanically controllable break junctions (MCBJ) has made it possible to create stable PCs with the diameter adjustable over a broad range, down to a single atom [5,6]. In the MCBJ experiments [7,8] the authors had studied the resistance of ultrasmall contacts with magnetic impurities as a function of the PC diameter d. In contrast to the prediction of the quasiclassical theory [4], Yanson at el. [7,8] observed that the Kondo scattering contribution to the contact resistance is nearly independent of the contact diameter d for small d. This behavior was explained by the authors [7,8] as being due to an increase of the Kondo impurity scattering cross section with decreasing contact size.

It has been shown in theoretical works [9] that in very small contacts the discreteness of impurity positions must be taken into account, and the experiments [7,8] may be explained by the «classical» mesoscopic effect of the dependence of the point contact conductance on the spatial distribution of impurities. This effect is essential in «short» contacts, and in the quasiclassical approximation it disappears with increasing contact length. Zarand and Udvardi [10] considered a contact in the form of a long channel and suggested that the Kondo temperature T_K is changed due to the strong fluctuations of the local density of states generated by the reflections of conduction electrons at the surface of the contact. As a result of that, the effective cross section of electrons has a maximum if the position of the impurity inside the contact corresponds to the maximum in the local electron density of states. But the mesoscopic effect of the spatial distribution of impurities in quantum contacts was not analyzed in that paper [10].

In ultrasmall contacts the quantum phenomena known as the quantum size effect occur. The effect of the $2e^2/h$ conductance quantization has been observed in experiments on contacts in the two-dimensional electron gas [11,12] and in ultrasmall three-dimensional constrictions, which are created by using scanning tunneling microscopy [13,14] and mechanically controllable break junctions [15]. Defects produce backscattering of electrons and thus break the quantization of the conductance. On the other hand, the impurities situated inside the quantum microconstriction produce a nonlinear dependence of the conductance on the applied voltage [16]. This dependence is the result of the interference of electron waves reflected by these defects [17,18].

In this paper we present a theoretical solution of this problem for the conductance of a quantum microconstriction in the form of a long ballistic channel containing single magnetic impurities. We study the first- and second-order corrections to the conductance of the ballistic microconstriction in the Born approximation. The effect of impurity positions is taken into account. Within the framework of the long-channel model the quantum formula for the conductance G is obtained. By using the model of a cylindrical microconstriction, the nonlinear conductance as a function of voltage V and the width of constriction d is analyzed numerically for different positions of a single impurity.

Let us consider a quantum microconstriction in the form of a long and perfectly clean channel with smooth boundaries and a diameter d comparable to the Fermi wavelength $\lambda_F = h/\sqrt{2m\varepsilon_F}$, where ε_F is the Fermi energy. We assume that this channel is smoothly (over the Fermi length scale) connected with bulk metal «banks». As was shown in [19,20], in such a constriction an accurate quantization can be obtained in the zeroth approximation in the adiabatic parameter $|\nabla d| << 1$. The corrections to the tunneling and reflection coefficients of electrons due to deviation from the adiabatic constriction are exponentially small, except near the points where the modes are switched on and off [21].

When a voltage V is applied to the constriction, a net current I start to flow. In the limit $V \to 0$, the ballistic conductance of the quantum microconstriction is given by the formula

$$G = \frac{dI}{dV} = G_0 \sum_{\beta} f_F(\varepsilon_\beta) \ , \tag{1}$$

where f_F is the Fermi function, ε_β is the minimal energy of the transverse electron mode, and β is the full set of transverse discrete quantum numbers. The ballistic quantum PC displays the specific nonlinear properties, such as the conductance jumps e^2/h. For the two-dimensional PC these effects were considered in the papers [22,23]. The aim of this study is to analyze the zero-bias Kondo minimum in the PC conductance. We assume that the bias eV is much smaller than not only the Fermi energy ε_F but also the distances between the energies ε_β of quantum modes. In this case the influence of the applied bias on the transmission is negligibly small.

Impurities and defects scatter the electrons, decreasing the transmission probability. In accordance with the standard procedure [24,25], the decrease of the electrical current ΔI due to the electron-impurity interaction is connected with the rate of dissipation of the energy E by the relation:

$$V\Delta I = \frac{dE}{dt} = \frac{d\langle H_1\rangle}{dt} \ . \tag{2}$$

The Hamiltonian H of the electrons contains the following terms:

$$H = H_0 + H_1 + H_{\text{int}} \ , \tag{3}$$

where

$$H_0 = \sum_{k,\sigma} \varepsilon_k \, c^+_{k\sigma} c_{k\sigma} \tag{4}$$

is the Hamiltonian of free electrons, and

$$H_1 = \frac{eV}{2} \sum_{k,\sigma} \text{sign}\,(v_z)\, c^+_{k\sigma} c_{k\sigma} \tag{5}$$

describes the interaction of electrons with electric field. The Hamiltonian of the interaction of electrons with magnetic impurities H_{int} can be written as

$$H_{\text{int}} = \sum_{j,k,k'} \mathbf{J}_{j,k,k'} \, [S_z(c^+_{k'\uparrow} c_{k\uparrow} - c^+_{k'\downarrow} c_{k\downarrow}) + $$

$$+ S^- c^+_{k'\uparrow} c_{k\downarrow} + S^+ c_{k'\downarrow} c_{k\uparrow}] \ . \tag{6}$$

Here the operator $c^+_{k\sigma}$ ($c_{k\sigma}$) creates (annihilates) a conduction electron with spin σ, wave function φ_k, and energy ε_k; $\mathbf{S}$ denotes the spin of the impurity; v_z is the electron velocity along the channel; $\mathbf{J}_{j,k,k'}$ is the matrix element of the exchange interaction of an electron with an impurity at the point $\mathbf{r}_j$; $k\sigma$ is the full set of quantum numbers; and,

$$\mathbf{J}_{j,k,k'} = \int d\mathbf{r}\, J(\mathbf{r}, \mathbf{r}_j)\varphi_k(\mathbf{r})\varphi^*_{k'}(\mathbf{r}) \ . \tag{7}$$

The electron wave functions and eigenvalues in the long channel in the adiabatic approximation are

$$\varphi_k(\mathbf{r}) = \psi_\beta(\mathbf{R}) \exp\left(\frac{i}{\hbar} p_z z\right); \tag{8}$$

$$\varepsilon_k = \varepsilon_\beta + \frac{p_z^2}{2m_e}, \tag{9}$$

where $k = (\beta, p_z)$, p_z is the momentum of an electron along the contact axis; m_e is the electron mass; $\mathbf{r} = (\mathbf{R}, z)$, with $\mathbf{R}$ the coordinate in the plane perpendicular to the z axis.

Differentiating $\langle H_1 \rangle$ over the time t, we obtain the equation for the change ΔI of the current as a result of the interaction of electrons with magnetic impurities:

$$V\Delta I = \frac{1}{i\hbar} \langle [H_1(t), H_{\text{int}}(t)] \rangle, \tag{10}$$

where

$$\langle \ldots \rangle = \text{Tr}\,(\rho(t) \ldots). \tag{11}$$

All operators are in the interaction representation.

The density matrix $\rho(t)$ satisfies the equation

$$i\hbar \frac{\partial \rho}{\partial t} = [H_{\text{int}}(t), \rho(t)], \tag{12}$$

which can be solved using perturbation theory:

$$\rho(t) = \rho_0 + \frac{1}{i\hbar} \int_{-\infty}^{t} dt' [H_{\text{int}}(t'), \rho_0] + \frac{1}{(i\hbar)^2} \int_{-\infty}^{t} dt' \int_{-\infty}^{t'} dt'' \, [H_{\text{int}}(t'), [H_{\text{int}}(t''), \rho_0]] \ldots \tag{13}$$

By means of Eq. (13) the change in the electric current due to magnetic impurities can be determined as

$$\Delta I = I_1 + I_2 + \ldots = -\frac{1}{\hbar^2 V} \int_{-\infty}^{t} dt' \, \text{Tr}\,(\rho_0 [[H_1, H_{\text{int}}(t)], H_{\text{int}}(t')]) - \frac{1}{i\hbar^3 V} \times \int_{-\infty}^{t'} dt'' \int_{-\infty}^{t} dt' \, \text{Tr}\,(\rho_0 [[[H_1, H_{\text{int}}(t)], H_{\text{int}}(t')], H_{\text{int}}(t'')]) + \ldots \tag{14}$$

After simple but cumbersome calculations, we find the first- and second-order corrections to the PC current

$$I_1 = -\frac{\pi e}{\hbar} s(s+1) \sum_{n,m} \sum_{i,j} (\text{sign}\, v_{zk} - \text{sign}\, v_{zn}) \times (f_m - f_n) \delta(\varepsilon_n - \varepsilon_m) \, \mathbf{J}_{j,n,m} \mathbf{J}_{i,m,n}. \tag{15}$$

$$I_2 = \frac{\pi e}{\hbar} s(s+1) \sum_{n,m,k} \sum_{i,j,l} (\text{sign}\, v_{zk} - \text{sign}\, v_{zn}) \times \left[\delta(\varepsilon_n - \varepsilon_k) \, \text{Pr} \frac{1}{\varepsilon_m - \varepsilon_k} + \delta(\varepsilon_m - \varepsilon_k) \, \text{Pr} \frac{1}{\varepsilon_n - \varepsilon_k} \right] \times [\mathbf{J}_{j,n,k} \mathbf{J}_{i,m,n} \mathbf{J}_{l,k,m} + \mathbf{J}_{j,k,n} \mathbf{J}_{i,n,m} \mathbf{J}_{l,m,k}] \times (f_m - f_k)(1 - 2f_n), \tag{16}$$

where $f_n = f_F[\varepsilon_n + (eV/2)\, \text{sign}\, v_z]$. The first addition I_1 to the PC current describes a small spin-dependent correction (of order $(J/\varepsilon_F)^2$) to the change of the current due to the usual scattering. The second addition I_2 is also small too, but contains the Kondo logarithmic dependence on the voltage, and it is the most important for the analysis of the nonlinear conductance of constrictions with magnetic impurities.

The expressions (15) and (16) can be further simplified in the case of a δ-function potential of the impurities

$$J(\mathbf{r}) = \frac{J}{n_e} \delta(\mathbf{r}), \tag{17}$$

where n_e is the electron density. In this case the addition I_2 to the ballistic current has the form:

$$I_2 = \frac{2\pi e^2}{\hbar} \left(\frac{J}{n_e}\right)^3 s(s+1) \sum_{n,m,k} \sum_{i,j,l} (\text{sign}\, v_{zk} - \text{sign}\, v_{zn}) \times \left[\delta(\varepsilon_n - \varepsilon_k) \, \text{Pr} \frac{1}{\varepsilon_m - \varepsilon_k} + \delta(\varepsilon_m - \varepsilon_k) \, \text{Pr} \frac{1}{\varepsilon_n - \varepsilon_k} \right] \times (f_m - f_k)(1 - 2f_n) \times \text{Re}\, [\varphi_k^*(\mathbf{r}_j) \varphi_n^*(\mathbf{r}_i) \varphi_m^*(\mathbf{r}_l) \varphi_k(\mathbf{r}_l) \varphi_m(\mathbf{r}_i) \varphi_n(\mathbf{r}_j)]. \tag{18}$$

It follows from Eqs. (16), (18) that the current I_2 depends on the positions of the impurities. Two effects influence the value of I_2 : the effect of quantum interference of scattered electron waves, which depends on the distances between impurities, and effect of the electron density of states at the points where the impurities are situated. The nonlinear part of the conductance can be easy obtained after differentiation of Eq. (18) with respect to the voltage $G_2 = dI_2/dV$. In the case of a single impurity and at zero temperature $T = 0$ this equation can be integrated analytically over the momentum p_z, and the conductance G_2 takes the form

$$G_2 = -\frac{\pi e^2 m_e^3}{\hbar^4}\left(\frac{J}{n_e}\right)^3 s(s+1) \sum_{\alpha,\beta,\gamma} \sum_{\kappa=\pm} |\psi_\alpha(\mathbf{R})|^2 |\psi_\beta(\mathbf{R})|^2 |\psi_\gamma(\mathbf{R})|^2 [p_\alpha^{(\kappa)} p_\beta^{(\kappa)} p_\gamma^{(\kappa)}]^{-1} \times$$

$$\times\left[\ln\left|\frac{p_\gamma^{(\kappa)} - p_\gamma^{(-\kappa)}}{p_\gamma^{(\kappa)} + p_\gamma^{(-\kappa)}}\left(\frac{p_\alpha^{(\kappa)}}{p_\gamma^{(\kappa)}}\right)\right| + (1-\delta_{\alpha\beta}) \ln\left|\frac{p_\alpha^{(\kappa)} p_\beta^{(-\kappa)} - p_\alpha^{(-\kappa)} p_\beta^{(\kappa)}}{p_\alpha^{(\kappa)} p_\beta^{(-\kappa)} + p_\alpha^{(-\kappa)} p_\beta^{(\kappa)}}\right| + \delta_{\alpha\beta} \ln\left|\frac{(p_\alpha^{(\kappa)})^2 - (p_\beta^{(-\kappa)})^2}{(p_\alpha^{(-\kappa)})^2}\right|\right], \quad (19)$$

where

$$p_\alpha^{(\pm)} = \left[2m_e\left(\varepsilon_F \pm \frac{eV}{2} - \varepsilon_\alpha\right)\right]^{1/2}, \quad (20)$$

and the transverse parts of the wave function $\psi_\alpha(\mathbf{R})$ and the electron energy ε_α are given by Eqs. (8), (9).

Carrying out the numerical calculations, we use the free electron model of a point contact consisting of two infinite half spaces connected by a long ballistic cylinder of a radius R and length L (Fig. 1). In the limit $L \to \infty$ the electron wave functions $\psi_\alpha(\mathbf{R})$ and eigenstates ε_α can be written as

$$\psi_\alpha(\mathbf{R}) = \frac{1}{\sqrt{\pi}\, R J_{m+1}(\gamma_{mn})} J_m(\gamma_{mn}\rho/R) \exp(im\varphi);$$
$$\varepsilon_\alpha = \frac{\hbar^2}{2m_e R^2}\gamma_{mn}^2, \quad (21)$$

where we have used cylindrical coordinates $\mathbf{r} = (\rho, \varphi, z)$ with the z axis along the channel axis. Here γ_{mn} are the nth zero of the Bessel function J_m. Because of the degeneracy of the electron energy with respect to azimuthal quantum number m (as a result of the symmetry of the model), quantum modes with $\pm m$ give the same contribution to the conductance. In this model the ballistic conductance (1) has not only steps G_0, but also steps $2G_0$ [20,26].

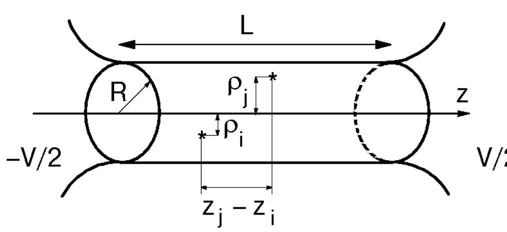

Fig. 1. Schematic representation of a ballistic microconstriction in the form of a long channel, adiabatically connected to large metallic reservoirs. Magnetic impurities inside the constriction are shown.

In Fig. 2 the dependence of the nonlinear conductance on the applied bias is shown for different positions of a single magnetic impurity inside the channel. The results obtained confirm that the nonlinear effect is strongly dependent on the position of the impurity. If the impurity is situated near the surface of the constriction, $\mathbf{r} = \mathbf{R}$, where the square modulus of the electron wave function is small, its influence on the conductivity is negligible. This conclusion is confirmed by the calculations of the dependence G_2 on the position of the impurity for different numbers of quantum modes (Fig. 3). The results indicate that the mesoscopic effect of the impurity position is more essential for ultrasmall contacts, which contain only a few conducting

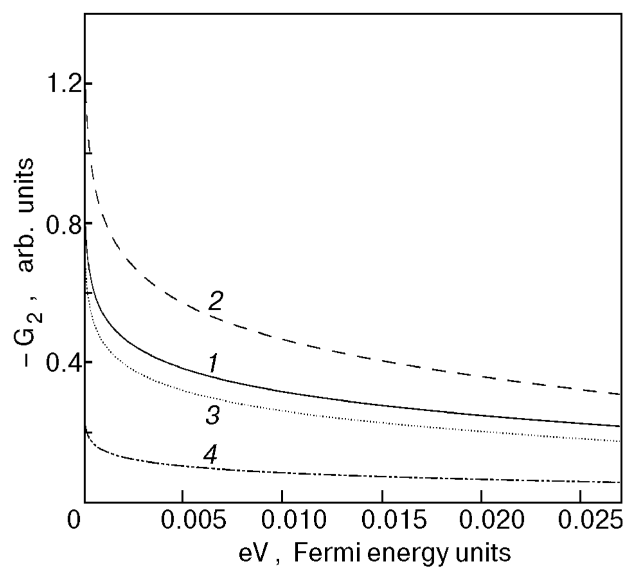

Fig. 2. The voltage dependence of the nonlinear part of the conductance G_2 (19) for different distances of the impurity from the contact axis ($2\pi R = 5.2\lambda_F$; $T = 0$; *1* — $2\pi\rho = 1.5\lambda_F$; *2* — $2\pi\rho = 2.5\lambda_F$; *3* — $2\pi\rho = 3.0\lambda_F$; *4* — $2\pi\rho = 3.5\lambda_F$).

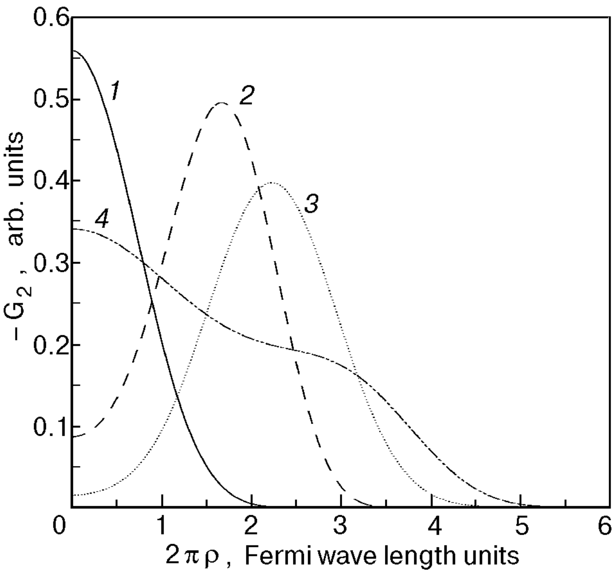

Fig. 3. The dependence of G_2 (19) on the position of the impurity for different numbers of quantum modes in the constriction ($V = 0.02\varepsilon_F$; $T = 0$; *1* — one mode ($2\pi R = 3\lambda_F$); *2* — three modes ($2\pi R = 4\lambda_F$); *3* — five modes ($2\pi R = 5.3\lambda_F$); *4* — six modes ($2\pi R = 6\lambda_F$).

modes, and G_2 has a maximum. Similar results are obtained for the dependence of G_2 on the radius R of the constriction (Figs. 4, 5). In the single-mode constriction (Fig. 4) the conductance G_2 displays a much stronger dependence on R than in the contact with five conducting modes (Fig. 5).

Thus we have shown that in long quantum microconstrictions the spatial distribution of magnetic impurities influences the nonlinear dependence of the conductance on the applied voltage. This

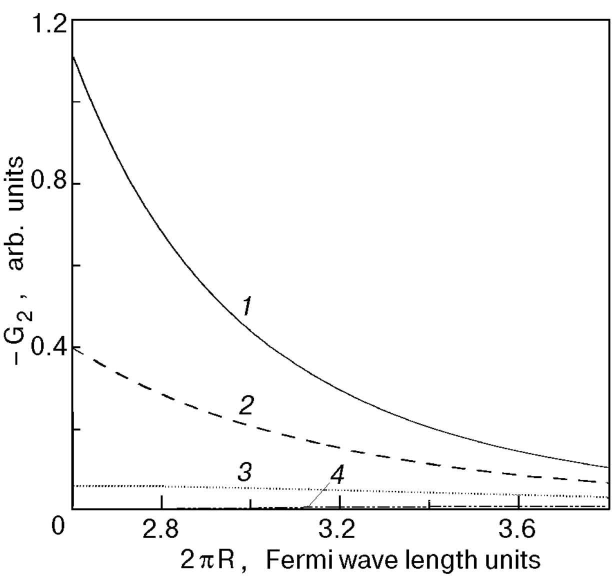

Fig. 4. The dependence of G_2 (19) on the radius of the constriction for a single-mode channel and different positions of the impurity ($V = 0.02\varepsilon_F$; $T = 0$; *1* — $2\pi\rho = 0.5\lambda_F$; *2* — $2\pi\rho = 1.0\lambda_F$; *3* — $2\pi\rho = 1.5\lambda_F$; *4* — $2\pi\rho = 2.0\lambda_F$).

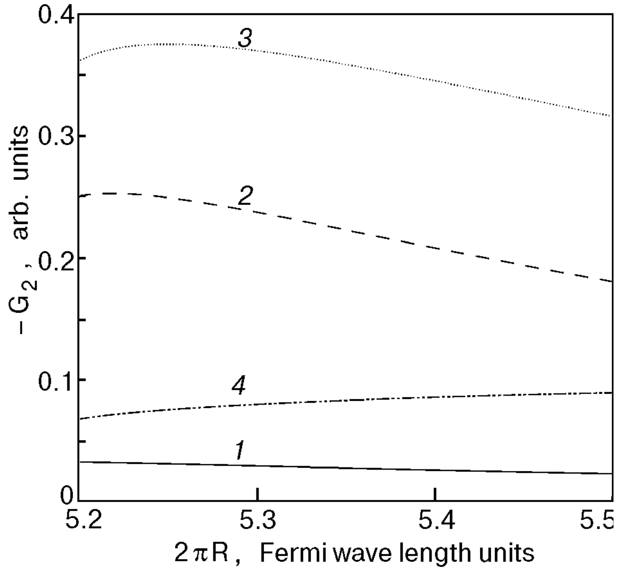

Fig. 5. The dependence of G_2 on the radius for a microconstriction with five quantum modes and different positions of the impurity ($V = 0.02\varepsilon_F$; $T = 0$; *1* — $2\pi\rho = 0.5\lambda_F$; *2* — $2\pi\rho = 1.5\lambda_F$; *3* — $2\pi\rho = 2.5\lambda_F$; *4* — $2\pi\rho = 4.5\lambda_F$).

mesoscopic effect is due to the strong dependence the electron scattering amplitude on the positions of the impurities. As a result of the reflection from the boundaries of the constriction, the electron wave functions corresponding to bounded electron motion in the direction transverse to the contact axis are standing waves. If the impurity is situated near a point at which the electron wave function is equal to zero (near the surface of the constriction or, for quantum modes with numbers $n > 1$, at some points inside), its scattering of electrons is small. The fact is that the amplitude of the Kondo minimum of the conductance of a quantum contact displays the mesoscopic effect of a dependence on the positions of single impurities. This effect is most important in the case when only few quantum modes are responsible for the conductivity of the constriction.

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