Nonlinear conductance of a quantum microconstriction with single slow two-level system

A. Namiranian
Physics Department, Iran University of Science and Technology, Narmak, 16844 Teheran, Iran and Institute for Advanced Studies in Basic Science, Gava Zang, Zanjan 45195-159, Iran

Ye. S. Avotina and Yu. A. Kolesnichenko
B. Verkin Institute for Low Temperature Physics and Engineering, National Academy of Sciences of Ukraine, 47 Lenin Avenue, 310164 Kharkov, Ukraine
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The nonlinear conductance of quantum microconstriction, which contains a single slow two-level system (TLS), was investigated. It is shown that the sign of zero bias anomaly in the point contact spectrum depends on the contact diameter and positions of TLS. This effect is due to the oscillation of local electron density of states inside the quantum microconstriction.

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The two-level system (TLS) is an atom (group of atoms or a dislocation) that can move between two different positions. They play an important role in the low-temperature properties of disordered metals. Historically, TLS's have been introduced by Anderson *et al.*[1] and their influence to different kinetic coefficients of metal glasses has been studied both theoretically and experimentally in many papers (for review, for example, see Ref. 2). Usually two types of TLS's are distinguished: slow and fast TLS's. In slow TLS atom has a transition between two energy states by quantum tunneling through a barrier or by thermal excitation over it. The transition rate in that case may be longer than seconds and an electron scattering by the TLS can be considered as the scattering by defect, which situated in a fixed position. If the electron experiences several transitions of atom during the interaction with it, such a TLS is called a fast TLS. Last TLS is responsible for a low temperature Kondo-like anomaly of kinetic coefficients.[3]

An investigation of bulk samples makes possible to find average characteristics of TLS's, such as an average distance between energy levels and a relaxation time. In mesoscopic conducting systems the electron scattering by a single TLS may significantly change the transport properties and hence the characteristics of certain TLS can be found. One of the classes of mesoscopic systems is point contacts and microconstrictions. The most important feature of ballistic microconstriction is the splitting of the Fermi surface by applied bias for opposite directions of electron velocity along the contact axis.[4] The nonelastic relaxation of this strongly nonequilibrium electron state results in singularities on the second derivative of the current-voltage characteristics d^2I/dV^2 [point-contact spectrum (PCS)[4,5]].

Experimentally it was observed that the electron-TLS interaction leads to a zero bias anomaly (ZBA) of the PCS. This anomaly can have a different sign.[6,7] The positive ZBA may be explained as the nonmagnetic Kondo-like effect.[3] Experiments of Ralph and Buhrman[8] investigating the ZBA in Cu nanoconstrictions are complied with the explanation[9] based on the two-channel Kondo model.[3] In some cases the ZBA appears as a negative peak in the differential resistance curve, which is only predicted in the theory of Kozub and Kulik.[10,11] In the quasiclassical approximation they have calculated the derivative d^2I/dV^2 for the point contact containing the slow TLS. For slow TLS's the sign of the PCS depends on the difference of electron elastic scattering cross-sections by the defect in different positions. If the scattering cross section in the upper state of TLS is less than in the lower state, the PCS has negative ZBA. The negative ZBA's were experimentally observed by Keijers, Sklyarevskii and van Kempen.[12] An intensity of PCS is defined by a position of TLS near the point contact.[11,13] The contact size dependence of the ZBA and the PCS in point contacts containing TLS's were studied in the experiments.[12,14] The different effects in metallic point contacts containing slow TLS's were reviewed in the paper.[7]

In mesoscopic systems the quantum effects are essentially influenced the manifestation of the electron scattering in conducting properties. Therefore the quantum oscillations of local density of states (LDOS's) of electron result in the size dependence of Kondo anomaly in quantum microconstrictions containing single magnetic impurities.[15,16] The reason of this dependence is the changing of the matrix element value of electron-magnetic impurity interaction as diameter of microconstriction is changed. The same effect should be taken into account in quantum constrictions with slow TLS's. In the difference with an impurity in a fixed position, the TLS atom changes its position inside the constriction. For such a TLS a distance between two positions in the perpendicular contact axis direction may be of the order of Fermi wave length. In this case the matrix elements of electron-TLS interaction for two positions could be distinctly different.

In this paper the nonlinear conductance of a long quantum constriction containing a slow TLS inside it is studied theoretically. We obtain different voltage and contact size dependencies of the conductance as well as its dependence on the TLS positions. The effect of atom's position changing after electron nonelastic scattering is taken into account. We predict the quantum analog of Kulik-Kozub effect: the resistance may decrease, as a result of the difference of local density of states for different positions of the defect and show that the ZBA in the PCS can change its sign with

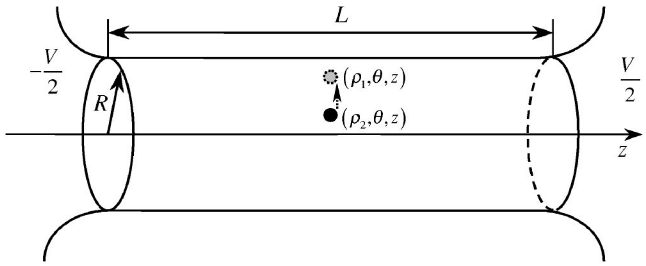

FIG. 1. The model of the quantum microconstriction in the form of a long channel of the radius R, which smoothly (on the Fermi length scale) connects two massive metallic reservoirs. Two positions of the TLS inside the constriction is shown schematically.

changing of the diameter of the constriction. Let us consider the quantum microconstriction in the form of a long ballistic channel with smooth boundaries and a diameter $2R$ comparable with the Fermi wavelength λ_F (Fig. 1). We assume that the channel is smoothly (over Fermi length scale) connected with bulk metal banks. Inside the microconstriction a single TLS is situated. As was shown,[17,18] in such constriction in the zeroth approximation on the adiabatic parameter $|\nabla R| \ll 1$ accurate quantization can be obtained.

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

$$\Psi_j(\mathbf{r}) = \psi_{nm}(\mathbf{r}_\perp)\exp(ik_z z), \quad \varepsilon_j = \varepsilon_{nm} + \frac{\hbar^2 k_z^2}{2m_e}, \tag{1}$$

where $j=(k_z,n,m)$ and (n,m) is the set of discrete transverse quantum numbers; k_z is the wave vector of an electron along the channel axis; m_e is an electron effective mass; $\mathbf{r}=(\mathbf{r}_\perp,z)$, $\mathbf{r}_\perp$ is a coordinate in the plain, perpendicular to the contact axis z; ε_{nm} is the energy of the transverse electron mode, which corresponds to the full set of transverse discrete quantum numbers m and n.

The general formula for a current I through the quantum contact at a arbitrary voltage V was obtained by Bagwell and Orlando.[19] They have shown that the transmission coefficient of electrons through a quantum microconstriction T depends on the applied voltage V because the electron scattering leads to the appearance inside it the nonuniform electrical field. In an almost ballistic microconstriction containing few scatterers the mentioned electrical field is small and we neglect its effect. For a pure ballistic microconstriction the conductance is given by the Landauer-Büttiker formula (for a review see Ref. 20). Below we assume that the applied bias eV is much smaller not only the Fermi energy ε_F, but also the distances between the energies ε_{nm} of quantum modes.

The effect of electron-TLS scattering leads to the decreasing of the transmission probability. In accordance with the standard procedure the changing of the electrical current ΔI due to the presence of TLS in the main on $H_{e-\mathrm{TLS}}$ can be written in the following form:[21,22]

$$\Delta I = -\frac{1}{\hbar^2 V}\int_{-\infty}^{t} dt' \,\mathrm{Tr}\{\rho_0[(H_1(0),H_{e-\mathrm{TLS}}(t)),H_{e-\mathrm{TLS}}(t')]\}, \tag{2}$$

where $\rho_0=f_F(H_0+H_1)$ is the statistical operator for electrons in the channel, f_F is the Fermi function,

$$H_0 + H_1 = \sum_j \varepsilon_j a_j^\dagger a_j + \sum_j \frac{eV}{2}\mathrm{sgn}(k_z) a_j^\dagger a_j; \tag{3}$$

the operator $a_j^\dagger(a_j)$ creates (annihilates) a conduction electron with wave function Ψ_j and energy ε_j. All operators is written in the interaction representation. The TLS can be modeled by a two-well potential, describing the system as occupying one of the two local minima whose energy difference is assumed to be Δ and the tunnelling probability for crossing the barrier between them is Δ_0. In this model the TLS Hamiltonian, H_{TLS} is written as

$$H_{\mathrm{TLS}} = \frac{1}{2}\sum_{\alpha,\beta=1}^{2}(\Delta\sigma^z_{\alpha\beta} + \Delta_0\sigma^x_{\alpha\beta}) b_\alpha^\dagger b_\beta, \tag{4}$$

where α labels the energy minima of TLS, and $b_\alpha^\dagger(b_\alpha)$ is the fermionic operator, which creates (annihilates) an atom in this state, $\sigma^i_{\alpha\beta}$ is the element of ith Pauli matrix. The TLS Hamiltonian can be diagonalized and one can obtain its eigenstates.[7]

The splitting of energy between the two eigenstates is $E=\sqrt{\Delta^2+\Delta_0^2}$. The occupation numbers for the upper and lower eigenstates of the TLS n_+ and n_- satisfy the relation $n_+ + n_- = 1$. The Hamiltonian of electron-TLS interaction can be written as[3]

$$H_{e-\mathrm{TLS}} = \sum_{\alpha,\beta,i,j} b_\beta^\dagger a_j^\dagger V_{ij,\alpha\beta} a_i b_\alpha. \tag{5}$$

The matrix elements $V_{ij,\alpha\beta}$ in general case can be written in terms of Pauli matrices:

$$V_{ij,\alpha\beta} = \sum_{k=x,y,z} V^k_{ij,\alpha\beta}\sigma^k_\alpha. \tag{6}$$

The diagonal matrix V^z describes the process, in which the atom stays in a given position during the scattering. The off-diagonal electron-TLS interaction $V^{x,y}$ induces a transition of atom between two energy minima. It is proportional to Δ_0 and in most real systems $V^{x,y}/V^z \simeq 10^{-3}-10^{-4}$.[2,3] In the slow TLS $\Delta_0 \ll \Delta$, and dealing with this system, in the main approximation on Δ_0, we neglect off-diagonal interaction in the full Hamiltonian.

The diagonal interaction potentials are given by

$$V^z_{ij,\alpha\beta} = \int d\mathbf{r}\Psi_i^*(\mathbf{r})\Psi_j(\mathbf{r}) \int d\mathbf{r}' U(\mathbf{r}'-\mathbf{r})\phi_\alpha^*(\mathbf{r}')\phi_\beta(\mathbf{r}'),$$

where ϕ_α is the atom (TLS) wave function, which is strongly localized and can be considered as the wave function of a particle confined in a spherical box; $U(\mathbf{r}'-\mathbf{r})$ is the potential of the interaction between the electron and atom in the position $\mathbf{r}'$.

Using Eq. (2) we find the first order corrections to the current through the microconstriction

$$\Delta I = \frac{e\pi}{\hbar}\sum_{j,j'} (\mathrm{sgn}\ k_z - \mathrm{sgn}\ k_z')(f_{j'} - f_j)\delta(\varepsilon_j - \varepsilon_{j'})\Gamma_{jj'},$$

where $f_j = f_F[\varepsilon_j + (eV/2)\mathrm{sgn}(k_z)]$, is the Fermi distribution function for conducting electrons and

$$\Gamma_{jj'} = n_+(|V^z_{jj',22}|^2 - |V^z_{jj',11}|^2) + |V^z_{jj',11}|^2.$$

In order to calculate conductance, one needs to differentiate the current over voltage. In this step the voltage dependence of the occupation number for the upper eigenstate of TLS, n_+ should be well established. Under the assumption that the transition probability between eigenstates of TLS by electron scattering process is a constant parameter, the stationary part of solution of time-dependent equation for the occupation number of the upper eigenstate in the model of long channel can be given by[11]

$$n_+ = \frac{1}{2} - \frac{2E}{2E\ \coth\dfrac{E}{2T} + (E+eV)\coth\dfrac{E+eV}{2T} + (E-eV)\coth\dfrac{E-eV}{2T}}.$$

It should be noted although the nonequilibrium dependence of $n_+(V)$ is due to the tunneling process but it does not depend on the value of Δ_0.[11]

Highlighting the novel quantum mesoscopic effect, let us use a simplified model: consider that during the scattering process, the atom is localized either at points $(\mathbf{r}_{\perp 1}, z)$ or $(\mathbf{r}_{\perp 2}, z)$. Also we assume a point like electron-atom interaction as $U(\mathbf{r}'-\mathbf{r}) = g\delta(\mathbf{r}'-\mathbf{r})$, where g is the constant of interaction. Within these approximations, the changing in the conductance for the elastic interaction is given by

$$\Delta G = \frac{e\pi}{\hbar} g^2 \sum_{j,j'} (\mathrm{sgn}\ k_z - \mathrm{sgn}\ k_z')\delta(\varepsilon_j - \varepsilon_{j'}) R_{mn,m'n'}(\mathbf{r}_{\perp 1}) \times \frac{d}{dV}(f_{j'} - f_j) + \frac{e\pi}{\hbar} g^2 \sum_{j,j'} (k_z - k_z')\delta(\varepsilon_j - \varepsilon_{j'}) \times Q_{mn,m'n'}(\mathbf{r}_{\perp 1}, \mathbf{r}_{\perp 2}) \frac{d}{dV}[n_+(f_{j'} - f_j)], \qquad (7)$$

where

$$R_{mn,m'n'}(\mathbf{r}_{\perp 1}) = |\psi_{mn}(\mathbf{r}_{\perp 1})|^2 |\psi_{m'n'}(\mathbf{r}_{\perp 1})|^2$$

and

$$Q_{mn,m'n'}(\mathbf{r}_{\perp 1}, \mathbf{r}_{\perp 2}) = |\psi_{mn}(\mathbf{r}_{\perp 1})|^2 |\psi_{m'n'}(\mathbf{r}_{\perp 1})|^2 - |\psi_{mn}(\mathbf{r}_{\perp 2})|^2 |\psi_{m'n'}(\mathbf{r}_{\perp 2})|^2.$$

The value $Q_{mn,m'n'}(\mathbf{r}_{\perp 1}, \mathbf{r}_{\perp 2})$ specifies the sign of last term in the conductance ΔG. Obviously this value depends on the local electron density of states in the position of TLS. By changing the diameter of channel, these densities change and this may change the sign of conductance too. This is the quantum analog of the effect has been predicted by Kuzob and Kulik in point contacts containing the single TLS.[10,11]

To illustrate the results we use the free electron model of a channel like contact consisting of two infinite half-spaces connected by a long ballistic cylinder of a radius R and a length L (Fig. 1). In a limit $L \to \infty$ the transverse part of electron wave functions $\psi_{mn}(\mathbf{r}_\perp)$ and eigenenergies ε_{mn} can be obtained analytically (see, for example, Ref. 20). Figure 2 shows the voltage dependence of correction to the conductance due to the presence of a slow TLS for three microconstrictions with different diameters whereas all other characteristic parameters of TLS and its position are the same. In Fig. 3 the PCS for these constrictions is plotted. This figure illustrates the possibility of changing of the sign of point contact spectrum with changing of diameter of microconstriction. The extremum of PCS occurs at $eV = E$,a TLS characteristic parameter.

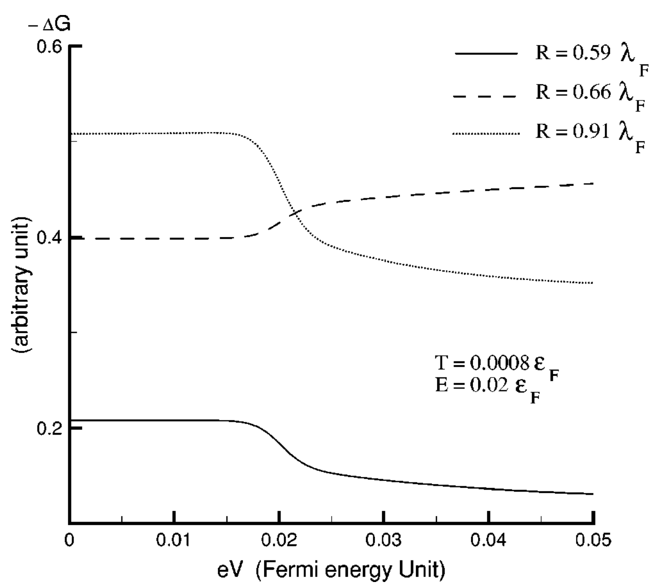

FIG. 2. Change in the conductance of quantum microconstrictions due to the presence of a slow TLS is plotted versus the bias voltage for different values of the radius.

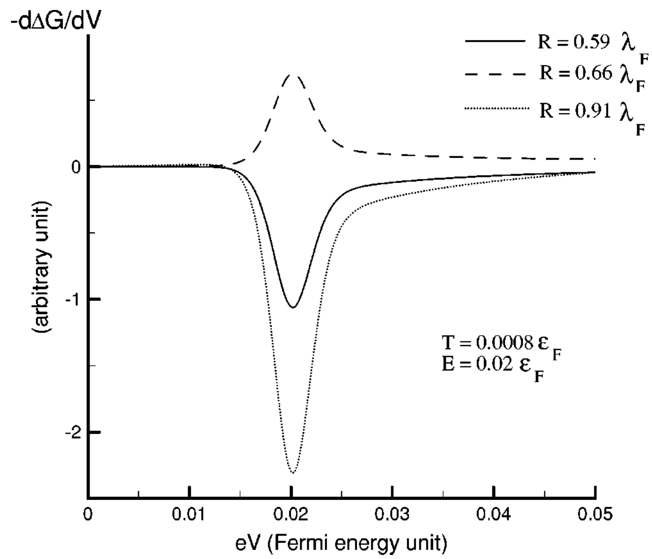

FIG. 3. The point contact spectrum for three quantum microconstrictions with different diameters each one including a single slow TLS. The sign of PCS changes with changing the diameter of microconstriction as the manifestation of a novel quantum mesoscopic effect.

Thus, we have shown that the influence of slow TLS on the conductance of quantum microconstriction depends on the space positions of atom inside it. This effect is due to the essential inhomogeneity of the local density of states (LDOS) of electrons across the constriction $\nu_{mn}(\mathbf{r}_\perp,\varepsilon) = \sqrt{m_e}|\psi_{mn}(\mathbf{r}_\perp)|^2/[\hbar\sqrt{2(\varepsilon-\varepsilon_{mn})}]$. This inhomogeneity results in different values of matrix element of electron-atom interaction for the same value of scattering potential for the two positions. The increasing of applied bias leads to increasing of probability to find the TLS in the upper state. The sign of the correction to the conductance of ballistic microconstriction depends on the difference of the LDOS of electrons in two positions of the atom. If the LDOS for upper energy state is smaller than for the lower state, the conductance decreases with the increasing of the voltage. Changing the diameter of the constriction makes it possible to change the pattern of the LDOS oscillations inside the constriction. We have shown that correction to the conductance due to such effect can change its sign. The quasiclassical theory[7,10,11] does not take into account the difference in the atom position in the Fermi wavelength scale, and the possibility of different sign of PCS related to the difference between effective electron scattering cross section by slow TLS in two quantum states. For a channel with $2R \gg \lambda_F$, the number of quantum modes (m,n) is large and after summation over all of them, the mesoscopic effect, which has been considered in this paper, becomes negligible. Note that conductance G of the microconstriction containing one usual pointlike defect depends on its position due to inhomogeneity of LDOS, but in such a case G does not depend on the voltage. The nonlinear dependence $G(V)$ may result from an interference of electron waves, which are scattered by different defects. This effect was analyzed in Ref. 22.

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