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0.7 ANOMALY IN QUANTUM POINT CONTACT, MODELLING BASED ON ANDERSON MODEL

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Abstract: The so-called 0.7 anomaly in conductance through quantum point contact is analyzed within Anderson Hamiltonian with energy dependent hybridization. In the non-interacting case the broad conductance plateau at $2e^2/h$ is caused by step-like increase of hybridization of the bound state inside quantum point contact with electrodes when the gate voltage is increased. In the interacting case the Kondo conductance enhancement is observed at low temperatures. The plateau at non-integer values of conductance appears when temperature increases and Kondo effect is diminished. The shape of the conductance curves and the non-integer value of conductance plateau strongly depend on the location of the hybridization step in the energy scale.

1. INTRODUCTION

An unusual temperature behavior of the conductance *vs.* gate voltage in quantum point contact (QPC) has been observed for years [1, 2] without satisfactory theoretical explanation. The deviations from conductance quantization in units of $2e^2/h$ have caused years lasting debate. Recently, the enlightening experiments of Cronenwett *et al.* [3] gave strong evidence that Kondo effect is responsible for this effect. They have shown the existence of the so-called zero-bias anomaly peak in the differential conductance and logarithmic temperature dependence of its width. The value of the first step in conductance *vs.* gate voltage curve has also this dependence. Moreover, the conductance curves can be scaled with single parameter corresponding to Kondo temperature. The results have been interpreted recently [4] in the frame of Anderson model with two parameter correlated hopping regulating probability of the occupancy of first and second electron of the quasi-bound state present in the constriction. Our approach is the simplest one possible, we utilize the single impurity Anderson Hamiltonian and the only modification we introduce is the energy step-like dependence of hybridization of the quasi-bound state with electrodes.

2. MODEL AND CALCULATIONS

We model a QPC by localized spin-degenerate bound state (LBS) located inside the constriction between two 2D-dimensional electron seas which form the electrodes. Electrons occupying localized ε_d level interact with the strength of Coulomb repulsion U, and LBS is hybridized with electrodes by the matrix element v_α. Such a system can be described in the frame of the Anderson Hamiltonian:

$$H = \sum_{k,\sigma,\alpha=L,R} \varepsilon_{k,\alpha} c^{+}_{k\sigma,\alpha} c_{k\sigma,\alpha} + \sum_{\sigma} \varepsilon_d d^{+}_{\sigma} d_{\sigma} + U n_{\uparrow} n_{\downarrow} + \sum_{k,\sigma,\alpha=L,R} v_\alpha \left[c^{+}_{k\sigma,\alpha} d_{\sigma} + d^{+}_{\sigma} c_{k\sigma,\alpha} \right] \quad (1)$$

The hybridization $\Gamma = \pi v^2 \rho_{el,\alpha}$ ($\rho_{el,\alpha}$ is the density of states in the α = Left, Right electrode) is assumed to have a step-like profile to simulate the potential barrier present inside QPC. When the gate voltage is large and negative, the QPC is fully closed for electrons and LBS is decoupled from the electrodes. As the gate voltage increases electron current begins to flow through the contact and the quasi-bound state in the QPC gets finite hybridization width, the transparency of the QPC increases. QPC is fully transparent when, in the non-interacting case, the hybridization with electrodes is so large that the conductance reaches its unitary limit $2e^2/h$. The potential barrier inside QPC is simulated by the function: $\Gamma(\varepsilon_d) = \{\exp[(-\varepsilon_d + \delta)/\tau] + 1\}^{-1}$, where τ – parameter controls the sharpness of the hybridization step (it is taken as unity in the course of calculations) and δ regulates the position of the step in the energy scale. These two parameters depend on the experimental details of the QPC fabrication. The hybridization step is most likely located in the vicinity of Fermi surface because the conduction electrons have the largest mobility in this region. We assume that the Fermi level is located at zero energy.

Strong electron correlations present on the QBS are analyzed within the Interpolative Perturbative Scheme (IPS) [5] which is an extension of the second order perturbation in U to the atomic limit [6]. We have modified the method to be applicable for the case when hybridization increases in step-like fashion. The method is applied both for strong (resonant Kondo regime) and weak (Coulomb blockade regime) hybridization. Such crossover from one regime to another indeed takes place in QPC when the hybridization of QBS with electrodes increases while increasing of the gate voltage.

Following Meir and Wingreen [7], conductance can be related to the spectral density of the central region and its coupling $\Gamma_{\alpha,\sigma}(\omega) = \pi t_\alpha^2 \rho_{\alpha,\sigma}(\omega)$ with electrodes. For the symmetric coupling and in zero limit of drain-source voltage conductance can be written in the form:

$$G = \frac{2\pi e^2}{h} \sum_\sigma \int_{-\infty}^{+\infty} \Gamma(\varepsilon) \left(-\frac{\delta f(\varepsilon)}{\delta \varepsilon} \right) \rho_\sigma^{\mathrm{LBS}}(\varepsilon) d\varepsilon \tag{2}$$

where $f(\varepsilon)$ is the Fermi distribution function and $\Gamma(\varepsilon) = \Gamma(\varepsilon)_L \, \Gamma(\varepsilon)_R / [\Gamma(\varepsilon)_L + \Gamma(\varepsilon)_R]$. Spectral density of the nanodevice is calculated from the appropriate retarded Green function: $\rho_\sigma{}^{\mathrm{LBS}}(\omega) = -(1/\pi) Im G_\sigma{}^{\mathrm{LBS}}(\omega + i\delta)$. In the non-interacting case the LBS single particle level gets finite width due to hybridization with electrodes Γ:

$$G_\sigma^{\mathrm{LBS}}(\omega) = \left[\omega - \varepsilon_{d,\sigma} + i\Gamma_\sigma \right]^{-1}. \tag{3}$$

When strong electron correlations within QBS are included the Green function is additionally dressed and the selfenergy Σ^{IPS} is calculated within IPS method beyond Hartree-Fock approximation:

$$G_\sigma^{\mathrm{LBS}}(\omega) = \left[\omega - \varepsilon_{d,\sigma} - n_{-\sigma} U - \Sigma_\sigma^{\mathrm{IPS}}(\omega) + i\Gamma_\sigma \right]^{-1}. \tag{4}$$

3. RESULTS AND DISCUSSION

We start our modeling when the bound state is initially weakly coupled to electrodes. It corresponds to the Coulomb blockade regime for quantum dots.

Non-interacting case

Without interactions the Hamiltonian, Eq. (1), is quadratic in operators and can be solved exactly. The conductance *vs.* LBS level position is shown in Fig. 1 for various hybridization strengths described by α multiplier. The strength of $\alpha = 1$ is taken as hybridization reference typical for quantum dot (QD). For $\Gamma > (\varepsilon_F - \varepsilon_d)$ the step-like behavior of conductance with saturation of $2e^2/h$ can be observed, thus QPC becomes fully transparent. For comparison two conductance curves for QD ($\alpha = 1$ and $\alpha = 30$) with constant (lorentzian in ω-dependence) hybridization with electrodes are also plotted. In this case G reaches unitary limit when the bare QD level crosses Fermi surface. As can be seen, the broad step-like plateau in conductance through QPC is produced when hybridization of the bound state with electrodes for the fully transparent QPC is one order of magnitude larger as compared to QD. This has its

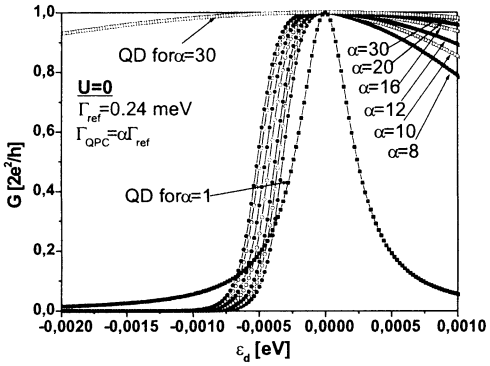

Fig. 1. Conductance *vs.* LBS level position in the non-interacting case for step-like profile of hybridization with increasing strength. For comparison conductance for constant hybridization, as in QDs, is plotted

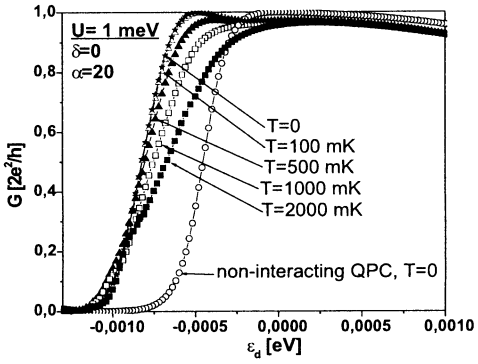

Fig. 2. Conductance *vs.* LBS level position in the interacting case, $U = 1$ meV, for increasing temperature; the curve for non-interacting electrons at $T = 0$ is also plotted

confirmation in experiments; QDs are nanostructures with well defined electrostatic confinement and QPCs are rather open systems. The calculations are made for $\delta = 0$ i.e. when the hybridization step is located at zero energy.

Interacting case

Conductance curves for interacting QPC are presented in Fig. 2 when the hybridization step is located at zero energy. The shoulder present in the conductance step is caused by the Kondo effect; it gradually decreases with increasing temperature. The curves are obtained for hybridization step placed at zero energy (i.e. for $\delta = 0$). A curve for non-interacting QPC is also plotted. Comparison of both cases shows the modification of the curves by Kondo effect. The calculated dependences are similar to those obtained experimentally by Kristensen *et al.* [8]. In QPCs fabricated by this group a positive gate voltage is required to open them,

differently to QPCs obtained by Cronenwett *et al.* which are activated already for negative gate voltage. This suggests that the potential barrier step present in the constriction forming QPC is located in different ranges of energy in contacts fabricated by both groups. The location of the QPC sub-bands with respect to the resultant average chemical potential is possibly also different.

In Figures 3a, b we present conductance curves calculated for δ = 0.5 meV and δ = 0.4 meV, i.e. when the hybridization step of the QPC with electrodes is shifted above zero energy. In this case the shoulder in the conductance curves caused by Kondo effect develops into clear maximum, which decreases with the increase of temperature and transforms into plateau at non-integer value of conductance. The value of the plateau depends on the location of the LBS hybridization step in energy scale. A further increase of conductance towards the unitary limit is caused by increasing transparency of QPC. In Fig. 4 the curves are shown when the QPC becomes fully transparent earlier, i.e. when the hybridization step is located below zero energy. In this case the resonant Kondo enhancement of conductance is practically obscured by large hybridization, which already alone saturates the conductance at $G = 2e^2/h$.

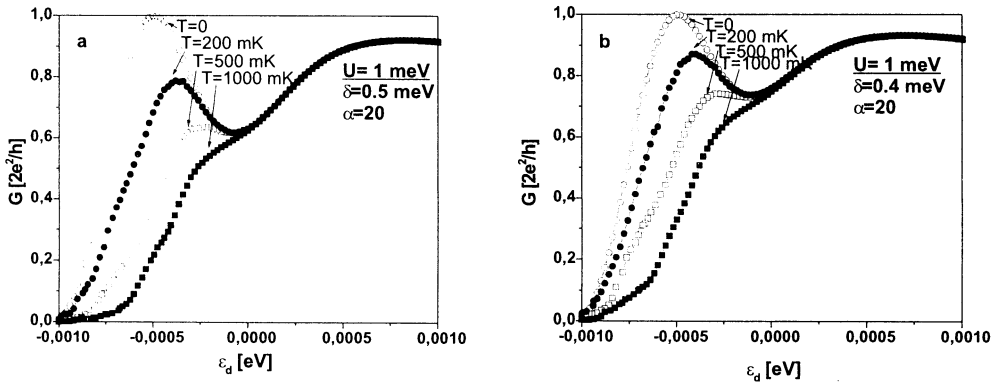

Fig. 3. Conductance *vs.* LBS level position in the interacting case, U = 1 meV for the hybridization step placed at δ = 0.5 meV. (a) and δ = 0.4 meV (b). The non-integer value of conductance depends on the location of the hybridization step

The selfconsistently calculated particle number located at the QPC level is presented in Fig. 5 and, for comparison, also for QD in Coulomb blockade (CB) and resonant Kondo regime (RR). Even for an infinitesimally small hybridization the level is fully occupied by two electrons with opposite spins when it lies well below Fermi surface at T = 0. Then, when the bare level is shifted towards Fermi surface, it enters the region where the level $\varepsilon_d + n_{-\sigma}U$ is pushed above the Fermi level and becomes empty. When ε_d is singly occupied (this is seen as a plateau around $n_{-\sigma} \sim 0.5$ for QD dependence in CB regime) the conductance is mainly enhanced by the Kondo effect. Then, the occupancy of the level ε_d decreases for QD when the level is shifted towards empty orbital regime. For QPC $n_{-\sigma}$ dependences are strongly modified by increasing hybridization. The occupation number decreases much slower, the LBS does not reach empty orbital regime so fast as the QD level due to its large width. The thick curve presents the calculations (for δ = 0.4 meV) according to Friedel sum rule (FSR) [9]

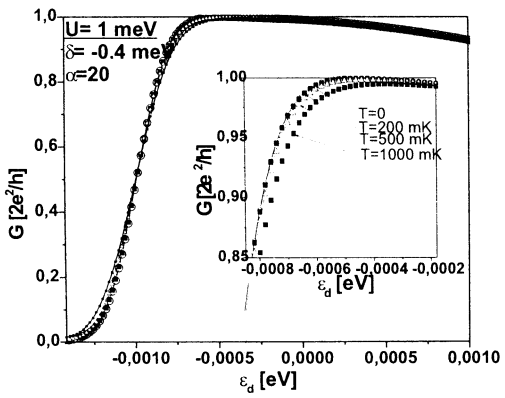

Fig. 4. Conductance *vs.* LBS level position in the interacting case, U = 1 meV for the hybridization step placed at δ = −0.4 meV. The curves for various temperatures nearly coincide (enlarged view of the shoulder is shown in the inset); Kondo effect is totally obscured by large hybridization

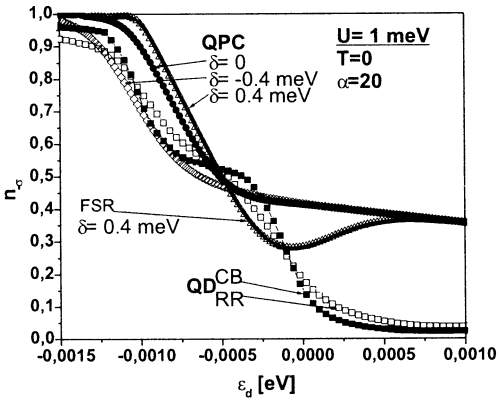

Fig. 5. Selfconsistently calculated particle number *vs.* localized level position for QPC and for QD. For QPC the calculations were made for hybridization step located at δ = 0, −0.4 and 0.4 meV. For QD Coulomb blockade (CB) and resonant regime (RR) curves were calculated for constant hybridization.

which describes the dependence of the phase shift acquired by conduction electrons scattered by localized QPC state and the charge on this site.

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