"0.7 anomaly" and magnetic impurity formation in quantum point contacts

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The origin of the 0.7-conductance anomaly in quantum point contacts (QPCs) has been a subject of lively discussions since its discovery more than 10 years ago [1]. In a recent letter, based on spin density functional theory (DFT), Rejec and Meir explained the origin of the 0.7-anomaly as being due to the formation of a magnetic impurity in the QPCs [2]. They did not, however, perform transport conductance calculations so the central question whether the 0.7-anomaly is indeed related to the formation of a magnetic impurity has remained unanswered. In this communication, we perform spin DFT transport calculations for the structures considered by Rejec and Meir. While we recover the findings reported by Rejec and Meir concerning the formation of localized spin-degenerate quasi-bound states, our transport calculations do not contain the 0.7 anomaly in the conductance. We suggest that the inability of the DFT to reproduce quantitatively the 0.7 anomaly may be due to the uncorrected self-interaction errors in the DFT calculation of electronic transport for the case when localization of charge is expected to occur, so that the magnetic impurity formation may be an artefact of DFT due to the spurious self-interaction.

We consider quantum point contacts defined by a split-gate in GaAs heterostructure similar to those studied by Rejec and Meir, see Fig. 1. We utilize the same Hamiltonian based on the spin DFT approximation (a detailed description of the Hamiltonian can be found in Refs. [3, 4, 5]). We calculate the scattering solutions of the Schrödinger equation in the open system using the self-consistent Green’s function technique where the whole device, including the semi-infinite leads, is treated on the same footing, i.e. the electron-electron interaction is accounted for both in the leads and in the QPC region within the spin DFT approximation. The detailed description of our method is given in Ref. [5]. Note that similar spin DFT conductance calculations reproduce quantitatively the measured spin-resolved magneto-conductance of quantum wires in the integer quantum Hall regime [6, 7].

Figures 1a, b show the spin resolved electron densities, the local density of states and the potentials for spin-up and spin-down electrons in the QPC of the lithographic length of 250 nm. These results agree very well with corresponding findings reported by Rejec and Meir [2]. (Note that spin DFT calculations predicting spin polarization in the QPC were reported in Refs. [8, 9, 10]). The calculated conductance is shown in Fig. 1c. Close to the pinch off a spin-degeneracy of the spin-up and spin-down conductance channels is lifted and the total conductance shows a broad feature peaked at \( \sim 0.5 \times 2e^2/h \). A similar feature is also present in the range of the gate voltages where a second step in the conductance develops. The calculated conductance clearly does not reproduce the 0.7 anomaly observed in almost all QPCs of various geometries. (We stress that the results presented here are generic: we studied QPCs with lengths in the range 40-400 nm and electron densities in the leads in the range \( 10^{15} \text{ m}^{-2} - 4 \times 10^{15} \text{ m}^{-2} \), with very similar results).

Why do DFT calculations fail to reproduce the 0.7 anomaly? Formation of the magnetic moment implies that electrons are trapped in the weakly coupled quasi-bound states in the center of the QPC [2]. It has been recently realized that a standard DFT approach in the case of the weak coupling suffers from the spurious interaction of the electron with its exchange and correlation potential [11, 12, 13, 14, 15]. This, for example, causes an orders-of-magnitude discrepancy between the calculated and measured currents through organic molecules coupled to metallic contacts [11, 12, 13, 14, 15]. (This is in contrast to the case of metallic atomic-scale wires for which the DFT-based calculations are in excellent agreement with the experiment [11, 12]). Several correction schemes have been recently suggested and implemented, restoring the agreement between the DFT calculations and the experiment for the case of the weak coupling [11, 12, 13, 14, 15]. A spurious self-interaction might well be the reason for the failure of the standard DFT for the case of the QPC and an accurate description of the 0.7 anomaly might require correction schemes eliminating the above errors.

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FIG. 1: Figure 1 | The conductance and the electron densities in the QPC. (a) The spin-up (left) and spin-down (right) electron densities in the quantum point contact for the gate voltage $V_g = -1.2$ V and (b) the corresponding local density of states (LDOS). The dotted lines indicate the self-consistent Kohn-Sham potential in the center of the wire (along $y = 0$). (c) The spin resolved and the total conductance of the QPC ($\uparrow$, $\downarrow$ stand for the spin-up and spin-down electrons). The dotted line corresponds to the spin-unpolarized conductance. The spin polarized conductance was obtained by applying a small magnetic field in the initial iterations of the self-consisted procedure. The parameters of the structure are as follows. The QPC is defined in the infinite quantum wire of the width of 500 nm. The lithographic position of the gates defining the QPC is indicated by the dashed lines in (a). The distance between the gates is 200 nm, and the gate length is 250 nm. The electrons are situated 50 nm below the surface of the GaAs heterostructure. The donor layer of the width of 36 nm and concentration of $7.2 \times 10^{23}$ m$^{-3}$ is situated 10 nm below the surface. The electron density in the quantum wire far away from the QPC is $2.5 \times 10^{15}$ m$^{-2}$ (which corresponds to 18 propagating modes in the leads). (A detailed description of the model for the heterostructure and the confining potential can be found in Refs. [3, 4, 5]). The calculations are performed for $T = 200$ mK.

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