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2008 J. Phys.: Condens. Matter 20 164208

(http://iopscience.iop.org/0953-8984/20/16/164208)

J. Phys.: Condens. Matter **20** (2008) 164208 (4pp) doi:10.1088/0953-8984/20/16/164208

The theory of the '0.7 anomaly' in quantum point contacts

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Received 15 October 2007, in final form 5 December 2007
Published 1 April 2008
Online at stacks.iop.org/JPhysCM/20/164208

Abstract
The phenomenology of the '0.7 anomaly' in quantum point contacts is fully explained in terms of a quasi-localized state, which forms as the point contact opens up. Detailed numerical calculations within spin-density functional theory do indeed confirm the emergence of such a state. Quantitative calculations of the conductance and the noise are obtained using a model based on these observations, and are in excellent agreement with existing experimental observations.

(Some figures in this article are in colour only in the electronic version)

1. Introduction and summary

The '0.7 anomaly', the subject of this collection, has been a long standing puzzle since it was first realized [1] that this is a generic phenomenon, which in fact had been already evident in the first experiments on conductance quantization in quantum points contacts (QPCs) [2, 3]. In this article I will demonstrate that existing experimental observations are consistent with a simple model, based on the formation of a quasi-bound state in the QPC as it opens up. I will first discuss the model and how it explains the '0.7 anomaly' rather briefly, and then in later sections will elaborate on a first principle calculation that indeed gives rise to the formation of such a state (section 2) and on quantitative calculations of the conductance and the noise using a model based on these observations (section 3).

The main assumption (to be substantiated in section 2) underlying the model is the emergence of a quasi-localized state at the QPC near pinch-off. With this assumption the following physics emerges:

- The conductance is reduced from its universal value of $G_0 \equiv 2e^2/h$, basically due to Coulomb blockade. As an electron is transferred through the quasi-localized state, it reduces the probability that another electron, with opposite spin, will be simultaneously transferred. Consequently, depending on parameters, the conductance will have a constant value between $0.5G_0$ and G_0 for any value of gate voltage in the Coulomb blockade regime.
- As the gate voltage is further increased the Coulomb blockade energy is overcome and the conductance reaches the value G_0. As we will see in section 2, the localized state disappears for such gate voltages.
- As magnetic field is increased the quasi-localized state energy splits. Similar to the physics of quantum dots, the conductance will decrease to $0.5G_0$ and the separation in gate voltage between the '0.7' step and the first plateau will increase linearly.
- The conductance around the '0.7' plateau may be thought of as carried by two channels, one with almost perfect transmission and one with reduced transmission. This leads to the reduction of the shot noise in this regime, compared to the situation where both channels carry the same conductance.
- At 'high' temperatures the spin of the quasi-localized state is fluctuating among all degenerate directions. As temperature is reduced below the Kondo temperature, at zero magnetic field, this local spin will be screened by the lead electrons—the Kondo effect—enhancing the conductance beyond its high temperature value towards the unitarity limit, G_0. A small magnetic field, such as the Zeeman splitting is of the order of the Kondo temperature, will polarize the spin.
- Formation of a quasi-localized state will also occur at large magnetic fields, where the lower spin branch of the second QPC mode crosses the higher spin branch of the first model, giving rise, in this case, to a '1.2' plateau. Due to the finite magnetic field, Kondo physics will not be relevant here at low temperatures.
- Sometimes a localized state is also formed at the opening of the second subband, giving rise to a '1.7' plateau. Unlike the generic situation in the first subband, we find the formation of this state in the second subband to be sensitive to parameters.

All these observations are in agreement with experiments.

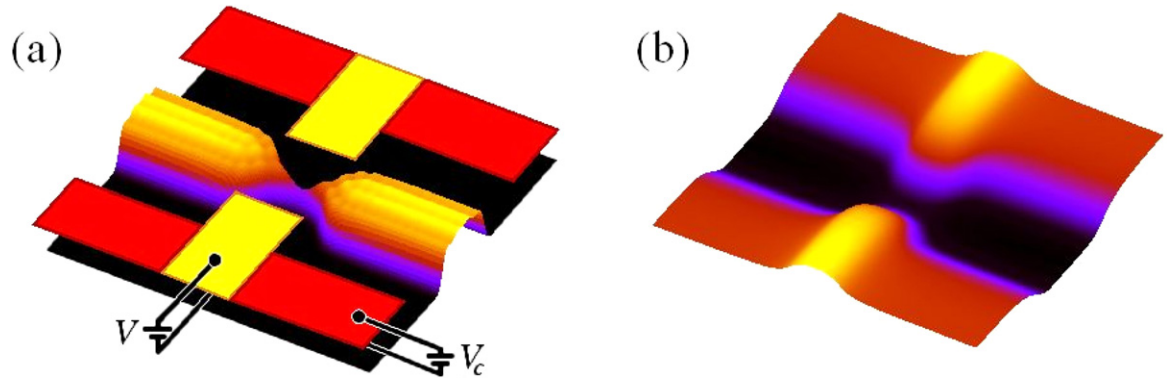

Figure 1. The gate electrodes for the SDFT calculation (a). The red (darker) gates define the maxima possible number of modes, while the yellow (brighter) gate define the QPC. An example of electron density in the wire is also depicted. (b) The effective potential in the 2DEG.

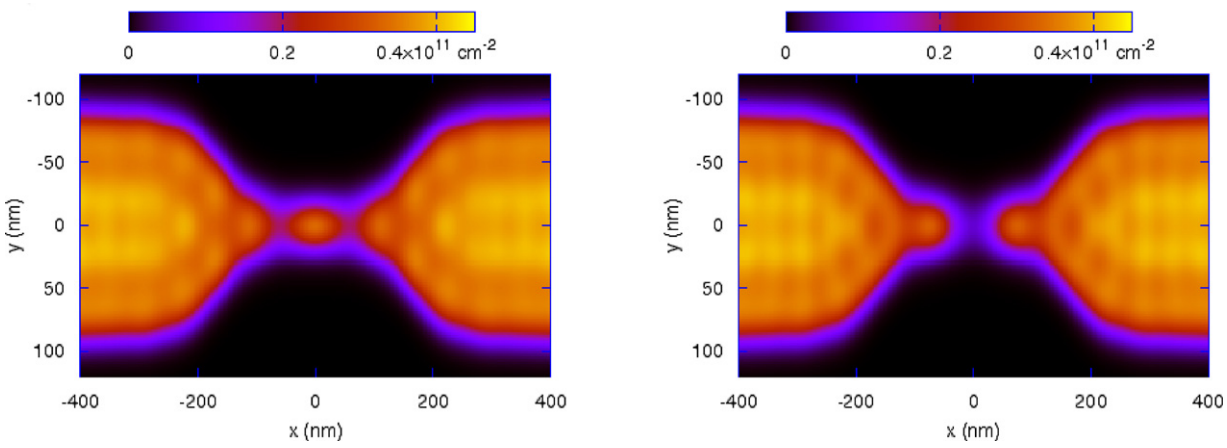

Figure 2. The spin up (a) and spin down (b) density distribution near the gate voltage corresponding to the 0.7 anomaly, indicating formation of a magnetic impurity on top of the QPC.

2. Formation of a magnetic impurity—a density functional calculation

In this spin-density functional calculation (SDFT) [4], which generalizes an earlier SDFT calculation [5], we treat the two-dimensional electron gas (2DEG), the electrodes and the donor layer as a set of three electrostatically coupled two-dimensional systems (figure 1(a)). We assume the donor layer is uniform and fully ionized, and the gates are kept in some voltage (gate voltage) with respect to the 2DEG. Then, according to spin-density functional theory (SDFT) [6], the properties of the system can be uniquely determined in terms of the spin densities of the 2DEG and of the distribution of charge on the electrodes. We treat the 2DEG quantum mechanically by including its kinetic energy and exchange–correlation energy in the energy functional, taking into account the GaAs effective mass and dielectric constant. We used the local spin-density approximation for the exchange–correlation functional, as parameterized in [7] (for more details see [4]). The effective self-consistent potential experienced by electrons in the 2DEG is depicted in figure 1(b).

We want to be able to include the possibility of a quasi-localized state in the calculations. If such a state indeed forms, it will necessarily be occupied by a single spin. To be able to incorporate such a solution within SDFT, we allow solutions of the Kohn–Sham equation [8] which break spin symmetry. Indeed the lowest energy solution, as the QPC opens up, is a spin-polarized state (though the spin direction is arbitrary)—as the effective QPC barrier is lowered the two semi-infinite electrons gases on its two sides start to overlap each other and the density on top of the QPC increases. Once this density is enough to support a full electron, the lowest energy solution describes a quasi-localized electron on top of the QPC (figure 2). This solution was found to be the ground state for all the range of parameters we have checked, thus supporting the idea that the formation of such a magnetic impurity in the opening of the first mode is a generic effect.

A similar solution is found sometimes, but not always, at the opening of the second mode (as electrons occupying the lowest mode screen out the Coulomb interactions), and the energy gained by the formation of the quasi-localized state is significantly lower, suggesting that a feature in the second plateau may be present, but sensitive to details. On the other hand we also find a generic localized state solution in large Zeeman fields, where the higher spin state in the lower mode and lower spin state in the next mode become degenerate (see figure 3). In this case we expect reduction of the conductance

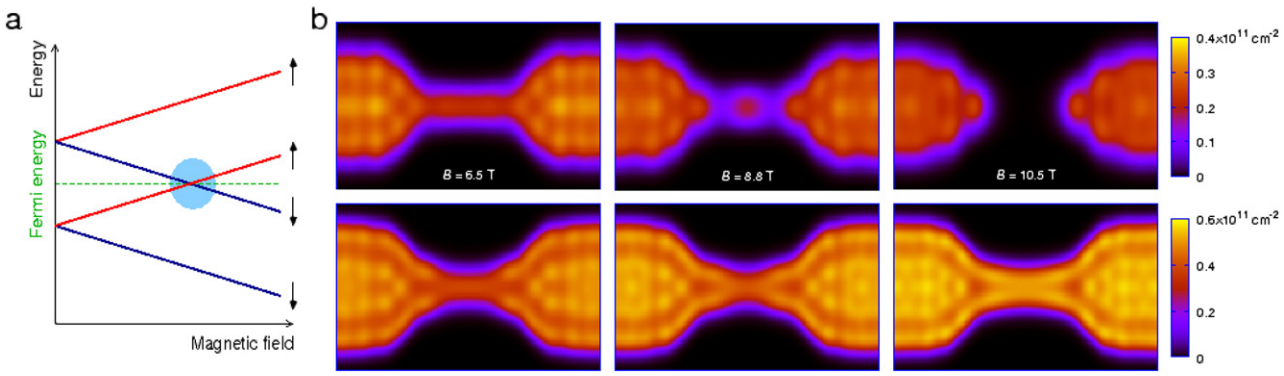

Figure 3. Formation of a quasi-localized state at the crossing of two spin subbands at large magnetic field. The two spin densities (top and bottom) are shown at three values of magnetic field, demonstrating the formation of that state only at a special value of the field.

from its $1.5G_0$ value, but no spin degeneracy. This is consistent with the observation of the 'analog' states [9].

While at high temperatures the localized electron fluctuates between all possible spin directions, so that the state is instantaneously polarized, one expects that as the temperature is lowered below the Kondo temperature, this spin will be screened by the electrons in the leads. Unfortunately, such a state is beyond the capability of SDFT in its local approximation (similar to the Hydrogen molecule problem). In addition, SDFT also cannot, in principle, give the correct dynamical properties of the system, in particular the conductance (see e.g. [10]). In order to evaluate transport properties and also include the Kondo effect, we use, in the next section, the static properties of the system, as obtained from SDFT, to write down an effective Hamiltonian from which one may calculate these properties using standard many-body techniques.

3. The effective model and transport properties

Our SDFT results indicate that even an initially smooth QPC potential can produce a narrow quasi-bound state, resulting in a spin bound at the center of the QPC. We [11] thus model the QPC and its leads by the generalized Anderson Hamiltonian [12]

$$H = \sum_{\sigma;k\in L,R} \epsilon_{k\sigma}\mathbf{c}^\dagger_{k\sigma}\mathbf{c}_{k\sigma} + \sum_\sigma \epsilon_\sigma \mathbf{d}^\dagger_\sigma \mathbf{d}_\sigma + U\mathbf{n}_\uparrow\mathbf{n}_\downarrow + \sum_{\sigma;k\in L,R}[V^{(1)}_{k\sigma}(1-\mathbf{n}_{\bar\sigma})\mathbf{c}^\dagger_{k\sigma}\mathbf{d}_\sigma + V^{(2)}_{k\sigma}\mathbf{n}_{\bar\sigma}\mathbf{c}^\dagger_{k\sigma}\mathbf{d}_\sigma + \text{H.c.}] \tag{1}$$

where $\mathbf{c}^\dagger_{k\sigma}(\mathbf{c}_{k\sigma})$ creates (destroys) an electron with momentum k and spin σ in one of the two leads L and R, $\mathbf{d}^\dagger_\sigma(\mathbf{d}_\sigma)$ creates (destroys) a spin-σ electron on 'the site', i.e. the quasi-bound state at the center of the QPC, and $\mathbf{n}_\sigma = \mathbf{d}^\dagger_\sigma\mathbf{d}_\sigma$. The hybridization matrix elements, $V^{(1)}_{k\sigma}$ for transitions between 0 and 1 electrons on the site and $V^{(2)}_{k\sigma}$ for transitions between 1 and 2 electrons, are taken to be step-like functions of energy, mimicking the exponentially increasing transparency (the position of the step defines our zero of energy). Physically, we expect $V^{(2)}_{k\sigma} < V^{(1)}_{k\sigma}$, as the Coulomb potential of an electron already occupying the QPC will reduce the tunneling rate of a second electron through the bound state. In the absence of magnetic field the two spin directions are degenerate, $\varepsilon_\downarrow = \varepsilon_\uparrow = \varepsilon_0$.

To obtain a quantitative estimate of the conductance we note that the relevant gate voltage range corresponds to the singly occupied state regime. We therefore perform a Schrieffer–Wolff transformation [13] to obtain the Kondo Hamiltonian [14]

$$H = \sum_{k\sigma\in L,R}\varepsilon_{k\sigma}c^\dagger_{k\sigma}c_{k\sigma} + \sum_{k,k'\sigma\in L,R}(J^{(1)}_{k\sigma;k'\sigma} - J^{(2)}_{k\sigma;k'\sigma})c^\dagger_{k\sigma}c_{k'\sigma} + 2\sum_{k,k'\sigma\sigma'\in L,R}(J^{(1)}_{k\sigma;k'\sigma'} + J^{(2)}_{k\sigma;k'\sigma'})c^\dagger_{k\sigma}\vec\sigma_{\sigma\sigma'}c_{k'\sigma'}\cdot\vec S$$
$$J^{(i)}_{k\sigma;k'\sigma'} = \frac{(-1)^{(i+1)}}{4}\left[\frac{V^{(i)}_{k\sigma}V^{(i)}_{k'\sigma'}}{\varepsilon_{k\sigma}-\varepsilon^{(i)}_\sigma} + \frac{V^{(i)}_{k\sigma}V^{(i)}_{k'\sigma'}}{\varepsilon_{k'\sigma'}-\varepsilon^{(i)}_{\sigma'}}\right]. \tag{2}$$

The potential scattering term (first line), usually ignored in Kondo problems, is crucial here, as it gives rise to the large background conductance at high temperature. The magnetic field B, defining the z-direction, enters the problem via the Zeeman term, S_zB. The couplings are assumed to be exponentially increasing as the QPC is opened. (In the above and in the following B and T denote the corresponding energies, $g\mu_BB$ and k_BT, respectively, where k_B is the Boltzmann constant, μ_B is the Bohr magneton, and with the appropriate g-factor.) Since $V^{(1)} \gg V^{(2)}$ then also $J^{(1)} \gg J^{(2)}$.

The main calculational problem is that $J^{(1)}$ is not small and thus cannot be used as a small expansion variable. To overcome this we note that the model can be solved exactly in the large B limit, where the spin channels are decoupled. Thus we [15] perform an expansion around large fields (the small parameter is $\exp(-B/T)$), which merges with the perturbation expansion in small J for zero magnetic field. Interpolating between these limits, the conductance can be written

$$G = \frac{e^2}{h}(T_1+T_2)$$
$$T_i = \frac{\tilde{g_i^2}}{1+\tilde{g_i^2}}, \tag{3}$$

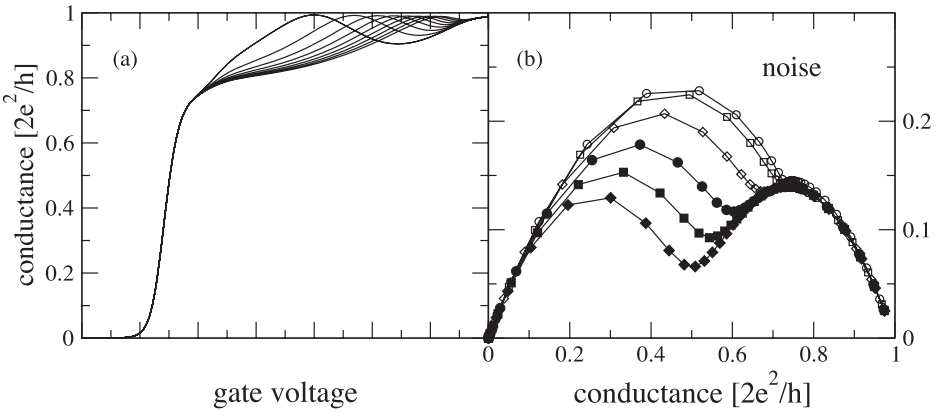

Figure 4. The conductance and the noise, resulting from the approximate calculations presented here and in [15].

where

$$\tilde{g_i^2} \equiv g_i^2 + \frac{B}{T \sinh \frac{B}{T}} \frac{(g_1 + g_2)^2}{1 + (g_1 + g_2)^2}, \tag{4}$$

and $g_i = 4\pi \nu J^{(i)}$.

At low temperature the Kondo effect develops, which leads to

$$\tilde{g_2^2} \to \tilde{g_2^2} + g_2^2 \left(\frac{1}{2} - \frac{B}{T \sinh \frac{B}{T}} \right) + G_2^{\mathrm{RG}}, \tag{5}$$

with

$$G_2^{\mathrm{RG}} = \frac{1}{\left(\ln \frac{\sqrt{B^2 + T^2}}{T_{\mathrm{K}}} \right)^2} \frac{\pi^2}{8} \left(1 + \frac{2B}{T \sinh \frac{B}{T}} \right) \tag{6}$$

with the Kondo temperature $T_{\mathrm{K}} \simeq U \exp(-\pi/g_2)$. The Kondo contribution enhances the contribution of the second channel, and gives rise to the merging of the '0.7' feature with the first $2e^2/h$ conductance step. As pointed out in [11], the resulting T_{K} increases exponentially with ϵ_{F}, in agreement with the experimental observation that T_{K} increases exponentially with the gate voltage [16]. The resulting conductance is plotted in figure 4(a), giving rise, as expected, to plateaus in the conductance around $G \simeq 0.7 G_0$, which increase with decreasing temperature (due to the perturbative nature of the calculation a spurious nonmonotonicity appears in the conductance). Since the latter is due to the Kondo effect, a zero-bias anomaly in the nonlinear conductance will develop at low temperatures, as seen experimentally [16].

Using the values of the transmission for the two channels, equation (3), one can also evaluate the shot noise, which is depicted in figure 4(b), giving rise to a dip in the noise around the '0.7' anomaly, again consistent with experiments [17].

4. Conclusions

We have demonstrated that all the experimental data, as far as we know, can be explained using a simple model that invokes the localization of an electron in the QPC near pinch-off. The emergence of such a quasi-localized state has been corroborated by spin-density functional calculations.

Acknowledgment

This work was supported by the Bi-National US–Israel Science Foundation.

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