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Spin-dependent electron behaviour in quantum point contacts and dots

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Abstract. We investigate theoretically the effect of spontaneous electron spin polarisation in quantum point contacts and quantum dots. Self-consistent calculation process has been developed in the framework of Kohn-Sham LSDA scheme. The existence of the detected spin-polarised states in the low-density regime can be used to explain an anomalous 0.7-structure in the conductance of quantum point contacts. The properties of the potential device based on such an effect are briefly discussed.

Introduction

The physics of interacting electrons in reduced dimensions has begun to unfold in ultra clean systems. In short 1D wires (quantum point contacts — QPCs) a major breakthrough in interaction studies has been achieved by the discovery of spontaneous spin polarisation of the 1D electron gas in the low-density regime. In addition to the quantised plateaux at multiples of $(2e^2/h)$ an anomalous structure at $0.7(2e^2/h)$ has been discovered at zero magnetic field [1, 2]. This structure was found to evolve into the spin-split conductance plateau at (e^2/h) in a strong in-plane magnetic field. More recent measurements on high-mobility double-layers QPCs have revealed that the anomaly in conductance may occur at half-integer values already at zero magnetic field.

1. Theoretical model and calculations

The anomaly in the conductance has been interpreted within the Kohn-Sham local-spin-density approximation (LSDA). For one-channel conduction in a model system, it was found in an earlier work [3] that the electron gas aquires local ferromagnetic order as the electron density is decreased towards pinch-off. By sweeping the gate voltage (i.e. transforming the geometry of the QPC channel) one effectively changes the density of electrons filling a higher energy sub-band. When the density reaches a certain threshold value, an effect of spin-polarisation spontaneously occurs in the channel due to the interplay between electron kinetic and exchange energies. At that very moment, the transmission barrier suddenly becomes different for electrons having up- and down-spin projections. The spin-aligned electrons still conduct current through propagating states in a normal way, while the electrons with opposite spins now have to tunnel from source to drain. Thus an anomaly in the channel conductance repeatedly takes place at certain values of the gate voltage.

We study this problem using proper modelling of the QPC device including a patterned gate, doping, surface states, etc. In this way we consider the case of higher sub-band conduction and predict how the anomalous conduction may depend on the channel geometry. In our approach, the QPC is simulated by a system of two large quantum dots (source and

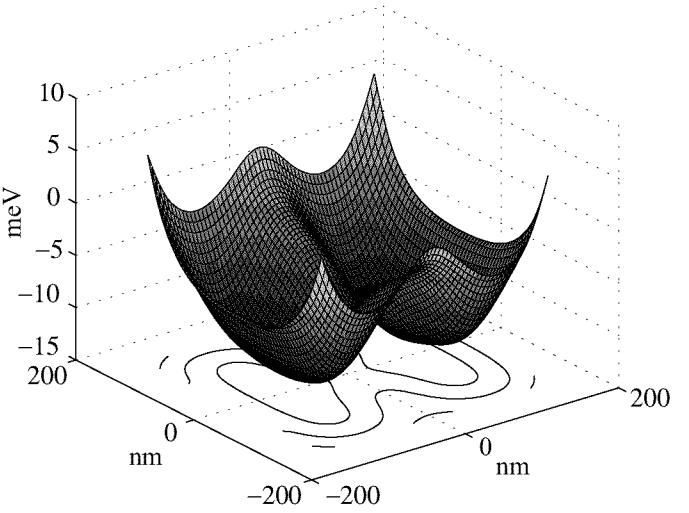

Fig. 1. Total potential of a QPC in the Thomas-Fermi approximation. The QPC is formed by two large quantum dots (source and drain) with a small quantum dot (channel) in between. Gate voltage is −0.5 V.

drain pads) with a smaller dot (the channel) in between, the dots being formed in 2DEG using the split-gate technique (Fig. 1). Thus, modelling a QPC we study magnetic properties of single and coupled quantum dots and how these may be monitored by external means. The topic is currently under active investigation, both theoretically and experimentally [4–7].

The system is described by the Schrödinger equation:

$$-\frac{\hbar^2}{2m^*}\left(\frac{d^2}{dx^2}+\frac{d^2}{dy^2}\right)\varphi^\sigma(x,y)+\left[U^c(x,y)+U^e(x,y)+U^\sigma_{\text{exch}}(x,y)\right.$$
$$\left.+g\mu_{\text{B}}B\sigma\right]\varphi^\sigma(x,y)=E^\sigma\varphi^\sigma(x,y) \tag{1}$$

where $\sigma = \pm\frac{1}{2}$ refers to spin, $U^c(x,y)$ and $U^e(x,y)$ are the confinement and Hartree potentials. In the Kohn-Sham scheme, the exchange potential energy has the form:

$$U^\sigma_{\text{exch}}(x,y)=-\frac{e^2}{\epsilon\epsilon_0\pi^{3/2}}\left[n^\sigma(x,y)\right]^{1/2} \tag{2}$$

where ϵ is the dielectric constant of the heterostructure material and $n^\sigma(x,y)$ is the spatial distribution for σ-spin electrons. We have also included the Zeeman splitting ($g\mu_{\text{B}}B = 10^{-6}$ eV) from a weak external magnetic field in order to trigger the onset of spin polarisation. This splitting turns out to be much smaller than the one caused by exchange interaction.

In order to solve Eq. (1) we applied the self-consistent iterative process with the initial total potential derived from Thomas–Fermi approximation. The electron densities are calculated at each iteration as

$$n^\sigma(x,y)=\sum_{E_i\le E_{\text{F}}}\left|\varphi^\sigma_i(x,y)\right|^2. \tag{3}$$

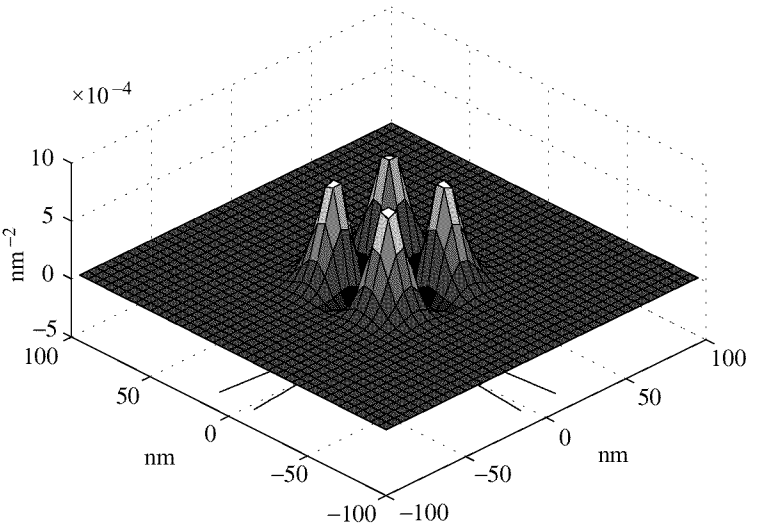

Fig. 2. Spin polarisation of a single quantum dot in the LSDA self-consistent scheme. At the gate voltage −0.58 V, the dot is occupied by four up-spin and three down-spin electrons.

The self-consistency is reached when the energy values and the potential in successive iterations are identical within an accuracy of (10^{-5} eV).

2. Results and discussion

We have shown the existence of spin-polarised states at low densities in a quantum dot and in a QPC formed by a system of coupled quantum dots. In such a situation the electron exchange energy dominates over the kinetic energy thus favouring electron spin-alignment according to the Hund's first rule. The spin-polarisation of a single quantum dot

$$p = n^{(\sigma=\frac{1}{2})} - n^{(\sigma=-\frac{1}{2})} \tag{4}$$

is shown in Fig. 2. One can see the maximum polarisation occurs at the dot periphery where the electron density is low. In the case of a QPC, the spin-polarisation shows reach texture but again is more pronounced at the QPC edges and in the channel area, i.e. in the regions of low electron density. More thorough interpretation of the numerical data for QPCs is currently underway.

We have also found the system properties, in particular the total number of up- and down-spin electrons, strongly dependent on the parameters of the heterostructure, e.g. its donor density. This implies the operation of the potential device based on such a structure would be very sensitive to the quality of the materials used for its fabrication. On the other hand, this enables to flexibly adjust the device characteristics within a wide parameter range, thus making it feasible for various applications.

The models will also allow us to search for more esoteric states like spin-density wave and antiferromagnetic groundstates in 1D channels.

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